Classical waves on nonlinear lattices

G. D. Mahan
Department of Physics, Pennsylvania State University, 104 Davey Laboratory, University Park, Pennsylvania 16802, USA
(Received 12 May 2005; revised manuscript received 28 July 2005; published 19 October 2005)

We discuss the solution to classical vibrations on several nonlinear lattices in one dimension. One lattice has nearest-neighbor potential energy with both quadratic and quartic terms in the relative displacements q. Another lattice has the potential energy terms going as $\cosh(q)$. Exact analytical solutions are derived for periodic waves that have a period of two, three, and four lattice constants. Several of these cases employ Jacobian elliptic functions, while one solution uses ordinary cosines. The quadratic term in the potential energy can have either sign, and a double well occurs when it is negative and the quartic is positive. Solutions are also found for this double-well potential.

DOI: 10.1103/PhysRevB.72.144302 PACS number(s): 63.20.Ry, 63.22.+m, 05.45.−a

I. INTRODUCTION

We discuss the solution to classical waves on one-dimensional lattices whose potential energy terms contain several kinds of nonlinear forms. One case has both quadratic and quartic terms

$$\mathcal{V}_{\pm}(q_n) = \pm \frac{K_2}{2} q_n^2 + \frac{K_4}{4} q_n^4, \quad q_n = Q_{n+1} - Q_n, \tag{1}$$

where $Q_n(t)$ is the displacement of an atom at site n and q_n is the relative displacement between two neighboring sites. We have found exact analytical solutions to lattices waves that have a period of two, three, or four lattice sites. Another case has

$$\mathcal{V}_c(q_n) = K[\cosh(bq_n) - 1], \tag{2}$$

where (b,K) are constants. In this case we find exact analytical solutions to lattice waves with a period of two or four lattice sites.

There has been much interest in solutions to waves on nonlinear lattices. The Toda lattice[1,2] has a potential energy that is an asymmetric exponential. It has exact solutions for both soliton waves[3] and lattice waves. This important result has been an impetus to finding exact solutions to excitations on other nonlinear lattices. The solutions are given in terms of Jacobian elliptic functions, which are called cnoidal waves.[4–6] Our solutions use the same functions.

The quadratic-quartic lattice has been the topic of numerous analytical and numerical calculations.[7–20] The analytical solutions are always approximate and make assumptions such as a small amplitude or the rotating-wave approximation.[7,8,10,12,14,18] Our solutions are exact and contain no approximations.

We found no prior work on lattices with a potential given by Eq. (2). However, the symmetric exponential is a natural extension of Toda's work on the asymmetric exponential.

Numerical solutions have identified numerous excitations.[9,13,15–17] Some are solitons, while others are quite localized. This numerical work has been our inspiration to find analytical solutions.

Another important kind of numerical work has been the study of heat transport in one-dimensional lattices with nonlinear potentials. Some use the potential in Eq. (1).[19,20] Generally it is found that Fouriers law is not obeyed. Perhaps nonlinear waves contribute to the heat flow in a way different than Fourier's law. The usual method of solving for the thermal conductivity, using the Boltzmann equation,[21] assumes that the harmonic potential gives harmonic phonons and the anharmonic parts of the potential cause the scattering which gives the phonon lifetime. Toda's result—that a nonlinear lattice has modes that have an infinite lifetime—casts doubt on this entire procedure, at least in one dimension.

II. LATTICE WAVES

The general description of classical vibrations on a one-dimensional lattice assumes only interactions between first neighbors. The displacement of an atom at site n is called $Q_n(t)$. The potential energy and equations of motion are

$$V = \sum_n \mathcal{V}(Q_n - Q_{n+1}), \tag{3}$$

$$m\frac{d^2}{dt^2}Q_n = F(Q_n - Q_{n+1}) - F(Q_{n-1} - Q_n), \quad F(q) = -\frac{d}{dq}\mathcal{V}(q). \tag{4}$$

Define the relative displacement as

$$q_n = Q_{n+1} - Q_n, \tag{5}$$

$$m\frac{d^2}{dt^2}Q_n = -F(q_n) + F(q_{n-1}). \tag{6}$$

Subtract the similar equation for $m\ddot{Q}_{n+1}$ and obtain the final equation

$$m\frac{d^2}{dt^2}q_n = 2F(q_n) - F(q_{n+1}) - F(q_{n-1}). \tag{7}$$

For example, a harmonic lattice has

$$\mathcal{V}(q_n) = \frac{K_2}{2}q_n^2, \quad F(q_n) = -K_2 q_n. \tag{8}$$

Then the solution to Eq. (7) is given in terms of sines or cosines:

$$q_n = Q_0 \cos(\mu n - \omega_0 t), \tag{9}$$

$$\omega_0^2 = \frac{K_2}{m} 4 \sin^2(\mu/2). \tag{10}$$

These harmonic waves are well known. Our interest here is to find solutions to cases where the potential function is not just parabolic. One problem we consider is

$$m\frac{d^2}{dt^2}q_n(t) = \pm K_2[q_{n+1} + q_{n-1} - 2q_n] + K_4[q_{n+1}^3 + q_{n-1}^3 - 2q_n^3], \tag{11}$$

which is a mixture of quadratic and quartic potential functions. The quadratic term can have either sign. When it is negative the potential function has a double well. Another problem we consider is for the $\cosh(bq)$ potential:

$$m\frac{d^2}{dt^2}q_n(t) = Kb[\sinh(bq_{n+1}) + \sinh(bq_{n-1}) - 2\sinh(bq_n)], \tag{12}$$

$$m\frac{d^2}{dt^2}Q_n(t) = Kb[\sinh(bq_n) - \sinh(bq_{n-1})]. \tag{13}$$

Either of these two equations describes lattice waves.

