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NONLINEARITY AND IRREVERSIBILITY IN LATTICE DYNAMICS

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0. **Contents.**

1. **Introduction.** In these lectures I am going to describe several complimentary methods which have been used in the past to analyze lattice dynamics, to indicate some of the ways these methods have been applied to study irreversibility in simple lattices, and to contrast these approaches with more recent nonlinear results. One of my objectives will be to point out that the recent successes in nonlinear lattice dynamics has so far proved to be a mixed blessing in clarifying several aspects of irreversibility. The two aspects of irreversibility I will consider are those related to the temporal relaxation to equilibrium and the spatial problem of lattice thermal conductivity. Both of these are, of course, closely (if mystically) connected with the classic ergodic and mixing problems of statistical mechanics, as well as to each other, at least according to the Kubo [8], [18b], fluctuation-dissipation concepts. It is in this context that many of the recent advances in both stochastic dynamics and soliton concepts may offer an opportunity for significant advances in our understanding of the origin of irreversibility.

While conceptual difficulties associated with the relationship between analytical dynamics and statistical irreversibility have been evident since the work of Boltzmann (see, e.g., [5]) the case of lattice dynamics presents both unique problems as well as analytic opportunities. A lattice is distinguished from a gas or liquid by the fact that the atoms maintain their relative spatial order in the course of time. This property permits nearest-neighbor interaction approximations, which yield a simple linear normal mode description of lattice dynamics, and is also

responsible for the one-to-one (nonlinear) transcription from the Lagrangian to the Eulerian representation of lattice dynamics. This latter continuum description, involving nonlinear partial differential equations, has generated a major area of mathematical research in recent years, centering around coherent nonlinear disturbances ("solitons"). The rediscovery of these nonlinear disturbances, originally studied in hydrodynamics, had its genesis in the present context in the nonergodic behavior of one-dimensional lattices, noted in computer calculations made by Fermi, Pasta, and Ulam [61] before 1955. It is interesting to note the interplay here between the question of the temporal relaxation to equilibrium (the FPU problem) and the spatial transport of energy (soliton picture). This field of continuum research has, of course, expanded greatly during the past ten years with the discovery of many beautiful analytic results, such as the inverse scattering technique (Gardner, Greene, Kruskal, Miura [43], [44]) and a wide variety of applications—as is attested to by this conference. Fortunately many of these results have been reviewed quite clearly in the literature (see references) and need not be discussed here.

My concern here will be to discuss some of the ways in which these results have clarified (or mystified!) our understanding of irreversibility in lattices. It does not require any great insight to appreciate that solitons are in fact the antithesis of a "resistance" to the energy flux through a lattice, in analogy to a gas of free particles (Knudsen gas), because they describe noninteracting collective degrees of freedom. Thus the occurrence of "perfect" nonlinear dynamics is as "non-mixing" as harmonic motion, so the origin of irreversibility in a lattice depends upon the demise of the simplistic picture of noninteracting coherent disturbances traveling through a nonlinear lattice. This statement, of course, rests upon the assumption that the conventional wisdom (as expressed for example by Fourier's Law of heat conduction) is indeed valid for *perfect* infinite lattices. In any case these nonlinear results should yield in the future important insights into the origin of statistical irreversible lattice dynamics, which will complement the historic linear techniques.

To clarify the contributions of these nonlinear results, as well as their present limitations, it is necessary to begin with a brief review of the methods used to analyze the harmonic lattice. It is from this basis that most of the detailed theories of irreversibility and stochastic behavior have been developed, with the aid of various perturbation methods. To simplify matters the description which will be presented will be largely (but not entirely) limited to one-dimensional lattices. The extension of some of these results to higher dimensions and more general lattice

structures is *not* generally a trivial affair, particularly in the nonlinear aspects (for harmonic generalizations, see the general references). The mathematical problems however are already quite formidable in the one-dimensional system, and the question as to the "realistic behavior" of such models can be viewed as somewhat secondary to the primary conceptual problem of understanding their irreversible properties. It is largely in that spirit that the following discussion will be conducted.

§ 2 contains an elementary introduction to lattice dynamics, primarily to introduce notation. § 3 contains some of the historic concepts concerning energy transport through lattices which have dominated past theoretical considerations (I might add that I have not done justice to theories of the past five to ten years. See, e.g., reviews in Horton and Maradudin [7]). In § 4 various results from computer calculations of energy transport are presented, with a brief examination of soliton effects and contributions. The famous Fermi-Pasta-Ulam problem, the grandfather of this conference, is discussed in § 5. Because I believe that this is a very fundamental problem, I have examined it from several points of view. The very interesting and basic area of stochastic dynamics is touched on only briefly in § 6. Its interface with soliton dynamics is presently a nearly virgin field of research. In § 7 I have attempted to summarize a number of questions and comments raised in these lectures, which I feel are of particular interest for future research. Perhaps this potpourri will be of some assistance to mathematicians looking for further applications of soliton concepts and needed generalizations.

2. **One-Dimensional Lattices.** As mentioned above, much of the following will be limited to one-dimensional lattices (chains). For more general descriptions, involving higher dimension, various lattice structures, boundary and disorder effects, etc., see the general references. Some limited references will be made below concerning higher dimensional cubic lattices, but it is a matter of some optimistic faith that one-dimensional systems should contain *many* of the "essential features" required to produce ergodicity, irreversibility, and the like. It is very doubtful, because of the severely limited dynamical freedom imposed by one-dimensional motion, that *all* irreversible properties can be properly accounted for in such systems. Thus the present discussion should be viewed with some reservation concerning its relevance to real solids. Nonetheless such investigations are basic to a more fundamental understanding of irreversibility.

In the Lagrangian description of a lattice the position, $x_n(t)$, and velocity, $\dot{x}_n(t) \equiv dx_n/dt$, of the nth particle are functions of the indepen-

dent variable t. Let h be the interparticle distance, and $y_n(t)$ the displacement from its equilibrium position, so that

$$\begin{aligned} x_n(t) &= nh + y_n(t) \qquad (n = 1, \cdots, N) \\ y_{n+1} - y_n &\geqq -h \qquad \text{(ordering condition)} \end{aligned} \tag{2.1}$$

where there are N degrees of freedom. If m_n is the mass of the n'th particle, and there are only nearest neighbor forces (see below) which are all the same, then the equations of motion are

$$\begin{aligned} m_n \ddot{y}_n(t) = F(y_{n+1} - y_n) \\ - F(y_n - y_{n-1}) \ (n = 1, \cdots, N). \end{aligned} \tag{2.2}$$

Note the order of the displacement variables in the force $F(z)$. It should perhaps be emphasized at this point that these equations are time reversible (e.g., they contain no dissipative friction), and that the "irreversibility" used throughout has only a statistical (ensemble) significance. The most common forms of the forces which have been used to study nonlinear lattices are:

(2.3) *Polynomial:* $F(z) = \mu(z + K_2 z^2 + K_3 z^3 + \cdots)$
Lennard-Jones approximation: $K_2 = -10.5$, $K_3 = 371/16$

(2.4) *Piecewise linear:* $F(z) = \mu_\ell z \ (z_\ell \leqq z \leqq z_{\ell+1};\ \ell = 1, 2, \cdots)$

(2.5) *Harmonic-plus-Hard-core (HHC):* $F(z) = \mu z, \quad z > -b$
$= -\infty, \quad z = -b$

(2.6) *Exponential (Toda Lattice):* $F(z) = a\,(1 - \exp(-bz))$
(i.e., $\mu = ab$, $K_n = (-b)^{n-1}/n!$ in (2.3))

A remarkable feature of the exponential lattice (among many remarkable results, see Toda 14]) is that this nonlinear system is apparently completely integrable for suitable boundary conditions. This integrability arises because the N analytic constants of the motion discovered by Hénon [85] are in involution, and can therefore yield the remaining N constants (see [17, p. 323]). It is not obvious, however, that these additional constants are analytic or single-valued functions—which is presumably relevant with regards to irreversible behavior. This offers a unique opportunity to probe the relationship (and folklore) between constants of the motion and irreversibility. This topic will be discussed below.

An extension of (2.2) to longer range forces (which, for example, are of critical importance in explaining compressibility properties of real solids) would be

$$m_n\ddot{y}_n = \sum_{k=1}^{N-n+1} F_k(y_{n+k} - y_n) - \sum_{k=1}^{n} F_k(y_n - y_{n-k}). \tag{2.7}$$

A basic constant of the motion (the energy) is

$$H = \sum_{n=1}^{N} \tfrac{1}{2}m_n\dot{y}_n^2 + \sum_{k,n} V_k(y_{n+k} - y_n) \tag{2.8}$$

where $V_k(z)$ is the potential energy, related to the function $F(z)$ by

$$F_k(z) = +dV_k/dz. \tag{2.9}$$

The use of such extended forms of the equations of motion appears to have been very limited to date, and may represent a very interesting future line of research.

The harmonic lattice corresponds to the case $K_n = 0$ in (2.3), and if one introduces the dimensionless time

$$\tau = 2\sqrt{\mu/m}\ t \equiv \omega_0 t \tag{2.10}$$

for the monatomic lattice ($m_n = m$), then (2.2) reduces to

$$\ddot{y}_n(\tau) = \tfrac{1}{4}(y_{n+1} + y_{n-1} - 2y_n). \tag{2.11}$$

A normal mode solution of these equations consists of the special solution $y_n = a_k(\tau)e^{ikn}$ where the normal mode, $a_k(\tau)$, is simple harmonic

$$\ddot{a}_k = -\omega_k^2 a_k; \qquad \omega_k = \sin(k/2). \tag{2.12}$$

If one sets $k = \kappa h$ (h given in (2.1)), then κ is called the wave number, and the group velocity of the waves is given by

$$v_g = \frac{d}{d_\kappa}\bar{\omega}_k \equiv \frac{d}{d_\kappa}\omega_0 \sin({}_\kappa h/2) = v_s \cos({}_\kappa h/2) \tag{2.13}$$

where $v_s = h\sqrt{\mu/m}$ is the sound speed. It will be noted that the group velocity decreases with large κ (shorter wavelength)—a phenomena which disperses a localized spatial disturbance because it must contain large values of k. The property is fundamental to harmonic lattices, and has numerous repercussions, as will be seen (e.g., Figure 2.3).

The general solution of (2.11) is

$$y_n = \sum_k a_k(t)e^{ikn}. \tag{2.14}$$

Note that $a_{-k} = a_k^*$ is required by the reality of y_n. The allowed values of k in the summation (2.14) are determined by the boundary con-

ditions $y_0(t)$ and $y_{N+1}(t)$. Several common boundary conditions, and resulting values of k, are:

Free Ends: $y_0(t) = y_1(t)$; $y_{N+1}(t) = y_N(t)$

$$k = \ell\pi/N \ (\ell = 0, 1, \cdots, N-1); \tag{2.15}$$

$$y_n = \sqrt{2/N}\,\Sigma a_k \cos((2N-1)k).$$

Periodic (Born-von Karman): $y_{n+N}(t) = y_n(t)$

$$k = 2\pi\ell/N, \ (-N/2 \leqq \ell \leqq N/2); \tag{2.16}$$

$$y_n = 1/\sqrt{N}\ \Sigma a_k e^{ikn}.$$

Fixed Ends: $y_0 \equiv 0 \quad y_{N+1} \equiv 0$

$$k = \ell\pi/(N+1) \ (\ell = 0, \cdots, N); \tag{2.17}$$

$$y_n = \sqrt{2/(N+1)}\ \ \Sigma\ a_k \sin(kn).$$

Several elementary points should be noted. The boundary conditions do not influence the functional form of the frequencies ω_k, (2.12), but only slightly shift the values of k—a feature of presumably little irreversible consequence. The periodic boundary condition, which is very popular due to its simplicity, is clearly inappropriate for the description of heat conduction (where the two ends of the lattice are in contact with thermal reservoirs at different temperatures, and hence not equivalent). This point is frequently ignored, but it is an example of the difficulty which arises in describing spatial inhomogeneity, while at the same time trying to ignore the necessary correlations which must thereby exist between *these* normal modes.

It is possible to introduce modes which have a certain degree of inhomogeneity incorporated in their definition (through their boundary condition). An example which I considered ten years ago is the "viscous-antiviscous" boundary conditions.

$$\begin{aligned} y_o - y_1 &= \mu_1 \dot{y}_1; & y_{N+1} - y_N &= \mu_N \dot{y}_N \\ \mu_1\mu_N &= -1; & (\mu_1 + \mu_N &\neq 0). \end{aligned} \tag{2.18}$$

In the physical terms, one end particle is in a frictional fluid (negative μ) whereas the other end continually *receives* energy ("antiviscous"). This can be seen by substituting (2.18) into (2.11) for $n = N$ and $n = 1$. This model has a dynamical irreversible coupling to the outside world, in contrast to a statistical coupling to a thermal reservoir. An application of this model will be given below.

If the normal modes (2.15–2.17) are substituted into the appropriate Hamiltonian (2.8), and the dimensionless time (2.10) is used, one obtains

$$\frac{H}{4\mu} = \sum \frac{1}{2}\left(\frac{dy_n}{d\tau}\right)^2 + \frac{1}{2}(y_{n+1} - y_n)^2 = \sum E_k \tag{2.19}$$

where the quantities

$$E_k \equiv \tfrac{1}{2}[\dot{a}_k\dot{s}_{-k} + \omega_k{}^2 a_k a_{-k}], \text{ for (2.16)};$$
$$\text{or } E_k \equiv \tfrac{1}{2}(\dot{a}_k{}^2 + {}_{\omega k}{}^2 a_k{}^2), \text{ for (2.15) and (2.17)} \tag{2.20}$$

are frequently referred to as the energy of the normal modes, even in the cases where there are nonlinear forces (and hence there is an interaction energy between the normal modes). Much of the computer analysis of nonlinear lattices has been presented in terms of the behavior of the functions E_k, which are constant in the harmonic lattice. The ratio $N_k = E_k/\hbar\omega_k$ is the (semi-classical) representation of the "number of phonons", with wavenumber k.

If the more general harmonic interaction, corresponding to nonlocal forces (2.7), is used so that (2.11) is generalized to

$$\ddot{y}_n = \frac{1}{4}\sum_{\ell=1}^{N-n+1} \gamma_\ell(y_{n+\ell} - y_n) - \frac{1}{4}\sum_{\ell=1}^{n} \gamma_\ell(y_n - y_{n-\ell}) \tag{2.21a}$$

the frequencies of the normal modes $a_k(\tau)$ are formally given by

$$\omega_k{}^2 = \sum_\ell \gamma_\ell \sin^2(k\ell/2). \tag{2.21b}$$

The satisfaction of boundary conditions, however, now becomes a much more complicated proposition. This form of the frequency begins to exhibit some of the complexity of real solids. In particular, it is not necessarily a monotonic function of k—a point of possible importance in the theory of heat conduction (e.g., see the L curve in Figure 2.2). It clearly can also have a considerable effect on the group velocity, (2.13).

Another description of the dynamics of harmonic lattices which is frequently used is in terms of the action-angle variables (J_k, θ_k), defined by

$$\dot{a}_k = (2\omega_k J_k)^{1/2}\cos\theta_k, \quad a_k = (2J_k/\omega_k)^{1/2}\sin\theta_k. \tag{2.22}$$

The harmonic Hamiltonian is then simply $H = \Sigma_k \omega_k J_k$, and the equations of motion are

$$\dot{J}_k = -\frac{\partial H}{\partial \theta_k} = 0, \qquad \dot{\theta}_k = \frac{\partial H}{\partial J_k} = \omega_k. \tag{2.23}$$

Thus the action is constant, and the angle is proportional to the time. Since the physical state is identical modulo 2π in the angle variable, the action-angle description can be viewed as an N-dimensional

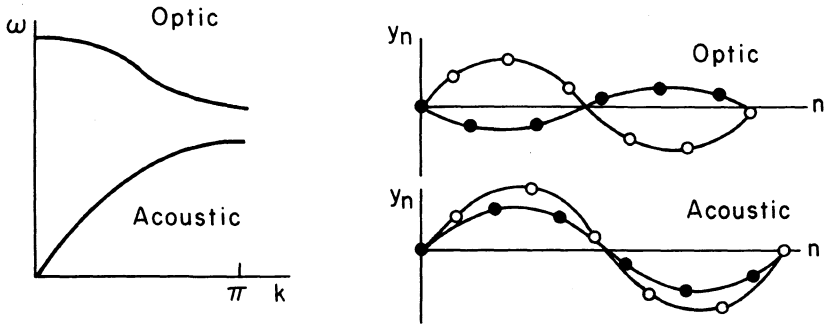

Figure 2.1. Normal mode frequency spectrum for a one-dimensional diatomic lattice.

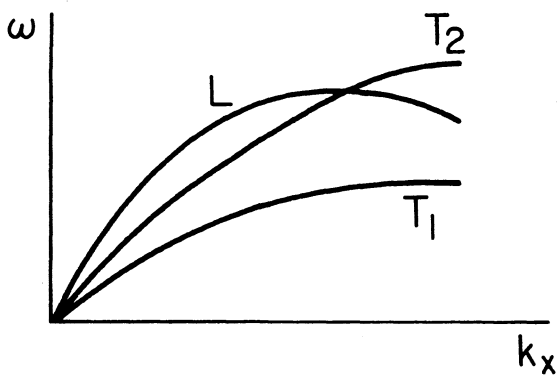

Figure 2.2. Schematic frequency spectrum for the longitudinal and transverse modes of a three-dimensional lattice as a function of one component of the wave vector.

torus—a point of view frequently emphasized in the Russian literature.

A generalization of the frequency spectrum (2.12) is illustrated in Figure 2.1. In the case of a diatomic one-dimensional lattice, there are two modes of oscillation called the optic and acoustic branch. A typical displacement, (2.14), is illustrated in each case. The expression for the (dimensional) frequencies is now

$$(2.24)\quad \omega_k^2 = \mu\left[\frac{1}{m_1}+\frac{1}{m_2} \pm \sqrt{\left(\frac{1}{m_1}-\frac{1}{m_2}\right)^2 + \frac{(1+\cos k)^2}{m_1 m_2}}\right].$$

which reduces to a "folded" version of (2.12) if $m_1 = m_2$ (see general references). It will be noted that the group velocity of the optic branch is very small, and hence these modes are not *directly* effective in transferring energy through a lattice. Another generalization is shown in Figure 2.2. In this case the lattice is a monatomic three dimensional lattice, so that there are two transverse and one longitudinal branches. These frequency spectra are at the heart of much of the historic development of irreversible results, as I will outline below.

In considering lattice systems involving large numbers of particles, two limiting situations should be clearly distinguished, namely the *thermodynamic limit*

$$\begin{gathered} \mathrm{N} \to \infty,\ L \to \infty,\ L/N = h \text{ (finite)} \\ \omega_k \leqq \omega_0 = 2\sqrt{\mu/m} \text{(frequency spectrum becomes dense);} \end{gathered} \tag{2.25}$$

and what I will call a *continuum limit:*

$$\begin{gathered} N \to \infty,\ m \to 0 \quad Nm = M \text{ (finite)};\quad h \to 0 \quad Nh = L \text{ (finite)} \\ \mu \to \infty,\quad \mu h^2/m = v_s^2 \text{ (finite)};\quad \omega_k \to \omega_0 k/2 \\ (\omega_k \text{ become uniformly spaced, hence commensurable}). \end{gathered} \tag{2.26}$$

The effect of these two limits on the frequency spectrum is illustrated in Figure 2.3 (note that the l intervals are uniformly spaced, and the k intervals become dense). The thermodynamic limit simply consists of a

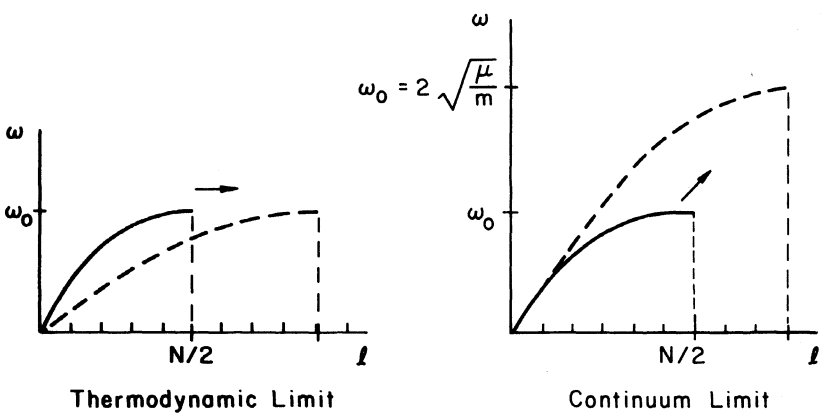

Figure 2.3. Frequency spectrum in the two limits (2.25) and (2.26).

larger system, thereby hopefully reducing the influence of boundary effects. It is this limit which is normally considered in the study of statistical (e.g., irreversible) properties. It is also the limit in which phonons can be treated semiclassically (because the energy spectrum, $\hbar\omega_k$, becomes dense). The continuum limit on the other hand involves changing properties of the system (m, μ, h) so as to remove its discrete particle characteristics, and making it closer (in some sense) to a fluid system. It is this limit (or some generalization) which has been used in recent years to obtain the Korteweg-deVries, the Boussinesq, and other nonlinear partial differential equations from the lattice equations (2.2). This limiting process will be considered in greater detail below. In particular, note that (2.26) does not specify what limits should be used for the nonlinear coefficients K_n in (2.3) and (2.6), and hence does not fully define a limiting process.

