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Thermal conductivity of one- and two-dimensional lattices

E Atlee Jackson and Antonis D Mistriotis†
Department of Physics, University of Illinois at Urbana-Champaign,
1110 West Green Street, Urbana, IL 61801, USA

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Abstract. Numerical experiments were conducted to study the energy transfer through one- and two-dimensional non-linear lattices, with various anharmonicities and diatomic mass ratios, when they are placed between two thermal reservoirs. The existence and dependence of normal thermal conductivity on the number of particles in the lattice ($N \leqslant 400$) and the mass ratio is studied. In these lattices, an approximate transition is found to be related to the decay of a pulse travelling across the finite lattice. The threshold for the transition from infinite to normal thermal conductivity is also found to coincide with the value of these parameters for which the divergence of trajectories in every region of the phase space of the system becomes non-linear with time, in an interval shorter than the time a pulse needs to travel through the lattice. It is also found that the thermal conductivity of the two-dimensional lattices that were examined differs from that of similar one-dimensional lattices only quantitatively and not qualitatively as predicted by Peierls' 'Umklapp' analysis.

1. Historical background

A first attempt to explain the thermal conductivity of solids (lattices) was made by Peierls [1] in 1929. He applied the concepts that had been developed by Boltzmann for the gas dynamics to phonons. This theory lacks the intuitive transparency of the original Boltzmann equation, because phonons cannot be localised with definite velocity as can the molecules in a classical gas. Nevertheless, the Boltzmann–Peierls equation has been widely used as a basis for understanding lattice thermal conductivity.

Peierls' theory, which is based upon Boltzmann's *Stosszahlansatz*, assumes that phonons behave in a stochastic way without justifying the origin of such behaviour. The first attempts to verify the validity of the stochastic hypothesis in lattices were the numerical experiments conducted by Fermi and co-workers [2] in 1953. They searched for energy sharing between the linear normal modes, which is characteristic of irreversible behaviour in non-linear lattices. Their discovery of the lack of the energy sharing among the modes raised a variety of questions. These early numerical experiments were followed by others, such as the one performed by Northcote and Potts [3], who discovered energy sharing among the normal modes in a lattice that consists of particles interacting with their first neighbours by means of a harmonic force plus a repulsive core.

Later, other computations attempted to verify the validity of Fourier's law (Fick's law) of heat conduction and to determine the coefficient of thermal conductivity K of lattices

$$\langle \boldsymbol{J} \rangle = -K \nabla T \tag{1}$$

† Current address: Research Centre of Crete, PO Box 1527, Heraklio 71110, Crete, Greece.

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where $\langle J \rangle$ is the total time-average energy flux. Among the earliest studies were those by Jackson and co-workers [4] and by Payton and co-workers [5]. In these studies, one-dimensional non-linear lattices were coupled at their ends with two heat reservoirs of constant temperature. The temperature difference between the two reservoirs imposed an external temperature gradient on the lattice. If Fourier's law is satisfied, the lattice has a coefficient of thermal conductivity, K, which is an intensive property of the system (i.e., is independent of the size of the system). It also exhibits an internal temperature gradient, where the temperature of a particle is defined as its average kinetic energy. In the next 15 years many similar computations were conducted [6], [7]. A summary of these results is presented in [8]. The conclusion presented there is that the 1D non-linear (anharmonic) lattices, on which numerical experiments had until that time been performed, were not known to exhibit normal thermal conductivity. Another review of the molecular dynamical calculations of energy transport in lattices is given in [9]. A general review of relationships between non-linearities and irreversibility of non-linear lattices is given in [10].

This series of disappointing results, which failed to present examples of non-linear lattices satisfying Fourier's law, ended only recently. Mokross and Büttner [11] studied the thermal conductivity of one-dimensional diatomic ordered Toda lattices. They presented results that strongly indicate that this type of lattice has a normal thermal conductivity if the mass ratio is 0.50. Nevertheless, they did not sufficiently study the dependence of the total energy flux on the number of particles in the lattice to establish that the coefficient of thermal conductivity is, in fact, an intensive property of the lattice. We study this question in detail in § 2. In addition to Mokross and Büttner's results, Casati and co-workers [12] proposed another type of lattice that, as they showed by numerical calculations, also satisfied Fourier's law, and they determined its thermal conductivity. This lattice consists of hard point particles, half of which (the even-numbered ones) are harmonic oscillators bound to their equally spaced lattice sites, while the odd-numbered particles are free particles (the 'ding-a-ling' model). This model, however, cannot be taken as a serious physical example because it is an extreme case, where the interaction between the particles in the lattice is not described by a potential that is a differentiable function. Hence, the KAM theorem [13] does not apply.

The thermal conductivity of lattices was also studied from a different point of view by Miura [14] (reviewed in [10]), who tried to interpret the Jackson–Pasta–Waters results by studying the decay of a pulse ('soliton') as it travels through the lattice. A discussion on the relationship between solitons and heat conduction in lattices can also be found in [15]. Extending these ideas in §3, we study the relationship between the thermal conductivity of the diatomic Toda lattice and the rate of decay of one pulse or two interacting pulses travelling through the lattice.

Despite these numerous numerical and analytical studies of lattice thermal conductivity, there still remained a number of unresolved questions. An extended discussion of these questions can be found in [10]. For example, the transition from an infinite to a finite thermal conductivity in the 'thermodynamic limit' (the number of particles N in the lattice is large, i.e., $N \rightarrow \infty$), which takes place as a parameter of the lattice changes, has not up to now been sufficiently studied. We therefore examine this question in § 2. Another unanswered question is 'What type of dynamics produces the irreversible behaviour of systems that exhibit normal thermal conductivity?' A consistent theory that relates the irreversibility of such systems to their dynamical behaviour in the phase space should also give a microscopic interpretation of their thermal conductivity. In particular, the prediction of the threshold for the transition from infinite to normal

thermal conductivity is a critical test for a theory that claims to present a dynamical justification of irreversibility. We examine this question in § 4, where it is proposed that thermal conductivity is related to the local τ-averaged rate of divergence of trajectories initiating in a neighbourhood of point $(\boldsymbol{q}, \boldsymbol{p})$ in the phase space, where τ is a finite time interval. The numerical results presented in § 4 suggest that the thermal conductivity is infinite if there is a region of finite measure in the phase space of the system such that the divergence of two trajectories starting close to a point $(\boldsymbol{q}, \boldsymbol{p})$ in that region is linear with time for a time period τ. The period τ is the sound-transit time for the lattice. This criterion differs fundamentally from those based on Lyapunov exponents, which characterise the (irrelevant) asymptotic ($t \rightarrow \infty$) characteristics of nearby solutions.

Finally, in § 5, we compare the thermal conductivity of a two-dimensional lattice to the thermal conductivity of a 1D lattice with the same type of interaction between their particles. In this way we check how important the influence of the dimensionality of the system is on its irreversible behaviour.