III. CNOIDAL WAVES

Some of the periodic solutions are based upon the properties of Jacobian elliptic functions,[4] which are also called cnoidal waves. They are reviewed in the Appendix. Here we just summarize a few of their basic properties.[1,4–6]

The integral for the arcsine is

$$u = \int_0^z \frac{dt}{\sqrt{1-t^2}} = \arcsin(z), \quad z = \sin(u). \tag{14}$$

In a similar way, introduce another function that depends upon the parameter k and its inverse

$$u = \int_0^z \frac{dt}{\sqrt{(1-t^2)(1-k^2t^2)}}, \quad z = \mathrm{sn}(u). \tag{15}$$

The quantity $\mathrm{sn}(u)$ is a Jacobian elliptic function. Using it, one can define a family of related functions

$$\mathrm{cn}^2(u) = 1 - \mathrm{sn}^2(u), \quad \mathrm{dn}^2(u) = 1 - k^2\mathrm{sn}^2(u), \tag{16}$$

$$\mathrm{sd}(u) = \frac{\mathrm{sn}(u)}{\mathrm{dn}(u)}, \quad \mathrm{cd}(u) = \frac{\mathrm{cn}(u)}{\mathrm{dn}(u)}, \quad \mathrm{nd}(u) = \frac{1}{\mathrm{dn}(u)}. \tag{17}$$

Other elliptic functions are the inverse of these. However, the ones we list have nice periodic properties and could be solutions to lattice waves. The inverses all contain divergences and are not possible solutions. So we restrict our attention to these functions.

They are periodic, with the period determined by multiples of the first elliptic integral $K(k)$,

TABLE I. First and second derivatives of some cnoidal functions. $k_1^2 = 1 - k^2$.

$\mathrm{fn}(u)$	$\frac{d}{du}\mathrm{fn}(u)$	$\frac{d^2}{du^2}\mathrm{fn}(u)$
$\mathrm{sn}(u)$	$\mathrm{cn}(u)\mathrm{dn}(u)$	$-\mathrm{sn}(u)[1+k^2-2k^2\mathrm{sn}^2(u)]$
$\mathrm{cn}(u)$	$-\mathrm{sn}(u)\mathrm{dn}(u)$	$-\mathrm{cn}(u)[1-2k^2+2k^2\mathrm{cn}^2(u)]$
$\mathrm{dn}(u)$	$-k^2\mathrm{sn}(u)\mathrm{cn}(u)$	$\mathrm{dn}(u)[2-k^2-2\mathrm{dn}^2(u)]$
$\mathrm{sd}(u)$	$\mathrm{cd}(u)\mathrm{nd}(u)$	$-\mathrm{sd}(u)[1-2k^2+2k^2k_1^2\mathrm{sd}^2(u)]$
$\mathrm{cd}(u)$	$-k_1^2\mathrm{sd}(u)\mathrm{nd}(u)$	$-\mathrm{cd}(u)[1+k^2-2k^2\mathrm{cd}^2(u)]$
$\mathrm{nd}(u)$	$k^2\mathrm{sd}(u)\mathrm{cd}(u)$	$\mathrm{nd}(u)[2-k^2-2k_1^2\mathrm{nd}^2(u)]$

$$K(k) = \int_0^1 \frac{dt}{\sqrt{(1-t^2)(1-k^2t^2)}} = \int_0^{\pi/2} \frac{d\theta}{\sqrt{1-k^2\sin^2\theta}}, \tag{18}$$

and the period of $\mathrm{dn}(u)$ is $2K(k)$, while that for $\mathrm{sn}(u)$ and $\mathrm{cn}(u)$ is $4K(k)$. All of these functions also depend upon k, although that dependence is not highlighted in the notation. In the limit of small values of k,

$$\lim_{k\to 0}\begin{cases} \mathrm{sn}(u) \to \sin(u), \\ \mathrm{cn}(u) \to \cos(u), \\ \mathrm{dn}(u) \to 1. \end{cases} \tag{19}$$

The derivatives of the functions are important. Start with the definition (15) and take its derivative

$$\frac{du}{dz} = \frac{1}{\sqrt{(1-z^2)(1-k^2z^2)}}, \tag{20}$$

$$\frac{dz}{du} = \frac{d\mathrm{sn}(u)}{du} = \sqrt{(1-z^2)(1-k^2z^2)} = \mathrm{cn}(u)\mathrm{dn}(u). \tag{21}$$

The others can be derived from this result. All the first and second derivatives are shown in Table I. The first derivatives are given in numerous references, but we had to obtain the second derivatives ourselves. Second derivatives are needed for the equations of motion. Note that they all have, on the right, a term with a single power of a cnoidal function and a term with a cubic power. Those are exactly the type of terms needed for equations of motion of quadratic-quartic springs. Additional properties are given in the Appendix.

The last three functions in Table I are simply related to the first three. The period of $\mathrm{sn}(u)$, $\mathrm{cn}(u)$ is $4K$, so that K is a quarter wave. An exact identity is[4]

$$\mathrm{sn}(u \pm K) = \pm\mathrm{cd}(u), \tag{22}$$

$$\mathrm{cn}(u \pm K) = \mp k_1\mathrm{sd}(u), \tag{23}$$

$$\mathrm{dn}(u \pm K) = k_1\mathrm{nd}(u). \tag{24}$$

Any solution that contains $\mathrm{sn}(u)$ is also solved by the function $\mathrm{cd}(u)$: the same for $\mathrm{cn}(u)$ and $k_1\mathrm{sd}(u)$, and $\mathrm{dn}(u)$ and $k_1\mathrm{nd}(u)$. Note, in Table I, that $\mathrm{cd}(u)$ has exactly the same second derivative as does $\mathrm{sn}(u)$. So we will only give solutions involving the first three of the functions in Table I, since the other cases are just a quarter-wave difference in phase.

IV. SINGLE-WELL QUADRATIC-QUARTIC SPRING

This section discusses the solution to Eq. (1) for the potential $\mathcal{V}_+(q)$. This potential function has a single minimum as a function of the displacement q.

A. Single spring

For a single spring we can get an exact solution to the classical equation of motion. This section discusses the solution for positive quadratic spring: the potential function for a mass attached to a single spring is

$$\mathcal{V}_+(Q) = \frac{K_2}{2}Q^2 + \frac{K_4}{4}Q^4, \tag{25}$$

$$m\frac{d^2}{dt^2}Q = -K_2Q - K_4Q^3. \tag{26}$$

Examine Table I, and notice that the second derivative of $\mathrm{cn}(u)$ looks like the equation of motion for potential (25) with quadratic and quartic terms. Let $u=\omega_0 t$ and then equate coefficients to get

$$Q = Q_0\mathrm{cn}(\omega_0 t), \tag{27}$$

$$\frac{K_2}{m\omega_0^2} = 1 - 2k^2, \quad \frac{K_4Q_0^2}{m\omega_0^2} = 2k^2. \tag{28}$$

Solving gives that

$$\omega_0^2 = \frac{1}{m}[K_2 + K_4Q_0^2], \quad 2k^2 = \frac{K_4Q_0^2}{K_2 + K_4Q_0^2} \leqslant 1. \tag{29}$$

The amplitude Q_0 is a free parameter, and it determines the frequency ω_0 of the wave. The last inequality requires that $k^2 \leqslant 1/2$.