Finally I would like to review briefly a solution of (2.11) apparently known to Hamilton (but unpublished) and discovered by Schrödinger, among others (see [12, p. 668 *ff*], for a historical survey). This solution contrasts with the normal mode solution in that it is appropriate for the description of a localized disturbance, rather than the nonlocal normal modes. This is particularly interesting in light of the localized nonlinear solutions which are now known. The connection between these soliton solutions and the following localized solutions has not been made to date, and represents an interesting and possibly enlightening study. The solutions result from introducing the functions

$$z_{2n} = \sqrt{m}\dot{y}_n; \qquad z_{2n+1} = \sqrt{\mu}\ (y_n - y_{n+1}) \tag{2.27}$$

in the harmonic equations

$$m\ddot{y}_n = \mu(y_{n+1} - y_n) - \mu(y_n - y_{n-1})$$

and showing that these functions satisfy the equations

$$\dot{z}_n(\tau) = \tfrac{1}{2}(z_{n-1} - z_{n+1}) \qquad \text{(all } n\text{)} \tag{2.28}$$

where τ is the dimensionless time (2.10). The equations (2.28) will be recognized as the recurrence relation for Bessel functions, so that the solution which is finite at $\tau = 0$ is

$$z_n(\tau) = \sum_{m=-\infty}^{\infty} x_m(0)\, J_{n-m}(\tau).$$

Thus, for example, if only one particle is initially disturbed, so that $\dot{y}_n(0) = v_0\delta_{n0}$, then $z_{2n}(0) = \sqrt{m}\ v_0\delta_{n0}$, and $y_n(\tau) = v_0 J_{2n}(\tau) \sim v_0/\sqrt{\tau}$. Such a simple result would be quite difficult to obtain using normal modes. The beauty of the solution (2.29) is somewhat complicated when

boundary conditions are taken into account. Thus, if particle $n = 1$ is free, then $Y_1(t) - y_0(t) = 0 = z_1(\tau)$ must hold. This condition will be satisfied for all times if the initial conditions

$$z_{1-m}(0) = (-1)^{m+1} z_{1+m}(0) \quad (m = 1, 2, \cdots) \tag{2.30}$$

are imposed in (2.29). To illustrate this with the above example, assume that the *end* particle initially receives an impulse, so that $\dot{y}_n(0) = v_1 \delta_{n1}$ and all $y_n(0) = 0$. One finds that in this case

$$\dot{y}_n(\tau) = v_1 2(2n - 1) J_{2n-1}(\tau)/\tau \tag{2.31}$$

which asymptotically proportional to $2v_1(2n - 1)/\tau^{3/2}$. This is very different from the infinite lattice result noted above ($\tau^{-1/2}$). This difference is a consequence of the fact that the harmonic lattice does not "forget" its boundary condition, even in the thermodynamic limit (2.25)—a point which will recur below. This solution is illustrated in Figure 2.4, and it exhibits the dispersive character of the harmonic lattice due to the variable group velocity, (2.13). It is this dispersive prop-

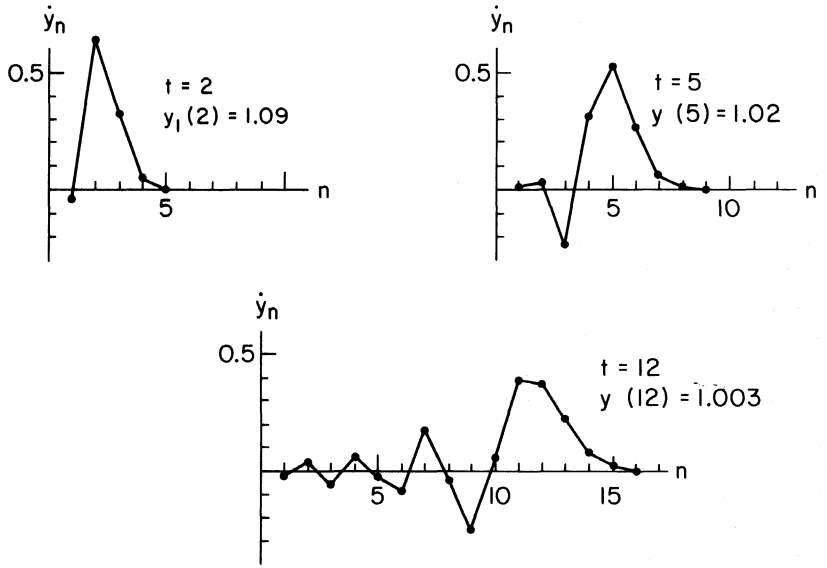

Figure 2.4. The Schrödinger solution (2.29) in a semi-infinite lattice for an initial impulse on the left end ($v_1 = 1$). Here $t \equiv \tau/2$ is used, to compare with the sound velocity which is one unit per (t) seconds.

erty which is counteracted by the nonlinear forces in forming solitons. The figure also contains the value of $y_1(t) = \Sigma n J_{2n}(t)$, showing that the harmonic lattice remains compressed—a point that also occurs with reservoir interactions (§ 4).

We note finally that the equations (2.28) admits the following constants of the motion (for an infinite system)

$$I_m = \sum_{n=-\infty}^{\infty} z_n z_{n+m}. \tag{2.32}$$

These constants were used by Brout and Prigogine [4] and will be relevant in the discussion of energy transport through harmonic lattices. We now turn to the transport considerations.

3. **Classic Concepts of Energy Transport.** One of the major applications of lattice dynamics which interests physicists is in the problem of energy flux due to the lattice motion. Historically this field dealt mostly with the problem of lattice thermal conductivity, but in recent years interest has also extended to large amplitude coherent excitations, second sound, and other "exotic" problems (see the references for a few examples). Actually some of the "exotic" problems are more easily analyzed than the historic problem of lattice thermal conductivity, which not only involves nonlinear dynamics, but statistical considerations, spatial inhomogeneity, and coupling of the lattice with thermal reservoirs (for a stationary state). Indeed this transport problem has the unique complication, both analytical and conceptual, of involving a spatial inhomogeneity in a statistical quantity, the "temperature"—which is an equilibrium concept. While such difficulties are presumably of little pragmatic concern, they have recurred repeatedly in various disguises in theoretical treatments ever since the classic theory was developed by Peierls [33] in 1929. This theory was a clever application (to phonons) of the concepts which had been developed by Boltzmann so successfully in the theory of gas dynamics. However this theory loses a great deal of the intuitive appeal enjoyed by Boltzmann's theory due to the nonlocal nature of normal modes, as contrasted with gas molecules. Thus for example, the introduction of localized wave packets to define local properties encounters difficulties if "mean free paths" are shorter than normal mode wave lengths (see, e.g., Ziman [18] for some discussion and references). The recent development of solitons reintroduces this feature of localization, but at the expense of much of the "interactions" in the lattice—and hence a loss of irreversibility. It thus appears that the theory of lattice thermal conductivity is damned if it does and damned if it doesn't localize the lattice disturbances. This point will be encountered in several mathematical problems below.

The energy flux can be established most completely through the use of the conservation of energy. If $\mathscr{E}(x, t)$ is the energy density and $J(x, t)$ is the energy flux density, then the conservation of energy is expressed through the equation

$$\frac{\partial \mathscr{E}}{\partial t} + \frac{\partial}{\partial x} J = 0. \tag{3.1}$$

Following Hardy [22], if one introduces a differentiable, localized δ-type function $\Delta(x - x_i) > 0$ which is normalized to unity, $\int_{-\infty}^{\infty} \Delta(x - x_i)\, dx = 1$, then the energy density can be written in the transparent form

$$\mathscr{E}(x, t) = \sum_{n=1}^{N} \Delta(x - x_n(t)) \left\{ \frac{1}{2} m_n \dot{x}_n^2 + \frac{1}{2} \sum_{\ell \neq n} V(x_\ell - x_n) \right\}. \tag{3.2}$$

If this is substituted into (3.1), then it can be shown that, for the potential $V(z) = \mu(1/2\, z^2 - k/3\, z^3)$ (corresponding to the polynomial force (2.3)), the *total* energy flux in the entire lattice

$$\mathscr{J}(t) = \int_{-\infty}^{\infty} J(x, t)\, dx \tag{3.3}$$

is given by

$$\begin{aligned} \mathscr{J}(t, N) = & \sum^{N} \frac{1}{2} \dot{y}_n^3 \sum_{n=1}^{N-1} (\dot{y}_{n+1} + \dot{y}_n) \left\{ \frac{1}{4} (y_{n+1} + y_n)^2 \right. \\ & \left. - \frac{K}{3} (y_{n+1} - y_n)^3 \right\} \\ & - \sum^{N-1} \frac{1}{2} (\dot{y}_{n+1} + \dot{y}_n)\{y_{n+1} - y_n - K(y_{n+1} - y_n)^2\} \end{aligned} \tag{3.4}$$

where the dimensionless time (2.10) has been introduced, and the flux normalized to mv_s^3 (v_s, the sound speed, (2.13)). One of the consequences of lattice ordering is that the first two summations in (3.4) do not contribute significantly to the lattice thermal conductivity (as they do in gases), so that one can consider only the total "lattice energy flux", defined as

$$\begin{aligned} \mathscr{J}_L(t, N) &= - \sum \frac{1}{2} (\dot{y}_{n+1} + \dot{y}_n) F(y_{n+1} - y_n) \\ &= - \sum_{n=1}^{N-1} \frac{1}{2} (\dot{y}_{n+1} + \dot{y}_n)\{(y_{n+1} - y_n) - K(y_{n+1} - y_n)^2\}. \end{aligned} \tag{3.5}$$

Moreover, historically (e.g., in Peierls' theory) only the *harmonic portion* of (3.5) was considered,

$$\hat{f}_{HL}(t, N) = -\sum_{n=1}^{N-1} \frac{1}{2}(\dot{y}_{n+1} + \dot{y}_n)(y_{n+1} - y_n)$$

$$= \sum \omega_k \frac{\partial \omega_a}{\partial h} a_k \dot{a}_{-k}. \tag{3.6}$$

As can be seen from a computer calculation of $\hat{f}_L$ and $\hat{f}_{HL}$, shown in figure 3.1, the harmonic contribution to the energy flux, $\hat{f}_{HL}$, need *not* be the dominant contribution to the total lattice energy flux, $\hat{f}_L$, which casts doubts on some theories from the outset. This also shows up dra-

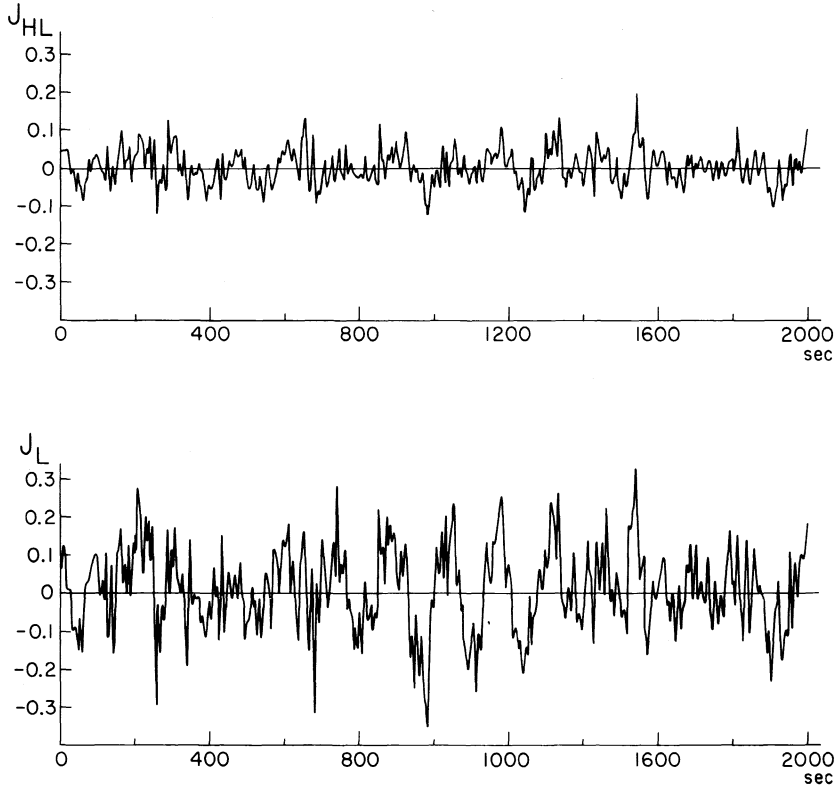

Figure 3.1. The total energy flux in an equilibrium nonlinear lattice, $\hat{f}_L$, and the usual harmonic approximation, $\hat{f}_{HL}$, at concurrent times.

matically in the comparison of the time averaged equilibrium values of $\hat{f}^2$, (3.4), and $\hat{f}^2_{HL}$ (Jackson, Pasta, and Waters [**24**]), namely $\langle \hat{f}^2 \rangle = 5.2 \langle \hat{f}^2_{HL} \rangle$. This fact does not seem to be widely appreciated in the literature.

Irreversibility, as it occurs in lattice thermal conductivity is presumably expressed through Fourier's *statistical* law of heat conduction

$$\langle J \rangle = -K_T \nabla T(x) \tag{3.7}$$

where K_T is called the coefficient of heat conductivity. Here the quantity $\langle J \rangle$ signifies a "short" time average of the J appearing in (3.1). It is the time averaged energy flux of course which is observed experimentally.

One implication of (3.7) is that $K_T(N)$ associated with a finite lattice should become an *intrinsic* ("intensive") property of the lattice as N goes to infinity (the *thermodynamic* limit, (2.25)), that is

$$\begin{aligned} \lim_{N\to\infty} K_T(N) &\equiv \lim_{N\to\infty} \langle J_L(t, N)\rangle/(\triangle T/N) \\ &= \lim_{N\to\infty} \langle \hat{J}_L(t, N)\rangle/\triangle T = K_T \text{(finite)} \end{aligned} \tag{3.8}$$

where $\triangle T$ is the temperature difference between the two thermal reservoirs at the ends of the lattice and $\langle J \rangle$ again represents a time averaged flux. The basic problem is to understand for what lattice systems (3.7) is indeed satisfied, and to predict the values of K_T in terms of the interparticle forces.

Presumably the "temperature" in (3.7) should be defined dynamically in terms of the time averaged energy density (3.2) by the relationship (for the one-dimensional system)

$$k_B T(x)/h = \langle \mathscr{E}(x, t) \rangle \tag{3.9}$$

where k_B is the Boltzmann constant and h is the interparticle spacing (2.1). Legitimate questions can be raised as to whether this is the temperature actually measured in any experiment, which is normally sensitive only to the local kinetic energy. The condition (3.8) avoids this problem by using the reservoir temperatures. However (3.8) is thereby only a necessary and not sufficient condition for (3.7) to be valid, because the latter involves the internal temperature gradient. Indeed (3.8) is not even necessary unless the boundary thermal resistance, $R_b \equiv (\triangle T)_b/\langle J \rangle$ (b = boundary), is also an intrinsic property of the lattice reservoir interface. These points are raised not to complicate matters, but simply to show that the matter *is* complicated—even to de-

fine! This is unfortunate, because the dynamic origin of irreversibility is sufficiently baffling in itself without having the additional weight of indecisive definitions. These difficulties are, of course, usually bypassed so that practical theories suitable for real solids, which presumably contain many generators of irreversibility (defects, impurities, boundary scattering, etc.), can be roughly estimated (e.g., see the recent book by Parrott and Stuckes [3]).

The present concern centers on the detailed dynamic behavior of (possibly unrealistic) one-dimensional lattices, and the degree to which they satisfy Fourier's law (3.7). It does not appear to me that this question has been clarified significantly since, for example, Kirkwood asked Brout "Does a one-dimensional crystal have a finite thermal conductivity?" some twenty years ago (in [34, p. 139]). Or, to be more accurate, it does not appear that any basic theory can answer "yes" to the above question, despite computer calculations which give *some* evidence that it *might* be true.

The most elementary picture of heat conductivity (Debye) yields, in analogy with the kinetic theory of gases, $K_T = Cv_s\ell/3$, where C is the specific heat capacity, v_s the velocity of sound and ℓ a "mean free path". In terms of a "relaxation time" $\tau = \ell/v_s$ of a normal mode, and taking into account their differing group velocities, (2.13), this becomes

$$K_T = \tfrac{1}{3} \int C(\omega) v_g^2(\omega) \tau(\omega) g(\omega)\, d\omega \tag{3.10}$$

where $g(\omega)$ is the density of normal modes.

In this type of expression, the fundamental problems rest on the combined use of the harmonic normal modes and the adequacy of the concept of their "relaxation time", $\tau(\omega)$. This concept has its origin in transition probabilities obtained frequently from second order perturbation theory (Fermi's "golden rule") and is closely associated with Fermi's interest in the computer calculations made by Fermi, Pasta and Ulam to be discussed below (§ 4).

In a harmonic lattice the normal modes do not interact so that their relaxation time is infinite. This gives rise to the misleading statement that a harmonic lattice has an infinite heat conductivity, when in fact it simply means that Fourier's law (3.7) is not valid. The correct statement is that $J_L(r, N)$ is finite, so that the limit in (3.8) is infinite. In an infinite harmonic lattice this lack of "resistance" to an energy flux is clear from the first constant of the motion in (2.32), because

$$d I_1/dt \equiv d \hat{J}_{HL}(t, \infty)/dt = 0$$

where J_{HL} is given in (3.6).

The fact that the energy transport through a harmonic lattice is not

related to the local kinetic energy is nicely illustrated by the "viscous-antiviscous" boundary conditions (2.18). Using

$$\langle J_H \rangle \equiv \lim_{\tau \to \infty} \frac{1}{2\tau} \int_{-\tau}^{\tau} (\dot{y}_1 + \dot{y}_0)(y_0 - y_1)\, dt \tag{3.11}$$

it is easy to show that

$$\begin{aligned} &\text{(a)} \qquad \operatorname{sign} \langle J_H \rangle = \operatorname{sign} \mu_1; \\ &\text{(b)} \qquad \langle \dot{y}_1^2 \rangle / \langle \dot{y}_N^2 \rangle = \mu_N^2 \cdot \qquad (\mu_1 \mu_N = -1). \end{aligned} \tag{3.12}$$

Thus the direction of the energy flow, given by (a), is independent of which end of the lattice is "hotter", given by (b)! Such "anomalous" (nonirreversible) properties of harmonic lattices can be found in many examples.

An outstanding case in point is the exact results obtained by Rieder, Lebowitz, and Lieb [38] for an ensemble of harmonic lattices coupled to two thermal reservoirs at different temperatures T_L (left) and T_R (right). They found that in the thermodynamic limit,

$$\langle J(N, \lambda) \rangle \to C(\lambda)(T_L - T_R) \tag{3.13}$$

that is, $\langle J \rangle$ is proportional to $(T_L - T_R)$ rather than $(T_L - T_R)/N$, required for a finite K_T in (3.8). The parameter λ in (3.13) is essentially the collision frequency between the lattice and the thermal reservoirs. A similar dependence on $(T_L - T_R)$ was found by Helleman [23] in the exact solution for the two-dimensional harmonic lattice. They also found an interesting effect which amounts to a boundary (coupling) resistance with the reservoir, namely $C(\lambda)$ takes on a maximum value for $\lambda = \sqrt{3}\,\omega_0/2$. The reason for this is due to the fact that a lattice is a low pass filter (transmitting frequencies only within its normal mode range—see Figures 2.1 and 2.2). Thus if the interaction with the reservoir is too frequent, λ becomes too large, the lattice cannot respond (accept the energy), so $C(\lambda)$ decreases. If λ is too small there is no coupling to the reservoirs, so $C(\lambda)$ goes to zero—hence $C(\lambda)$ has a maximum.

This coupling to the reservoirs is not an academic point but one of both practical interest, and a difficulty which arises in computer calculations of lattice thermal conductivity. Their rigorous result (for their reservoir coupling) moreover yielded a totally anomalous interior temperature distribution, T_i, shown in Figure 3.2. Although $T_L > T_R$ they found $T_2 < \overline{T} < T_{N-1}$, where $\overline{T}$ is the mean temperature, $(T_L - T_R)/2$. Thus near the hot reservoir there are relatively cold particles, and vice versa! Such anomalous results, like (3.12), obviously defy intuition, and certainly Fourier's law.

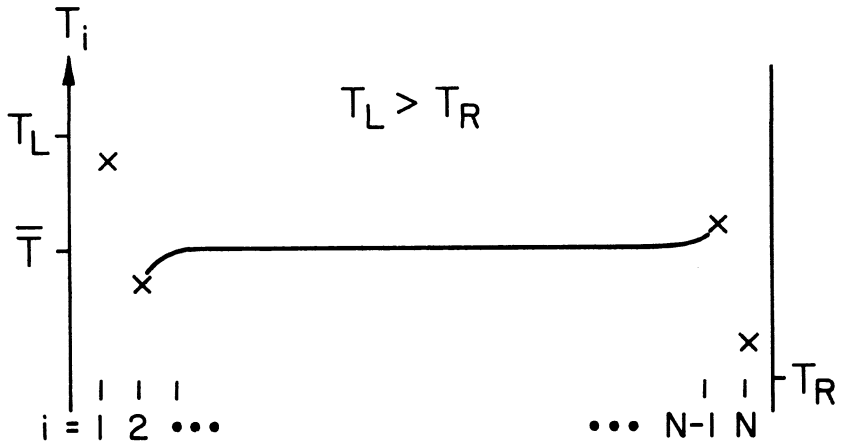

Figure 3.2. Theoretical temperature distribution in a harmonic lattice between two thermal reservoirs (Rieder, Lebowitz, and Lieb).