Before presenting our results, we would like to discuss the question of whether the computer simulations of lattice dynamics are relevant to the real phenomena. Even though a high accuracy was maintained during our calculations, (e.g. the energy is conserved with an error of the order 10^{-4}), one can argue that, if the divergence between two trajectories in a region of the energy surface is exponential with time, a computer-produced trajectory cannot stay close to a physical trajectory for a long period of time. However, this argument is not relevant in the present systems, both because of the very finite sound-transit time noted above and the continual stochastic interaction with the reservoirs. A computer simulation reproduces the stochastic behaviour of such a system and all related phenomena, which is all that is required.

2. Numerical experiments on one-dimensional diatomic Toda lattices

Recently, Mokross and Büttner [11] claimed that a diatomic Toda lattice exhibits an internal temperature gradient when its left- and right-end particles are coupled with two reservoirs of temperature, T_L and T_R, respectively, if the ratio of the masses of the two different types of particles in the lattice is $r = m_1/m_2 = 0.50$. The same system was previously studied by Casati and Ford [16], who showed that for certain values of r and its total energy this system has large chaotic regions in its phase space. This strongly suggests that irreversible effects might be found in that system. Indeed, the internal temperature gradient shown in figure 1 is an indication that this lattice has normal thermal conductivity. Nevertheless, Mokross and Büttner only computed the total average energy flux through a few lattices, all of which had a small number of particles. Therefore, they did not establish that the thermal conductivity is an intensive property of the lattice, which is a basic feature of Fourier's law. We will demonstrate this property here and, in the process, obtain information concerning the size of the lattice that is required for Fourier's law to be valid.

The lattice we study in this section consists of two types of particles with different masses. The odd-numbered particles have mass m_1 and the even-numbered have mass m_2. They interact with their nearest neighbours with an exponential force. The end particles of this lattice are fixed. In other words, $q_0 = q_{N+1} = 0$. The equations of motion for this system are, therefore,

$$\dot{q}_i = p_i/r_i \qquad \dot{p}_i = -\exp -(q_{i+1} - q_i) + \exp -(q_i - q_{i-1}) \tag{2}$$

where $i = 1, \ldots, N$, $r_i = m_1/m_2$, if i is odd and $r_i = 1.00$, if i is even. The particles $i = 1$

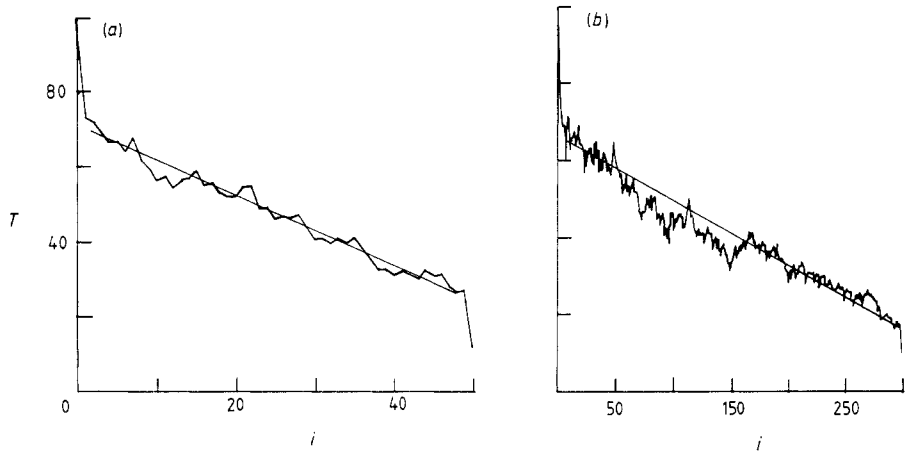

Figure 1. Internal temperature gradient for a diatomic Toda lattice: (*a*) $N = 51$, $r = 0.50$, $T_L = 100$, $T_R = 10$, max $\delta t = 0.20$; (*b*) $N = 299$, $r = 0.65$, $T_L = 100$, $T_R = 10$, max $\delta t = 0.20$.

and $i = N$ are coupled with two thermal reservoirs of temperature, T_L and T_R, respectively. This means that these particles collide with the particles of the corresponding reservoir at the times t_i. The velocity of each of the two end particles at time t_i is given from a velocity distribution of the type

$$f(v) = (|v|/T_k)\exp(-v^2/2T_k) \tag{3}$$

where k is R and L, respectively. The sign of this velocity is determined randomly such that the two possible signs have the same probability. The factor $|v|$ in formula (3) takes into account the fact that the fastest particles in the reservoirs have greater probability of interacting with the end particles of the lattice. Notice that the end particles of the lattice are constrained by the fixed boundary conditions to move close to its equilibrium point. Therefore, the probability of a particle in the reservoir colliding with the end particle of the lattice does not depend on their relative velocity, but only on the velocity of the particles in the reservoir. The interval $\delta t = t_{i+1} - t_i$ is determined from a uniform distribution, $g(\delta t) = 1/\max \delta t$, defined for the values $0 < \delta t < \max \delta t$. The numerical method used for the integration of the equations of motion is the Nyström method, which was suggested as the most appropriate for this case by Miura [13]. The initial velocities of the particles in the lattice were chosen such that their kinetic energy satisfies the temperature gradient, which is expected to be the steady state. In this way we reduce the time needed to reach the steady state.

The first question we investigate is whether the system described in the previous paragraph has a thermal conductivity that is an intensive property. This means that the coefficient of thermal conductivity is independent of the number of particles in the lattice. For this reason we study the total time-averaged energy flux $\langle J \rangle$ through the lattice as a function of the number of particles N in the lattice. For these numerical calculations, $T_L = 100$, $T_R = 10$, $r = m_1/m_2 = 0.50$, and max $\delta t = 0.20$. In this way the average temperature in the lattice is the same in all our computations. In table 1 and figure 2 the values of the coefficient of thermal conductivity K, which is defined as $K = \langle J \rangle N/(T_L - T_R)$ for lattices of different number of particles N, are shown. Notice that in this paper the term 'coefficient of thermal conductivity' will be used for K, even in the case where it is not an intensive property of the lattice. The error bars shown in figure 2 correspond to the amplitude of fluctuations of $\langle J \rangle$ around its mean value after the system

Table 1. The values of the coefficient of thermal conductivity $K = \langle J \rangle N/(T_L - T_R)$ for the diatomic Toda lattice as a function of the number of particles N in the lattice and the mass ratio r. $T_L = 100$, $T_R = 10$, max $\delta t = 0.20$.

N	0.50	0.65	0.75	0.85
99	21 ± 1	31 ± 1	42 ± 2	60 ± 6
199	25 ± 2	36 ± 3	55 ± 2	91 ± 3
249	34 ± 3	43 ± 4	58 ± 6	101 ± 5
299	34 ± 3	43 ± 3	58 ± 5	108 ± 7
349	35 ± 3	50 ± 5	68 ± 4	118 ± 2
399	34 ± 3	48 ± 3	64 ± 6	133 ± 2

had reached the equilibrium (figure 3). (Results corresponding to other values of r are also presented in the same figure; they will be discussed in the following paragraph.) Our results show that the values of K are independent of the lattice length for $N \geq 250$. This means that the coefficient of thermal conductivity is an intensive property of the lattice for large N. Therefore, the diatomic Toda lattice with mass ratio $r = 0.50$ exhibits normal thermal conductivity. In other words, it obeys Fourier's law.

