Nonlinear dynamics of the diatomic Toda lattice and the problem of thermal conductivity of quasi-one-dimensional crystals

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(Submitted 1 April 1991)
Zh. Eksp. Teor. Fiz. **102**, 511–521 (August 1992)

The process of thermal transport in insulating quasi-one-dimensional crystals is studied using a well-known model—the diatomic Toda lattice. It is established that all the characteristics of this process discovered earlier through numerical modeling can be explained by analyzing the dynamical behavior of limiting systems corresponding to high and low temperatures. Such an approach, which can be generalized to other model systems, leads to a number of conclusions on the nature of the finite thermal conductivity of dielectric crystals.

INTRODUCTION

At present the diatomic lattice with exponential interaction has become an object of close attention in connection with modeling thermal conductivity in nonmetallic crystals.[1–3] The anomalies in thermal conductivity in substantially nonlinear systems were well known from the time of the notable work of Fermi, Pasta and Ulam.[4] But it has only recently been realized that nonlinearity does not lead to the inelastic phonon-phonon interaction taken into account in the classical theory of thermal conductivity. Thermal solitons in the quasi-one-dimensional system, experimentally observed in the work of Ref. 5, can radically change the character of this process. Moreover, there has been no success in finding an expression for the coefficient of thermal conductivity from first principles—the problem of the finite thermal conductivity of nonmetallic crystals remains open.[3]

The only lattice model with nearest-neighbor interactions for which a normal finite thermal conductivity has been numerically determined is the diatomic Toda lattice. The remarkable properties of the model considered are its complete integrability for the case of equal masses[6] and the transition to a stochastic regime for a certain mass ratio.[2] The finite thermal conductivity of the diatomic Toda lattice, discovered in numerical simulations,[1,2] is also a consequence of this transition.

To understand the special features of the dynamical behavior of this system and the mechanism of thermal conductivity, it is desirable to have an analytic representation of the elementary excitations of the lattice. The first attempts at deriving such representations were undertaken in Ref. 7. However, the results of Ref. 7 were wrong, as was shown in Ref. 8 by direct substitution of the solutions obtained into the equations of motion.

In Refs. 8 and 9 the correct asymptotic expansions are obtained for the limiting cases of long-wavelength acoustic and optic waves. In the case of acoustic waves the displacements are assumed sufficiently small, and the limiting system is found to be completely integrable. However, this constraint, as will be shown, does not permit one to explain the normal thermal conductivity of the system considered.

In the present work we carry out a classification of the elementary excitations of the diatomic Toda lattice, including both long and short waves of small and large amplitude. Using these results and the numerical modeling results, we discuss the problem of thermal conductivity in nonmetallic crystals.

1. THE EQUATIONS OF MOTION; BASIC LIMITING CASES

The system of equations of motion for the diatomic Toda lattice is written in the following form:

$$\begin{aligned} m_1\partial^2 y_{2n}/\partial t^2&=\exp(y_{2n-1}-y_{2n})-\exp(y_{2n}-y_{2n+1}),\\ m_2\partial^2 y_{2n+1}/\partial t^2&=\exp(y_{2n}-y_{2n+1})-\exp(y_{2n+1}-y_{2n+2}), \end{aligned}\tag{1.1}$$

where y_{2n+1} is the displacement of a particle of mass m_2, and y_{2n} is the displacement of a particle of mass m_1. The usual Toda potential is used:

$$\Phi(r_n)=(a/b)\exp(-br_n)+ar_n.\tag{1.2}$$

Everywhere in the following we take $a = b = 1$, except where specifically noted. The equations in terms of the deformations are often useful:

$$\begin{aligned} m_1m_2\partial^2 r_{2n}/\partial t^2&=(m_1+m_2)\exp(-r_{2n})-m_2\exp(-r_{2n-1})\\ &\quad-m_1\exp(-r_{2n+1}),\\ m_1m_2\partial^2 r_{2n+1}/\partial t^2&=(m_1+m_2)\exp(-r_{2n+1})-m_2\exp(-r_{2n+2})\\ &\quad-m_1\exp(-r_{2n}). \end{aligned}\tag{1.3}$$