In an attempt to discover a system for which Fourier's law could be rigorously established in a system not involving nonlinear forces, O'Connor and Lebowitz [30] investigated heat conduction through isotopically disordered harmonic lattices, considering the influences of various boundary conditions. Visscher, who has made extensive computer studies with his co-workers, has recently [41] given a nice review of these results for isotopically disordered lattices. The fact that a harmonic lattice has variable masses does not, of course, alter the fact that it still possesses harmonic normal modes, and hence is still nonergodic. It is thus perhaps to be expected that such lattices also do not satisfy Fourier's law. Indeed the limit (3.8) vanishes for a lattice with fixed ends, and diverges if the ends are free (it is conjectured that $K_T \sim N^{-1/2}$ and $\sim N^{+1/2}$ respectively), again indicating the "abnormal" influence of the boundaries on a harmonic lattice. In any case, $\langle J(N)\rangle \to 0$ as $N \to \infty$ in contrast with (3.13).

The first theory to take into account the effects due to the nonlinear coupling within the lattice was due to Peierls [33], who obtained a "Boltzmann equation" for the "distribution function" $N_k(\underset{\sim}{r}, t)$ for the probable number of phonons (energy of the normal mode, (2.2)) of wave number k around $\underset{\sim}{r}$ at the time t. Obviously some limitations are required for the simultaneous use of $\underset{\sim}{k}$ and $\underset{\sim}{r}$ descriptions—a point usually left vague. This nonlinear integrodifferential equation is of the form (e.g., Ziman [18, p. 293 ff.]).

$$\frac{\partial N_k}{\partial t} + V_k \frac{\partial N_k}{\partial x} = \int\int [\{N_k N_k (1 + N_{k''}) - (1 + N_k)(1 + N_{k'}) N_{k''}\} Q_{kk'}^{k''} + \frac{1}{2}\{N_k (1 + N_{k'})(1 + N_{k''}) - (1 + N_k) N_{k'} N_{k''}\} Q_{kk'}^{k''}] dk' dk''. \tag{3.15}$$

Not only is it impossible to solve this equation, but its original derivation was essentially based on second order perturbation theory (through the kernel Q), involving the use of random phase assumptions between the normal modes, which is certainly less appealing than the stosszahlansatz used by Boltzmann in the case of molecular collisions (see the discussion in the FPU problem, § 5). Studies have been made to extend Peierls' equation to long times without the repeated use of the random phase approximation (e.g., Brout and Prigogine [4]) as well as basic studies of the application of perturbation theories to such collective many-body problems (e.g., Van Hove [15]). More recent derivations of the phonon Boltzmann equation, with corrections, have been given by Horie and Krumhansl [6] and Kwok [9]. Despite these efforts some basic questions remain about the conditions necessary for irreversibility, and particularly about stationary nonequilibrium states, as in thermal conductivity (see, e.g., the review by Carruthers [21], and more recent reviews in [7]).

Without getting unduly involved in these considerations, it is perhaps useful to point out one feature that all of the perturbation theories find essential to irreversibility in lattices, but which so far has played no role in the soliton picture of energy conduction. This can be illustrated if the anharmonic forces only involve second and third order nonlinearities, so the normal modes satisfy equations of the form

$$\ddot{a}_k = -\omega_k^2 a_k - \sum V_{-k\ell m} a_\ell a_m + \sum W_{-k\ell mn} a_\ell a_m a_n. \tag{3.16}$$

It is not difficult to show that the rate of change of the total harmonic energy flux, (3.6) is then given by

$$\frac{d\hat{f}_{LH}}{dt} = \frac{i}{3} \sum \left[\omega_k \frac{\partial \omega_k}{\partial k} + \omega_\ell \frac{\partial \omega_\ell}{\partial \ell} + \omega_m \frac{\partial \omega_m}{\partial m} \right] V_{k\ell m} a_k a_\ell a_m$$

$$- \frac{i}{4} \sum \left[\omega_k \frac{\partial \omega_k}{\partial k} + \omega \frac{\partial \omega_\ell}{\partial \ell} + \omega_m \frac{\partial \omega_m}{\partial m} + \omega_k \frac{\partial \omega_n}{\partial_n} \right] W_{k\ell mn} a_k a_\ell a_m a_n \tag{3.17}$$

a result first obtained by Peierls. Note that (3.17) is not a statistical equation, and is therefore not subject to any irreversibility interpretations. The first and second sum in (3.17) are sometimes referred to as three- and four-phonon processes. In a *perfect lattice*

$$\begin{aligned} V_{k\ell m} &\neq 0 \text{ only if } k + \ell + m = 0, \pm 2\pi \\ W_{k\ell mn} &\neq 0 \text{ only if } k + \ell + m + n = 0, \pm 2\pi. \end{aligned} \tag{3.18}$$

If there is no dispersion, so that $\omega_k = k v_s$, then both the three- and four-phonon contributions to (3.17) will vanish unless

$$k + \ell + m = \pm 2\pi, \text{ or } k + \ell + m + n = \pm 2\pi. \tag{3.19}$$

This follows because the [ ] coefficients in (3.17) will vanish otherwise. Peierls called the terms (3.19) "Umklapp" processes, in contrast to the "normal" processes (e.g., $k + \ell + m = 0$), and emphasized their importance in producing thermal resistance (e.g., $d\hat{f}_{LH}/dt \neq 0$). An interesting situation arises however when one considers the time average of (3.17) *and* uses the *harmonic* solutions (2.13) for the $a_k(t)$. It follows immediately that the three- and four-phonon contributions do not vanish when time averaged only under the following conditions:

$$\begin{aligned} \langle d J_{LH}/dt \rangle_{3p} &\neq 0 \text{ only if } \omega_k + \omega_\ell + \omega_m = 0 \\ \langle d J_{LH}/dt \rangle_{4p} &\neq 0 \text{ only if } \omega_k + \omega_\ell + \omega_m + \omega_n = 0. \end{aligned} \tag{3.20}$$

Now, because of the dispersive behavior of the ω_k, Figure 2.1, it follows that if

$$k + \ell + m = 0, \pm 2\pi \text{ then } \omega_k + \omega_\ell + \omega_m \neq 0 \quad \text{(in one-dimensional lattices).} \tag{3.21}$$

However it *is* possible for

$$k + \ell + m + n = 0, \pm 2\pi \text{ and } \omega_k + \omega_\ell + \omega_m + \omega_n = 0 \quad \text{(in one dimension).} \tag{3.22}$$

The net result of this analysis due to Peierls is to conclude that there is only resistance to heat conduction in a one-dimensional system due to four-phonon umklapp processes—which is obviously a rather restricted class of the nonlinear interactions. In higher dimensions the situation changes because it is possible for $\omega_{\underset{\sim}{k}} + \omega_{\underset{\sim}{\ell}} + \omega_{\underset{\sim}{m}} = 0$ if $\underset{\sim}{k} + \underset{\sim}{\ell} + \underset{\sim}{m} = \underset{\sim}{K}$ (called a reciprocal lattice vector, which has the property $\exp[i(\underset{\sim}{k} + \underset{\sim}{K}) \cdot \underset{\sim}{r}_n] = \exp[i\underset{\sim}{k} \cdot \underset{\sim}{r}_n]$ for all atomic locations $\underset{\sim}{r}_n$. In the simple case (2.14) this corresponds to 2π). Moreover because of the different (longitudinal-transverse) branches of the frequency spectrum (see figure 2.2) it is possible to satisfy both (3.20) and (3.18) for even three phonon interactions. This is the basis for much of the belief that there should be a significant difference in the thermal conduction of one- and two-dimensional perfect lattices—a result so far *not* found in any computer calculations (see, e.g., Rich, Visscher, and Payton [36], and Nakazawa [28]).

These results concerning the influence of the nonlinear forces on the energy flux are subject to a number of doubts. Thus the *harmonic* solution was used in the time averages (3.20)—a point noted before by MacDonald [26] in obtaining zero resistance to the energy flux in a one-dimensional system. MacDonald obtained this result even when the *total* lattice energy flux, (3.5), is considered. Indeed the result is entirely altered if $\hat{f}_L$ is used instead of $\hat{f}_{LH}$, (3.6), for then

$$\begin{aligned} \hat{f}_L = i \quad & \omega_k \frac{\partial \omega_k}{\partial k} \dot{a}_k a_{-k} \\ & - 1 \sum V_{k\ell m} \frac{1}{\omega_k} \frac{\partial \omega_k}{\partial k} \dot{a}_k a_\ell a_m \\ \dot{a}_k a_\ell \, a_m a_n \quad & + i \sum W_{k\ell mn} \frac{1}{\omega_k} \frac{\partial \omega_k}{\partial k} \end{aligned} \tag{3.23}$$

and one finds from (3.16) that

$$\begin{aligned} d\hat{f}_L/dt = & - 2i \sum V_{k\ell m} \frac{1}{\omega_k} \frac{\partial \omega_k}{\partial k} \dot{a}_k \dot{a}_\ell a_m \\ & + 3i \sum W_{k\ell mn} \frac{1}{\omega_k} \frac{\partial \omega_k}{\partial k} \dot{a}_k \dot{a}_\ell a_m a_n \end{aligned} \tag{3.24}$$

and this bears essentially no resemblance to the expression (3.17). MacDonald's result would indicate that the time average of (3.24) should vanish for harmonic $a_k(t)$. Thus these theoretical considerations of the influence of nonlinear forces has been considerably less than satisfactory. There is still plenty of room for good basic research in this area.

An entirely different approach to coefficient of heat conduction is in terms of the energy flux autocorrelation (see, Kubo [8], [18])

$$K_T = \lim_{t\to\infty} \lim_{N\to\infty} \frac{1}{kT^2L} \int_0^t \langle \hat{J}(N, t')\hat{J}(N, 0)\rangle \, dt' \tag{3.25}$$

where $L = Nh$, and

$$\langle \hat{J}(t)\hat{J}(0)\rangle \equiv \lim_{\tau\to\infty} \frac{1}{\tau} \int_0^\tau \hat{J}(N, t')\hat{J}(N, t + t') \, dt'. \tag{3.26}$$

In (3.25) the limit $N \to \infty$ is to be taken before the long time limit so as to avoid the problems associated with the Poincaré recurrence effect (for an estimate of the recurrence time in lattices, see the discussion in § 5). While this theory appears to be very "clean" compared with the above discussion, it too suffers from some significant problems. Even aside from questions relating to the validity of (3.25) (see Visscher [**40**] for a recent defense), the expression (3.26) appears to be unusable in any direct computer experiment, where N must remain *very* finite. Thus this formalism has not shed much light to date on the origin of thermal resistance in lattices. In fairness, however, one should point out that this same limiting difficulty arises in the (theoretical!) definition (3.8) of K_T.

In this section I have attempted to present a few of the theoretical ideas and results concerning the energy flux through lattices which have historically dominated this field. The lack of contact, much less agreement, between these ideas and either computer calculations or soliton concepts will be quite obvious in what follows.

4. **Computer Studies of Energy Transport.** In recent years there have been a number of numerical investigations of the energy flux through a lattice between two thermal reservoirs. These calculations have been made for both one- and two-dimensional systems, with and without isotopic disordering, and with a limited variation of the anharmonicity. One of the more complete reviews of these computations has been given recently by Visscher [**41**] who is responsible for much of the computational results in this area. The computations for one-dimensional systems involve a lattice shown in Figure 4.1, where the reservoirs are

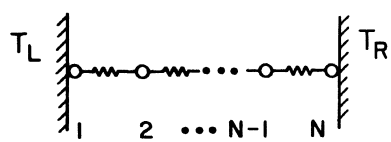

Fig. 4.1a

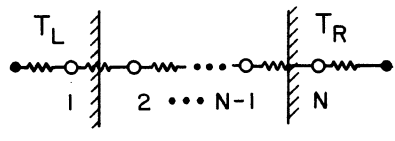

Fig. 4.1b

Figure 4.1. Two models for coupling a lattice to thermal reservoirs.

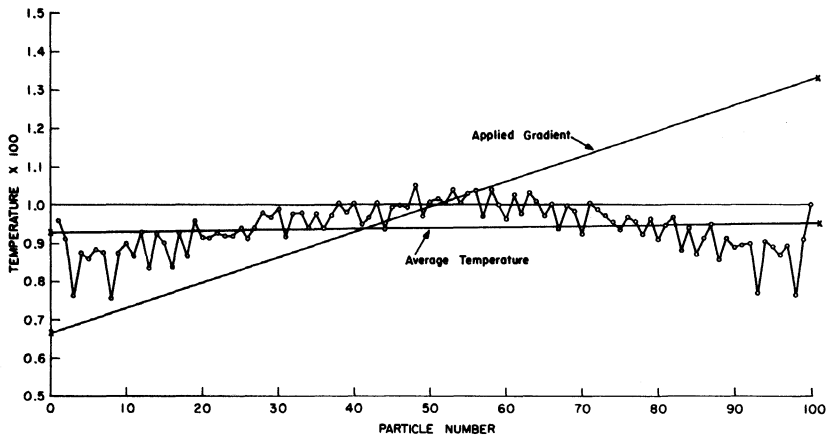

Figure 4.2. The time averaged kinetic energy ("temperature") of the particles in a non-equilibrium harmonic lattice (Jackson, Pasta, and Waters).

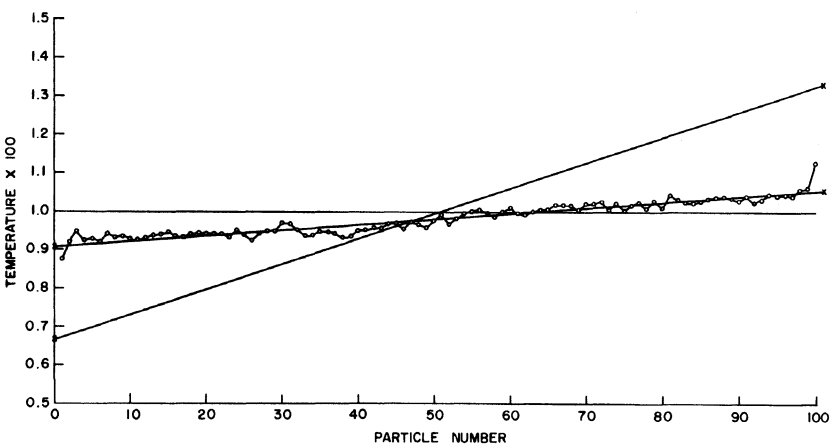

Figure 4.3. The same as Figure 4.2, except that lattice is now very anharmonic.

characterized by statistical energy distributions appropriate to two temperatures, T_L and T_R. The lattice can be coupled to the reservoirs by different methods, as illustrated in the two figures 4.1a and 4.1b. In the former case, the lattice interacts with the reservoir only when it reaches the reservoir wall, whereas in Figure 4.1b, the end partice interacts with the reservoir regardless of its location. Another model involving N "self-consistent" reservoirs along the lattice has also been employed by Visscher. The interior reservoir temperatures are fixed so that, in the steady state, no heat flows in or out of them.

Characteristically, for a harmonic lattice the internal time-averaged energy ("temperature") bears no relationship to the applied temperature difference, $T_R - T_L$. Thus Jackson, Pasta, and Waters [24] using the boundary condition shown in Figure 4.1a, found the spatially *periodic* (!) "temperature" distribution shown in Figure 4.2. The applied temperature gradient is shown by the sloping straight line (the optimum Fourier coupling between the reservoirs). By way of contrast, compare the theoretical Figure 3.2, which is more closely related to the coupling 4.1b. A result similar to this was obtained in computations made by Nakazawa [28]. For a sufficiently nonlinear lattice ($K_2 = 10$, $K_3 = 2\,K_2{}^2/3$) one finds an internal temperature gradient, but with very large boundary resistance effects (temperature jumps), as shown in Figure 4.3. These boundary effects are naturally influenced by the details of the coupling (Figure 4.1) to the reservoir, but Nakazawa [28] and Helleman [23] also found similar discontinuities. The important fact to note here is that a one-dimensional monatomic lattice *can* support an energy (real temperature?) gradient. The inclusion of defects increases this gradient (Jackson, Pasta, and Waters [24]), as does isotopic impurities (Visscher, et al., [32], [35], [36], [37], [40], [41]). However, whether any of these systems obey Fourier's law, with an intensive coefficient of heat conduction, (3.8), is not clear at present. Most computations of $K_T(N)$ have been for $N \leqq 100$, except for some results due to Helleman [23] with $N \leqq 200$, and Visscher involving N as large as 1000.

The displacements of 100 particles in a harmonic lattice as a function of time is illustrated in Figure 4.4. Note that, because of the coupling shown in Figure 4.1a, there are periods of time when the end particle is not in contact with the thermal reservoir. This is similar to the compression noted in Figure 2.4. It will be noted that, despite the dispersion of the harmonic modes, the reservoir impulses can propagate across the system and even interact with each other as coherent pulses, much like the nonlinear solitons (presumably due to the limited time it takes to cross the lattice). The corresponding picture for a nonlinear lattice is shown in Figure 4.5. The contact with the reservoir is now

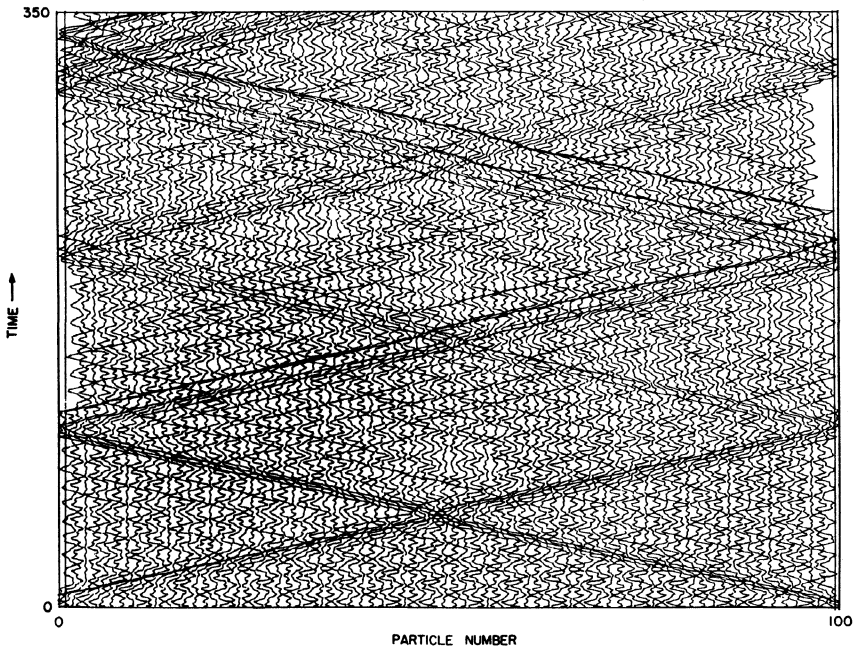

Figure 4.4. The locations, $x_n(t)$, of the particles in a harmonic lattice between two thermal reservoirs. Crossing pulses *slow down* during interaction because of the bulk displacements of lattice sections (Jackson, Pasta, and Waters).

improved (a stiffer lattice), which should reduce the temperature jump at the boundary.

What is of more interest in Figure 4.4 and 4.5 is that the pulses interfere with each other (have a velocity change where they cross) in the *harmonic* lattice, and interfere relatively little in the anharmonic lattice. One might expect that disturbances should superimpose in a harmonic lattice, and hence not exhibit this interference. The origin of this effect (as noted by K. Miura [27]) is that the Figures 4.4 and 4.5 show the displacement in physical space, x, (so that one observes the Eulerian density $n(x, t)$), rather than the values of the Lagrangian displacements, $x_n(t)$, (2.1). It is, of course the Lagrangian equations which are linear (for a harmonic lattice) and thereby enjoy the superposition property. The transcription from the Lagrangian to Eulerian picture is a nonlinear mapping (see below), which accounts for this interference effect. (I am indebted to F. Tappert for raising this point at the confer-

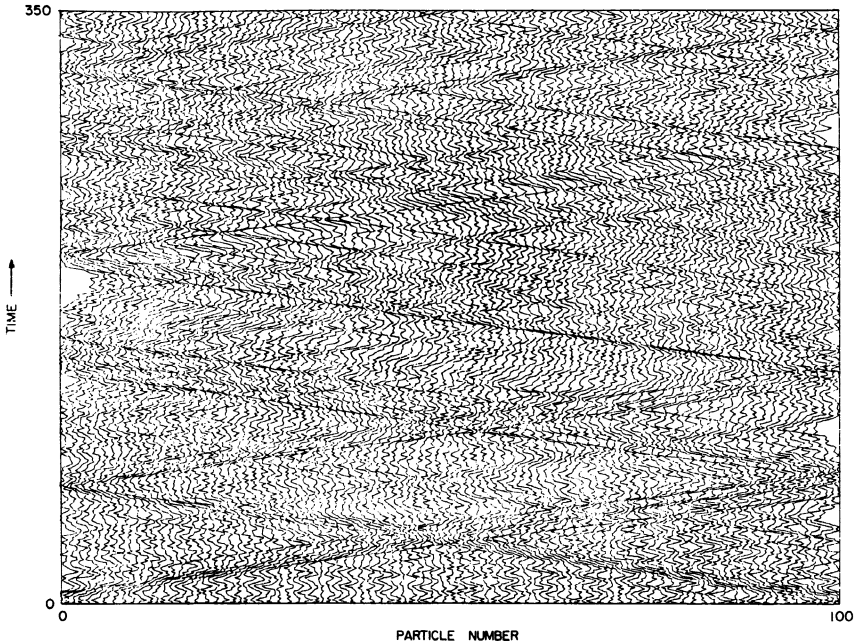

Figure 4.5. The same as Figure 4.4, except the lattice is now very anharmonic.

ence, and for subsequent discussions with him, K. Miura, and J. Pasta, clarifying this effect.)