It is known that the 1D monatomic Toda lattice ($r = 1.00$) is an integrable system, so it does not obey Fourier's law, and it has infinite thermal conductivity. Hence, a transition takes place from infinite to normal thermal conductivity as the parameter changes

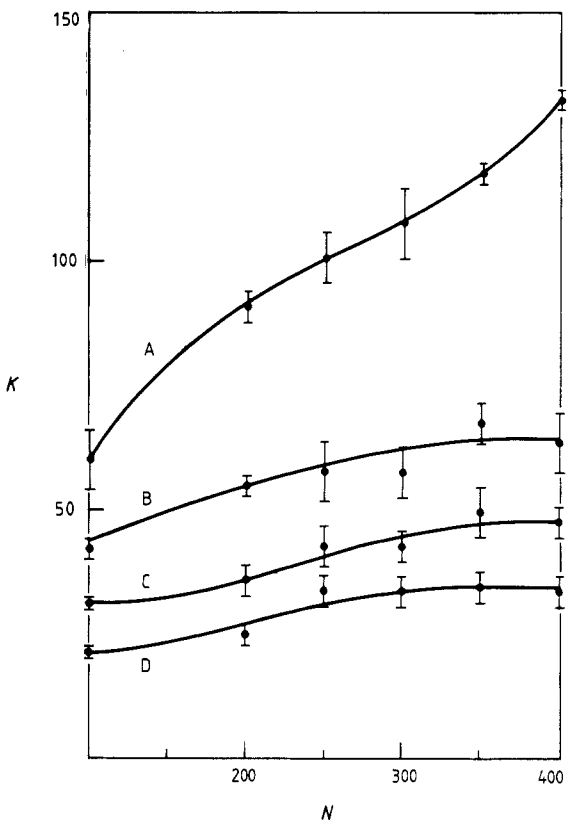

Figure 2. The coefficient of thermal conductivity $K = \langle J \rangle N/(T_L - T_R)$ for the diatomic Toda lattice as a function of N for several values of the mass ratio r. $T_L = 100$, $T_R = 10$, max $\delta t = 0.20$.

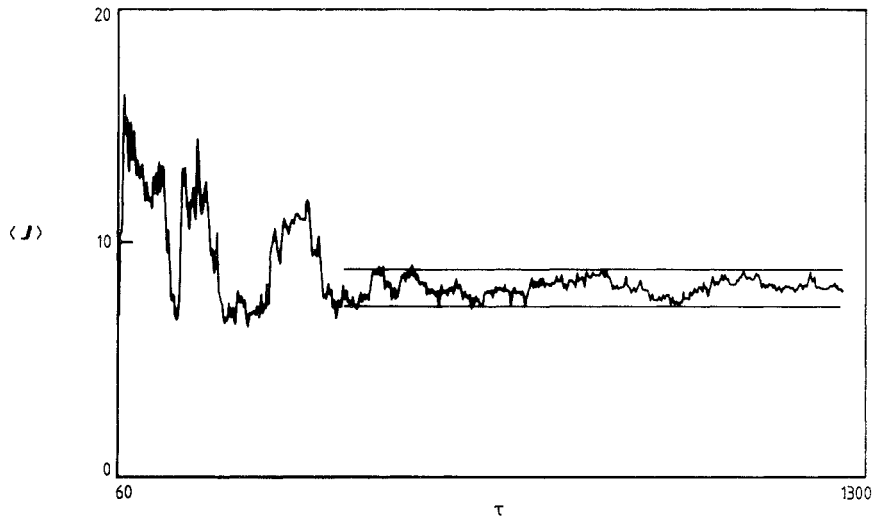

Figure 3. The function $\langle J\rangle(\tau) = (1/t)\int_0^t J(t)\,\mathrm{d}t$ for a diatomic Toda lattice, where $r = 0.50$, $N = 399$, $T_L = 100$, $T_R = 10$, $\max \delta t = 0.20$. $J(t)$ is the total instantaneous energy flux through the lattice. The half distance between the two parallel lines in the figure corresponds to the error for the value of $\langle J\rangle$.

from 1.00 to 0.50. To study this transition, we repeated the computations that we had conducted for the case $r = 0.50$ for the cases $r = 0.65$, $r = 0.75$, and $r = 0.85$, keeping $\max \delta t$, T_L, T_R the same. The results of these numerical calculations are presented in table 1 and are pictorially shown in figure 2. There we see that as r increases the curves are gradually transformed in such a way that the value of K diverges as N increases. This clearly appears to be the situation when $r = 0.85$, while for the cases $r = 0.65$ and $r = 0.75$, K shows a tendency towards a saturation value, but the existence of normal thermal conductivity cannot be proved unless longer lattices are considered. This suggests that there may be a critical value, $r = r_c$, such that $K(N) \to \infty$ as $N \to \infty$, when $r > r_c$. It is not possible to determine whether r_c is smaller than 1.00 for $N \to \infty$ because this requires computing the total time-averaged energy flux $\langle J\rangle$ passing through very long lattices for many values of r. Nevertheless, figure 2 gives a probable estimate for r_c; namely, that it lies close to 0.75 if the results only up to $N = 400$ are taken into account.

In the next two sections, we shall analyse and try to explain the transition from infinite to normal thermal conductivity in terms of the dynamical behaviour of the system. In other words, we will discuss the possible correlation between dynamical characteristics of the system and the value of its thermal conductivity.

3. Decay of a pulse travelling through a diatomic Toda lattice

It was suggested in [14] and [15] that information about the way in which energy is transferred through a lattice (diffusively or not) can be obtained by studying the decay of a solitary pulse travelling in the lattice. The basis of this idea is that the decay of a pulse takes place because of 'irreversible' energy sharing among the particles in the lattice and that the rate of decay indicates how fast the energy sharing occurs. If the lifetime of the pulse is shorter than the time it needs to travel through the lattice, then the energy is transferred by a diffusion process and the system is expected to satisfy