Note that a purely quartic spring has $K_2=0$, which is achieved by setting $k^2=1/2$, and then

$$\omega_0^2 = \frac{K_4}{m}Q_0^2. \tag{30}$$

The purely quadratic lattice has $k=0$. Values in the range $0<k^2<1/2$ contain a mixture of quadratic and quartic potential energies. One can show that the total energy in the oscillation is

$$E = \frac{1}{2}K_2Q_0^2 + \frac{1}{4}K_4Q_0^4. \tag{31}$$

B. Period four lattice waves

A quartic lattice also has a solution in terms of elliptic functions. Still consider the single well with $K_2>0$, which is the potential $\mathcal{V}_+(q_n)$ in Eq. (1).

Treat the case where the wave has a period of four lattice sites. The addition theorem for $\mathrm{cn}(u)$ is[4–6]

$$\mathrm{cn}(u+v) = \frac{\mathrm{cn}(u)\mathrm{cn}(v) - \mathrm{sn}(v)\mathrm{dn}(v)\mathrm{sn}(u)\mathrm{dn}(u)}{1 - k^2\mathrm{sn}^2(u)\mathrm{sn}^2(v)}. \tag{32}$$

The period of this function is $4K$, where $K(k)$ is the elliptic integral of the first kind. For a quarter period $\mathrm{cn}(K)=0$, $\mathrm{sn}(K)=1$, and $\mathrm{dn}(K)=\sqrt{1-k^2}\equiv k_1$, so that

$$\mathrm{cn}(u+K) = -k_1\frac{\mathrm{sn}(u)\mathrm{dn}(u)}{1 - k^2\mathrm{sn}^2(u)} = -k_1\mathrm{sd}(u), \tag{33}$$

$$\mathrm{cn}(u-K) = k_1\frac{\mathrm{sn}(u)\mathrm{dn}(u)}{1 - k^2\mathrm{sn}^2(u)} = -\mathrm{cn}(u+K). \tag{34}$$

We find

$$\mathrm{cn}(u+K) + \mathrm{cn}(u-K) = 0, \tag{35}$$

$$\mathrm{cn}^3(u+K) + \mathrm{cn}^3(u-K) = 0. \tag{36}$$

We assume that the solution to Eq. (11) is

$$q_n(u_n) = q_0\mathrm{cn}(u_n), \quad u_n = nK - \omega_4 t, \tag{37}$$

where ω_4 is the frequency of a wave of period four lattice sites. Using the above identities (35) and (36), Eq. (11) becomes

$$m\omega_4^2\frac{d^2}{du^2}q_0\mathrm{cn}(u_n) = -2K_2q_0\mathrm{cn}(u_n) - 2K_4q_0^3\mathrm{cn}^3(u). \tag{38}$$

This equation has exactly the form of our cnoidal equation of motion in Table I. The solution is

$$\frac{2K_2}{m\omega_4^2} = 1 - 2k^2, \quad \frac{2K_4q_0^2}{m\omega_4^2} = 2k^2, \tag{39}$$

$$\omega_4^2 = \frac{2}{m}[K_2 + K_4q_0^2]. \tag{40}$$

Again $k^2=1/2$ for a purely quartic lattice ($K_2=0$) and $k=0$ for a purely quadratic lattice ($K_4=0$). In either case the lattice wave has a period of four lattice sites.

The energy of the wave, per atomic site, is

$$\frac{E}{N} = \frac{1}{2}K_2q_0^2 + \frac{1}{4}K_4q_0^4. \tag{41}$$

The other interesting quantity is the atom displacement Q_n. We wish to determine the function f_n, which obeys $Q_n=Q_0f_n$, and

$$q_n = q_0\mathrm{cn}(u_n) = Q_0[f_{n+1} - f_n]. \tag{42}$$

The solution to the above equation uses the feature that $\mathrm{cn}(u+2K)=-\mathrm{cn}(u)$ to find

$$f_n = \mathrm{cn}(u_n) + \mathrm{cn}(u_{n+1}), \tag{43}$$

$$f_{n+1} = \mathrm{cn}(u_{n+1}) + \mathrm{cn}(u_{n+2}) = \mathrm{cn}(u_{n+1}) - \mathrm{cn}(u_n), \tag{44}$$

$$q_0\mathrm{cn}(u_n) = -Q_0 2\mathrm{cn}(u_n), \quad q_0 = -2Q_0. \tag{45}$$

Thus we have derived the atomic displacement $Q_n(t)$, which exactly solves the problem of a lattice wave with a period of four sites.

An interesting feature is the absolute value Q_x of the atomic displacements, which is not obvious from Eq. (43). Define $\phi = u_n + K/2$, and we find

$$f_n = \mathrm{cn}(\phi - K/2) + \mathrm{cn}(\phi + K/2) \tag{46}$$

$$= 2\mathrm{cn}(K/2)g(\phi), \tag{47}$$

$$g(\phi) = \frac{\mathrm{cn}(\phi)}{1 - k^2\mathrm{sn}^2(K/2)\mathrm{sn}^2(\phi)} = \frac{\mathrm{cn}(\phi)}{1 - (1-k_1)\mathrm{sn}^2(\phi)}, \tag{48}$$

$$\mathrm{sn}^2(K/2) = \frac{1}{1+k_1}, \quad \mathrm{cn}^2(K/2) = \frac{k_1}{1+k_1}. \tag{49}$$

The result depends upon the maximum value of $|g(\phi)|$ as a function of ϕ. There are two regimes.

(i) For $k_1 > 1/2$ the largest value is when $\phi=0$ or $2K$, where $|g(0)|=1$. In this case the maximum atomic displacement is

$$Q_x = 2Q_0\sqrt{\frac{k_1}{1+k_1}}. \tag{50}$$

(ii) For $k_1 < 1/2$, the maximum of $g(\phi)$ is at an intermediate value of ϕ. In this case, the maximum atomic dispslacement is $Q_x = Q_0/k$, where $k \geqslant \sqrt{3}/2$.

At $k=0$ ($k_1=1$) the atomic displacment is $Q_x = \sqrt{2}Q_0$. For nonzero values of k it decreases monotonically down to $k=1$ ($k_1=0$) where it is $Q_x = Q_0$.