In the limiting case of the monatomic Toda lattice ($m_1 = m_2 = m$) the two equations (1.3) become identical, and travelling-wave solutions exist:[6]

$$\exp(-r_n)-1=m\omega^2(dn^2(qn\pm\omega t)-K/E),\tag{1.4}$$

where ω is the wave frequency, q is the wavenumber, K and E are the complete elliptic integrals of the first and second kind, and dn is the Jacobian elliptic function. The wavenumber and frequency are connected by the dispersion relation

$$\omega=(m(1/sn^2q-1+E/K))^{-1/2}.\tag{1.5}$$

For $q=$ constant, $k\to 1$ the periodic wave of (1.4) transforms to the single-soliton solution:

$$\begin{aligned} \exp(-r_n)-1&=\mathrm{sh}^2 q/\mathrm{ch}^2(qn-\omega t),\\ \omega&=\mathrm{sh}\, q/m^{1/2}. \end{aligned}\tag{1.6}$$

However, in the case of unequal masses, exact solutions analogous to (1.5) and (1.6) cannot be constructed. Therefore analysis of the elementary excitations in such a system is carried out below on the basis of approximate relations obtained using such small parameters as the deviation of the wavenumber from limiting values. In considering a complete classification of the elementary excitations it is reasonable to also consider the mass ratio as a small parameter.

 0038-5646/92/080271-06$05.00

TABLE I.

Wavenumber	Type of motion	Equations of motion	Temporal characteristic
		Case 1	
$q=0$	$y_{2n}=y_{2n+2}=0$ $=y_{2n+1}=y_{2n-1}$	$(y_{2n})_{tt}=0$ $(y_{2n+1})_{tt}=0$	$y_k=0$ for all k
		Case 2	
$q=0$	$y_{2n}=y_{2n+2}=v$ $y_{2n-1}=y_{2n+1}=w$	$m_1v+m_2w=0$ $(v-w)_{tt}=-2\text{sh}\,(v-w)/\mu$	$\exp(-v+w)_2$ $=(K/E)\,dn\,(\omega_0t+\varphi_0)$ $\omega_0=(K/2E\mu)^{1/2}$
		Case 3	
$q=K/2$	$y_{2n-1}=-y_{2n+1}=p$ $y_{2n}=y_{2n+2}=0$	$(y_{2n})=0$ $(m_2p)_{tt}=-2\text{sh}\,(p)$	$\exp(-p)$ $=(K/E)\,dn^2\,(\omega_2t+\varphi_2)$ $\omega_2=(K/2Em_2)^{1/2}$
		Case 4	
$q=K/2$	$y_{2n}=-y_{2n+2}=s$ $y_{2n+1}=y_{2n-1}=0$	$(y_{2n+1})=0$ $(m_1s)_{tt}=-2\text{sh}\,(s)$.	$\exp(-s)$ $=(K/E)\,dn^2\,(\omega_1t+\varphi_1)$ $\omega_1=(K/2Em_1)^{1/2}$

Then the asymptotes corresponding to near and strongly differing masses are complementary cases. The spatial and temporal characteristics of the motion, as well as the system of equations corresponding to the limiting cases, are presented in the Table. Here $\mu=m_1m_2/(m_1+m_2)$; $m_1<m_2$.

We note that in the linearized system obtained from (1.3), cases 1 and 3 correspond to acoustic, and cases 2 and 4 to optical vibrations.

Thus, in the vibrational spectrum of the diatomic Toda lattice, as in the linear case, there exist acoustic and optical branches. The gap between their left- and right-hand boundaries is given by the relations

$$\Delta\omega_L=(K/2E\mu)^{1/2},\quad \mu=m_1m_2/(m_1+m_2),$$
$$\Delta\omega_R=(K/2E)^{1/2}(1/(m_1)^{1/2}-1/(m_2)^{1/2}). \tag{1.7}$$

We now turn to an anaylsis of the elementary excitations based on the limiting cases in the table.

2. LONG-WAVELENGTH WAVES

For long-wavelength acoustic waves, to which limiting case 1 corresponds, we arrive at the well-known Boussinesq equation, which is completely integrable:[9]

$$u_{tt}=b(r^2u_{xx}-r^3u_xu_{xx}+\tfrac{1}{3}r^4(1-3\mu/M)\cdot u_{xxxx}, \tag{2.1}$$
$$b=2/(1+m_1/m_2),\quad \mu=m_1m_2/(m_1+m_2),\ M=m_1+m_2;$$

here r is the lattice parameter, and u is the continuous variable describing frequency shift.