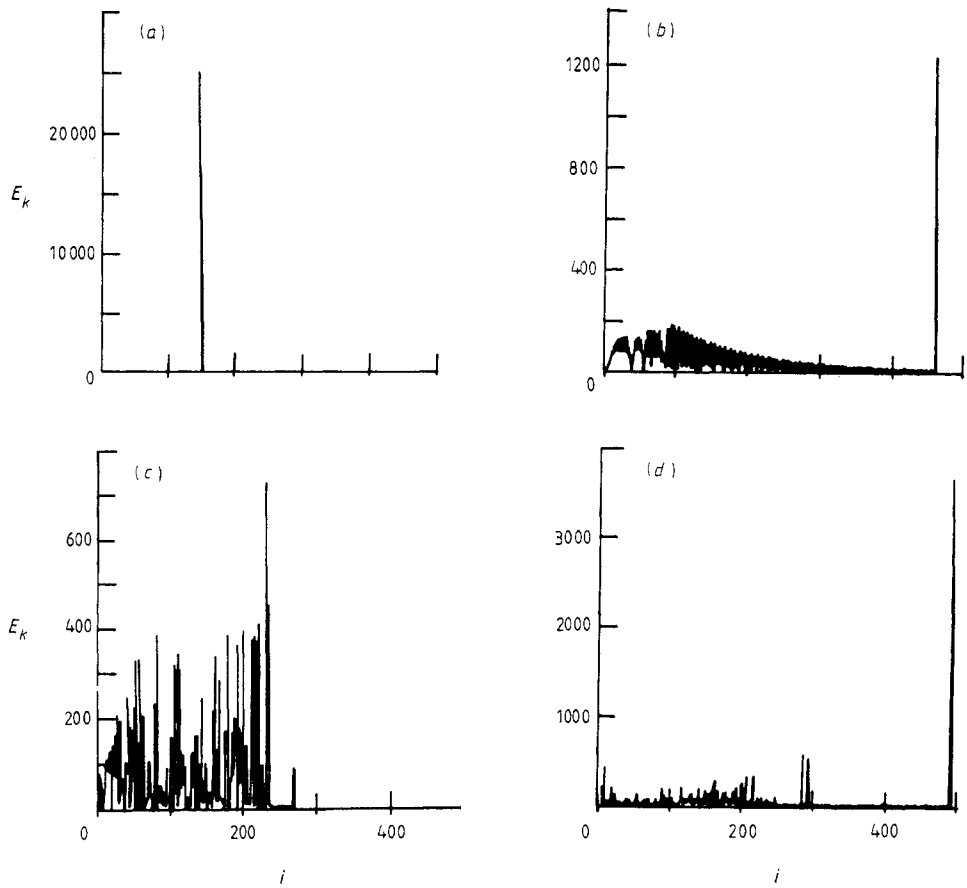

Figure 4. Decay of a pulse travelling through a diatomic Toda lattice $N = 499$: (*a*) $r = 1.00$; (*b*) $r = 0.85$; (*c*) $r = 0.75$; (*d*) $r = 0.50$.

Fourier's law. This idea is particularly applicable to systems that are perturbations of an integrable system that has soliton (non-dispersive, spatially localised) solutions. This is the case with the diatomic Toda lattice, which is examined here, if the mass ratio is used as the perturbation parameter, because the monatomic Toda lattice ($r = 1.00$) is known to have soliton-like solutions.

The system for which we study the decay of a soliton is a 1D diatomic Toda lattice with fixed ends. It consists of $N = 499$ particles. The even-numbered particles have mass 1 and the odd-numbered, mass r. At time $t = 0$, particle $i = 1$ is given a large kinetic energy ($E = N(T_L + T_R)/2$), where $T_L = 100$ and $T_R = 10$. We then record the kinetic energy of every particle in the lattice after a time period $t = 40$. In this way we obtain figure 4(*a–d*), corresponding to $r = 1.00$, 0.85, 0.75, 0.50, respectively. Figure 4(*a*) shows a non-decaying pulse travelling through the lattice. This corresponds to a pulse that consists of essentially one soliton, which is a solution of the system for the case $r = 1.00$. As r decreases, the rate at which the pulse decays increases. Figure 4(*b*) shows that for the case $r = 0.85$, the original pulse still retains a large part of its energy and can be recognised at $t = 40$. For $r = 0.75$ (figure 4(*c*)) at time $t = 40$, the pulse has decayed such that it cannot be distinguished from the other peaks of the kinetic energy when it is plotted as a function of the particle number. For $r = 0.50$ (figure 4(*d*)), we see that a large peak compared with the background still appears at $t = 40$, even though this lattice

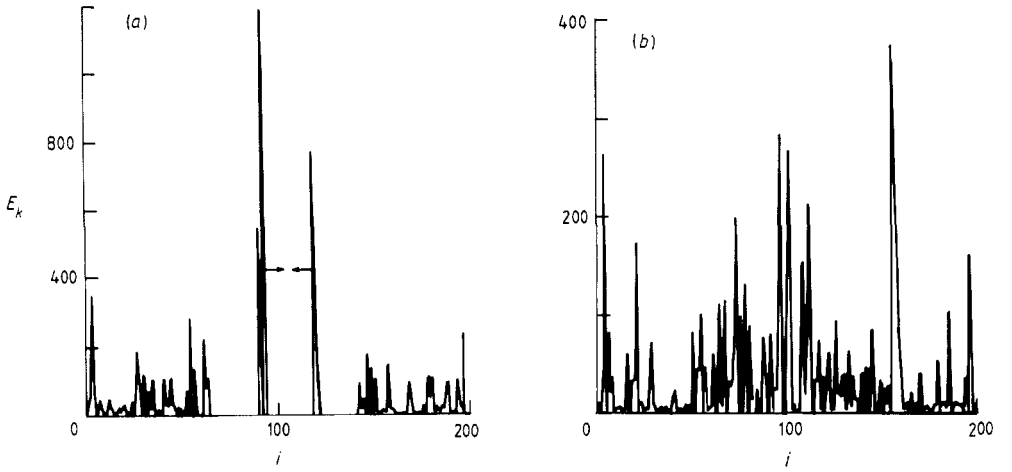

Figure 5. Decay of two pulses because of their collision in a diatomic Toda lattice. $N = 199$, $r = 0.50$: (*a*) before the collision at $t = 12$; (*b*) after the collision at $t = 20$.

exhibits normal thermal conductivity, as was shown in § 2. This result raises the question of why this pulse does not contribute to the transfer of energy through the lattice in a non-diffusive way.

To answer this question, we study the effect of collisions between two pulses. In figure 5 we see two pictures of a diatomic Toda lattice with 199 particles and $r = 0.50$ at $t = 12$ and $t = 20$. This shows that the collision between the two pulses moving in opposite directions, shown in figure 5(*a*), results in their destruction (figure 5(*b*)). Figure 6 shows that this remains a strong effect when $r = 0.75$. In contrast, if $r = 0.85$ the two pulses survive the collision between them, as it is shown in figure 7. Therefore, the process of the decay of a pulse travelling through a lattice is more complicated than the situation that is studied in figure 4, where a pulse is travelling through a previously unperturbed lattice. In fact, collisions between pulses play an important role in the rate at which the lattice approaches its equilibrium state.