C. Period two waves

Cnoidal waves also exist with a period of two lattice sites. Note that $\mathrm{sn}(2K)=0$ and $\mathrm{cn}(2K)=-1$ which gives

$$\mathrm{cn}(u \pm 2K) = -\mathrm{cn}(u), \tag{51}$$

$$\mathrm{cn}^3(u \pm 2K) = -\mathrm{cn}^3(u). \tag{52}$$

Therefore, using a cnoidal wave of period two gives the following equation from Eq. (11):

$$q_n = q_0\mathrm{cn}(u_n), \quad u_n = 2Kn - \omega_2 t, \tag{53}$$

$$m\omega_2^2 \frac{d^2}{du^2} q_0\mathrm{cn}(u) = -4K_2 q_0\mathrm{cn}(u) - 4K_4 q_0^3\mathrm{cn}^3(u). \tag{54}$$

Compare this equation with the second derivative of $\mathrm{cn}(u)$ in Table I and find

$$\frac{4K_2}{m\omega_2^2} = 1 - 2k^2, \quad \frac{4K_4 q_0^2}{m\omega_2^2} = 2k^2, \tag{55}$$

$$\omega_2^2 = \frac{4}{m}[K_2 + K_4 q_0^2] = 2\omega_4^2. \tag{56}$$

So there is an exact solution to Eq. (11) with a period of two lattice sites in terms of cnoidal functions. These modes are at the edge of the Brillouin zone. Since the period is $4K$, then the allowed wave vector p, in the Brillouin zone, runs in the range $-2K \leqslant pa \leqslant 2K$ where a is the lattice constant. The energy per site is still Eq. (41).

The atomic displacement must still solve Eq. (42), which in this case is acomplished by the choice

$$Q_n = Q_0\mathrm{cn}(u_n), \quad Q_{n+1} = Q_0\mathrm{cn}(u_n + 2K) = -Q_0\mathrm{cn}(u_n), \tag{57}$$

$$q_n = -2Q_0\mathrm{cn}(u_n), \quad q_0 = -2Q_0. \tag{58}$$

We have derived the atomic displacement $Q_n(t)$, which exactly solves the lattice wave of period two sites.

D. Period three waves

The quartic potential has a cosine solution which gives a periodic wave. Use the identity

$$\cos^3(\theta) = \frac{1}{4}[\cos(3\theta) + 3\cos(\theta)] \tag{59}$$

to get the lattice solution

$$\begin{aligned} &\cos^3(\theta_n + \mu) + \cos^3(\theta_n - \mu) - 2\cos^3(\theta_n) \\ &\quad = \frac{1}{2}\{\cos(3\theta_n)[\cos(3\mu) - 1] + 3\cos(\theta_n)[\cos(\mu) - 1]\}. \end{aligned} \tag{60}$$

Therefore, the lattice equation (11) has a cosine solution when choosing $\cos(3\mu)=1$ and $\mu = \pm 2\pi/3$. Then Eq. (11) becomes

$$q_n = q_0\cos(\theta_n), \quad \theta_n \equiv \frac{2\pi}{3}n - \omega_3 t, \tag{61}$$

$$-m\omega_3^2 q_0\cos(\theta_n) = -3K_2 q_0\cos(\theta_n) - \frac{9}{4}K_4 q_0^3\cos(\theta_n), \tag{62}$$

$$\omega_3^2 = \frac{3}{m}\left[K_2 + \frac{3}{4}q_0^2 K_4\right]. \tag{63}$$

The frequency depends upon the relative strength of the two spring constants (K_2, K_4). Note that this solution also permits negative values of K_2, as long as $\omega_3^2 > 0$. Page[8] obtained a different value of ω_3^2 when using the rotating-wave approximation.

The energy in the wave, per site, is

$$E/N = \frac{1}{2}K_2 q_0^2 + \frac{9}{32}K_4 q_0^4. \tag{64}$$

The atomic displacements are

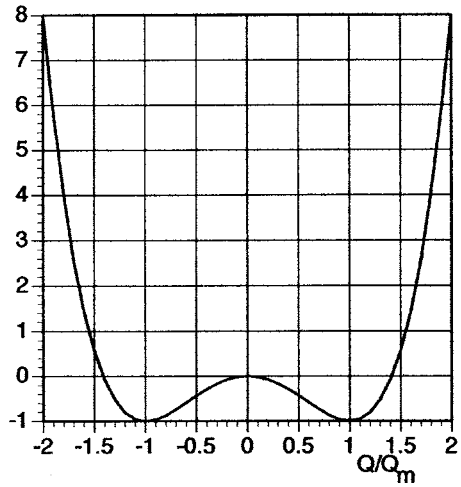

FIG. 1. Double-well potential $f(x)$ graphed as a function of $x = Q/Q_m$.

$$Q_n = Q_0 \sin(\theta_n - \pi/3), \tag{65}$$

$$\begin{aligned} q_n &= Q_0[\sin(\theta_n + \pi/3) - \sin(\theta_n - \pi/3)] \\ &= 2Q_0 \sin(\pi/3)\cos(\theta_n), \end{aligned} \tag{66}$$

$$q_0 = \sqrt{3}Q_0, \tag{67}$$

where we used $\sin(\pi/3) = \sqrt{3}/2$. This solution has a period of three lattice sites. So when the wave has a period of three sites, the solution is a cosine function, but when the period is two or four lattice sites, it is a Jacobian elliptic function.

V. DOUBLE-WELL POTENTIAL

Now consider the solution when the quadratic spring constant is negative. For a lattice, we solve using $\mathcal{V}_-(q_n)$ in Eq. (1). For a single spring, we solve using the potential

$$\mathcal{V}_-(Q) = -\frac{K_2}{2}Q^2 + \frac{K_4}{4}Q^4, \tag{68}$$

$$m\frac{d^2}{dt^2}Q = K_2 Q - K_4 Q^3 = -F(Q). \tag{69}$$

The potential has a double well. The force $F(Q)$ is zero at three points $Q=0$, $Q=\pm Q_m$, where the latter are the minima of the double well:

$$Q_m = \sqrt{\frac{K_2}{K_4}}. \tag{70}$$

Figure 1 shows the double well graphed as a function of $x = Q/Q_m$:

$$\mathcal{V}_-(Q) = \frac{K_4 Q_m^4}{4} f(Q/Q_m), \quad f(x) = x^2(x^2 - 2). \tag{71}$$

The potential minima are at $x = \pm 1$, and the potential is zero at $x = \pm\sqrt{2}$. If the total energy of vibration is negative, then the particle oscillates in one of the two minima. If the total energy is positive, the oscillations is over both sides of the double well.