It is easy to see that for any mass ratio the signs of the coefficients in the equations, that is, the character of the solutions, does not change. The elementary excitations, as in the case of the monatomic lattice, are photon-type excitations and supersonic solitons.

It is extremely important that in order to describe a given system using equations (2.2), we require not just small wavenumber and the acoustic character of the excitations; the transition to the continuum description can be successfully carried out only on the assumption that the amplitudes of the particle displacement are small.[9] The description of the case of large amplitudes, which up to now has not been studied for the diatomic system, requires another approach, using the approximation of hard spheres. We first explain the essential points of such an approximation applied to the monatomic Toda lattice, for which this very approximation was introduced in Ref. 6.

The potential (1.2) in the limit $a\to0$, $b\to\infty$ transforms to a potential barrier at $r=0$ (for $r>0$ there is no interaction). In other words, in this case the monatomic Toda lattice reduces to a system of hard spheres of a single mass in a straight line. The integrals of motion here acquire an especially simple meaning: the interaction between particles reduces to an exchange of momentum, the magnitude of which does not change with time. The single-soliton solution in such a system corresponds to the case when at each moment in time one particle is moving, and all the rest are stationary.

An analogous situation arises in the case when the amplitude of excitation in the system is very large. In fact, the single-soliton solution (1.6) with an infinitely small width (localization on a single site) and an infinitely large propagation speed corresponds to the motion of a single particle in the hard-sphere potential.

Let us examine the equation of motion of the Toda lattice in the dual variables $f_n=a[\exp(-br_n)-1]$ (see Ref. 6):

$$\partial^2(\ln(1+f_n/a))/\partial t^2=b(f_{n-1}-2f_n+f_{n+1})m. \tag{2.2}$$

Taking as the initial approximation for s_n

$$s_n{}^0=\begin{cases}-A, & \xi<0,\\ 0, & \xi=0,\\ A, & \xi>0,\end{cases} \tag{2.3}$$

where $\xi=n-vt$, $\partial s_n/\partial t=f_n$, we obtain after the first iteration

$$s_n{}^1=\begin{cases}-A, & \xi<-1.\\ A\{-1+2\exp(\xi\ln(\varepsilon))\}, & -1<\xi<0,\\ 0, & \xi=0,\\ A\{1-2\exp(-\xi\ln(\varepsilon))\}, & 0<\xi<1,\\ A, & 1<\xi.\end{cases} \tag{2.4}$$

Substitution of (2.5) in equation (2.3) gives

$$A\approx(am/b)^{1/2}\varepsilon^{1/2}/2,$$
$$v\approx-2Am/(b\ln(\varepsilon)). \tag{2.5}$$

The expression (2.5) actually corresponds to the expansion of the exact solution for s_n

$$s_n = (am/b)^{d/2}\,\mathrm{sh}(\lambda)\,\mathrm{th}(n\lambda+\beta t) \tag{2.6}$$

with $\beta=(ab/m)\sinh(\lambda)$ for the case $\lambda\to 1$ with $\varepsilon=\exp(-\lambda)$.

It is easy to verify that the second of the relations (2.6) corresponds to an expansion of the dispersion relation (1.6) in that same small parameter. Thus, the given approach is consistent and gives the correct asymptotic relation in the case of large amplitudes.

It is obvious that an analogous process can be followed for the cnoidal wave, taking as the zeroth approximation a sequence of momenta.

In the case of the diatomic lattice the system of hard spheres may also be taken as limiting for large amplitudes. However, now the system is nonintegrable. The nonintegrability is very intuitive—when particles with different masses collide an energy redistribution takes place which quickly leads to obliteration of the initial conditions. In a certain sense this case is the opposite of the long-wavelength acoustic oscillations, which are described by the integrable Boussinesq equation.

Naturally, an exact solution for the diatomic lattice similar to the single-particle excitation (2.3) does not exist; therefore it is not possible to construct an asymptotic limit like (2.6). Nonetheless, in the cases of near and strongly differing masses it is possible to estimate the rate of decay of an excitation initially concentrated at one particle. Analysis of these cases, as will be shown below, is important in explaining effects connected with the thermal conductivity.

a) The case of nearly equal masses

Let a particle of unit mass propagate at speed u_0 toward a stationary particle of mass $1+\varepsilon$, $|\varepsilon|\ll 1$:

$$\begin{aligned} u&=u_1+(1+\varepsilon)v_1,\\ u^2&=u_1^2+v_1^2(1+\varepsilon), \end{aligned} \tag{2.7}$$

where u_1, v_1 are the speeds of the spheres with masses 1 and $1+\varepsilon$ after the first collision.