The importance of the collisions between pulses to the energy sharing between the

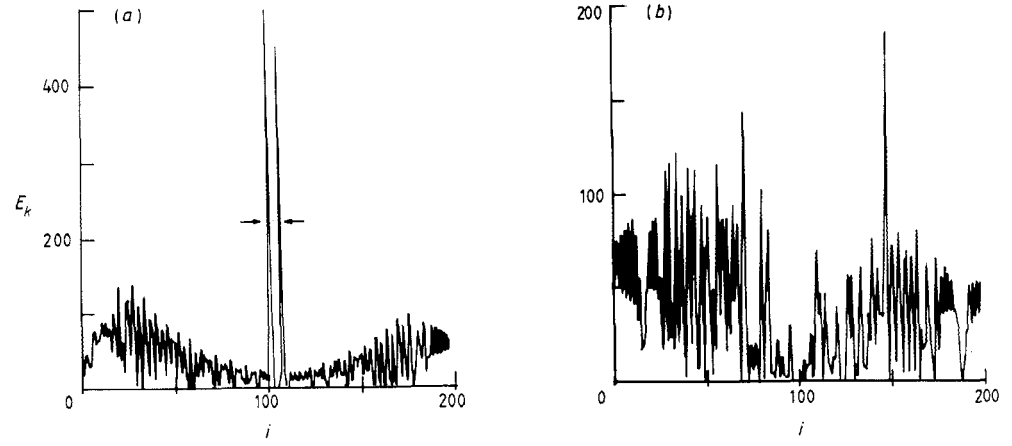

Figure 6. Two pulses travelling through a diatomic Toda lattice had already substantially decayed before their collision. The collision intensifies even more the energy sharing. $N = 199$, $r = 0.75$: (*a*) before the collision at $t = 12$; (*b*) after the collision at $t = 20$.

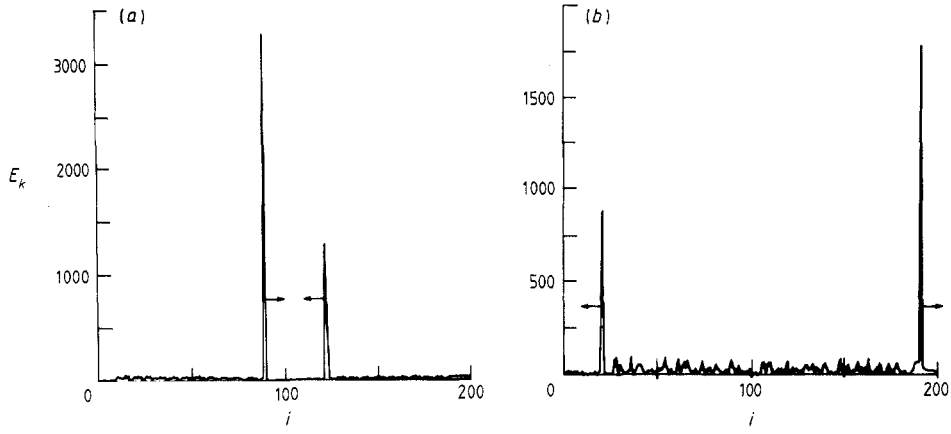

Figure 7. Two pulses colliding in a diatomic Toda lattice. $N = 199$, $r = 0.85$: (*a*) before the collision at $t = 8$; (*b*) after the collision at $t = 20$.

particles in the lattice can also be shown in a quantitative way. Two pulses, with initial energy E_0 and $2E_0/3$, respectively (where $E_0 = 6567$), are considered travelling in a lattice that consists of $N = 199$ particles. The largest values, E_1 and E_2, of the kinetic energy as a function of the particle number at $t = 12$ and $t = 20$, respectively, are computed for several values of r (0.90, 0.85, 0.80, 0.75, 0.70, 0.65, 0.60, 0.55, 0.50, 0.40, 0.30. 0.20, 0.10). In figure 8, the graphs of the functions $E_1(r)/E_0$ and $E_2(r)/E_0$ are presented. At $t = 20$, the collision between the two pulses has already taken place, while for $t = 12$, the two pulses have not yet collided for most values of r. For the cases where the collision of the pulses occurs before $t = 12$, the correct value for $E_1(r)$ is taken to be the largest value of the kinetic energy at $t = 12$ in a lattice where only one pulse with energy equal to E_0 is considered as the initial condition. In this way, the influence of the collision on the decay of the pulses can be studied. Figure 8 shows that the function

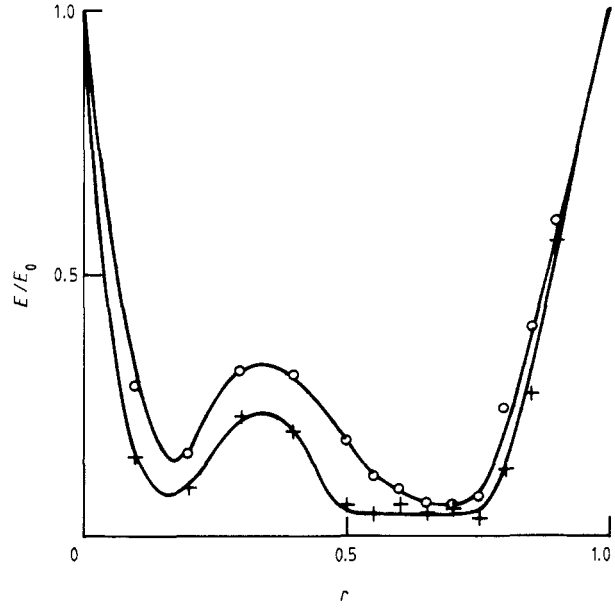

Figure 8. The functions $E_1(r)/E_0$ (circles) and $E_2(r)/E_0$ (crosses). E_1 and E_2 are the largest values of the kinetic energy as a function of the particle number at $t = 12$ (before the collision) and $t = 20$ (after the collision). E_0 is the kinetic energy of the largest of the two original pulses.

$E_1(r)/E_0$, which corresponds to $t = 12$, exhibits a strange behaviour. For $0.70 < r < 1.00$, it decreases when r decreases, but for $r < 0.70$, it increases. The large value of $E_1(0.50)/E_0$ does not correlate with the fact that this lattice exhibits normal thermal conductivity for $r = 0.50$. On the contrary, the function $E_2(r)/E_0$, which corresponds to $t = 20$ when the collision has already occurred, is almost constant for $0.50 < r < 0.75$ fluctuating around 0.04 and then increases rapidly towards 1.00 when $r > 0.75$. This shows that a transition takes place for r just larger than 0.75. This is a good agreement with the value of r_c, found in § 2.

The study of pulses that travel without decaying through a previously unperturbed lattice, but which interact with each other, is clearly an interesting subject that requires further investigation. In the next section, we present another way to analyse the results of § 2 about the thermal conductivity of the diatomic Toda lattice.

4. The relationship between the thermal conductivity and the local rate of divergence of trajectories

The rate of divergence of trajectories close to each other in the phase space has frequently been used to describe quantitatively the stochastic dynamical behaviour that is believed to be related to irreversibility. This relationship has been established for the asymptotic case $t \to \infty$, where the rate of divergence is described by the Lyapunov characteristic exponents. Nevertheless, thermodynamic behaviour far from equilibrium is related to the dynamic behaviour of the system during a finite time period of length τ. The period τ is a characteristic time for the examined system. For example, in the case we study, the lattice thermal conductivity, τ, is the sound-transit time of the lattice.