A. Single spring

Examine the second derivative of the third elliptic function $\mathrm{dn}(u)$ in Table I. Compare it to Eq. (93) and note that the first term on the right has the sign appropriate to be a solution to Eq. (69). The function $\mathrm{dn}(u)$ is a solution to this equation. The exact solution is

$$Q(t) = Q_0 \mathrm{dn}(\omega_0 t), \quad u = \omega_0 t, \tag{72}$$

$$\omega_0^2 = \frac{K_4 Q_0^2}{2m}, \quad k^2 = 2\left[1 - \frac{K_2}{K_4 Q_0^2}\right] = 2\left[1 - \frac{Q_m^2}{Q_0^2}\right]. \tag{73}$$

This solution applies to the case that the atom is vibrating in one of the two potential minima: here we have chosen the sign for the right-hand minimum. The minimum occurs at the displacement Q_m.

The restriction that $k^2 > 0$ is that $Q_0 > Q_m$ which is natural. In the bottom of the well, the particle oscillates in the range $Q_0 > Q > k_1 Q_0$, where $k_1^2 = 1 - k^2$. The solution is only valid for $k^2 \leqslant 1$. At $k^2 = 1$, then $\mathcal{V}_-(Q_0) = 0$ and $\mathrm{dn}(u) = \mathrm{sech}(u)$, and the particle oscillates in the range $Q_0 > Q > 0$ and $Q = 0$ is approached only asymptotically at large time.

Another solution is needed for the case that the particle in the double well has sufficient energy to oscillate through both wells. In this case we again use the equation for the second derivative of $\mathrm{cn}(u)$. Rewrite this equation as

$$\frac{d^2}{du^2}\mathrm{cn}(u) = (2k^2 - 1)\mathrm{cn}(u) - 2k^2 \mathrm{cn}^3(u). \tag{74}$$

Whenever $1 > k^2 > 1/2$ the factor of $(2k^2 - 1) > 0$. In this case,

$$Q(t) = Q_0 \mathrm{cn}(\omega_0 t), \tag{75}$$

$$2k^2 - 1 = \frac{K_2}{m\omega_0^2}, \quad 2k^2 = \frac{K_4 Q_0^2}{m\omega_0^2}, \tag{76}$$

$$\omega_0^2 = \frac{K_4}{m}(Q_0^2 - Q_m^2), \quad k^2 = \frac{1}{2}\frac{Q_0^2}{Q_0^2 - Q_m^2} < 1, \tag{77}$$

which requires $Q_0^2 > 2Q_m^2$. The function $\mathrm{dn}(u)$ is the solution for $Q_m < Q_0 < \sqrt{2}Q_m$, while $\mathrm{cn}(u)$ is the solution when $Q_0 > \sqrt{2}Q_m$. The energy of the oscillation is

$$E = -\frac{1}{2}K_2 Q_0^2 + \frac{1}{4}K_4 Q_0^4. \tag{78}$$

Equation (69) also has a solution that is purely decaying in time. Try a solution of the form

$$Q(t) = \frac{A}{\cosh(\omega t)}. \tag{79}$$

This equation is an exact solution of Eq. (69) when

TABLE II. Three solutions with values of $k^2=1/4,1/2,3/4$. The case $k^2=1/2$ is a purely quartic lattice ($K_2=0$). The case $k^2=3/4$ is a double well.

	$k^2=1/4$		$k^2=1/2$		$k^2=3/4$	
n	pa	ω_n/Ω	pa	ω_n/Ω	pa	ω_n/Ω
2	2K=3.708	2	2K=3.372	$\sqrt{8}$	2K=4.313	$\sqrt{8/3}$
3	$2\pi/3=2.094$	3/2	$2\pi/3=2.094$	$\sqrt{21/4}$	$2\pi/3=2.094$	$\sqrt{5/4}$
4	K=1.854	$\sqrt{2}$	K=1.686	2	K=2.157	$\sqrt{4/3}$

$$\omega^2 = \frac{K_2}{m}, \quad A = \sqrt{2}Q_m. \tag{80}$$

At $t=0$ the amplitude is $Q=\sqrt{2}Q_m$. That is the amplitude of a wave with zero potential energy. So if the double well starts with that amplitude and zero kinetic energy, it does not oscillate, but the amplitude decays to zero.

B. Period four lattice wave

The solution for the period four lattice wave can be extended to cover the double-well solution. For $1>k^2>1/2$ the quadratic spring constant K_2 changes sign. The solution (37) also applies to this case, where the quadratic spring has a negative constant as in Eq. (68):

$$\frac{2K_2}{m\omega_4^2} = 2k^2 - 1, \quad \frac{2K_4 q_0^2}{m\omega_4^2} = 2k^2, \tag{81}$$

$$\omega_4^2 = \frac{2}{m}[K_4 q_0^2 - K_2], \tag{82}$$

$$2k^2 = \frac{q_0^2}{q_0^2 - Q_m^2}. \tag{83}$$

We have found an exact solution for the potential $\mathcal{V}_-(Q)$ with a double-well potential. This solution applies when $q_0^2 > 2Q_m^2$. The energy per site is

$$E/N = -\frac{1}{2}K_2 q_0^2 + \frac{1}{4}K_4 q_0^4. \tag{84}$$

The atom displacement is the same as in Eq. (43).

C. Period two lattice wave

The double well $\mathcal{V}_-(q_n)$ also has a lattice wave with a period of two lattice sites. The earlier solution using $\mathrm{cn}(u_n)$ can be extended to include the double-well potential. For $1>k^2>1/2$ the quadratic spring constant K_2 changes sign. The solution (53) also applies to this case, where the quadratic spring has a negative constant as in Eq. (68).

$$\frac{4K_2}{m\omega_2^2} = 2k^2 - 1, \quad \frac{4K_4 q_0^2}{m\omega_2^2} = 2k^2, \tag{85}$$

$$\omega_2^2 = \frac{4}{m}[K_4 q_0^2 - K_2] = 2\omega_4^2, \tag{86}$$

$$2k^2 = \frac{q_0^2}{q_0^2 - Q_m^2}. \tag{87}$$

We have found another exact solution for the potential $\mathcal{V}_-(Q)$ with a double-well potential. This solution applies when $Q_0^2 > 2Q_m^2$. The energy is Eq. (84). The atom displacement is the same as in Eq. (57).