The solution for this system has the form

$$\begin{aligned} v_1&=u(2/(2+\varepsilon)),\\ u_1&=-u(\varepsilon/(2+\varepsilon)). \end{aligned} \tag{2.8}$$

Let us now examine the following collision:

$$\begin{aligned} (1+\varepsilon)v_1&=(1+\varepsilon)v_2+u_2,\\ (1+\varepsilon)v_1^2&=(1+\varepsilon)v_2^2+u_2^2. \end{aligned} \tag{2.9}$$

We find

$$\begin{aligned} u_2&=u(1-\varepsilon^2/(2+\varepsilon)^2),\\ v_2&=2\varepsilon u/(2+\varepsilon)^2. \end{aligned} \tag{2.10}$$

To terms of order ε^3 we have

$$u_2=u(1-(\varepsilon/2)^2). \tag{2.11}$$

After transmission over $2k$ interatomic distances we have

$$u_{2k}=u(1-(\varepsilon/2)^2)^k. \tag{2.12}$$

For $k\gg 1$ we obtain

$$u(k)=u(0)\exp(-k\varepsilon^2/4). \tag{2.13}$$

b) The case of strongly differing masses

In this case momentum transfer proceeds differently, by means of multiple collisions of light particles with the preceeding and succeeding heavy ones. These collisions occur until the speed of the light particle becomes less than that of the succeeding heavy one. It is not possible, because of the large number of collisions, to evaluate the energy in the "tail" of the initial excitation directly, as in case (a). However, this very fact allows us to assume that after propagation of the momentum, the energy is already equally distributed between light and heavy particles, and the speed of the light particles is of the order of the speed of the initial excitation.

Let $m_1=\varepsilon$, $m_2=1$, and $\varepsilon\ll 1$. Then in the "tail," in a primitive cell (two neighboring particles), the energy

$$E\approx\varepsilon u^2 \tag{2.14}$$

remains, where u is the initial speed of the heavy particle. The speed of the next particle of mass 1 is

$$u_2\approx u(1/2-\varepsilon). \tag{2.15}$$

The corresponding decay law is

$$u_{2k}=u\exp(-k\varepsilon). \tag{2.16}$$

Therefore, exponential extinction is observed in this case also, but the exponent depends on the small parameter ε.

The second limiting case in the Table is that of long-wavelength optical waves. According to Ref. 8, they are described by the following relationships:

$$\begin{aligned} \exp(-r_{2n})&=(K/E)dn^2(z)\,(1+2qm_1k^2\,\mathrm{sn}(z)\mathrm{cn}(z)/M\\ &\times dn(z)+q^2(-3m_1^2dn^2(z)/M+m_1(4m_2-m_1)(1\\ &-k^2)M^2dn^2(z)+2m_1^2(2-k^2-2m_2E/m_1K)/M^2));\\ \exp(-r_{2n-1})&=(K/Edn^2(z))\,(1+2m_1qk^2\,\mathrm{sn}(z)\\ &\times\mathrm{cn}(z)/Mdn(z)+q^2(-3m_1^2(1-k^2)/Mdn^2(z)\\ &+m_1(4m_2-m_1)dn^2(z)/M^2+2m_1(2-k^2\\ &-2m_2E/m_1K)/M^2)). \end{aligned} \tag{2.17}$$

Here, $z=2nq-\omega t$, and sn and cn are the Jacobian elliptic functions.