In this section we present a method that uses the average rate of divergence over a time interval τ between trajectories initiating in a neighbourhood of a point $(\boldsymbol{q}, \boldsymbol{p})$ of the phase space to determine whether a system exhibits irreversible behaviour. This rate of divergence between trajectories is called local because it depends on the point $(\boldsymbol{q}, \boldsymbol{p})$ and the magnitude of τ. By defining this local rate of divergence we can study the short-time dynamical behaviour of the system, which is essential for thermodynamics far from equilibrium. If there is a region of positive measure in the phase space where any two trajectories diverge linearly with time for a time period of τ, the loss of correlation between an initial and the corresponding final state of this system takes place slowly for time periods less than τ. Therefore we expect that such systems do not exhibit normal irreversible behaviour. In particular, they do not obey Fourier's law. This is not a rare situation. Nearly integrable systems have trajectories that diverge at a very slow rate. Therefore they exhibit a persistence of regular motion even in the chaotic region of their phase space. This persistence of regularity was observed in several numerical experiments [17, 18], and is discussed in a more general approach in [19] in relation to Nekhoroshev's theorem [20].

We can test this idea by numerically calculating the size of the regions in the phase space of a lattice with a large number of particles, N, where the divergence is approximately linear with time over an interval, τ. τ is taken to be the sound-transit time across this lattice. For longer time intervals the correlation function is dominated by external effects and, therefore, equation (4) cannot be used.

Whether the local rate of divergence is approximately linear with time can be determined numerically by the following method. The distance, $d(t)$, between two trajectories starting in the neighbourhood of a point, $(\boldsymbol{q}, \boldsymbol{p})$, is approximated for $0 < t < \tau$

by a function of the form $A(\boldsymbol{q}, \boldsymbol{p}, \tau) \exp(k(\boldsymbol{q}, \boldsymbol{p}, \tau)\, t)$ using the least-squares method. We also approximate the function $d(t)$ by a linear function of the form $B(\boldsymbol{q}, \boldsymbol{p}, \tau)\, t + C(\boldsymbol{q}, \boldsymbol{p}, \tau)$. In this way the rate of increase of the function $d(t)$ is compared with two possible extreme cases of rate of divergence, the linear and the exponential. If $d(t)$ is approximated better by the linear function than by the exponential; in other words, if

$$\int_0^\tau \mathrm{d}t\, |d(t) - B(\boldsymbol{q}, \boldsymbol{p}, \tau)t - C(\boldsymbol{q}, \boldsymbol{p}, \tau)|^2 < \int_0^\tau \mathrm{d}t\, |d(t) - A(\boldsymbol{q}, \boldsymbol{p}, \tau) \exp(k(\boldsymbol{q}, \boldsymbol{p}, \tau)t)|^2 \tag{4}$$

then the τ-averaged divergence is considered linear with time. This test is performed numerically for a large number, M, of points, $(\boldsymbol{q}, \boldsymbol{p})$, lying in the chaotic part of a surface of section. The ratio, M_0/M, where M_0 is the number of points out of the total, M, for which the τ-averaged rate of divergence is linear with time, gives an estimate of the measure of the part of the phase space where the local rate of divergence is linear. We expect to find $M_0 = 0$ for the lattices that satisfy Fourier's law and $M_0 \neq 0$ otherwise.

We apply this idea to the lattice examined in § 2. Figure 2 suggests that N should be larger than 300 in order to approach the 'thermodynamic limit', which means that τ should be taken to be larger than 60. Unfortunately, this computation requires very long computing time and it was beyond the capability of the facilities used. For this reason, N is reduced to 11 and τ was taken to be 10. A lattice of length $N = 11$ is the shorter size system, which we expect to retain lattice characteristics. The time length $\tau = 10$ is chosen, longer than the sound-transit time of the lattice with $N = 11$, but of the same order of magnitude with the sound-transit time for the long lattices ($N = 300$). By this choice we attempt to find results valid also for the longer lattices and, on the other hand, to avoid allowing the distance between the two trajectories to become the same size as the boundaries of the lattice phase space. We expect that the ratio M_0'/M, found this way, will be larger than the $N = 300$ result M_0/M, because the larger the number of particles in the lattice, the easier it is for the chaotic behaviour to appear. Hence, the function $M_0'(r)/M$ is an upper bound for the function $M_0(r)/M$.

The ratio M_0'/M is computed for several values of r (0.30, 0.40, 0.50, 0.65, 0.75, 0.85). The energy, E, was taken equal to $11(T_L + T_R)/2 = 605$. The M points were produced in the following way. A trajectory on this energy surface was numerically integrated for a time period long enough to produce a set of a few thousand points on a 20D surface of section. Then, $M = 150$ points were chosen randomly from this set. Figure 9 shows the results of this computation. This figure shows that the function $M_0'(r)/M$ remains almost constant for $r < 0.65$, fluctuating around the value 0.10. When r becomes larger than a critical value r_c', which is close to 0.75, $M_0'(r)/M$ starts increasing rapidly toward the value 1.00 at $r = 1.00$. It appears, therefore, that the graph of the function $M_0'(r)/M$ presents a transition that takes place at $r = r_c'$. This result correlates with the results presented in figure 2, which indicates that there may be a transition from infinite to normal thermal conductivity for a value of $r = r_c$, close to 0.75. As we explained earlier, $M_0(r)/M$ is expected to be smaller than $M_0'(r)/M$. Therefore, $M_0(r)/M$, which corresponds to $N \geqslant 300$, is expected to be similar to the broken curve of figure 9. Notice also, the broken curve of figure 9 is very similar to the graph of the function $E_2(r)/E_0$ of figure 8 for $r > 0.5$. It appears, therefore, that there is an approximate agreement between the ideas presented in this section and the numerical results presented in §§ 2 and 3. Notice that if $k(\boldsymbol{q}, \boldsymbol{p}, \tau)\, \tau \ll 1$, the test described by equation (4) has no meaning,

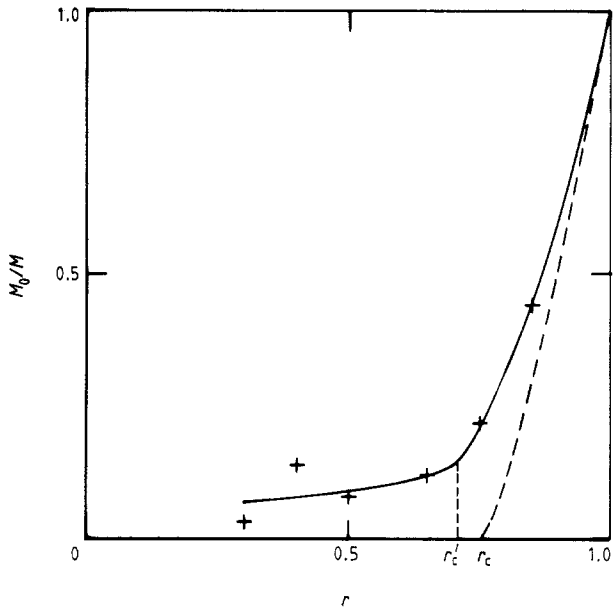

Figure 9. The measure M_0/M of the part of the chaotic region where the local rate of divergence is linear with time as a function of the mass ratio r for a diatomic Toda lattice for $N = 11$ and $t = 10$.

because an exponential with small exponent differs little from a linear function. This influences the value of the function $M_0'(r)/M$, but not the value of r_c'.