This transcription from the Lagrangian to the Eulerian description will be outlined briefly here, not only because it clarifies the above effect, but because it makes clear the fact that the space variable in the usual continuum equations, obtained from the lattice equation (e.g., the Korteweg-deVries equation), is *not* the spatial coordinate x. To show this, consider the usual continuum limit ($h \to 0$) and write the spatial location of a particle (2.1) in the form

$$x(x_0) = x_0 + y(x_o, t) \tag{4.1}$$

where $x_0 = n\,h$ represents the continuous *undisplaced* locations of the particles (particle labels). In figures such as 4.4 and 4.5, what one notices is the Eulerian density of lines, $n(x, t)$. Because of the conservation of particles, this density satisfies

$$n_0 dx_0 = n(x, t)\, dx \tag{4.2}$$

where n_0 is the unperturbed density, and (dx, dx_0) are related by (4.1). Actually (4.2) holds only if the particles retain their spatial ordering, (2.1), which I will assume is the case. From (4.1) and (4.2) one readily obtains

$$n(x, t) = \frac{n_0}{1 + \partial y/\partial x_0}\Bigg|_{x_0(x,t)} \tag{4.3}$$

where $x_0(x, t)$ is given implicitly by (4.1). Spatial ordering is maintained if $\partial y/\partial x_0 > -1$. Obviously the relationship between this density, which is observed in the above displacement figures, and the particles' locations, is very nonlinear. (Another application of these ideas arose in nonlinear plasma oscillations; see, J. Dawson, Phys. Rev. **113**, 383 (1959), and E. A. Jackson, Phys. Fluids, **3**, 831 (1960)).

In the usual derivation of the continuum equations from the lattice equations (Zabusky [69], [57], or see the review by Toda [14]), the replacement

$$y_{n+1} = y \pm h\frac{\partial y}{\partial x} + \frac{1}{2}h^2\frac{\partial^2 y}{\partial x^2} + \cdots \tag{4.4}$$

is made, where $x = n\,h$. As is clear from (4.1), a change in the value of n corresponds to a proportional (h) change in x_0, rather than a proportional change in the spatial coordinate x. Thus, if we wish to retain that meaning for the symbol x, one should write instead of (4.4)

$$y_{n\pm1} = y \pm h\,\frac{\partial y}{\partial x_0} + \frac{1}{2}h^2\,\frac{\partial^2 y}{\partial x_0^{\,2}} + \cdots \tag{4.5}$$

This makes it quite clear that the displacement, y, is expressed in terms of the undisplaced locations ("labels") of the particles. In this sense these continuum equations are *not* the usual Eulerian (field) equations, and care must be taken in the physical interpretation of phase shifts (e.g., of interacting solitons), as well as the application of boundary conditions for such equations.

Perhaps this is an appropriate place to also mention another aspect of these "continuum equations" which could use further elucidation. The lattice equations

$$m\,\ddot{y}_n = F(y_{n+1} - y_n) - F(y_n - y_{n+1}) \tag{4.6}$$

or the related equations

$$m\,\ddot{u}_n = F(u_{n+1}) - 2\,F(u_n) + F(u_{n-1}) \tag{4.7}$$

where

$$u_n = y_{n+1} - y_n \tag{4.8}$$

can be used as the basis for deriving continuum equations. Thus, for example, using

$$u_{n\pm1} = u(x_0) \pm h\frac{\partial u}{\partial x_0} + \frac{1}{2}h^2\frac{\partial^2 u}{\partial x_0^2} + \cdots \tag{4.9}$$

equation (4.7) can be written in the form

$$m\,\ddot{u}(x_0, t) = 4\sinh^2\left(\frac{h}{2}\frac{\partial}{\partial x_0}\right) F(u(x_0,t)) \tag{4.10}$$

if $F(z)$ is a polynomial force. The continuum limit (2.26), $h \to 0$, can not be simply employed, since it would lead to the *linear* wave equation (note: $u(x_0, t) = O(h)$, by (2.1), and $F = O(\mu u)$ in this limit).

What has been done in the past is to make a judicious selection of derivative terms from the infinite number generated by (4.5) (e.g., in (4.10) or the corresponding equation from (4.6)). Such a selection *may* be equivalent to increasing select nonlinear coefficients, K_n in equation (2.3) as $h \to 0$, but this clearly has no physical basis. It would be of considerable interest to better understand the physical content of these continuum equations, and under what conditions they adequately represent the lattice dynamics. Some discussion along these lines has been given recently by Toda [14].

One of the interesting features found by Payton, Rich and Visscher [32] was that the "thermal conductivity" of an isotopically disordered one-dimensional lattice is *increased* as the anharmonic strength is increased. This feature is illustrated in Figure 4.6, taken from their paper. The lattice was 50% disordered with masses in the ratio 3:2. The anharmonic force constant K_2 was varied, retaining a constant ratio K_3/K_2 (equation (2.3)). As K_2 is increased, both $\langle J\rangle$ and $K_T(N)$ increase, whereas ∇T is relatively constant. They interpreted this increase in $K_T(N)$ (also see Visscher [41]) as being due to the fact that the nonlinar forces break down the spatially localized character of many of the disordered lattice modes which do not transport energy effectively, thereby increasing the flux $\langle J\rangle$. Zabusky [59] proposed that this increase in conductivity could be viewed as being due to the increased importance of solitons in the transport of energy through the lattice. While both pictures appear consistent, the soliton interpretation is clouded somewhat by the relatively unknown influence which isotopic disorder has on their behavior. Thus both Payton, Rich and Visscher as well as Jackson, Pasta, and Waters [24] found that the addition of different defects caused $K_T(N)$ to decrease, for constant anharmonicity, as one would ex-

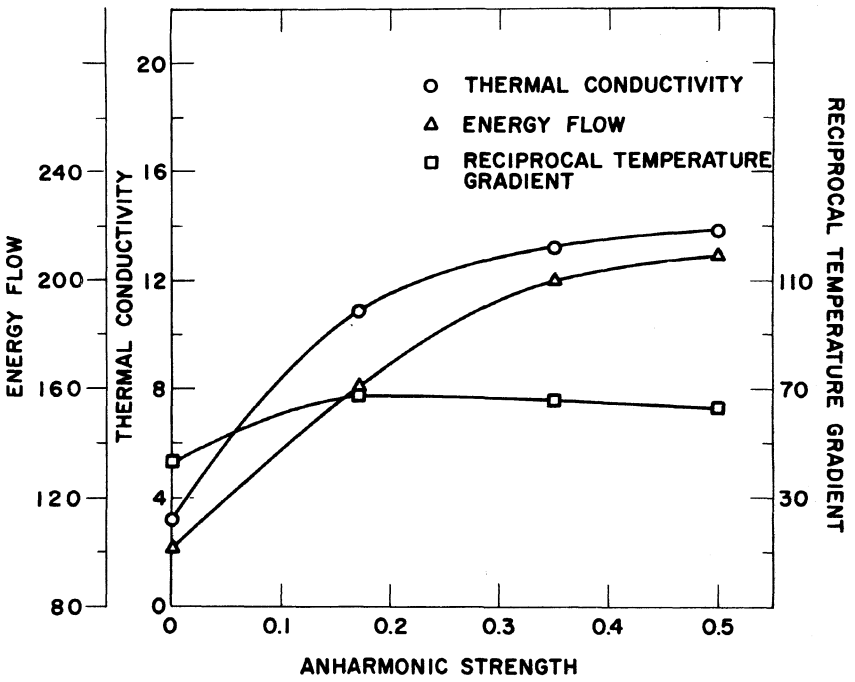

Figure 4.6. The energy flow, $(\nabla T)^{-1}$, and K_T for a one-dimensional lattice with random 50% mass mixture (3:2) as a function of the anharmonic strength (Visscher).

pect from phonon arguments. This would also seem to imply that solitons lose their effectiveness with increased defects.

An example which avoids this uncertainty is a calculation carried out in [24] in which the only change that was made was in the cubic force coefficient (both cases without defects). When K_3, equation (2.3), was changed from $K_3 = (2/3)\ K_2{}^2$ to $K_3 = (1/4)\ K_2{}^2$ (and $K_2 = -10$) then $(\nabla T \times 10^5$, $\langle J \rangle \times 10^4$, and $K_T(N))$ were found to change from (1.48, 7.53, 51) respectively to (2.58, 8.19, 31.7). Thus a reduction in the cubic force caused a *decrease* in $K_T(N)$, which is certainly not what one expects from the phonon scattering picture of the last section. The "explanation" of this decrease in K_T being due to the less efficient production of solitons when K_3 is smaller, is probably too simplistic however. Thus $\langle J \rangle$ increases as K_3 decreased, so that the energy flux did not decrease as one might expect if there were fewer solitons. Moreover in other (limited) calculations it was found that if $K_3 = (2/3)\ K_2{}^2$, and K_2 was increased from 5 to 10 the energy flux *decreased* by a factor of

two, while the temperature gradient increased by less than 1.3, again implying a decreased $K_T(N)$. Neither of these results would appear to be consistent with a simple picture that the soliton flux should become more important with increasing (K_2, K_3). Another feature clouding the issue is the role which the temperature jumps at the boundary thermal resistance (temperature discontinuities) may play in these comparisons (see, Nakazawa [28] and K. Miura [27].)

Another very basic difficulty with the soliton explanation of the above increase in K_T, is that solitons are not related in any obvious fashion with a temperature gradient, on which K_T is based. This is true even if there are phase shifts due to interactions, and different average soliton velocities coming from the two reservoirs. The solitons indeed form a "Knudsen gas" of noninteracting excitations, which is the antithesis of thermal resistance. To obtain a temperature gradient requires some "breakdown" of the solitons—possibly a "stochastic" breakdown when sufficiently energetic solitons interact, or a nonsoliton (dispersive wave) production at the boundary. In an attempt to find such a source of temperature gradient, K. Miura [27] investigated the propagation and interaction of pulses generated by impulses at the end of a finite lattice. As an example, the initial velocity, V_i, was given to the end particle in a polynomial force lattice ($K_2 = -10$, $K_3 = 2/3\, K_2^2$ in (2.3)), and the percentage of that energy which was propagated in the form of a "soliton" (a nondispersive pulse) was determined, as indicated in the following table:

TABLE 4.1

V_i	V_sSoliton velocity	A_s:Soliton amplitude	% Energy in soluton
.08	1.13	.0364	91.1
.10	1.19	.0465	93.4
.20	1.39	.0900	98.0
.30	1.57	.1252	99.0
.40	1.75	.1550	99.4
.50	1.89	.1819	99.6
.60	2.02	.2066	99.67
.80	2.27	.2482	99.8
1.00	2.51	.2840	99.99

where the velocity is in units of the sound velocity of the lattice, C_s. The velocity of the soliton is found to be somewhat greater than the theoretical value

$$V_s^2 = C_s^2[1 + (2K_2/3)A_s + (K_3/2)\,A_s^2] \tag{4.11}$$

predicted from the continuum equation

$$\ddot{u} = C_s^2 \frac{\partial^2}{\partial x_0^2} \left[u + K_2 u^2 + k_3 u^3 + (h^2/12) \frac{\partial^2 u}{\partial x_0^2} \right] \tag{4.12}$$

obtained from a truncated version of (4.10). If $K_3 = 0$, then (4.12) would be the usual Boussinesq equation. The above table shows rapid increase in the efficiency of the energy conversion to solitons as V_i is increased. This increase in efficiency is also evident in the displacement profiles for $u_n(t)$ shown in Figure 4.7. The smaller impulse ($V_i = .05$)

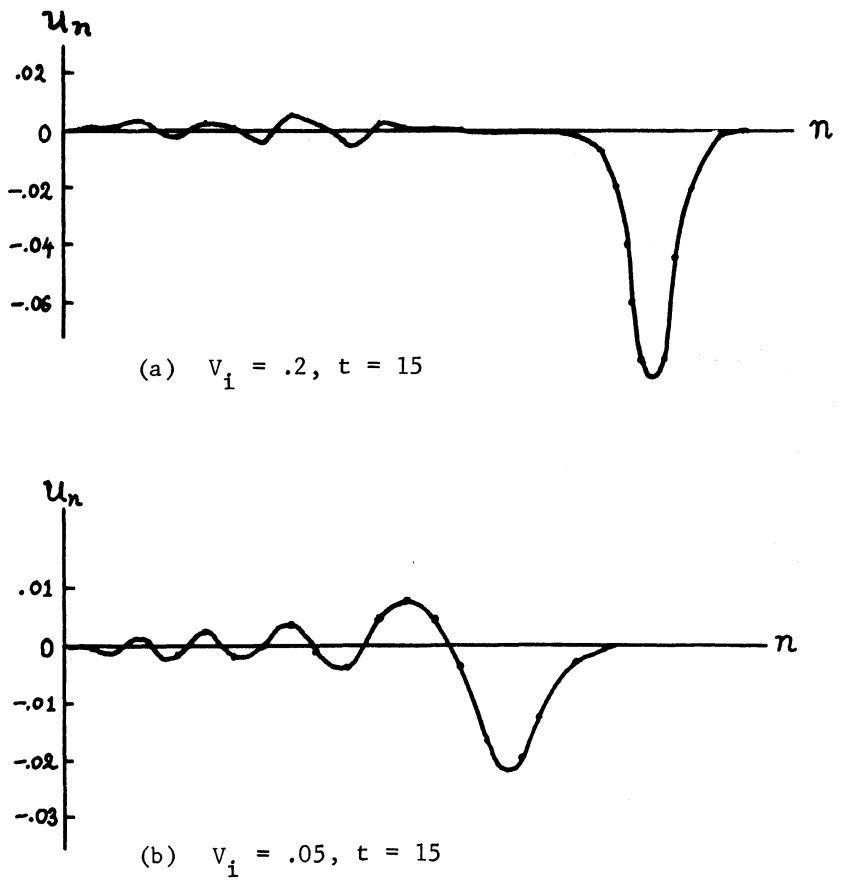

Figure 4.7. The disturbance produced in an semi-infinite anharmonic lattice by a strong and weak impulse at the left end (K. Miura).

produces a significant amount of dispersive "tail" to the soliton. In the interaction with a reservoir, it seems very reasonable therefore that a substantial fraction of the energy is deposited in these dispersive modes (because most V_i *are* small). It would be very nice to have a theoretical prediction of $E_s(V_i)$, the energy of the soliton vs. V_i, but that has yet to be obtained. It appears quite possible that such a source of dispersive energy might be responsible for the "temperature" gradient observed in *computer calculations*. K. Miura also found that a *major* portion of the energy flux between the reservoirs was carried by the solitons. This clearly leads to the possibility of a totally different explanation for the relationship between $\langle J \rangle$ and ∇T, from the "classic" (i.e., historical) theory described in the last section. The degree to which this boundary production may be a significant source for the energy gradient, possibly only in the one-dimensional lattice, remains for future studies to determine. It is rather difficult to see how this can lead to an intrinsic coefficient of heat conductivity as N is increased, unless there is some internal resistance phenomenon.

To study this further within the context of solitons, K. Miura looked for the possible breakdown of solitons when they interact. Thus the two end atoms of the above 50 atom lattice were given initial velocities $V_i = 0.5$ and -0.5. The result of their encounter at $n = 25$, is to leave behind a very small amount of dispersive energy (0.3% of the initial energy). Miura also investigated the production and interaction of "solitons" in harmonic-plus-hardcore potential (HHC, equation (2.5), with $b = 0.5$), and also the piecewise linear force, (2.4), with various values of b. As might be expected solitons are not formed in such lattices unless the impulse velocity at the end is sufficiently large to induce the nonlinearity (now requiring a minimum displacement). The result for various V_i in the HHC lattice are given in the following table:

TABLE 4.2

V_i	V_s	E_s	E_{tail}	Energy lost in collision
.79	(decays at $n = 12$)			
.80	1.19	(decays at $n = 38$)		
.90	1.60	.4043	.0007	.01502
1.00	1.82	.4999	.0001	—
1.5	3.07	1.125	2×10^{-6}	.00248
2.0	4.0	2.00	5×10^{-8}	—

In the case of the solitons created by $V_i = .90$ (note that it requires a $V_i > 0.5$ before there can be *any* hardcore interactions), one sees that

nearly 4% of the energy is lost when they interact, which is quite substantial. The more energetic "soliton" however is quite stable. Indeed, for very large V_i, the "soliton" is simply a moving particle which exchanges all its momentum with the next particle through a hard core collision. Fairly similar results were also found for the piecewise linear force lattice, which K. Miura analyzed in some detail.

A potentially very important phenomenon was indicated in calculations made by Ooyama and Saito [46]. They observed that a soliton passing through random disturbances in an exponential lattice ($a = .471$, $b = 2.121$ in (2.6) experienced a frictional drag, *apparently* of the form

$$\dot{V}_s = -\zeta(\epsilon)V_s. \tag{4.13}$$

Here the frictional coefficient, $\zeta(\epsilon)$, increases as the fraction of the total energy, ϵ, in the background disturbances increases. Moreover there appears to be a critical value, $\epsilon = \epsilon_c$, below which $\zeta(\epsilon) = 0$. Unfortunately the energy *density* of disturbances, which is presumably the governing quantity, could not be established from their data. The slow down of the soliton is correlated, of course, with a loss in its energy. It would be very interesting to have information about this "irreversible" relaxation time $\tau(\epsilon) \equiv \zeta^{-1}(\epsilon)$, or "mean-free-path", $\lambda(\epsilon) = V_s(\epsilon)/\zeta(\epsilon)$, of solitons in this situation.

Finally, because of the results of Northcote and Potts [66] indicating that the harmonic-plus-hardcore model *may* be ergodic (see § 5), it would appear that this lattice is one of the more likely candidates to have an intensive K_T within the constraint of a one-dimensional system. Visscher has noted however that, depending on the local energy in the lattice, it can vary from a harmonic behavior to a system of free hard-core particles, as noted above. Both of these limits certainly do not have the desired irreversible behavior so that, on this basis, Visscher argues that such a lattice could give a normal K_T only over a limited temperature range (which does not encompass either of the above extremes). While the argument is appealing, the fact that one is dealing with an energy *distribution* may always introduce a sufficient number of (ergodic type) interactions to produce the desired irreversibility. While both Visscher and Helleman have made initial studies of thermal conduction in such systems, additional calculations are needed to settle this matter.

5. **The Fermi-Pasta-Ulam Recurrence Problem.** Much of the present activity in the solution of nonlinear partial differential equations is due to extensions of the novel approach which was taken by Kruskal and Zabusky to explain the computer calculations made by Fermi, Pasta,

and Ulam [61] before 1955. The subsequent beautiful inverse scattering technique, originally proposed by Greene, Gardner, Kruskal, and Miura [43], [44] and its generalizations are well known to the mathematical community (e.g., see Whitham [55], Scott, Chu, McLaughlin [48], and papers by Flaschka, Kruskal, and Newell in [18a]. What is perhaps not as well known to this community is why physicists were interested, surprised, or concerned with a phenomenon such as the FPU recurrence, and the fact that the above beautiful results have yet to clarify some of the original questions! Indeed there is an example which raises questions about the continuum soliton picture of FPU recurrence, which I will discuss below. I make these latter statements in the spirit of a future challenge to our understanding lattice dynamics, not to detract from past successes, which are obvious!