D. Period three lattice wave

Again use a cosine function and find

$$q_n = q_0 \cos(\theta_n), \quad \theta_n \equiv \frac{2\pi}{3}n - \omega_3 t, \tag{88}$$

$$-m\omega_3^2 q_0 \cos(\theta_n) = 3K_2 q_0 \cos(\theta_n) - \frac{9}{4}K_4 q_0^3 \cos(\theta_n), \tag{89}$$

$$\omega_3^2 = \frac{3}{m}\left[\frac{3}{4}q_0^2 K_4 - K_2\right], \tag{90}$$

which is valid as long as $\omega_3^2 > 0$. The energy per site is identical to Eq. (64) after changing the sign of K_2. The atom displacement is still $Q_0 \sin(\theta_n - \pi/3)$.

Our solutions for the lattice waves of the double well only apply to the case of positive energy of the wave, so that the oscillations are over both sides of the double well. We do not have a solution for the case of negative total energy, where the periodic motion is restricted to one of the two well minima. For the single spring, the function $\mathrm{dn}(u)$ provided a solution to this case. This function does not work for the lattice, and we have not identified a function that does work.

E. Numerical examples

Here we wish to compare the properties of these three solutions. Table II shows the frequencies and wave vectors (pa) for three cases $k^2=1/4,1/2,3/4$. The case $k^2=1/2$ is a purely quartic lattice ($K_2=0$). The case $k^2=1/4$ has equal parts quadratic and quartic energies. The case $k^2=3/4$ is a double well. The frequencies are normalized to

$$\Omega^2 = \frac{K_4 q_0^4}{m}. \tag{91}$$

For $k^2=1/4,3/4$ we also set $\Omega^2 = K_2 q_0^2/m$. This choice is arbitrary. We could alternately define Ω^2 in terms of the maximum atomic displacements or else in terms of the average energy of each mode. In these cases the comparisons are slightly different. The above choice seems the most convenient, and the comparison is made only to show that the modes have a regular progression in terms of frequency versus wave vector.

The double-well case ($k^2=3/4, Q_0^2=3Q_m^2$) has a peculiar solution, since the lattice wave of period three has a lower frequency and a lower value of pa than does the lattice wave of period four. This feature is unavoidable, since the period three has a spacing of $2\pi/3$, while the period four has a spacing of $K(k)$. As k nears 1, then $K(k)$ gets very large and passes $2\pi/3$ in value.

VI. cosh(q) POTENTIAL

This section solves some of the properties of a lattice with the potential $K[\cosh(bq)-1]$ between neighboring atoms.

A. Single spring

For a single spring we can get an exact solution to the classical equation of motion. The potential function for a mass attached to a single spring is

$$\mathcal{V}(Q) = K[\cosh(bQ) - 1], \tag{92}$$

$$m\frac{d^2}{dt^2}Q = - bK \sinh(bQ), \tag{93}$$

$$\frac{d^2}{d\tau^2}\xi = - \sinh(\xi), \quad \xi = bQ, \quad \tau = \omega_0 t, \quad \omega_0^2 = \frac{b^2K}{m}. \tag{94}$$

The solution to the equation of motion is

$$\xi = \pm 2 \ln\left[\frac{\mathrm{dn}(u)}{\sqrt{k_1}}\right], \quad u = \beta\tau, \tag{95}$$

where dn(u) is a Jacobian elliptic function.[4–6] Evaluating the two sides of Eq. (94) gives

$$\frac{d^2}{d\tau^2}\xi = \mp 2\beta^2\left[\mathrm{dn}^2(u) - \frac{k_1^2}{\mathrm{dn}^2(u)}\right], \tag{96}$$

$$- \sinh(\xi) = \mp \frac{1}{2}\left[\frac{\mathrm{dn}^2(u)}{k_1} - \frac{k_1}{\mathrm{dn}^2(u)}\right]. \tag{97}$$

These two expressions are identical if

$$4\beta^2 k_1 = 1, \tag{98}$$

$$\beta = \frac{1}{2\sqrt{k_1}}, \tag{99}$$

$$u = \frac{\tau}{2\sqrt{k_1}}, \quad \omega = \frac{\omega_0}{2\sqrt{k_1}}, \tag{100}$$

which completes the exact solution for a single spring.

Equation (24) has a well-known property $\mathrm{dn}(u+K) = k_1/\mathrm{dn}(u)$. Define $X=\mathrm{dn}^2(u)/k_1$. At the time u, then $\xi=\ln(X)$. At the later time $u+K$, then $\xi=\ln(1/X)=-\ln(X)$. This sign alternation gives the oscillatory behavior. The function $X(u)$ oscillates in value around 1, and $\ln(X)$ oscillates in value around 0. At $u=0$, then $\mathrm{dn}(0)=1$, while at $u=K$, then $\mathrm{dn}(K)=k_1$. These two points are the limits of the oscillations $\pm\hat{q}_0$, where

$$\hat{q}_0 = - \ln(k_1), \tag{101}$$

$$E = \frac{K}{2k_1}(1 - k_1)^2 = K[\cosh(\hat{q}_0) - 1]. \tag{102}$$

The last equation gives the energy.

B. Period two lattice waves

The exponential lattice has periodic solutions in terms of elliptic functions. Exact solutions have been found for lattice waves with a period of two and four lattice sites.