These results provide one more indication that the non-linear divergence of trajectories in the phase space, if it takes place in a finite period of time, is an essential characteristic of the dynamics that produces irreversibility. It is essential that this non-linear divergence take place in finite time, comparable to the sound-transit time of the lattice, and not at the limit $t \to \infty$. This is true for several reasons. First, it is known that there are systems with positive Lyapunov exponents that do not exhibit normal thermodynamic behaviour (e.g. the billiard model with periodic boundary conditions has an infinite diffusion coefficient in the case of 'infinite horizon', even though its K-entropy is positive). Secondly, the asymptotic ($t \to \infty$) behaviour of a finite system cannot be responsible for its non-equilibrium behaviour.

5. Thermal conductivity of a two-dimensional lattice

The failure of many numerical experiments to verify Fourier's law was sometimes attributed to the fact that these experiments were conducted on 1D lattices. It is easy to show that the restriction to 1D lattices occasionally creates unnatural situations. A well known example is the case of free hard spheres that interact with each other only by elastic collisions and are bound in a box (gas model). If this system is 1D it is integrable, while in 2D it is chaotic. Correspondingly, the energy conduction through such a system is dramatically modified by the change in dimensions. On the other hand, we should not expect that dimensionality will dramatically influence all types of systems, as it does in the case of the gas model. Thus, a harmonic lattice is integrable, independent of its dimension. This is very important because for low energies all lattices behave approximately like a harmonic lattice and, therefore, do not exhibit irreversibility. Hence, if the average temperature, T, of the lattice is considered as a parameter, a transition from infinite to normal thermal conductivity takes place as T is increased, in a manner similar

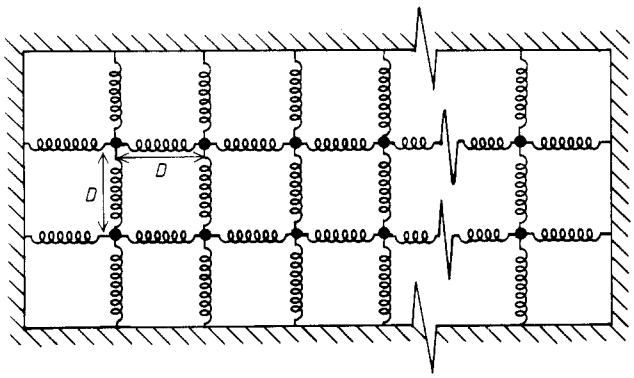

Figure 10. A 2D lattice with fixed boundary.

to that of the transition that was described for the diatomic 1D Toda lattice in § 2.

In this section, we investigate the influence of the dimensionality on the thermal conductivity for a special case. The system that is studied here is a $2 \times N$ lattice, where the particles interact only with their first neighbours by a harmonic plus quartic potential. The equilibrium distance between the particles is D. The boundary particles interact with fixed particles, which lie on outside neighbouring lattice sites (figure 10). The equations of motion for the system are therefore

$$\dot{q}_{x,ij} = p_{x,ij} \qquad \dot{q}_{y,ij} = p_{y,ij}$$

$$\begin{aligned}\dot{p}_{x,ij} = {} & -4q_{xij} + q_{x,(i+1)j} + q_{x,(i-1)j} + q_{x,i(j+1)} + q_{x,i(j-1)} \\ & + \varepsilon[(q_{x,(i+1)j} + D - q_{x,ij})^3 + (q_{x,(i+1)j} + D - q_{x,ij}) \\ & \times (q_{y,(i+1)j} + D - q_{y,ij})^2] - \varepsilon[(q_{x,ij} + D - q_{x,(i-1)j})^3 \\ & + (q_{x,ij} + D - q_{x,(i-1)j})(q_{y,ij} + D - q_{y,,(i-1)j})^2] \\ & + \varepsilon[(q_{x,i(j+1)} + D - q_{x,ij})^3 + (q_{x,i(j+1)} + D - q_{x,ij}) \\ & \times (q_{y,i(j+1)} + D - q_{y,ij})^2] - \varepsilon[(q_{x,ij} + D - q_{x,i(j-1)})^3 \\ & + (q_{x,ij} + D - q_{x,i(j-1)})(q_{y,ij} + D - q_{y,i(j-1)})^2]\end{aligned}$$

and

$$\begin{aligned}\dot{p}_{y,ij} = {} & -4q_{y,ij} + q_{y,(i+1)j} + q_{y,(i-1)j} + q_{y,i(j+1)} + q_{y,i(j-1)} \\ & + \varepsilon[(q_{y,(i+1)j} + D - q_{y,ij})^3 + (q_{y,(i+1)j} + D - q_{y,ij}) \\ & \times (q_{x,(i+1)j} + D - q_{x,ij})^2] - \varepsilon[(q_{y,ij} + D - q_{y,(i-1)j})^3 \\ & + (q_{y,ij} + D - q_{y,(i-1)j})(q_{x,ij} + D - q_{x,(i-1)j})^2] \\ & + \varepsilon[(q_{y,i(j+1)} + D - q_{y,ij})^3 + (q_{y,i(j+1)} + D - q_{y,ij}) \\ & \times (q_{x,i(j+1)} + D - q_{x,ij})^2] - \varepsilon[(q_{y,ij} + D - q_{y,i(j-1)})^3 \\ & + (q_{y,ij} + D - q_{y,i(j-1)})(q_{x,ij} + D - q_{x,i(j-1)})^2] \end{aligned} \tag{5}$$

where $j = 0, \ldots, 3$ and $i = 0, \ldots, N+1$. $q_{x,0j}$, $q_{y,0j}$, $q_{x,(N+1)j}$, $q_{y,(N+1)j}$, $q_{x,i0}$, $q_{y,i0}$, $q_{x,i3}$, and $q_{y,i3}$ are taken to be zero (fixed edges). The two ends of this lattice are coupled to two heat reservoirs with temperatures T_L and T_R, respectively. The x and y components

Table 2. The values of the coefficient of normal thermal conductivity for a 1D (K_{1D}), and a 2D (K_{2D}) lattice with harmonic plus quartic interaction, $\varepsilon = \frac{4}{3}$, $T_L = 1$, $T_R = 20$, max $\delta t = 0.70$, $D = 1.0$.