The dispersion relation for this system is of the following form:

$$\omega^2=\omega_0^2(1-4q^2\mu E/MK). \tag{2.18}$$

3. THE CASE OF SHORT WAVELENGTHS

We note that for $m_1=m_2$, the limiting cases 3 and 4 in the table are identical and correspond to a wave number $K/2$ in relation (1.4) for the monatomic Toda lattice. Taking into account that for short wavelengths in the diatomic lattice the wavenumbers must differ slightly from K, and transforming to the model variables

$$\begin{aligned} y_{2n-1}&=-w_{2n-1},\quad y_{2n+1}=w_{2n+1},\\ y_{2n}&=v_{2n},\quad y_{2n+2}=v_{2n+2}, \end{aligned} \tag{3.1}$$

we obtain the following system of equations:

$$m_1\partial^2 v_{2n}/\partial t^2=\exp(-w_{2n-1}-v_{2n})-\exp(v_{2n}-w_{2n+1}),$$
$$m_2\partial^2 w_{2n+1}/\partial t^2=\exp(v_{2n}-w_{2n+1})-\exp(w_{2n+1}+v_{2n+2}). \quad (3.2)$$

Since in the present case the model variables (in contrast to the initial variables) vary smoothly with index n, it is possible to transform to the continuum approximation, which in fact describes the behavior of the envelope of the actual displacements:

$$m_1\partial^2 v/\partial t^2=\exp(-w)(-2\,\mathrm{sh}\,v+2w_x\,\mathrm{ch}\,v+w_{xx}\,\mathrm{sh}\,v),$$
$$m_2\partial^2 w/\partial t^2=\exp(v)(-2\,\mathrm{sh}\,w-2\,v_x\,\mathrm{ch}\,w-v_{xx}\,\mathrm{sh}\,w). \quad (3.3)$$

This system of equations cannot be solved analytically for an arbitrary mass ratio. Also, it is obvious that in the case of nearly equal masses the behavior of the system will be practically the same as in the case of the monatomic lattice. Therefore subsequent investigation will be directed primarily towards the case of very diferent masses.

a) Acoustic waves

To treat the limiting case 3 from the table we introduce the parameter α such that

$$m_1/m_2=\varepsilon,\ \partial/\partial x\approx\varepsilon,\ v\approx\varepsilon^\alpha w. \quad (3.4)$$

The only consistent value is $\alpha = 1$.

In further analysis in this section it is more convenient to use the initial system of equations (1.1) as the equations of motion. Nonetheless, all the conclusions reached for (3.3) on orders of magnitude of terms are true for (1.1), because in the present case these systems differ only by terms of order ε^3. Keeping terms up to order ε^2 in system (1.1), we have

$$m_2\partial^2 y_{2n+1}/\partial t^2=\exp(y_{2n}-y_{2n+1})-\exp(y_{2n+1}-y_{2n+2}),$$
$$0=\exp(y_{2n-1}-y_{2n})-\exp(y_{2n+1}-y_{2n+2}). \quad (3.5)$$

Transformation leads obviously to the system

$$m_2\partial^2 y_{2n+1}/\partial t^2=\exp((y_{2n-1}-y_{2n+1})/2)-\exp((y_{2n+1}-y_{2n+3})/2),$$
$$y_{2n}=(y_{2n-1}+y_{2n+1})/2. \quad (3.6)$$

The first equation of this system formally agrees with the exact equation for the monatomic Toda lattice consisting only of the particles with larger masses. The second equation determines the displacements of the smaller masses.

From the above, it is obvious that the long-wavelength (close to $K/2$) solutions of equations (3.6) should first be investigated. They are very similar to those studied in Ref. 6; therefore we will not discuss them.

2) Optical waves

This type of motion corresponds to case 4 in the Table. We introduce parameters p and q such that

$$m_1/m_2\approx\varepsilon,\ \partial/\partial t\approx\varepsilon^{-1/2},\ \partial/\partial x\approx\varepsilon,\ w\approx\varepsilon^p v,\ v\approx\varepsilon^q. \quad (3.7)$$

We substitute (3.7) in (3.3). Consistent values are $p = 3$, $q = 1$.

Keeping terms up to order ε^2 inclusive in (3.3), we obtain

$$m_1\partial^2 v/\partial t^2=-2\,\mathrm{sh}\,v,$$
$$m_2\partial^2 w/\partial t^2=-2v_x\exp v. \quad (3.8)$$

The solution of this system in the class of travelling waves has the form

$$v=-\ln(K/Edn^2\xi), \quad (3.9)$$
$$w=2qm_1/m_2E^2/(K^2\varkappa^2)(Z(\xi)-k^2\,\mathrm{sn}\,\xi\,\mathrm{cn}\,\xi/dn\xi),$$
$$\xi=qx-\omega t,\ \omega=\omega_1,\ \varkappa^2=1-k^2.$$

Here, $Z(\xi) = \int dn^2\xi d\xi - E\xi/K$ is the Jacobian elliptic function.