The function dn(u) has a period of $u=2K$, so that $\mathrm{dn}(u+2K)=\mathrm{dn}(u)$. A period of two sites is obtained by choosing

$$\phi_n = Kn - \beta\tau, \tag{103}$$

$$\xi_n = bQ_n = \pm \ln\left[\frac{\mathrm{dn}(\phi_n)}{\sqrt{k_1}}\right]. \tag{104}$$

The $\pm$ sign is confusing, so omit it. However, a solution is found for either choice. Using the plus sign, the periodicity gives

$$\xi_{n+2} = \xi_n, \tag{105}$$

$$\xi_{n\pm1} = - \xi_n, \quad \xi_{n\pm1} - \xi_n = - 2\xi_n, \tag{106}$$

where the latter identity used Eq. (24). For this case, Eq. (13) can be written as

$$\frac{d^2}{d\tau^2}\xi_n = - 2 \sinh(2\xi_n). \tag{107}$$

This is the same equation we solved for the single spring, except for occasional factors of 2. The solution is Eq. (104) with

$$\beta = \pm \frac{1}{\sqrt{k_1}}, \tag{108}$$

$$\phi_n = Kn \pm \frac{\tau}{\sqrt{k_1}}, \quad \omega_2 = \frac{\omega_0}{\sqrt{k_1}}. \tag{109}$$

We have derived the atomic displacement $Q_n(t)$, which exactly solves the lattice wave of period two sites. The energy in the wave, per site, is

$$\frac{E}{N} = \frac{K}{2k_1}(1 - k_1)^2 = K[\cosh(\hat{q}_0) - 1]. \tag{110}$$

The maximum displacement in this case is $\hat{q}_0/2$.

C. Period four waves

Consider the case where the wave has a period of four lattice sites. The relative displacement has the expression

$$r_n = bq_n = 2\ \ln\left[\frac{\mathrm{dn}(\phi_n)}{\sqrt{k_1}}\right], \tag{111}$$

$$\phi_n = vn - \beta\tau, \quad v = \frac{K}{2}. \tag{112}$$

This choice gives $r_{n+4}=r_n$ for a period of four. In evaluating Eq. (12), the left-hand side is

$$\frac{d^2 r_n}{d\tau^2} = -2\beta^2 k_1\left(X - \frac{1}{X}\right), \quad X \equiv \frac{\mathrm{dn}^2(\phi_n)}{k_1}. \tag{113}$$

The first two terms in the force are

$$\sinh(r_{n+1}) + \sinh(r_{n-1}) = \frac{1}{2}\left[\frac{\mathrm{dn}^2(\phi_{n+1}) + \mathrm{dn}^2(\phi_{n-1})}{k_1}\right. \tag{114}$$

$$\left. - k_1\left(\frac{1}{\mathrm{dn}^2(\phi_{n+1})} + \frac{1}{\mathrm{dn}^2(\phi_{n-1})}\right)\right] \tag{115}$$

$$= \frac{1}{2}[\mathrm{dn}^2(\phi_{n+1}) + \mathrm{dn}^2(\phi_{n-1})]\Lambda, \tag{116}$$

$$\Lambda = \frac{1}{k_1} - \frac{k_1}{\mathrm{dn}^2(\phi_{n+1})\mathrm{dn}^2(\phi_{n-1})}. \tag{117}$$

When $v=K/2$, then an identity[4–6] for these functions is

$$\mathrm{dn}(u+v)\mathrm{dn}(u-v) = k_1. \tag{118}$$

This identity can be proved by using an equation in the Appendix and

$$\mathrm{sn}^2(K/2) = \frac{1}{1+k_1}, \quad \mathrm{cn}^2(K/2) = \frac{k_1}{1+k_1}, \quad \mathrm{dn}^2(K/2) = k_1. \tag{119}$$

In this case $\Lambda=0$ and the two terms in Eq. (114) cancel to zero. Therefore our equation of motion becomes, for period four,

$$\frac{d^2 r_n}{d\tau^2} = -2\ \sinh(r_n). \tag{120}$$

This equation is similar to that of a single spring. The solution has $2\beta^2 k_1=1$ or

$$\beta = \pm\frac{1}{\sqrt{2k_1}}, \tag{121}$$

$$\phi_n = \frac{K}{2}n \pm \frac{\tau}{\sqrt{2k_1}}, \quad \omega_4 = \frac{\omega_0}{\sqrt{2k_1}}. \tag{122}$$

The energy per site is again given by Eq. (110).

The single-site displacement is

TABLE III. Period four wave amplitudes when $\tau=0$.

n	ϕ_n	$\mathrm{dn}(\phi_n)$	q_n
0	0	1	$-\hat{q}_0/2$
1	$K/2$	$\sqrt{k_1}$	$+\hat{q}_0/2$
2	K	k_1	$+\hat{q}_0/2$
3	$3K/2$	$\sqrt{k_1}$	$-\hat{q}_0/2$
4	$2K$	1	$-\hat{q}_0/2$

$$\xi_n = -\ln\left[\frac{\mathrm{dn}(\phi_n)\mathrm{dn}(\phi_{n+1})}{k_1}\right], \tag{123}$$

$$\xi_{n+1} = -\ln\left[\frac{\mathrm{dn}(\phi_{n+1})\mathrm{dn}(\phi_{n+2})}{k_1}\right], \tag{124}$$

$$r_n = \xi_{n+1} - \xi_n = \ln\left[\frac{\mathrm{dn}(\phi_n)}{\mathrm{dn}(\phi_{n+2})}\right], \tag{125}$$

$$r_n = 2\ \ln\left[\frac{\mathrm{dn}(\phi_n)}{\sqrt{k_1}}\right], \tag{126}$$

where again we used Eq. (24) to evaluate $\mathrm{dn}(\phi_{n+2}) = \mathrm{dn}(\phi_n+K)$.

Table III shows the evaluation of this function at the moment when $\tau=0$. The last entry ($n=4$) is identical to the first ($n=0$). Table IV shows the evaluation when the time has advanced half a lattice step ($\beta\tau=K/4$), giving $\phi_n = (K/2)(n-1/2)$. The amplitude q_x is

$$q_x = \ln[\mathrm{dn}^2(K/4)/k_1], \tag{127}$$

$$\zeta^2 = \mathrm{dn}^2(K/4) = \sqrt{k_1}\left(\frac{\sqrt{1+k_1}+1}{\sqrt{1+k_1}+\sqrt{k_1}}\right). \tag{128}$$

Note that $q_x > \hat{q}_0/2$ and q_x is the maximum displacement at a site.

VII. DISCUSSION

We have examined classical waves on several nonlinear lattices. One lattice has potential energy terms which are quadratic and quartic. Another lattice has the symmetric exponential $\cosh(bq)$, where q is the relative displacement of

TABLE IV. Period four wave amplitudes when $\beta\tau=K/4$ and $n^*=n-1/2$.

n^*	ϕ_n	$\mathrm{dn}(\phi_n)$	q_n
1/2	$K/4$	ζ	0
3/2	$3K/4$	k_1/ζ	$+q_x$
5/2	$5K/4$	k_1/ζ	0
7/2	$7K/4$	ζ	$-q_x$
9/2	$9K/4$	ζ	0

two neighboring sites. Exact analytical solutions have been found for several periodic lattice waves for each potential. The quadratic-quartic potential has waves with a period of (i) two, (ii) three, and (iii) four lattice sites. Two of the solutions have been found using Jacobian elliptic functions, called cnoidal waves, and the third uses ordinary trigometric functions. For the symmetric exponential potential, we found analytical solutions for periodic waves with a period of two and four lattice sites.