Among Fermi's many interests was his long concern about ergodic questions in statistical mechanics [7], and the process of relaxation to thermal equilibrium. It should perhaps be emphasized that these problems are quite distinct in the sense that the knowledge that a system is ergodic gives no indication on how fast a system will approach equilibrium. This latter question is, of course, of great practical importance to physicists. Fermi's use of second order perturbation methods to arrive at time independent transition probabilities (relaxation times), still forms the backbone of much of the irreversible estimates which are made in quantum mechanics for example the relaxation time $\tau(\omega)$ which appears in the thermal conductivity expression (3.10). Another early example of the application of this estimate was the theory of sound absorption in solids, developed by Landau and Rumer [25]. Such estimates of transition probabilities are affectionately referred to as Fermi's "golden rule" (e.g., Bethe and Jackiw [2]), and certainly "golden" is an appropriate adjective for such a fruitful estimate. However, perhaps because such estimates were so easy to obtain, physicists tended to believe that nature must also find it as equally easy to approach equilibrium, given a little nonlinearity between the normal modes of a lattice. In the spirit of observing such a relaxation to equilibrium (i.e., an equipartition of energy among the normal modes of the lattice), Fermi, Pasta, and Ulam made their classic calculation illustrated in Figure 5.1 and 5.2. These figures show the energy in the modes, E_k in (5.2), as a function of $\omega_1 t/2\pi$, when initially all of the energy was placed into the lowest mode, $k = 1$. The lattice they used in these figures had $N = 32$ (hence 32 modes), and a polynomial force $F(z) = \mu(z + \alpha z^2)$, with $\alpha = 1/4$ and $\alpha = 1$ in the two figures respectively. The unexpected (and unwanted!) feature of these results is the lack of energy sharing among the modes the "rapid recurrence" (see below) of the initial values of E_k—namely

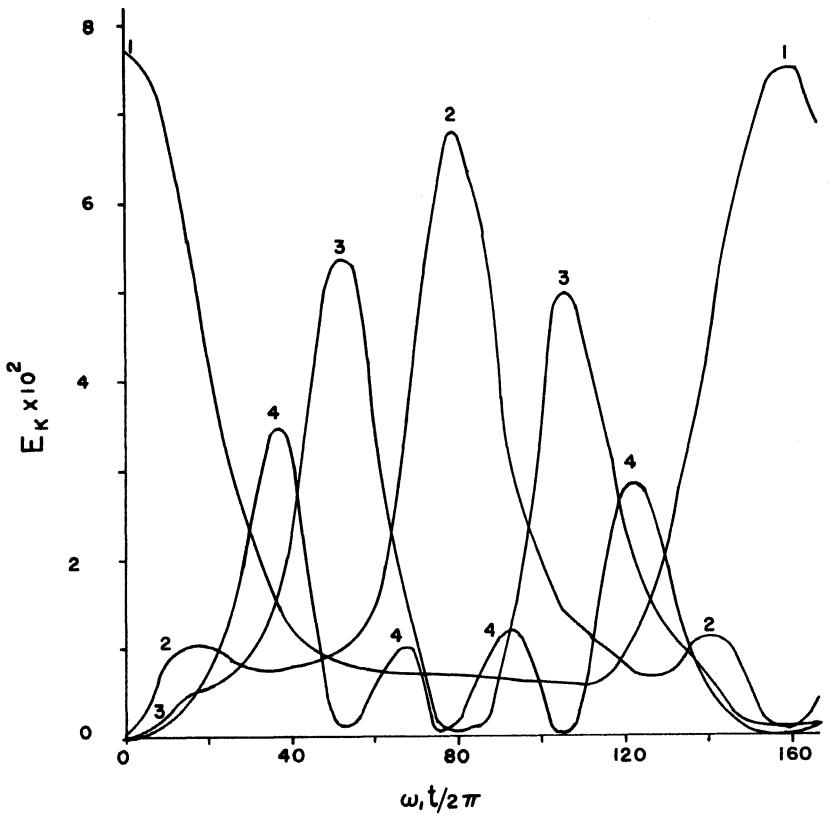

Figure 5.1. The FPU calculation of the normal mode energies, $E_k(t)$ ($k = 1, \cdots, 4$ are shown, and $E_5 < .015$), for the case $N = 32$, $\alpha = 1/4$ (lattice force $F(z) = z + \alpha z^2$).

in about 160 periods ($2\pi/\omega_1$) for $\alpha = 1/4$ and 80 periods for $\alpha = 1$. Even more disheartening from the historic point of view, is the *decrease* in this recurrence time with an *increase* in the nonlinear coupling, α, and nearly total lack of excitation of the modes $k \geqq 7$ (say). At the same time (1954) a proof was developed by Kolmogorov [89] which showed why such lack of energy sharing would indeed occur for most initial states *provided* that a suitable parameter is sufficiently small (*related* to the FPU α, see § 6).

Before turning to more exact treatments of this problem, I would like to give a "back of the envelope" derivation which shows how the FPU recurrence differs from the classic relaxation process, the role of the

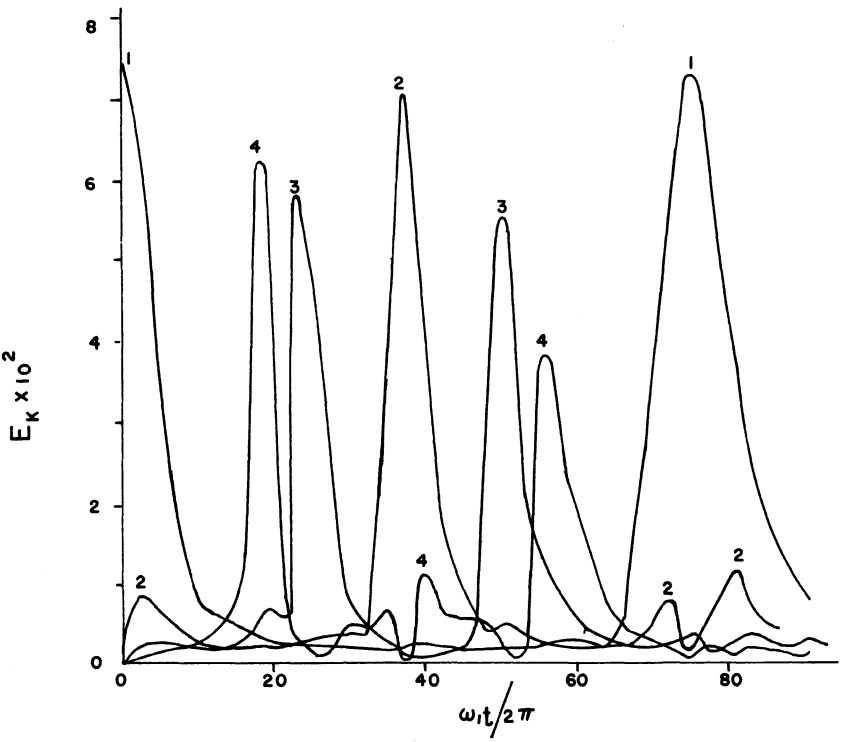

Figure 5.2. The same as Figure 5.1 except that $\alpha = 1$. Note the *decrease* in the recurrence time.

thermodynamic limit (2.25) in these types of considerations, and trivial estimates for the periods of time one would expect any relaxation process to break down. To do this consider the nonlinear normal mode Hamiltonian

$$\mathscr{H} = \sum \frac{1}{2}(a_k{}^2 + \omega_k{}^2 a_k{}^2) + \sum \frac{1}{3} V_{jk\ell} a_j a_k a_\ell. \tag{5.1}$$

Since the "normal mode energy"

$$E_k \equiv \frac{1}{2}(\dot{a}_k{}^2 + \omega_k{}^2 a_k{}^2) = \omega_k J_K \tag{5.2}$$

is the quantity of interest in the FPU problem, it is useful to transform (5.1) into the action-angle variables (2.22)

$$\mathcal{H} = \sum \omega_K J_K + \sum \frac{1}{3} V_{jk\ell} \left[\frac{8 J_j J_k J_\ell}{\omega_j \omega_k \omega_\ell} \right]^{1/2} \sin\theta_j \sin\theta_k \sin\theta_\ell \tag{5.3}$$

with the equations of motion

$$\dot{\theta}_K = \frac{\partial H}{\partial J_K} \; ; \; \dot{J}_K = - \frac{\partial H}{\partial \theta_k} \, . \tag{5.4}$$

In the harmonic approximation this gives

$$\dot{\theta}_K = \omega_k, \tag{5.5}$$

which will be assumed in all that follows (for simplicity). On the other hand, (5.4) yields in general

$$\dot{J}_j = - \sum_{k,\ell} V_{jk\ell} \left[\frac{8 J_j J_k J_\ell}{\omega_j \omega_k \omega_\ell} \right]^{1/2} \cos\theta_j \sin\theta_k \sin\theta_\ell. \tag{5.6}$$

Mathematicians may be amused by the fact that (5.6) does *not* satisfy the Lipschitz condition at $J_n = 0$. To examine a relaxation process appropriate for the FPU problem assume that at time $t = 0$ only one mode is initially excited, $J_i \neq 0$, then J_j changes according to (5.6) with both $k \equiv i$ and $\ell = i$. Moreover, because of (5.5), the slowest varying term arising from the trignometric factors is

$$\dot{J}_j \simeq V_{jii} \frac{J_i}{\omega_i} \left(\frac{J_j}{2\omega_j} \right)^{1/2} \cos(2\theta_i - \theta_j).$$

Refinements to this procedure are given below. In any case, for short times during which J_i is essentially constant, this yields

$$J_j^{1/2} \simeq \frac{V_{jii}}{2\sqrt{2\omega_j}} \frac{J_i}{\omega_i} \frac{\sin(2\theta_i - \theta_j)}{(2\omega_i - \omega_j)} \tag{5.7}$$

assuming, of course, that the denominator does not vanish, and one ignores the spurious second solution $J_j(t) \equiv 0$. The fate of the initial action, $J_i(t)$, is determined by substituting (5.7) into (5.6). Again retaining only the slowest varying terms yields for the energy (5.2).

$$\frac{dE_i}{dt} \simeq - \frac{d}{dt} \sum \frac{(V_{ii\ell} E_i)^2}{4\omega_\ell \omega_i^3} \frac{\sin^2(2\theta_i - \theta_\ell)}{(2\omega_i - \omega_\ell)^2} \, . \tag{5.8}$$

Using (5.5), it will be noted that for very short times (5.8) reduces to

$$\frac{dE_i}{dt} \simeq - \sum \frac{(V_{ii\ell}E_i)^2}{4\omega_\ell \omega_i{}^3}\, t. \tag{5.9}$$

This does *not* give $E_i{}^{-1}dE_i/dt$ which is independent of time explicitly (a time independent "relaxation time"). Instead τ^{-1} is explicitly proportional to t. One only obtains a time independent $E_i{}^{-1}dE_i/dt$ over a limited range of time, during which one can make the approximation

$$\sin^2(2\theta_i - \theta_\ell)/(2\omega_i - \omega_\ell)^2 = \pi t \delta(2\omega_i - \omega_\ell) \tag{5.10}$$

(see, e.g., D. Bohm, Quantum Theory (Prentice Hall, 1951)), where δ is the Dirac delta function. In this case (5.8) can be written

$$\frac{dE_i}{dt} \simeq - \left[\sum_\ell \frac{V_{ii\ell}^2 E_i}{4\omega_\ell \omega_i{}^3}\, \delta(2\omega_i - \omega_\ell) \right] E_i \equiv -E_i/\tau_i \tag{5.11}$$

which is not explicitly dependent on t. The last identity in (5.11) is clearly fanciful, since τ_i itself is a function of E_i (i.e., a nonlinear equation is made to "look" like a linear relaxation equation). Indeed the fact that the FPU *does* behave like a relaxation process over a limited period (see below) is *not* explained by this derivation (a model example is given in Jackson [**64**, Appendix B]). The use of (5.10) in (5.8) requires that t be neither too large nor too small. Specifically, one has as *necessary* conditions

$$\max(2\omega_i - \omega_\ell) \gg 2\pi/t \gg \min(2\omega_i - \omega_\ell) \tag{5.12}$$

in addition to other conditions which may be required to justify the perturbation approximation. The first inequality of (5.12) eliminates the result (5.9). The second condition is necessary in order to have a large number of terms in the summation lying inside the first minimum of $\sin(2\theta_i - \theta_\ell)$. It is this condition which is satisfied by taking the thermodynamic limit, (2.25), because the normal mode frequencies become dense, in contrast with the continuum limit (2.26). In addition to the conditions (5.12), it is clear, that (5.11) cannot be valid over times of the order of the Poincaré recurrence time. This is another reason for considering the limit $N \to \infty$ (e.g., in (3.25)), but even for quite finite values of N the Poincaré time is very large.

To be more specific consider, following Hemmer, Maximom, and Wergeland [**84**] (also see additional references), let

$$z_k \equiv \dot{a}_k + i\omega_k a_k = \sqrt{2\omega_k J}_k\, e^{i\theta_k}. \tag{5.13}$$

For a harmonic system the actions are constant, so a near recurrence only involves the near return of the angle variables. We assume, of course, that the frequencies $\dot{\theta}_K = \omega_k = \omega_o \sin(\pi k/2N)$ do *not* satisfy $\sum m_K \omega_K = 0$ for a nonzero set of integers $\{m_K\}$, since otherwise the system is periodic. Recurrence is now *defined* in terms of the allowable range of the angles from some specified values, i.e.,

$$\theta_k^0 \leqq \arg z_k \leqq \theta_k^0 + \Delta\theta_k. \tag{5.14}$$

The recurrence time is then given by

$$T_R = \prod_{k=1}^{N-1} (2\pi/\Delta\theta_k) \Big/ \sum_{k=1}^{N-1} (\omega_k/\Delta\theta_k). \tag{5.15}$$

The harmonic system just considered is not ergodic because each of the energies, E_k, are constants of the motion, implying that much of the energy surface, $E = \sum E_k$, does not contain the trajectory of prescribed initial state. Since one expects an anharmonic lattice to distribute its energy among all the modes, its recurrence time certainly should not be any less than (5.15). Assume that we now require $\Delta\theta_k = 2\pi/100$, then (5.15) becomes approximately

$$T_R \simeq (\pi/N)\, 10^{2N-24} (\textit{years}). \tag{5.17}$$

Based on this type of estimate, physicists obviously had no reason to be concerned with the Poincaré recurrence for macroscopic systems (say $N = 10^{20}$). This also lent vague support to the assumption that many of the mode interactions, neglected in a derivation such as given for (5.11), could be justified at least over experimental periods of time (usually much less than a day).

Unfortunately the above estimate of the recurrence time has essentially nothing to do with the recurrence of the *energies* in an *anharmonic* lattice. The recurrence time one is interested in here is the one *defined* by conditions

$$|z_k^0|^2 \leqq |z_k|^2 \leqq |z_k^0|^2 + \Delta |z_k|^2 \tag{5.18}$$

rather than (5.14). In the harmonic lattice the recurrence time defined only by (5.18) is of course zero! The only way to determine this recurrence time is to investigate the *nonlinear* lattice. Moreover it is obviously this recurrence time which is relevant to the limitation of the validity of (5.11). One should in fact distinguish between the *Poincaré recurrence time* for the anharmonic lattice (*defined* by the *simultaneous* satisfaction of (5.14) *and* (5.18)), and what probably should be referred

to as the *FPU recurrence time*, defined *only* by the requirement (5.18). Obviously the latter recurrence time will usually be much less than the Poincaré time.

Before turning to the question of determining the FPU recurrence time, let me point out that the time dependence of $E_1(t)$, shown in Figure 5.1, in fact *does* have a relaxation process behavior, and only in the time interval required by (5.12). This fact is illustrated in Figure 5.3,

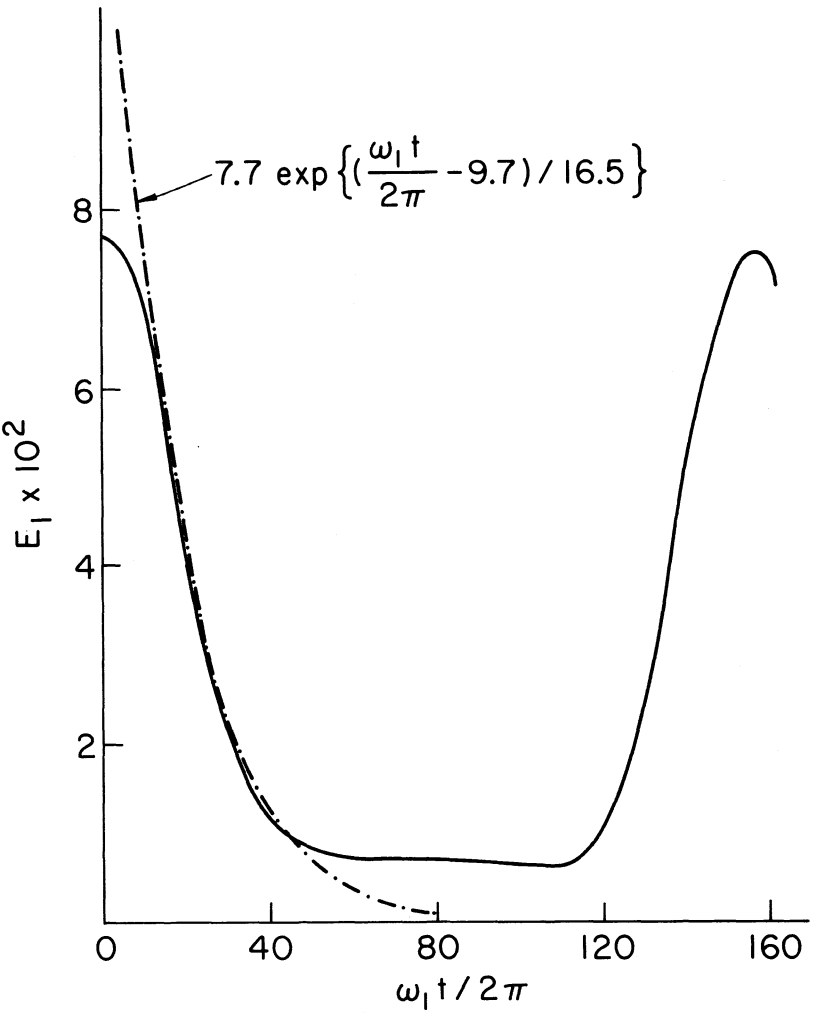

Figure 5.3. An exponential fit to the FPU result for $E_1(t)$ shown in Figure 5.1.

which is roughly the "breaking time" of Kruskal and Zabusky [70], to periods $(2\pi/\omega_1)$ *after* a suitable initial period (first inequality of (5.12)), which is roughly the "breaking time" of Kruskal and Zabusky [70] to be discussed below. The long time limit of (5.12) in the present case is $\omega_1/(2\omega_1 - \omega_2) = 415 \geqq \omega_1 t/2\pi$ which is far larger than the end of the relaxation behavior in Figure 5.3 (about 50 periods). Let me emphasize that this is curve fitting, not derived results, and is being presented as a curiosity because of the ubiquitous expectations of relaxation processes in physics. Indeed I think that one of the interesting future programs, pointed out at the end of § 4, is to see whether even solitons, under suitable background interactions, cannot exhibit a lifetime behavior (illustrating again perhaps how hard fixations die!).

It was soon shown by Northcote and Potts [66] that the FPU lack of equipartition between the E_k does not apply to the very nonlinear harmonic-plus-hardcore lattice, $F(z) = \mu z\,(z > -b), F(z) = -\infty(z = -b)$, with fixed ends $(x_0 = x_{N+1} = 0)$. They considered the same lowest mode excitation used by FPU, with an initial energy $E_1 = N\epsilon$, with $\epsilon = \mu/2\,b^2$ (the energy per particle equals the potential energy required for a hardcore collision). For $N = 15$ the percentage time averaged energy in the modes, $100\langle E_i\rangle/E$, is illustrated in the following table (only some typical modes are tabulated—see [66] for complete data). C indicates the number of hardcore collisions that have taken place up to that time.

TABLE 5.1

$\omega_1 t/2\pi$	C	$i=$ 1	2	3	7	8	9	13	14	15
0.0	0	100	0	0	0	0	0	0	0	0
.018	5	99	.1	.1	.1	.1	.1	0	0	0
.025	10	96.8	.5	.6	.1	.2	.2	.1	.1	.1
.037	15	93.1	1.7	1.5	.4	.6	.5	.2	.2	.1
.49	60	69.7	10.2	2.2	3.4	1.4	1.2	1.0	1.8	2.0
1.02	105	47.9	9.8	3.1	3.7	3.0	3.3	2.9	3.5	6.1
3.85	300	19.6	7.8	5.9	6.6	5.5	4.1	4.5	4.6	8.6
8.19	600	11.3	9.2	8.8	6.6	6.0	5.3	5.2	4.9	6.7
12.30	900	8.7	9.5	8.6	6.7	5.9	6.1	6.1	4.8	6.7
20.85	1500	7.2.	7.5	7.8	6.5	6.3	6.5	6.7	5.6	7.3

These results are presented on the same time scale used in Figures 5.1 and 5.2. It will be noted that the average $C(t)2\pi/\omega_1 t$ is 72, so that ω_1 has lost its physical significance. One can see that by 21 periods all the modes have roughly the same *time averaged* energy. The rapidity with which this system reaches an equipartition of energy is impressive when compared to the FPU weak coupling. Although it is not demonstrated

in the above table, the behavior which they found for $E_1(t)$ decidedly did *not* exhibit a relaxation time character (nor did $E_1(C)$), indicating this behavior may be more exceptional than characteristic.

The importance of the FPU recurrence, (5.18), (5.13), in contrast with more general problems of ergodicity and mixing, centers on the historic importance attached to the mode energy E_k (or the number of phonons, $N_k = E_k/\hbar\omega_k$) and how these quantities relax, or fail to relax. From this point of view, the recent emphasis on solitons is a study in the behavior of a *coherent* group of modes (phonons) which, of course, do not "relax" into the remaining modes. The fact that relaxation does not take place need *not* be obvious from a limited examination of the $E_k(t)$. This is illustrated rather nicely in Figure 5.4, due to K. Miura [27], which shows the energy in various modes at different times, when the end particle of the lattice is given an initial velocity $V_i = 0.5$ (similar to the situation shown in Figure 4.7). The system then has essentially only one soliton, yet it appears as if there is a "relaxation" to all of the available modes ($N = 25$). This masking of the mode correlation, which is obvious in the spatial representation $y(x_o, t)$, is a problem which may make it very difficult to delineate the onset of stochastic behavior in lattices which have more degrees of freedom than have been recently studied (e.g., see the review by Ford [81])—a point I will return to in § 6.