System (3.8) has no soliton solutions in this class of waves.

4. NUMERICAL MODELING OF THE THERMAL CONDUCTIVITY OF THE DIATOMIC TODA LATTICE

The first work on numerical modeling of heat transport in the diatomic Toda lattice was Ref. 1; however, substantial anomalies were apparent in the work of Ref. 2. It was shown that for a specific value of the mass ratio a transition occurred, from the infinite thermal conductivity characteristic of integrable systems to the usual picture of heat transport by a diffusion mechanism, the existence of which is indicated by the applicability of Fourier's law. In this work a method of computational study of stochastic processes in a system, based on scanning in phase space for regions in which the phase trajectories exponentially diverge, was applied. For parameter values which lead to normal thermal conductivity, the situation in phase space corresponded in fact to dynamic chaos.

In the work of Ref. 10 several new phenomena were detected. In particular, for a mass ratio of 1/2, which in Refs. 1 and 2 corresponded to the case of normal thermal conductivity, an anomalous thermal conductivity was detected a low temperatures. In addition, it was noted that in regions of stochastic behavior, a certain part of the energy is transmitted by so-called ballistic heat flux, which does not obey Fourier's law. This anomalous flow at sufficiently high temperatures of the ends of the lattice is negligibly small compared to the normal flow, which obeys the classical heat diffusion law. However, at low temperatures it becomes the principal carrier of energy. It has also been established that in the case of normal thermal conductivity its size is inversely proportional to the temperature of the system. The results of Ref. 2 were confirmed as regards the structure of phase space in the system.

We now turn to a discussion of results of these numerical experiments based on the information, obtained in sections 2 and 3, on the behavior of systems close to the limiting cases for the diatomic Toda lattice.

We will first examine the case of low temperatures. For this case, small deviations of the atoms from their equilibrium positions are characteristic; this makes it possible to limit the potential expansion to cubic terms, and thus to use the continuum approximation for acoustic waves of small wavenumber. These considerations lead to the Boussinesq equation, as noted above. The integrability of this system insures that it will have an anomalous thermal conductivity, due to transport of heat by supersonic compression solitons and phonon-type travelling waves. This mechanism is realized at low temperatures regardless of the mass ratio. Anomalous thermal conductivity is in fact observed in such a system even for a mass ratio of 1/2 (Ref. 10), that is, for the maximum deviation from the completely integrable case (the monatomic Toda lattice).

With reference to the case examined in Ref. 2, it can be asserted that it is describable as an asymptotic "potential wall" for the diatomic Toda lattice. This is confirmed by numerical analysis of the decay of a solitary excitation propagating across the lattice (see Fig. 8, Ref. 2), that is, of the inelastic interaction of a solition with phonons. In the figure it can be seen that the character of the decay of an excitation near the limiting values of the mass ratio (0 and 1) differs, and that the difference is well described by relations (2.13) and (2.16). This indicates that the interaction between particles can be approximated as a collision of hard spheres of different masses. It is evident that the long-wavelength approximation, good for small amplitudes, cannot describe such processes.

The question arises as to how the presence in the system of small-amplitude waves influences the decay of a strong excitation. The collisional mechanism of momentum transfer leads to the condition that the rate of decay of an excitation influences only the state of particles ahead of the region in which the excitation is localized. Their speed in this case is small compared to the speed of the excitation itself. In other words, in the case examined, the most important condition for stochastic behavior in the diatomic Toda lattice is that the limiting hard-sphere system is far from integrable.

It is also interesting to trace the decay of a soliton in a system of hard spheres from the point of view of the momentum conservation law. The initial momentum is redistributed among the particles located in the "tail" of the soliton. This means that a "big" soliton breaks up into a sequence of "small" ones, and their momentum is conserved. These small solitons are decribed by the long-wavelength approximation, and thus satisfy the Boussinesq equation and propagate without dissipation through the lattice. As noted in Ref. 6, as the amplitude of a soliton increases, its energy grows faster than its momentum. Therefore "small" solitons can transport a significant part of the momentum of the initial "big" soliton excitation, taking only an insignificant part of its energy. This fact allows us to associate with them the "ballistic flux" of heat observed in Ref. 10, which dominates at low temperatures and becomes negligibly small at high temperatures.