n	K_{1D}	K_{2D}
10	6.0 ± 0.3	7.1 ± 0.3
20	12.2 ± 0.5	12.1 ± 0.5
30	17.5 ± 0.8	18.0 ± 1.0
45	24.0 ± 1.0	24.0 ± 1.0
60	29.0 ± 2.0	27.0 ± 2.0
120	51.0 ± 3.0	42.0 ± 3.0
200	76.0 ± 4.0	
300	88.0 ± 4.0	

of the velocity of the two particles at each end of the lattice, at the moments when they collide with the particles of the reservoirs, are chosen from the distribution (3). The time of interaction of the end particles with the reservoirs is determined from a uniform distribution in the same way as in § 2. The total time-averaged energy flux, divided by the width of the lattice (here by 2), was calculated for several different lengths of the lattice. For these computations, $\varepsilon = \frac{4}{3}$, $T_L = 1$, $T_R = 20$, max $\delta t = 0.70$, and $D = 1$. These results are presented in table 2 and figure 11, where they are also compared with the total energy flux of a one-dimensional lattice with the same type of interaction. The equations of motion for the one-dimensional lattice are

$$\dot{q}_i = p_i \qquad \dot{p}_i = -2q_i + q_{i+1} + q_{i-1} + \varepsilon[(q_{i+1} + D - q_i)^3 - (q_i + D - q_{i-1})^3] \tag{6}$$

where $i = 0, \ldots, N+1$. q_0 and q_{N+1} are taken to be zero. The values of the parameters ε, T_L, T_R, D, and max δt for the 1D case are the same as for the 2D lattice.

The results presented in figure 11 and table 2 do not show any qualitative difference in the thermal behaviour between the 1D and the 2D lattice. For the lattice lengths examined, normal thermal conductivity was not observed in both cases. It is true that the coefficient of thermal conductivity is slightly smaller for the 2D lattice than for the 1D when the external temperature gradient is the same, but this is a slight, quantitative, difference.

We also briefly studied the dependence of the thermal conductivity of the 2D lattice on its width. For a short lattice ($N = 30$), it was found that the influence of the width is

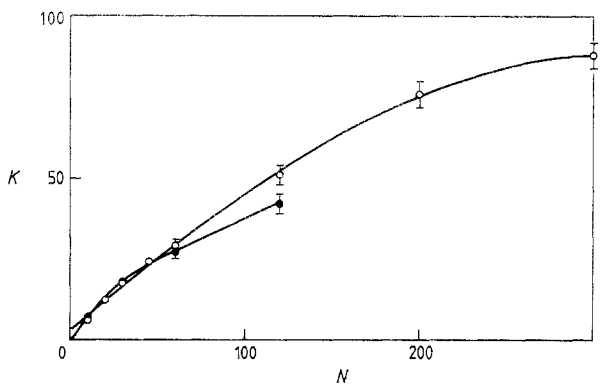

Figure 11. The coefficient of thermal conductivity as a function of the length of the lattice, N, for a 1D (open circles) and a 2D (full circles) lattice with harmonic plus quartic interaction: $\varepsilon = \frac{4}{3}$; $T_L = 1$; $T_R = 20$, max $\delta t = 0.70$; $D = 1$.

not very significant for the type of lattice we have studied. More specifically, the total time-averaged energy flux $\langle J \rangle$, divided by the width, is 10.9 for lattice which is five particles wide and 11.4 for a two-particle wide lattice. For these results, $\varepsilon = \frac{4}{3}$, $T_L = 1$, $T_R = 20$, max $\delta t = 0.70$, and $D = 1$.

Therefore, the importance of the dimensionality can vary for different types of interaction. In the example presented here, the result of the influence of the dimensionality on the thermal conductivity is quantitative, while for the hard-spheres system it is qualitative, and for the harmonic case dimensionality is not important at all. Nevertheless, we generally expect that higher dimensionality facilitates the appearance of normal thermal conductivity because it permits an easier diffusive transfer of energy through the lattice.

The results presented in this section have a direct bearing on Peierls' theory concerning the importance of Umklapp processes in lattice thermal conductivity [21]. His theory, based on the use of Boltzmann's *Stosszahlansatz*, predicts that 'Umklapp' processes are necessary for a finite coefficient of thermal conductivity in lattices. It can be easily shown that three-phonon 'Umklapp' processes, which were the basis of Peierls' theory, cannot occur in monatomic 1D lattices. However, the numerical calculations presented in § 2 show that there are 1D lattices that exhibit a regular thermal conductivity. The 'Umklapp' theory of heat conduction predicts a qualitative difference between the 1D and 2D systems, while the results presented in this section show only a small (about 20%) quantitative difference between these two dimensionalities. Similar insensitivities have been reported by Rich and co-workers [22] and Nakazawa [6] (see also the review in [10]).

'Umklapp' processes are not a realistic picture of the dynamics of lattices that exhibit irreversible behaviour. The supposed importance of this process arises from Peierls' attempt to apply Boltzmann's *Stosszahlansatz* for gases to a system of phonons. Even though this theory has great historical importance, and some gas-based intuitive appeal, it is now known that there are essential differences between the two systems. In other words, systems that exhibit approximate phonon solutions are nearly integrable systems. On the other hand, a gas model in two dimensions is a chaotic system. As a consequence, an analogy between the two systems cannot be established because near integrability can greatly influence the dynamical behaviour of a system in a finite period of time, as was also explained in § 4. It was pointed out there that for phenomena far from thermal equilibrium, like thermal conductivity, the short-time behaviour of the system is important. Hence, the description of the diffusion of energy through a lattice in terms of weakly interacting (random-phased) phonons can be misleading.

6. Conclusion

The purpose of this work was to investigate the thermal conductivity of lattices from several points of view. First, the thermal conductivity of 'long' ($N \leqslant 400$) 1D diatomic Toda lattices was studied numerically. It was shown that, for certain values of the ratio of the masses of the two types of particles in the lattice, the coefficient of thermal conductivity becomes an intensive property of the system for these lattices. These numerical results indicated a critical mass ratio, r_c, required for the transition from infinite to normal thermal conductivity in the present lattices. More research involving longer lattices is needed to determine whether r_c is actually bounded below one, or whether it tends to unity as N becomes very large.

An attempt was made to understand this transition by studying the decay of a pulse travelling through the lattice. A relationship exists between the lattice thermal conductivity and the rate of decay of pulses travelling through the lattice. Collisions between solitary pulses were found to influence their rate of decay critically. Figure 8 shows how the decay of pulses is influenced by the mass ratio.

Another attempt was made to analyse the transition from infinite to normal thermal conductivity by relating it to the local rate of divergence of trajectories in the phase space. The thermal conductivity is related to the local rate divergence of a very long lattice. To facilitate the computations, the lattices on which they were conducted were considerably shortened (11 particles long). Nevertheless, a fair quantitative agreement was found between the critical value of the mass ratio calculated this way and the one which was found from the direct computations of the thermal conductivity.

Finally, we studied the influence of both the dimensionality and the lattice length on the thermal conductivity. The thermal conductivity of a 2D lattice with harmonic plus quartic interaction was numerically calculated and it was compared to the thermal conductivity of a 1D lattice with the same type of interaction. The coefficient of thermal conductivity of the 2D lattice was found to be smaller (approximately 20%) than that of the 1D lattice, but neither case exhibits a normal thermal conductivity. These results give further evidence that Umklapp processes are not generally relevant to the study of thermal conductivity in lattices.

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