In addition to the reason cited above, the theoretical prediction of the FPU recurrence time is important because it represents a test of our understanding of the nonlinear dynamics in such lattices. It is also very instructive because it brings into contrast perturbative methods and the soliton picture of lattice dynamics. The initial perturbative analysis of this problem was made by Ford [62] (see also Ford and Waters ([63]), who drew attention to the importance of the combination frequencies $\omega(m) = \sum m_K\omega_K$ ($\{m_k\}$: integers). Because E_2 was directly excited by E_1, (5.7), the minimum time that would be required for recurrence is the "beat period" between these two modes, 2π $(2\omega_1 - \omega_2)$. This yields the *minimum* recurrence time *for weak coupling*

$$\min(\omega_1 T_R/2\pi) = \frac{\omega_1}{2\omega_1 - \omega_2} \simeq (2N/\pi)^2. \tag{5.19}$$

Later [64] I proposed a theory for analysing nonlinear coupled oscillators based on a generalization of the Brillouin-Wigner perturbation theory. This method introduces unknown frequencies, Ω_k, ab initio into the equations of motion, so that the original normal mode equations

$$\ddot{a}_k + \omega_k{}^2 a_k = -\lambda\, \partial H_1/\partial a_k \tag{5.20}$$

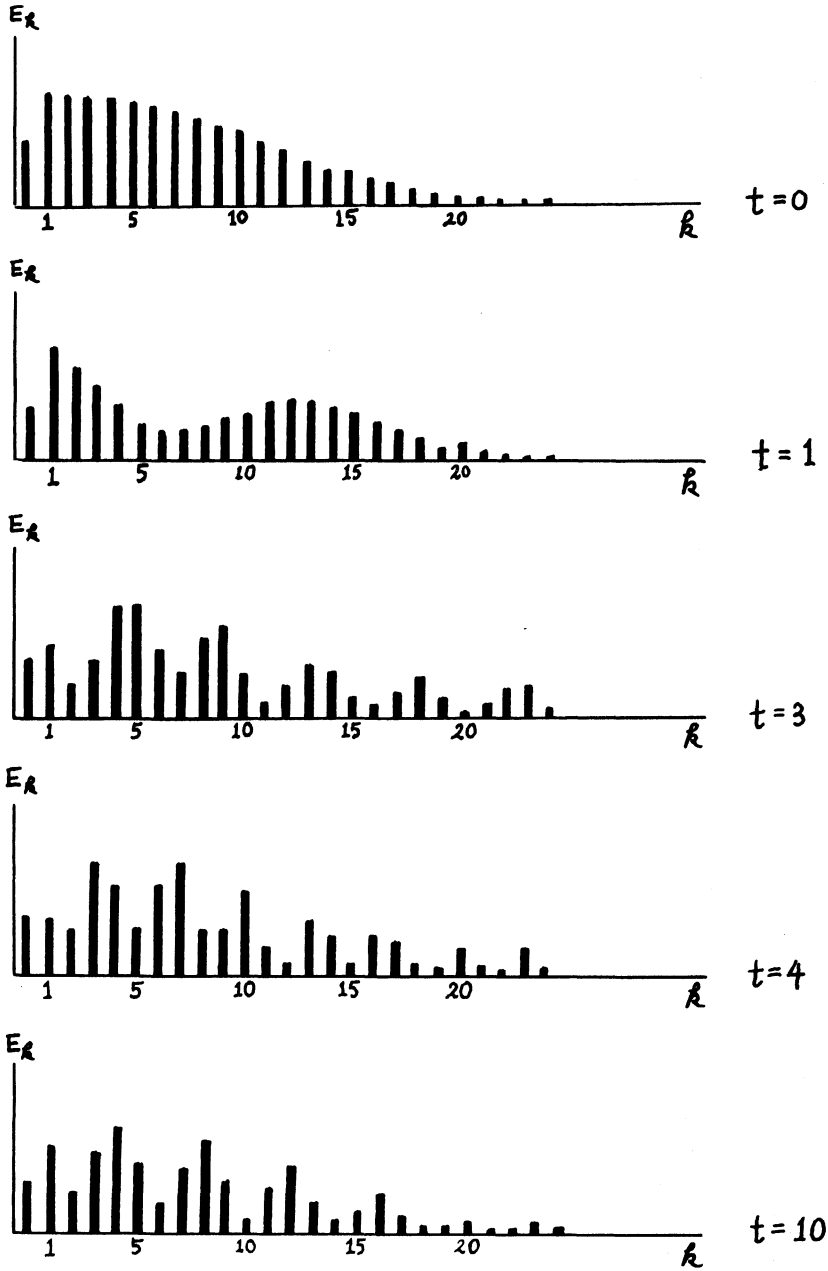

Figure 5.4. The normal mode energies corresponding to a single soliton generated by an impulse ($v_i = 0.5$) at one end of an $N = 25$ anharmonic lattice (similar to Figure 4.7; K. Miura).

are written formally as

$$\ddot{a}_k + \Omega_k{}^2 a_k = -\lambda \frac{\partial H_1}{\partial a_k} + \sum_{n=1} \lambda^n \mu_k{}^{(n)} a_k \tag{5.21}$$

where

$$\Omega_k{}^2 \equiv \omega_k{}^2 + \sum_{n=1} \lambda^n \mu_k{}^{(n)}(\lambda) \tag{5.22}$$

and λ is a formal ordering parameter. (5.22) is *not* an analytic expression in λ, since the functions are also dependent on λ. The unknown functions $\mu_k{}^{(n)}(\lambda)$ are determined in each *explicit* order of λ by the condition that the right side of (5.21) be orthogonal to the homogeneous solutions, $\alpha_k \cos(\Omega_k t + \phi_k)$

$$\int_{-\infty}^{\infty} \cos(\Omega_k t + \phi_k) \left(\frac{\partial H_1}{\partial a_k} - \sum \lambda^{n-1} \mu_k{}^{(n)} a_k \right) d = 0. \tag{5.23}$$

In this case the solution of (5.21) can be written

$$\begin{aligned} a_k &= \alpha_k \cos(\Omega_k t + \phi_k) \\ &- \lambda \int_{-\infty}^{\infty} G_k(t, t') \left[\frac{\partial H_1'}{\partial a_k} - \sum_{n-1} \lambda^{n-1} \mu_k{}^{(n)} a_k' \right] dt' \end{aligned} \tag{5.24}$$

where the Green's function contains only the unknown frequencies

$$G_k(t, t') = \sum_{\{m\}}{}' \frac{\cos(\Omega(m)t + \phi(m)) \cos(\Omega(m)t' + \phi(m))}{\Omega_k{}^2 - \Omega^2(m)} \tag{5.25}$$

where

$$\Omega(m) \equiv \sum_{\{m\}} m_K \Omega_K; \quad \phi(m) \equiv \sum_{\{m\}} m_K \phi_K.$$

The summation in the Green's function (5.25) is over all positive and negative integers $\{m_k\}$, such that $\Omega^2(m) \neq \Omega_k{}^2$, denoted by the prime on the summation. This perturbation method then consists of an iteration in the explicit powers of λ, using the a_k from (5.24) in (5.23) to determine the $\mu_k{}^{(n)}$, hence Ω_k (5.22). This then gives the new $G_k(t, t')$, (5.25), to yield the corrected a_k, (5.24). It is not difficult to show that this method always adjusts the frequencies Ω_k so that one never obtains the classic problem of small denominators. On the other hand the convergence of the method is totally unknown, probably being only an asymptotic method. Nonetheless this theory, at least for a limited range of α, gave fairly accurate results. It would be of considerable interest to

improve these calculations, or perhaps to use the more recent perturbative theory developed by Eminhizer, Helleman and Montroll [60], which has been shown to yield convergent series for *periodic* solutions. They use the clever method, similar in spirit to Kolmogorov's device [89] of readjusting the initial conditions at each order so as to retain a precisely periodic solution—and then showing that this leads to a con-

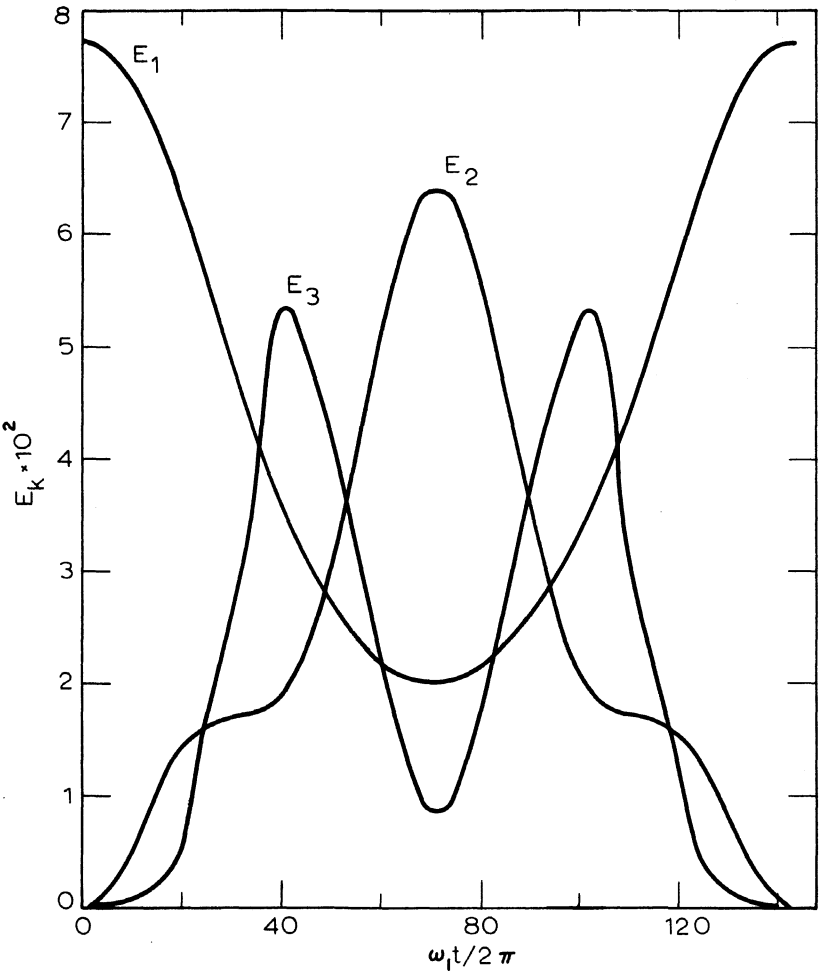

Figure 5.5. Rough theoretical calculation of the FPU problem shown in Figure 5.1, based on (5.22)–(5.25).

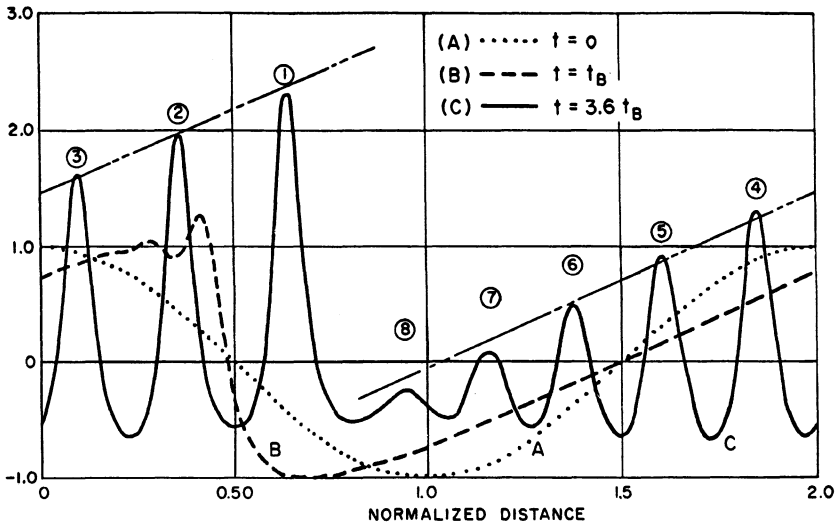

Figure 5.6. A solution of the Korteweg-deVries equation showing the development of eight solitons from an initial sine wave displacement (Zabusky).

vergent result. While it may be quite true that perturbation methods are the "conventional physicists" approach to such nonlinear problems, nonetheless they are the *only* methods to date to yield an accurate prediction of the recurrence times (see below), or a complete description of the intermediate dynamics of the lattice. As an illustration of the latter see Figure 5.5, which is a crude "hand calculation" of the $E_k(t)$, for $\alpha = 1/4$, using the above perturbation theory. Obviously it has its shortcomings when compared with the FPU Figure 5.1, yet it *is* recognizable. While perturbative methods are not the primary interest of this conference, I think it is worth pointing out that some of the recent successes in nonlinear methods may still have competition from more conventional methods, when it comes to *predicting* (rather than interpreting) nonlinear properties.

The above theory yields a minimum recurrence time as a function of the nonlinear coupling parameter α

$$\min(\omega_1/2\pi)T_R(\alpha) = \omega_1/[2\Omega_1(\alpha) - \Omega_2(\alpha)] \tag{5.26}$$

which reduces to Ford's result, (5.19), as $\alpha \to 0$. Whether (5.26) is the

actual recurrence time, depends on an examination of the other combination frequencies $\Omega(m) \equiv \sum m_K \Omega_K(\alpha)$ and ascertaining whether the relevant combinations are approximately commensurate with $(2\Omega_1 - \Omega_2)$. This was in fact the case over the ranges of α which were considered. Some values of $(\omega_1 T_R/2\pi)$ obtained from computer studies and approximate values using the above theory are listed in the following table (where $F(z) = \mu[z + \alpha z^2]$, $y_n(0) = \sin(n\pi/N)$, and $\omega_k = 2\sin(k\pi/2N)$). The last column will be discussed below. It will be noted that $T_R(\alpha)$ is predicted quite well by the above theory, despite the limited accuracy of the calculations, at least for small α. Note also how rapidly $T_R(\alpha)$ changes near $\alpha = 0$, particularly for large N.

TABLE 5.2

	$\omega_1 T_R/2\pi$	Theory (5.26)	R
$N = 64$			
$\alpha = 0$	–	1660	–
$\alpha = 1/4$	341	–	.333
$N = 32$			
$\alpha = 0$	–	415	–
$\alpha = 1/4$	156	142	.43
$\alpha = 1$	78	68	.43
$N = 9$			
$\alpha = 0$	–	32.9	–
$\alpha = 1/4$	21.6	22.1	.40
$N = 4$			
$\alpha = 0$	–	6.57	–
$\alpha = 1/4$	5.48	5.58	.34
$\alpha = 1/2$	4.14	.47	.37
$a = 3/4$	3.35	3.75	.36

The above perturbative method contrasts with the novel approach of Kruskal and Zabusky, which led to the interpretation of the FPU recurrence as consisting of a sequence of events, shown in Figures 5.6 and 5.7 (Zabusky and Kruskal [56], Zabusky [57]). The initial wave form ($t = 0$ in Figure 5.6) develops into a steep shock where its profile "breaks" into a number of solitons ($t = t_B = T_R/30.4$), labeled 1 through 8. As shown in Figure 5.7, these solitons then travel at different speeds, interact the experience rather complicated phase shifts, and finally collect back ("unbreak") into the first normal mode (not shown

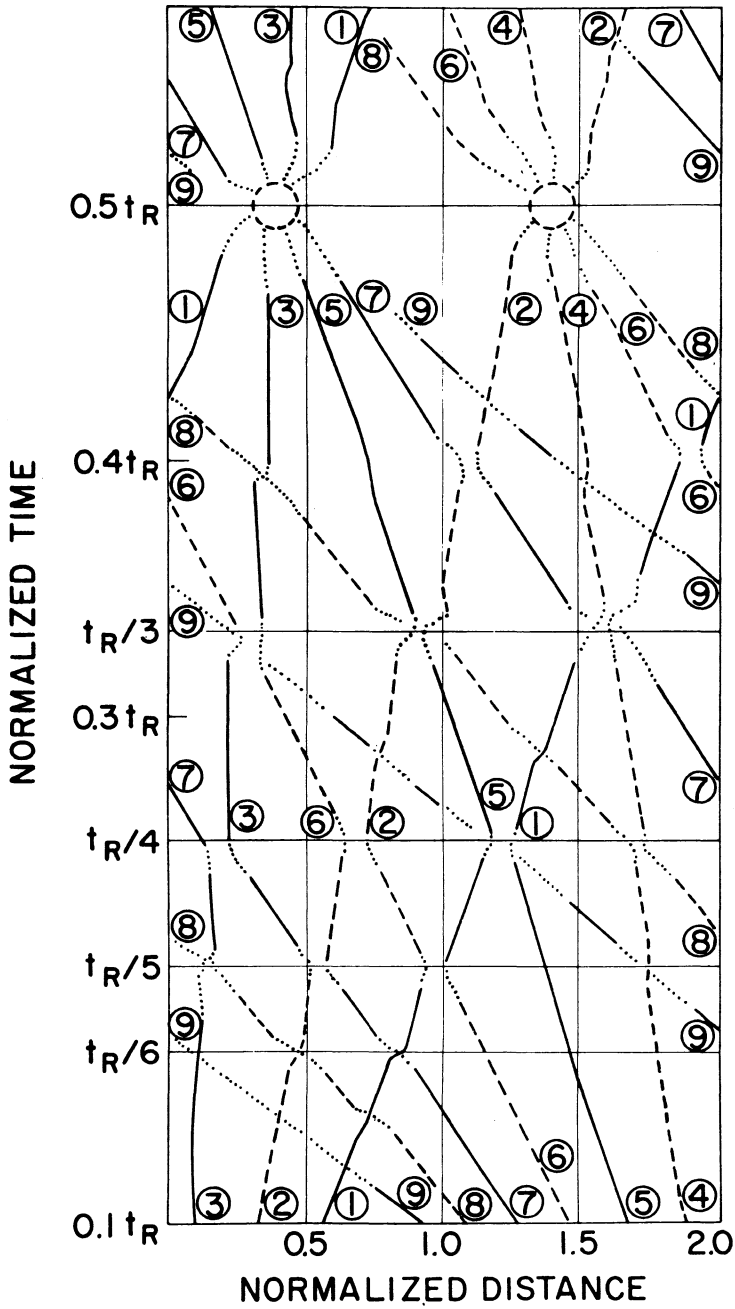

Figure 5.7. The propagation of the solitons shown in Figure 5.6 (Zabusky).

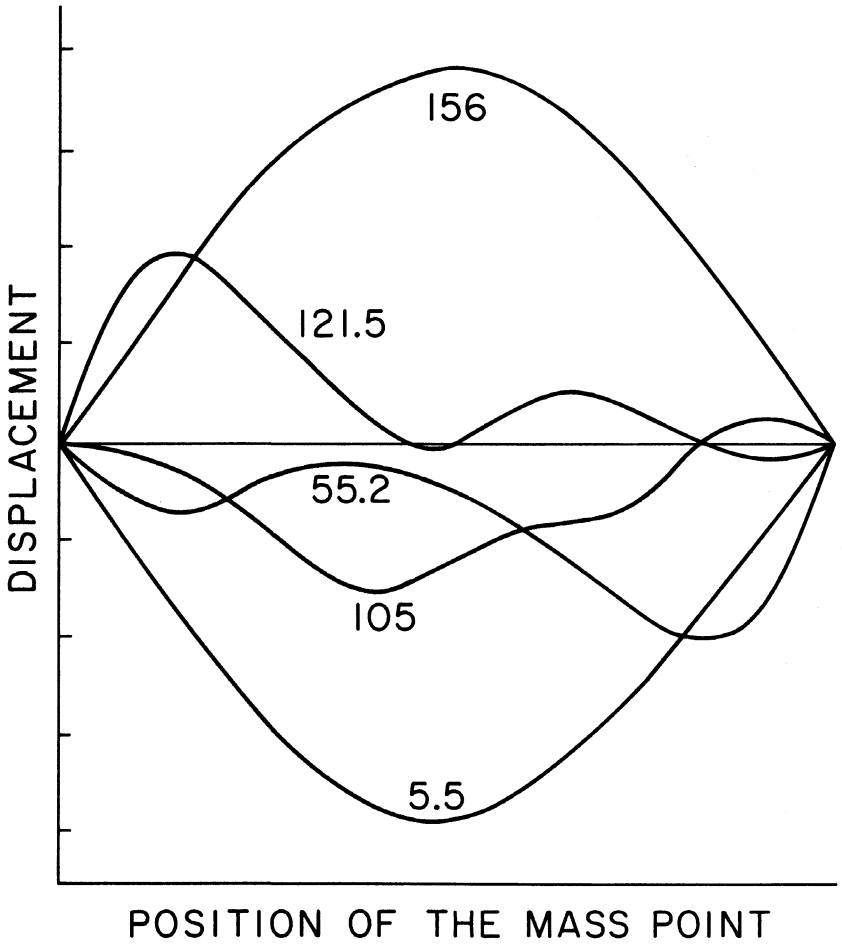

Figure 5.8. The displacement $y(n, t)$, of the particles in the FPU calculation corresponding to Figure 5.1. The numbers on the curves are values of $\omega_1 t/2\pi$ (after Fermi, Pasta, and Ulam).

in Figure 5.7; see Toda [14, p. 28]). As Zabusky noted, one of the remarkable features of this result is the persistence of the solitons' identities through many interactions. To me, an equally remarkable feature is that "unbreaking" in fact ever occurs, given the apparent chaotic shifts in some trajectories (a point I will return to below).