A simple estimate shows that the temperatures of the lattice ends in the numerical experiment of Ref. 3 are in fact rather high for the "potential wall" approximation to be applicable.

5. THE ROLE OF NONLINEARITY IN THE THERMAL CONDUCTIVITY OF REAL CRYSTALS

In the preceding sections we determined a series of features of the heat transport in a model system—the diatomic Toda lattice. The question naturally arises as to how the results obtained fit in with the generally accepted theories of the thermal conductivity of crystals.

The classical theory of thermal conductivity examines the two principal different limiting cases of low and high temperatures; the Debye temperature is taken to be the cutoff. The first case implies a quantum treatment taking account of phonon-phonon interaction as well as phonon scattering on boundaries and defects. The second case corresponds to the classical scattering of waves on lattice density fluctuations.

a) The high-temperature case

In the classical model it is assumed that dynamic chaos exists in the system, with equipartition of energy among the degrees of freedom. In this case the use of Boltzmann statistics for the vibrational spectrum is justified, and for the coefficient of thermal conductivity we get the relation

$$\varkappa \approx c v \lambda / 3, \tag{5.1}$$

where c is the lattice specific heat, v is the characteristic speed of the excitation, and λ is the mean free path. For λ we have the estimate

$$\lambda \approx (\Delta^2)^{-1}, \tag{5.2}$$

where Δ^2 is the mean square fluctuation of the relative expansion of the lattice. A well-known thermodynamic formula gives

$$(\Delta^2) = NkT\beta, \tag{5.3}$$

where β is the cyrstalline compressiblity. From (6.1), (6.2), and (6.3) we have

$$\varkappa \approx T^{-1} \tag{5.4}$$

for high temperatures. This conclusion is confirmed by numerical experiment for the diatomic Toda lattice as well.[10]

It is obvious that the mechanism of scattering on density fluctuations dominates at high temperatures independently of the nature of the excitations studied, since its applicability only requires that the system be stochastic.

However, from the above discussion it it clear that this is not always so, even for a system not showing complete integrability. In the diatomic Toda lattice, the chaos developed appears at acoustic timescales only if the mass ratio is less than a critical value.[2] For monatomic systems with a real interaction potential (a strong repulsion as atoms approach and a weak attraction at longer distances) the limiting system at high temperatures is one of hard spheres of identical mass in a straight line. Obviously chaotic behavior will not occur in this case.

b) The low-temperature case

The presently accepted microscopic thoery of crystalline thermal conductivity at low temperatures takes account of the following phonon scattering mechanisms:

(I) defect scattering,

(II) transfer processes upon phonon-phonon interaction,

(III) reflection from crystalline edges.

Mechanisms (I) and (II) also require energy equipartition among the degrees of freedom, i.e., dynamic chaos. However, taking account of anharmonicity in one-dimensional models does not lead to the same results. Thus, for example, in Ref. 11 the behavior of a lattice of atoms with cubic anharmonicity was studied. Solution of the quantum problem showed that the elementary excitations in such a system have primarily a solitonic, and not phonon, character. Scattering processes are determined by soliton interactions, i.e., by a higher-order effect.

Within the phonon model mechanism (III) results in a finite thermal conductivity even for the harmonic lattice, but it requires the existence of a large number of boundaries. Such systems are not discussed here.

From the above we may reach a conclusion: at low temperatures, for one-dimensional regular lattices with nearest-neighbor interactions, there is no mechanism that ensures normal thermal conductivity. Numerical experiments confirm this conclusion. It appears that the only way to obtain a normal thermal conductivity in this case involves taking account of long-range interactions in the lattice. The system can then no longer be described by the integrable Boussinesq equation.[12] A more detailed study of such systems lies in the future.

In the high-temperature case, long-range interactions do not "save" the situation—in the limit a hard-spheres system is still obtained. It is significant here that heat transport processes in real crystals can very rarely be described as quasi-one-dimensional. In fact, the two-dimensional system of hard spheres, in contrast to the one-dimensional case, is in general nonintegrable. This range of problems is also in need of study.

In conclusion, the authors express their gratitude to V. V. Smirnov and V. V. Ginzburg for useful discussions.

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Translated by I. A. Howard