Finding these solutions is always a bit of luck. One tries to solve the equation of motion using many different kinds of functions, and occasionally one works. Are there exact analytical solutions for other periods? We do not know, but continue to search. Our hypothesis is that there are periodic-wave solutions for all wavelengths, but only in a few cases are they expressed in known mathematical functions. In other cases we will need to derive a new function which gives the right solution. We are presently exploring methods of doing this, such as series expansions. Incidently, we started out trying to find analytical solutions to soliton waves on these lattices. We have not yet found any, but continue to search.

We believe all one-dimensional nonlinear lattices have both soliton waves and periodic lattice waves that travel without damping. If that hypothesis is correct, then thermal transport theories in one dimension need to include these excitations. First we need to find these solutions, which is our present quest.

ACKNOWLEDGMENT

Research support is acknowledged from Grant No. NSF-NIRT-DMR 03-04178.

APPENDIX: JACOBIAN ELLIPTIC FUNCTIONS

Here we list some addition theorems and other identities for elliptic functions, as found in Refs. 4–6:

$$\mathrm{sn}(u+v) = \frac{\mathrm{sn}(u)\mathrm{cn}(v)\mathrm{dn}(v) + \mathrm{sn}(v)\mathrm{cn}(u)\mathrm{dn}(u)}{1 - k^2\mathrm{sn}^2(u)\mathrm{sn}^2(v)}, \quad \text{(A1)}$$

$$\mathrm{cn}(u+v) = \frac{\mathrm{cn}(u)\mathrm{cn}(v) - \mathrm{sn}(v)\mathrm{dn}(v)\mathrm{sn}(u)\mathrm{dn}(u)}{1 - k^2\mathrm{sn}^2(u)\mathrm{sn}^2(v)}, \quad \text{(A2)}$$

$$\mathrm{dn}(u+v) = \frac{\mathrm{dn}(u)\mathrm{dn}(v) - k^2\mathrm{sn}(v)\mathrm{cn}(v)\mathrm{sn}(u)\mathrm{cn}(u)}{1 - k^2\mathrm{sn}^2(u)\mathrm{sn}^2(v)}, \quad \text{(A3)}$$

$$\mathrm{sn}(u+v)\mathrm{sn}(u-v) = \frac{\mathrm{sn}^2(u) - \mathrm{sn}^2(v)}{1 - k^2\mathrm{sn}^2(u)\mathrm{sn}^2(v)}, \quad \text{(A4)}$$

$$\mathrm{cn}(u+v)\mathrm{cn}(u-v) = \frac{\mathrm{cn}^2(v) - \mathrm{sn}^2(u)\mathrm{dn}^2(v)}{1 - k^2\mathrm{sn}^2(u)\mathrm{sn}^2(v)}, \quad \text{(A5)}$$

$$\mathrm{dn}(u+v)\mathrm{dn}(u-v) = \frac{\mathrm{dn}^2(v) - k^2\mathrm{sn}^2(u)\mathrm{cn}^2(v)}{1 - k^2\mathrm{sn}^2(u)\mathrm{sn}^2(v)}, \quad \text{(A6)}$$

$$\mathrm{dn}^2(u/2) = \frac{k_1^2 + \mathrm{dn}(u) + k^2\mathrm{cn}(u)}{1 + \mathrm{dn}(u)}. \quad \text{(A7)}$$

[1] M. Toda, *Nonlinear Waves and Solitons* (Kluwer, New York, 1989).

[2] M. Toda, *Theory of Nonlinear Lattices*, 2nd ed. (Springer-Verlag, New York, 1989).

[3] G. L. Lamb, *Elements of Soliton Theory* (Wiley, New York, 1980).

[4] *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. Stegun, Natl. Bur. Stand. Appl. Math. Ser. No. 55 (U.S. GPO, Washington, D.C., 1964), Chap. 16.

[5] E. H. Neville, *Jacobian Elliptic Functions* (Clarendon Press, Oxford, 1944).

[6] N. I. Akhiezer, *Elements of the Theory of Elliptic Functions* (American Mathematical Society, Providence, RI, 1990), Vol. 79.

[7] A. J. Sievers and S. Takeno, Phys. Rev. Lett. **61**, 970 (1988).

[8] J. B. Page, Phys. Rev. B **41**, 7835 (1990).

[9] R. Bourbonnais and R. Maynard, Phys. Rev. Lett. **64**, 1397 (1990).

[10] S. Takeno, J. Phys. Soc. Jpn. **59**, 1571 (1990).

[11] V. M. Burlakov, S. A. Kiselev, and V. N. Pyrkov, Phys. Rev. B **42**, 4921 (1990).

[12] S. R. Bickham and A. J. Sievers, Phys. Rev. B **43**, 2339 (1991).

[13] S. R. Bickham, A. J. Sievers, and S. Takeno, Phys. Rev. B **45**, 10344 (1992).

[14] G. X. Huang, Z. P. Shi, and Z. X. Xu, Phys. Rev. B **47**, 14561 (1993).

[15] R. F. Wallis, A. Franchini, and V. Bortolani, Phys. Rev. B **50**, 9851 (1994).

[16] R. Dusi, G. Viliani, and M. Wagner, Philos. Mag. B **71**, 597 (1995).

[17] R. Dusi, G. Viliani, and M. Wagner, Phys. Rev. B **54**, 9809 (1996).

[18] G. H. Zhou, Q. L. Xia, and J. R. Yan, Eur. Phys. J. B **17**, 207 (2000).

[19] S. Lepri, R. Livi, and A. Politi, Phys. Rev. Lett. **78**, 1896 (1997); Europhys. Lett. **43**, 271 (1998); Phys. Rev. E **68**, 067102 (2003).

[20] C. Giardina, R. Livi, A. Politi, and M. Vassalli, Phys. Rev. Lett. **84**, 2144 (2000).

[21] J. M. Ziman, *Electrons and Phonons* (Clarendon Press, Oxford, 1960).