Figures 5.6 and 5.7 are based on the Korteweg-deVries equation

(5.27) $$u_t + u\,u_x + \delta^2 u_{xxx} = 0$$

with $\delta = 0.022$ and $u(0, x) = \cos(\pi x)$, which Zabusky proposed as a continuum approximation of the lattice equations. Presumably the profile $y_n(t)$ (or $y(x, t)$?) shown at different times in the (modified) FPU Figure 5.8, should be understood to be a combination of the left and right traveling Riemann invariants considered by Zabusky. Figure 5.8 corresponds to the dynamics shown in Figure 5.1, with the curves labeled with values of $(\omega_1 t/2\pi)$. Of course many oscillations occur between each illustrated configuration of the lattice. While the derivative of $y(x_0, t)$, which corresponds to the $u(x_0, t)$ in Figure 5.6, does exhibit as many as five extrema in Figure 5.6 (corresponding to the excitation of five normal modes), it does not appear to contain the complexity exhibited by the soliton picture—a fact which is presumably due to the superposition of left and right traveling nonlinear wave forms (Zabusky [58]; Toda [14]). Obviously, regardless of this comparison, the revival of the Korteweg-deVries equation and the subsequent mathematical developments have proved to be a very fruitful area of research.

The question remains, nonetheless, as to how detailed one can *predict* such features as the FPU recurrence time from the soliton picture. From a number of computations, Zabusky proposed [57], [58] that the recurrence time could be expressed in terms of the empirical formula

(5.28) $$(\omega_1/2\pi)T_R = R\,N^{3/2}/\alpha^{1/2}$$

where $R \simeq 0.44$, $F(z) = z + \alpha z^2$, and $y_n(0) = \sin(n\pi/N)$; $\dot{y}_n(0) = 0$. As can be seen from the last column of Table 5.2, this expression does agree (within 25%) with the calculated values if $\alpha \geqq 1/4$. Clearly (5.28) cannot hold as $\alpha \to 0$, but its limitations for small α are unclear. A very nice explanation of the empirical relationship (5.28) has been proposed by Toda [14], using the fact that the soliton amplitudes (and hence velocities) arising from the initial state $u(0, x) = \cos(\pi x)$ form an arithmetic series. This feature of Figure 5.6 was also noted but not explained by Kruskal and Zabusky [56]. Because of this common difference in the velocities of the solitons, Δv_s, *if the solitons do not accelerate as they pass through one another,* then the *ordering* of the solitons will recur in a time $L/\Delta v_s$, where L is the length of the (periodic) system. Toda concluded that this *reordering* time is the *recurrence* time, $T_R = L/\Delta v_s$, leading to the *prediction*

(5.29) $$(\omega_1/2\pi)T_R = \frac{3N^{3/2}}{\pi^{3/2}\sqrt{\alpha}}$$

which corresponds to $R = 3/\pi^{3/2} \simeq .54$ in Zabusky's formula.

I feel that Toda's expression (5.29) is the closest that the soliton picture has come to date in the *prediction* of any of the FPU results. Unfortunately I do not believe that even this derivation can be considered complete at present, because of two reasons:

(i) It does not explain why the obvious shifts in Figure 5.7 play no role in this recurrence effect—or to put it more negatively, "how is it possible that recurrence occurs at all, in virtue of these apparent 'incommensurable' shifts?". The resolution of this problem *may* rest with the recognition that the shift *may* only occur in the "particle label" space x_0, rather than physical space, x, as noted in the last section (note again the lack of accelerations in Figure 4.5). This however has yet to be established.

(ii) The reordering time, $L/\Delta v_s$, is not generally, or even usually, a recurrence time. The latter requires a reordering between the solitons as well as with the ends of the lattice (simultaneously). This will only occur if $\min(v_s) = \Delta v_s/n > 0$, where n = integer, in which case

$$T_R = nL/\Delta v_s. \tag{5.30}$$

Toda's expression (5.29) comes from using $n = 1$.

In addition to these problems, there appears to be nothing in the derivation which limits the size of α. Clearly (5.28) and (5.29) cannot be correct as $\alpha \to 0$, for we know that in the present case

$$\lim_{\alpha \to 0} (\omega_1/2\pi)T_R = \omega_1/(2\omega_1 - \omega_2).$$

How this arises from a soliton picture is unclear at present.

I would like to conclude this section concerning the interrelation between the FPU recurrence and solitons, by discussing a result obtained by K. Miura during our investigations in 1973, but not included in his thesis. This result concerns a lattice with the polynomial force $F(z) = \mu[z + K_3 z^3]$ (i.e., with no quadratic term), which was one of the examples also studied by Fermi, Pasta, and Ulam [61] (with $K_3 = +8$, their Figure 4). The continuum equation usually retained from (4.10) for a polynomial force $F(z) = \mu[z + K_2 z^2 + K_3 z^3]$ is

$$u_{tt} = u_{xx} + K_2(u^2)_{xx} + K_3(u^3)_{xx} + u_{xxxx} \tag{5.31}$$

where t is in units of $h(12)^{-1/2}/C$, and x is in units of $(12)^{-1/2}h$. Now, if $K_2 = 0$, then (5.31) has a solitary wave solution

$$u(x, t) = w(x - vt) \equiv w(z); \quad \lim_{z \to \pm\infty} w(z) = 0 \tag{5.32}$$

only if $K_3 > 0$. This is easily proved after making three integrations of (5.31), using the boundary conditions (5.32), to obtain

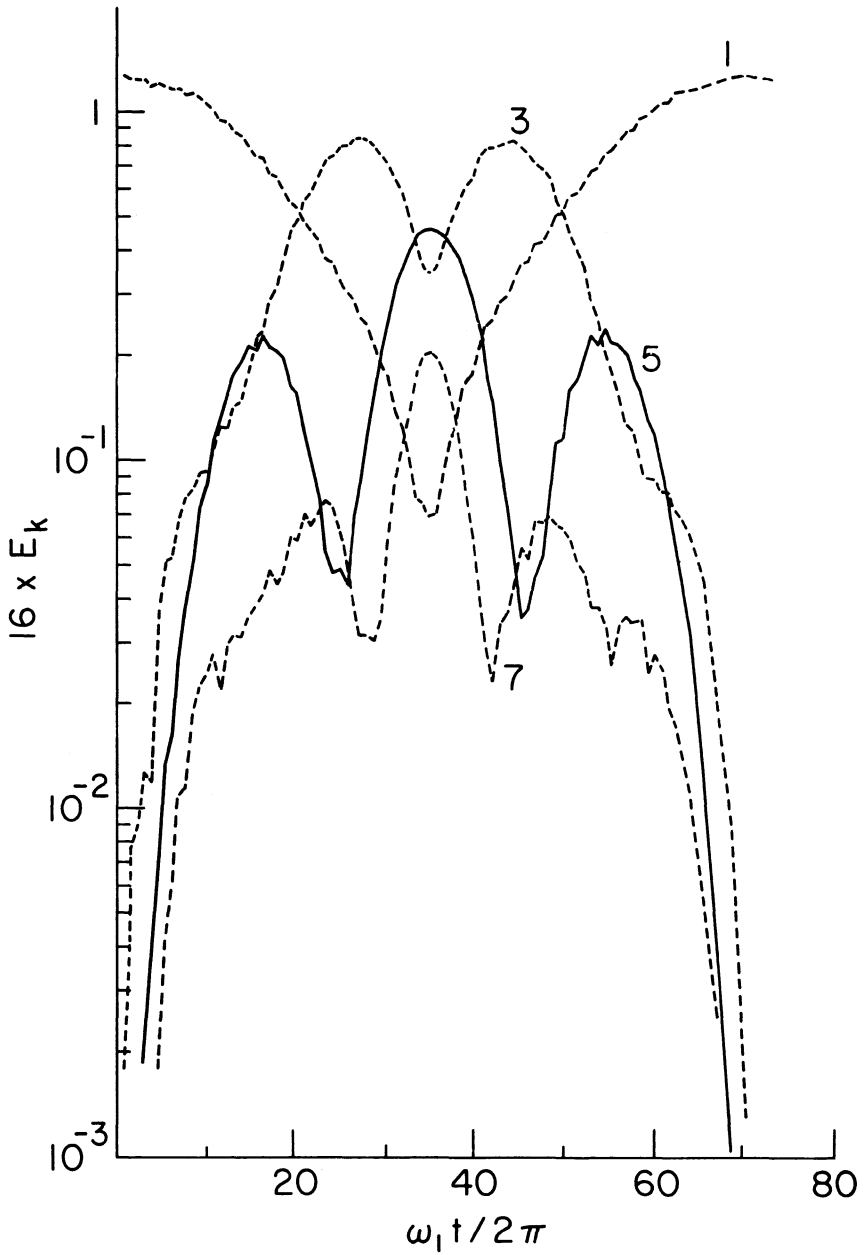

Figure 5.9. The mode energies for the lattice with a force $F(z) = z + 8z^3$, which has a continuum soliton solution, with the FPU initial condition (K. Miura).

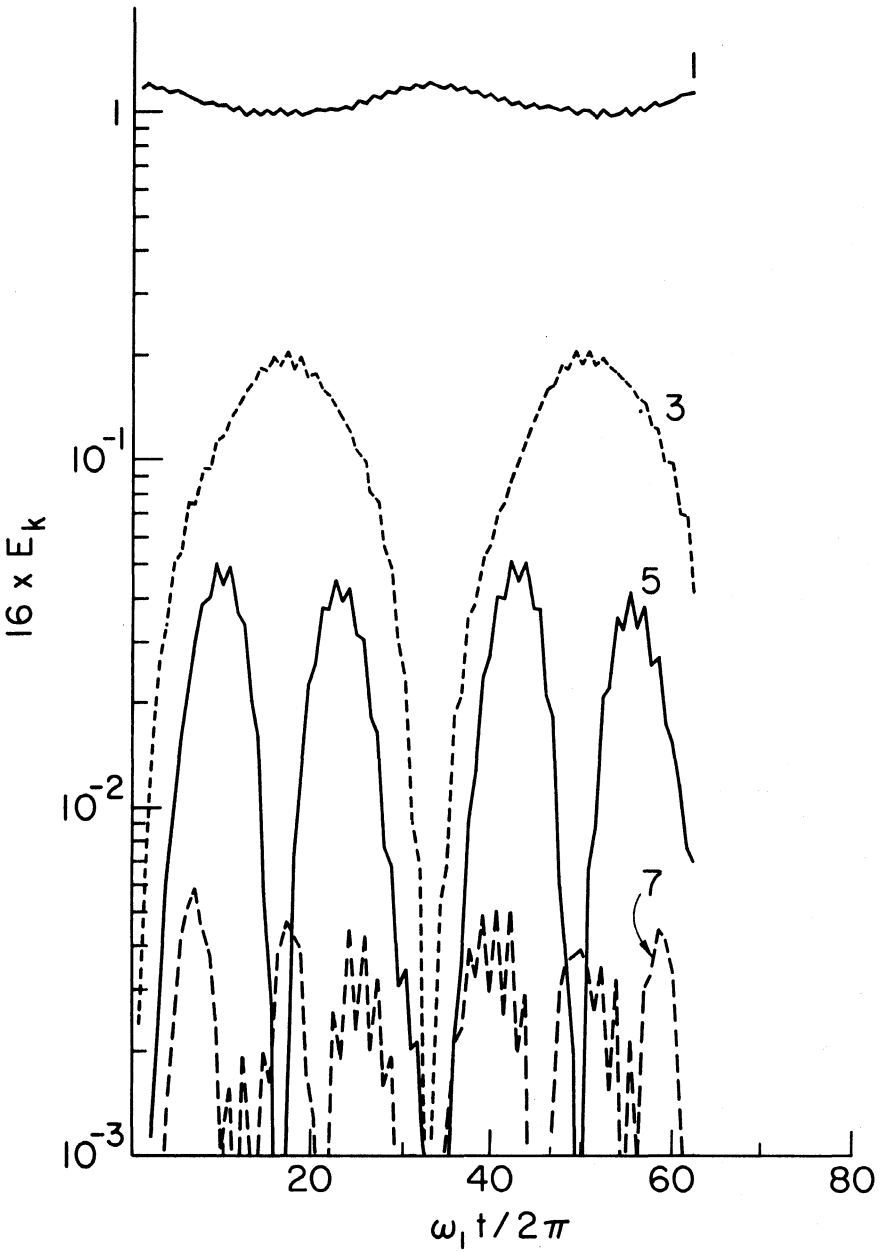

Figure 5.10. The mode energies for the lattice with a force $F(z) = z - 8z^3$, which has no continuum soliton solution (5.32) (K. Miura).

$$(w')^2 = [v^2 - 1 - \tfrac{1}{2}K_3 w^2]w^2 \equiv P(w). \tag{5.33}$$

Obviously $P(w) > 0$, which means that $v^2 > 1$, in order for $w^2 \to 0$ (as $z \to \pm\infty$). In order for (5.33) to have a nontrivial solution w' must vanish for some finite z, which can only happen if $K_3 > 0$. Indeed the solitary wave solution is found to be

$$U = \kappa(2/K_3)^{1/2} \operatorname{sech}[\kappa(x \pm \sqrt{1+\kappa^2}\, t)];\ (K_2 = 0) \tag{5.34}$$

which may be compared with the solution (5.32) of the Boussinesque equation ($K_3 = 0$, in (5.31))

$$u = \kappa^2(3/2K_2) \operatorname{sech}^2[1/2\, \kappa(x \pm \sqrt{1+\kappa^2}\, t)];\ (K_3 = 0). \tag{5.35}$$

K. Miura calculated the values of $E_k(t)$ for the polynomial force lattice with $K_2 = 0$ and $K_3 = \pm 8$, using fixed ends and the initial condition $y_n = \sin(n\pi/32)$, $\dot{y}_n = 0$ (there are $N = 31$ particles). The results of these calculations are shown in Figures 5.9 and 5.10 (the former may be compared with FPU Figure 4). The difference in the two results is dramatic, both in terms of the relative amount of energy exchanged between the modes, and the time scale over which the recurrence takes place. Only the odd modes are excited because of the odd powers of z in $F(z)$. Note that the energy exchange is much greater when $K_3 = +8$ (Figure 5.9), than when $K_3 = -8$, and that the time for recurrence in the latter case is about one half of that in the case $K_3 = +8$. The lack of energy exchange between the linear normal modes in the case $K_3 = -8$ is one way of expressing the fact that a solitary (localized) disturbance does *not* develop, which agrees with the above result. On the other hand there is clearly a significant energy exchange in Figure 5.10 (E_1 decrease by 15–20% of its initial value during part of the time), and a well defined recurrence time ($\sim 33(2\pi/\omega_1)$). This particular recurrence phenomenon is an example which cannot be interpreted in terms of *continuum* solitary waves, arising from equation (5.31). Whether there are discrete (lattice) solitons when $K_3 < 0$ is not known at present. On the other hand the difference between the cases $K_3 > 0$ and $K_3 < 0$ can be expected from the above perturbation theory. This is because H_1 contains factors $K_3 a^4$, so there is a frequency shift $\mu_k^{(1)}$ proportional to the *first* power of K_3. This *can* produce dramatic differences depending on the sign of K_3 (the details, however, have *not* been confirmed to date).

6. **Stochasticity, Ergodicity, and Solitons.** One of the fundamental areas of research in irreversible lattice dynamics is the study of the onset of "stochastic" behavior as the nonlinearity of the lattice is increased. "Stochastic" is a widely used, and rather imprecise term which

indicates the erratic, wild, and hopefully "statistical" behavior of at least some set of dynamic variables. The FPU recurrence phenomena is therefore a classic example of non-stochastic dynamics, as is the long-time existence of a soliton. The variables which have been usually considered are the (harmonic) normal mode energies, or the intersection of the phase trajectory with some Poincaré surface of section (see below), or a set of action-angle variables generated by a canonical transformation selected to make the Hamiltonian conform with the conditions of the KAM theorem (also see below). One of the interesting results that has been found (Ford, Stoddard, and Turner [82]) is that the "stochasticity" observed in computer calculations can be strongly influenced by the selection of the dynamic variables, and that several tests may be warranted before statistical conclusions can be anticipated.

Early investigations which indicated the onset of stochastic behavior in lattice systems were made by Izrailev and Chirikov [86], Chirikov [76], and Zaslavsky and Sagdeev [102]. These were followed by studies of one-dimensional lattices (Saito, Ooyama, Aizawa, and Hirooka [95]), two-dimensional lattices (Hirooka and Saito [94]) with varying amounts of nonlinear coupling. They found from computer experiments that, not only did energy sharing occur for larger coupling, but that there appeared to exist an "induction period" during which there is very little energy exchange, followed by an apparent equipartition of energy (see also, Saito et al. [95]). More recently Bivins, Metropolis, and Pasta [74] examined how this induction time is influenced by the number of modes used to describe the dynamics of the system, and to relate it to instability regions of the Mathieu equation. It is interesting to note that Northcote and Potts [66] also showed an example where their $E_1(t)$ exhibited such an induction period, before it rapidly lost energy (their Figure 2). The existence of an induction period is, of course, quite contrary to the usual "relaxation time" picture of energy loss noted in previous sections. Both the existence of this induction period, and the apparent stochastic nature of the equipartition of energy contrast sharply (at least in some cases) with another method of examining (small) lattice dynamics which has been widely used by Ford and his coworkers [75], [79]–[82], [101]. Since Ford [80], [81] has written very clear and extensive reviews on this method, I will discuss it only briefly in order to contrast it with other methods.

Their method is based on the use of Poincaré's surface of section, which had been applied by M. Henon and C. Heiles (Astron. J. 69, 73 (1964)) and others in astronomy, as well as applications in unimolecular dissociation in chemistry. (See Walker and Ford [101] for a very nice discussion and additional references. A recent application in chemistry

can be found in D. W. Noid and R. A. Marcus, J. Chem. Phys. **62**, 2119 (1975).) Henon and Heiles studied the bounded motion of a system with the Hamiltonian

$$H = \tfrac{1}{2}(p_1^2 + p_2^2 + q_1^2 + q_2^2) + q_1^2 q_2 - \tfrac{1}{3} q_2^3 \tag{6.1}$$

and used the Poincaré surface of section to determine whether the system has any other "well-behaved" constants of the motion besides H. To determine this they examined the points at which the system trajectory intersected the (p_2, q_2) plane when $q_1 = 0$ and $p_1 \geqq 0$. If these points fall on a "smooth" closed curve this indicates that there is another "regular" constant of the motion, $I(p_1, q_1, p_2, q_2)$ so that I and H restrict the trajectory motion to a smooth two-dimensional surface in the phase space (p_1, q_1, p_2, q_2). Figures 6.1 and 6.2 show some of the results presented by Walker and Ford for the Henon and Heiles' Hamiltonian (6.1), with the intersection points connected by freehand curves where appropriate. In Figure 6.1 $H = 1/12$, and it appears that, within computer accuracy, all initial states have trajectories lying on smooth two-dimensional surfaces (tori). In Figure 6.2 $H = 1/8$, and there is now a large region with dynamic states which exhibit instabilities, or "stochasticity". These observations were extended later to include the determination of the separation distance between pairs of trajectories which initially are very close to each other. They found that this separation, $S(t)$, is essentially proportional to time for those pairs which lie in the region with the smooth curves, but that $S(t)$ increases essentially exponentially with time if the pairs lie in the "stochastic" region. This latter property is one which is associated with C-systems, and therefore presumably very suggestive of ergodic behavior. Unfortunately, in a computer calculation it is not always possible to make a precise determination of when a system goes from a linear to an exponential behavior of $S(t)$, unless the growth rate of $S(t)$ is short compared with the computation time. Nonetheless, this added measure of stochasticity is a very important addition to the Poincaré plane "smooth curve" method, because the latter is probably only useful for systems with very few degrees of freedom. If the system has a large number of degrees of freedom then the intersection of its trajectory with such a two-dimensional surface can be very complicated, even if other "regular" constants of the motion do exist. The separation test however would appear to be usable with more degrees of freedom. Here the difficulty may be that $S(t)$ will behave like $S(t) = t\,P(t)$, or $S(t) = \exp(at)\,P(t)$, but where $P(t)$ is itself sufficiently erratic that it may be difficult to distinguish linear and exponential separations.

Regardless of these questions on the extension of this method to lat-

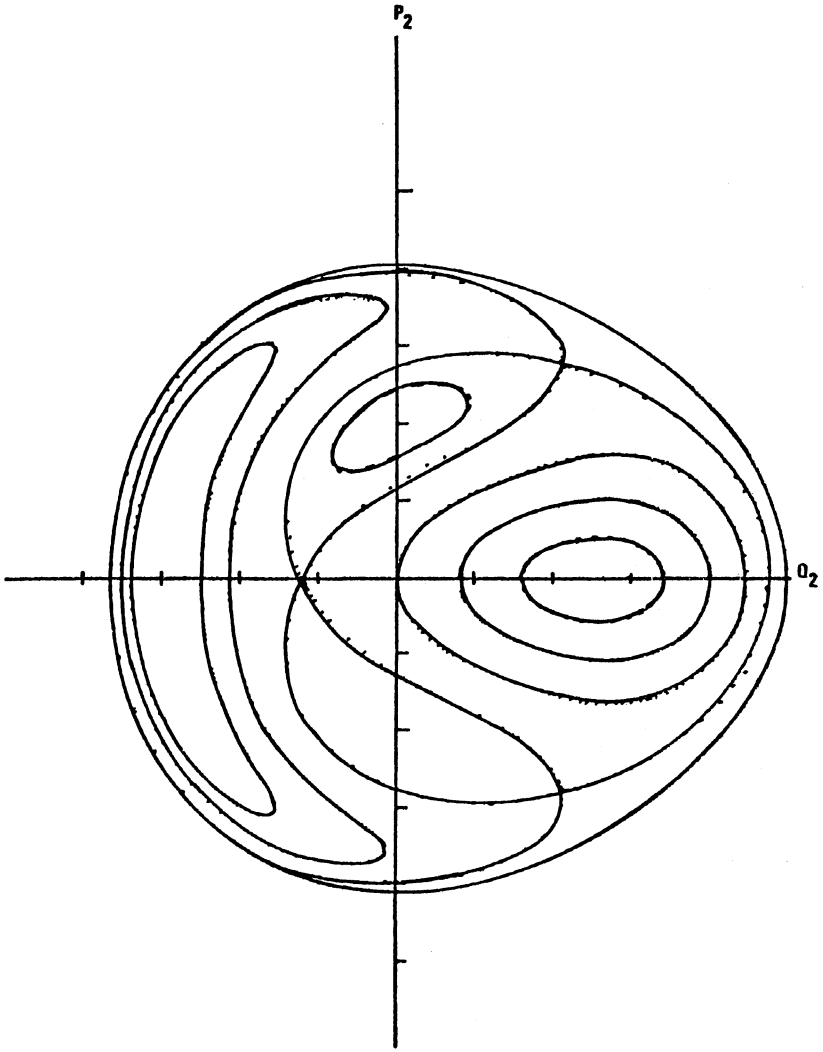

Figure 6.1. The intersection of several two-dimensional tori in phase space (p_1, q_1, p_2, q_2), associated with different dynamical trajectories, with a Poincaré surface of section. The Henon-Heiles system has energy $E = 1/12$. (Walker and Ford).

tices with more degrees of freedom, this approach was strikingly successful in predicting the existence of well-behaved (indeed analytic) integrals of the motion for the exponential lattice. Ford, Stoddard, and

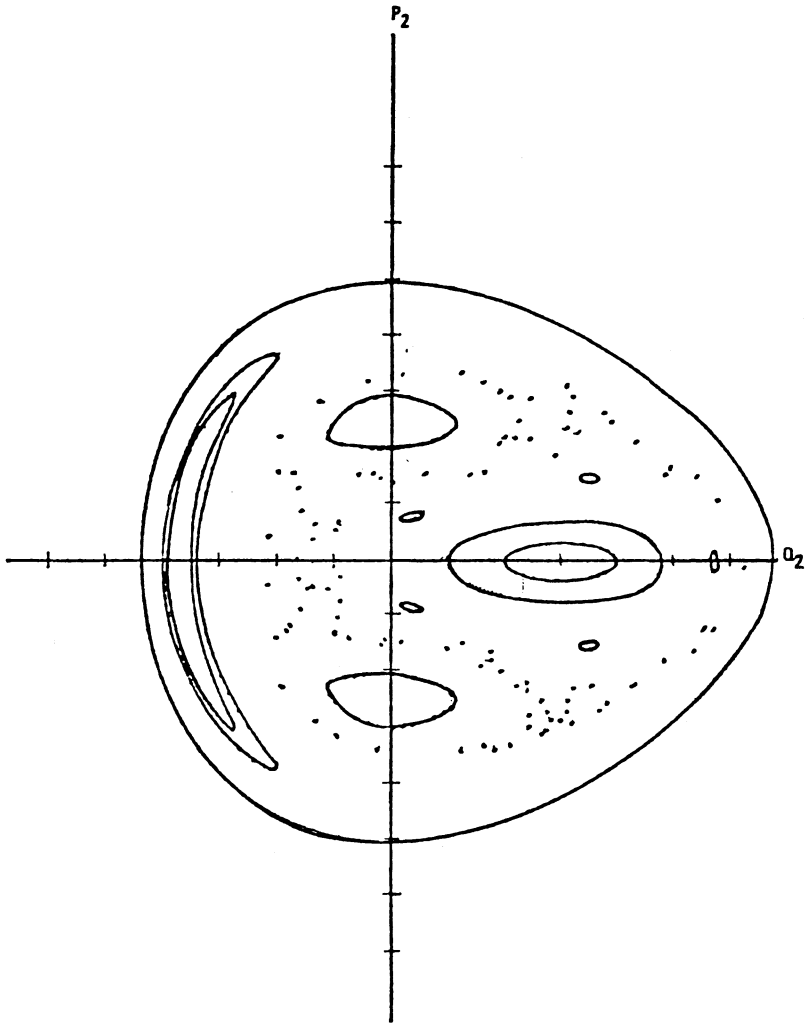

Figure 6.2. The surface of section for the Henon-Heiles system with a larger energy ($E = 1/8$) than in Figure 6.1. The unconnected dots are produced by the intersection of a single trajectory with this surface (Walker and Ford).

Turner [82] computed the surface of section for a three particle exponential "lattice" with periodic boundary conditions, characterized by

$$H = \tfrac{1}{2}(p_1^2 + p_2^2 + p_3^2) + e^{-(q_1-q_3)} + e^{-(q_2-q_1)} + e^{-(q_3-q_2)} - 3 \tag{6.2}$$

They concluded, both from the persistence of smooth intersection curves even at very large energies, and from the linear time dependence of the separation distance, $S(t)$, that the exponential lattice must possess well behaved integrals of the motion in addition to H (and another which they had accounted for). This computer prediction led Henon [**85**] (also see Flaschka [**78**]) to seek and find N analytic constants of the motion which are in involution (Whittaker [**17**]), and certainly is an outstanding example of the useful interplay which may result between computer calculations and theory.

One of the greatest benefits which may result from Toda's exponential lattice model is that it presents a clear distinction between ergodicity and FPU energy sharing. As noted by Ford, Stoddard, and Turner, the above result establishes the fact that the exponential lattice is certainly not ergodic. On the other hand, as shown in the computer studies by Saito, Ooyama, Aizawa, and Hirooka [**95**], the exponential lattice *can* exhibit energy sharing for sufficiently strong nonlinearity. (They used $N = 15$, $a = 0.471$, $b = 2.127$, and initially excited the eleventh mode, apparently with an amplitude $a_{11} = 2.0$). Also Ooyama and Saito [**46**] observed that solitons passing through a sufficiently energetic background of "ripples" experience a viscous drag, slow down, and hence must be losing energy (see the end of § 5). This deterioration of a soliton appears to be related to the stochastic energy sharing, in that a minimum background energy seems to be required before there is an observable drag. The important fundamental point to be learned here is that energy sharing and ergodicity are quite distinct. Nothing precludes a system which has a number of independent analytic integrals of the motion from exhibiting energy sharing, or a transition to this form of "stochasticity" as a nonlinear parameter is increased.

This question of whether "stochasticity" may not frequently be "in the eye of the beholder", depending on which dynamic variables (*not* a complete set) he chooses to examine, strikes me as a very important consideration in future research. Thus the breakdown of a physically interesting quantity, such as the soliton, may not require anything like ergodic behavior, to say nothing of mixing and other more exotic properties (e.g., Arnol'd and Avez [**73**]). Therefore, while the system may appear quite "regular" dynamically in one set of variables, the physically interesting variables may exhibit quite "irreversible" properties. This fact may be worth keeping in mind when one draws physical conclusions about limited variables from some mathematical theorems.

In this respect I would like to make a few comments about the very beautiful and important Kolmogorov-Arnol'd-Moser (KAM) theorem (e.g., Moser [**91**]), which is presumably closely related to the FPU re-

currence phenomena, and perhaps more directly to the existence of the regular regions in Figure 6.2 (see Ford [80], [81] for a discussion of this connection). The KAM theorem states roughly the following:

> Let the Hamiltonian $H(J, \theta, \lambda)$ be an analytic function of its arguments near $\lambda = 0$, and over some open set of values $(J, \theta) \in \mathscr{P}^{2N}$. Assume also that H has period 2π in each of the variables $\theta = (\theta_1, \cdots, \theta_N)$ and that, for $\lambda = 0$, the Ham iltonian depends only on $J = (J_1, \cdots, J_N)$, so that $H(J, \theta, 0) \equiv H_0(J)$. Consider the N-dimensional tori defined at $\lambda = 0$ by

$$\dot{\theta}_k = \frac{\partial H_0}{\partial J_k} \equiv \Omega_k(J); \quad J_k = J_k{}^0 \text{ (constants)}. \tag{6.3}$$

Assume that the frequencies $\Omega_k(J)$ are independent functions of J at J^0, so that the following Jacobian does not vanish at J^0

$$\partial(\Omega_1, \cdots, \Omega_N)/\partial(J_1, \cdots, J_N) \neq 0 \quad (J = J^0). \tag{6.4}$$

Then, for sufficiently small λ, most of these tori are invariant, in the sense that

$$\theta = \phi + f(\phi, \lambda), \quad J = J^0 + g(\phi, \lambda) \tag{6.5}$$

where $f(\phi, \lambda)$ and $g(\phi, \lambda)$ are analytic functions, periodic in ϕ, which vanish at $\lambda = 0$. Moreover $\dot{\phi} = \Omega_k(J^0)$.

These invariant tori therefore remain close to their surfaces at $\lambda = 0$ (i.e., they are "stable", not erratic, or "stochastic"). Thus the smooth curves in the surface of section in Figure 6.1 is an example of the intersection of two-dimensional invariant tori with this surface. The breakdown of this invariance is then demonstrated by the erratic region in Figure 6.2. This interpretation, and an analogous "explanation" of the FPU invariance of periodic motion, leaves some questions which would be useful to have clarified.

The difficulty centers on the condition (6.4), and the introduction of the parameter λ. Such a parameter does not occur naturally in a physical Hamiltonian, and is *introduced* usually as a measure of the nonlinearity of the system (for a fixed region $\mathscr{P}^{2N}$). Then, at $\lambda = 0$, one has a harmonic lattice, so $H_0 = \sum \omega_k J_k$, and $\Omega_k(J) = \omega_k$. Since the functions $\Omega_k(J)$ are all constants, they are not independent, and (6.4) is not satisfied. Note that this condition has nothing to do with whether the ω_k are commensurable. This means that, if the KAM theorem is to be associated with the FPU study, then the λ of this theorem cannot be simply the physical measure of nonlinearity (e.g., the α in the FPU force $F(z) = \mu[z + \alpha z^3]$). Indeed what is required, before the KAM theorem

can be applied, is to make a canonical transformation to another set of action-angle variables, $(\bar{J}, \bar{\theta})$, given by $\bar{J} = \partial K(J, \bar{\theta})/\partial\bar{\theta}$; $\theta = \partial K(J, \bar{\theta})/\partial J$, such that the new Hamiltonian $\bar{H}(\bar{J}, \bar{\theta})$ has an additive part which is at least quadratic in $\bar{J}$. One can then write

$$\bar{H}(\bar{J}, \bar{\theta}) = \bar{H}_0^{(s)}(\bar{J}) + \bar{H}_{s+1}(\bar{J}, \bar{\theta}) \tag{6.6}$$

where $\bar{H}_0^{(s)}(\bar{J})$ is of order s in $\bar{J}$. The process of carrying out such transformation was discussed by G. D. Birkhoff (Dynamical Systems, Amer. Math. Soc., 1927, p. 82ff.) and in the present contest by Arnol'd [71, p. 108ff]. To perform this transformation requires that the frequencies ω_k satisfy

$$\sum m_k\omega_k \neq 0 \quad \text{if} \quad |m| = \sum_{k=1}^{N} |m_k| \leqq 2s - 1. \tag{6.7}$$

If $\bar{H}_0^{(s)}$ $(\bar{J})$ satisfies (6.4), Arnol'd calls the system $\bar{H}(\bar{J}, \bar{\theta}) = \bar{H}_0^{(s)}(\bar{J})$ a general elliptic type. A system with this Hamiltonian is, of course, quite stable because the $\bar{J}_k$ are constants. However the system with the Hamiltonian $\bar{H}(\bar{J}, \bar{\theta})$ remains close to this stable trajectory only for a time of the order ϵ^{-s}, where ϵ is their initial distance from the origin. One cannot draw any conclusion about the stability of the original system by taking $s \to \infty$, because the Birkhoff series diverges in this limit, due to the classic problem of small denominators. What one can do instead is to stop at $s = 2$ (say), and then proceed to use the KAM theorem, assuming that its conditions are now met. A study establishing when this procedure satisfies the conditions of the KAM theorem has been made by Nishida [92] (I am indebted to J. Ford for bringing this reference to my attention). This theorem is again based on canonical transformations, but since the $\Omega(\bar{J})$ are now functions of $\bar{\mathrm{J}}$, one can use the result from the theory of Diophantine approximations to conclude that, in a region ϵ, nearly all $\Omega(\bar{J})$ satisfy (for $|m| > 0$)

$$\left| \sum^{N} m_k\Omega_k \right| \geqq K\epsilon|m|^{-\nu}(\nu = N + 1) \tag{6.8}$$

for some $K > 0$. Using this fact, one can then establish the convergence of the series of transformations, for nearly all initial states. This very pretty procedure has the disadvantage of introducing a parameter, and new canonical variables which have no direct physical significance. This presumably is of no consequence as long as one does establish stability, because everything is stable (so to speak). However, if one is interested in extending these results, and considers the destruction of the tori for larger nonlinearity, then the physical significance of the varia-

bles may be quite important in judging the statistical effect of some destroyed region. Thus, to return to Ford, Stoddard and Turner's result, they found stability for Toda's exponential lattice, yet the physically interesting normal mode energies can exhibit a "stochastic" behavior [**95**]. It would be very nice to understand better how such a stable system can exhibit such stochasticity in *some* variables. Similarly above, the fact that some tori in the $(\bar{J}, \bar{\theta})$ space are invariant may not indicate a "smooth" dynamical behavior in the original (J, θ) space. In a similar way the stability of such tori may not indicate the apparent stability of solitons. At present the connection between stochastic dynamics and the onset of soliton breakdown is nearly a totally virgin field.

POSTSCRIPT. Recently some very interesting calculations have been made by Casartelli, Diana, Galgani, and Scotti [**103**] and by Benettin, Galgani, and Strelcyn [**104**] which study the relationship between the onset of stochasticity and the Kolmogorov-Sinai dynamical entropy (or a related entropy). Previous important studies of this type have been made by Chirikov [**76**], Chirikov, Keil, and Sessler [**105**], and by Chirikov, Izrailev, and Tayursky [**106**].

7. **Suggestions for Future Research.** Perhaps, after this excursion through various irreversible thickets, one of the more useful exercises would be to extract some more or less specific problems which have been eluded to in the above discussion. While this represents one more distillation, nonetheless I apologize for the obvious vagueness and possible bias of some of these questions. Perhaps mathematicians can sharpen some of them, and thereby find a problem worthy of future research. In random order of importance:

1. What is the relationship (if any) between the "stochastic" temporal behavior of a lattice and its ability to support highly independent spatially localized disturbances? This, of course, involves the question of a bridge between the temporal and spatial behavior of a lattice.

2. Is there an N dependence to the stochastic behavior of a lattice (for given energy per particle)? That is, how does stochasticity change in the thermodynamic limit?

3. So far there is much more theoretical than computational reason to believe that a temperature gradient is easier to establish in a two-dimensional rather than a one-dimensional lattice. Is there a *non*existence proof of two-dimensional solitons (in a nondispersive, noninteracting sense) which would further support this contention?

4. How is the temperature gradient, observed in many computer calculations of one-dimensional lattices, compatible with soliton transport of energy? Is the temperature gradient correlated with the oscillatory "tails" of the solitons which are produced at the reservoirs, or does it represent a "local stochastic breakdown" produced by the interaction of two "solitons"? K. Miura's calculations indicate that in the interaction of less energetic solitons they lose both a larger percentage and absolute amount of energy to "thermal noise".

5. It appears to be an untested consensus that anything beyond nearest-neighbor interactions adds nothing essential to the irreversible properties of a lattice. Perhaps long range interactions can produce "dynamic transitions" (e.g., to stochastic behavior) in analogy to phase transitions in equilibrium statistical mechanics. It should be noted that for the long range interactions $V(r) = r^2 + r^{-2}$ (Collegro lattice) the system *is* integrable (J. Moser, Adv. Math., to be published), and does *not* exhibit stochasticity (G. Casati and J. Ford, J. Math. Phys., to be published). A less nebulous question is what is the influence of longer range interactions on the ability of lattices to maintain independent localized disturbances (nonsolitary solitons!)?

6. FPU recurrence can occur in lattices which have no "continuum" soliton solutions (in the standard continuum approximation). Do the corresponding discrete lattices support solitons? What does this result imply about the explanation of FPU recurrence in terms of solitons, or that solitons are more basic than periodic solutions (which these same lattices do possess).

7. Obtain an accurate prediction of the FPU recurrence time from continuum equations (if possible, or with accuracy related to the number of higher derivatives), or from the Toda lattice. In either case account should be taken of the phase delays introduced by interactions between solitons or with the fixed ends. Perhaps even more basic is to prove that FPU recurrence *should* occur, even with these phase delays. That already appears to be very mysterious, and may be related to the Euler vs. Lagrange descriptions (see problem 9). Also how does the soliton picture become modified as $\alpha \to 0$ in (5.28)?

8. Push the perturbation theory predictions of the FPU recurrence times to their convergence limits—whatever that may mean precisely. The calculations ten years ago were crude, being done by hand (without even a calculator!). It would be of great interest to see how these, or more recent methods (Eminhizer, Helleman, and Montroll [60]) may give indications of the onset of stochasticity (e.g., a rapid lengthening

of the recurrence time with increased energy or N—perhaps a "phase transition" to the Poncaré's time?). These perturbation calculations are still the only methods which have given answers accurate to (say) 20%.

9. A careful analysis of the continuum limit should be made, distinguishing carefully between the Lagrangian and Eulerian pictures ($x_n(t)$, and (x, t)). Much of the Eulerian nonlinearity can arise in a transcription of simple linear (harmonic) Lagrangian dynamics, and thus is trivial (Figure 4.4). For example, is it possible that a "lattice-shift" slowdown (e.g., Figure 4.4) can combine with the "Lagrangian speed-up" of $y(x_0, t)$ for crossing impulses (e.g., Toda [14]) to yield a net zero acceleration in space (e.g., Figure 4.5)?

10. It would be interesting to determine to what extent the local energy in a computer calculation of lattice thermal conductivity has in fact a local canonical distribution. This is a basic assumption of the Kubo formulation of thermal conductivity, and is distinct from the Hamiltonian modification used for other irreversible processes (e.g., electrical conductivity). Perhaps Fourier's "temperature" is not canonical, and the law thereby does not imply "strong mixing" of the modal energies (or solitons).

11. The coupling of a lattice to an outside source (e.g., thermal reservoir) presents several interesting problems (see the temperature jumps, Figure 4.3). What conditions insure the best energy exchange—e.g., in terms of collision frequencies, sound velocities, mass ratios, etc.?

12. The integrability of the Toda lattice affords a unique opportunity to clarify the importance of such integrability on macroscopic irreversible behavior. Good energy sharing can occur in such a system (Saito's calculations), but this may not imply Fourier's law (Visscher's observation about the energy sharing HHC lattice, found by Northcote and Potts). The important investigation of Casati and Ford (to be published in Phys. Rev. A) on the influence of the unequal mass Toda "molecule" ($N = 2$; $p_3 = q_3 = 0$ and $p_1 \to p_1^2/m_1$, $p_2 \to p_2^2/m_2$ in (6.2)), should be extended to larger systems, where thermal conductivity and solitons are meaningful.

13. Is stochasticity in nonlinear (say polynomial) lattices perhaps most simply understood in terms of the harmonic plus hardcore model (2.5)? This system, which is obviously nonergodic for small energies, is at least energy sharing for larger energies [66] and this division should be quite sharp. An apparent paradox arises however since only at the larger energies can the HHC lattice apparently support a nonergodic

disturbance similar to a soliton. Actually this is unclear since K. Miura's calculations were not over sufficiently long times to draw a definite conclusion about their dispersion, and the interacting pulses *did* show a loss of energy. The HHC model does however seem to give a particularly transparent example of exponentially diverging states (because of totally different futures, resulting from a few hardcore interactions).

14. What is the relationship between the velocity, V_i, imparted to the end of a finite lattice, and the energy (and velocity) of the resulting soliton (Figure 4.7)?

15. Is there a continuous transition from Schrödinger's (et al.) localized solution of the harmonic lattice (2.29, and Figure 2.4) to the nonlinear soliton? The exponential lattice offers an explicit example ($a \to \infty, b \to 0, ab =$ constant).

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