Heat conduction in one-dimensional chains

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We study numerically the thermal conductivity in several different one-dimensional chains. We show that the phonon-lattice interaction is the main ingredient of the Fourier heat law. Our argument provides a rather satisfactory explanation to all existing numerical results concerning this problem. [S1063-651X(98)10803-6]

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It is still an open and challenging problem to understand the macroscopic phenomena and their statistical properties in terms of deterministic microscopic dynamics. The crucial point is how to connect the irreversibility with the time reversible deterministic microscopic dynamics. One outstanding problem is whether or not the heat conduction in a one-dimensional (1D) chain obeys the Fourier heat law (normal thermal conductivity) and if so under what condition.

The first convincing result of the Fourier heat law in a classical system was given by Casati *et al.* [1]. They studied the so-called ding-a-ling model, which is a 1D chain consisting of the fixed equidistant hard-point particle harmonic oscillators, and in between two fixed particles there is a free particle. The particles have the same mass. The two ends of the chain are put into two thermal reservoirs. Classically, this system can be changed from integrable to fully chaotic by adjusting the system parameter. They found that the key ingredient for the normal thermal conductivity is chaos. Later on, Prosen and Robnik [2] studied the ding-dong model by three different numerical methods and verified the Fourier heat law. The ding-dong model is a modification of the ding-a-ling model. The only difference is that in the ding-dong model the fixed harmonic oscillators are allowed to collide and there is no free hard-point particles in between. Furthermore, they have studied the temperature dependence of the thermal conductivity and found that it increases monotonically with temperature.

Most recently, Lepri *et al.* [3] have studied the Fermi-Pasta-Ulam (FPU) β model. This model represents the simplest anharmonic approximation of a monoatomic solid. They have the Nosé-Hoover thermostats acting on the first and the last particle keeping constant temperature T_+ and T_-, respectively. They show that there exists a simple nontrivial scaling relation for the increasing number of particles. The thermal conductivity, however, diverges approximately as $N^{1/2}$. N is the number of particles. They claimed that chaos is not sufficient to ensure the Fourier heat law.

In this paper, we shall investigate the mechanism leading to the Fourier heat law. In other words, we would like to answer the following question: under what condition does the heat conduction of a 1D many-body Hamiltonian system have the Fourier heat law. To this end, we shall consider different models, such as the Frenkel-Kontorova (FK) model and the harmonic dissipative model for example. We will show that by invoking a simple mechanism we can obtain a rather satisfactory explanation to all existing numerical results, qualitatively and quantitatively. The possible connection with the experimental results is also discussed.

Normal thermal conductivity. — Both the ding-a-ling and the ding-dong model are more or less artificial models. We would like to turn to a more realistic model, which is close to a true physical system, i.e., the Frenkel-Kontoroval model. It describes a particle (atom) chain connected by harmonic springs subject to an external sinusoidal potential. It has been widely used to model crystal dislocation, charged density wave, magnetic spirals, absorbed epitaxial monolayers, etc. in condensed matter physics [4]. This model displays very rich interesting phenomena. However, we shall not discuss in detail all of these properties in this paper; for more details please see Refs. [4,5]. Our attentions in this paper are focused on thermal conductivity.

The existence of the thermal conductivity of this model has been proved by Gillan and Holloway by using different numerical techniques [6]. The classical Hamiltonian of the standard FK model is

$$\mathcal{H}=\sum_i \frac{P_i^2}{2m}+\frac{\gamma}{2}(X_i-X_{i-1}-a)^2-\frac{A}{(2\pi)^2}\cos\frac{2\pi X_i}{b}. \quad (1)$$

For convenience of numerical calculations, we shall scale this Hamiltonian into a dimensionless one,

$$H=\sum_i \frac{p_i^2}{2}+\frac{1}{2}(x_i-x_{i-1}-\mu)^2-\frac{K}{(2\pi)^2}\cos 2\pi x_i. \quad (2)$$

By doing this, we have obtained a new effective dimensionless temperature T. The real temperature T_r is related to T through the following relation:

$$T_r=\frac{m\omega_0^2 b^2}{k_B}T, \quad (3)$$

where m is the mass of the particle, γ the elastic constant, and b the period of external potential, which is unitary after scaling. a is the equilibrium distance of the particle; it is $\mu=a/b$ after scaling. $K=A/\gamma b^2$ is a rescaled strength of the external potential. $\omega_0^2=\gamma/m$ is the oscillator frequency. k_B is the Boltzmann constant. In this paper, the winding number in the FK model is kept at 1/3.

It is helpful to establish the above relationship (3). It can give us very useful information about the corresponding true temperature to that one we used and enable us to gain some physical insights. For instance, for the typical values of atoms,

$$b\sim 10^{-10}\ \text{m}, \quad \omega_0\sim 10^{13}\ \text{sec}^{-1},$$

$$m\sim 10^{-26}-10^{-27}\ \text{kg}, \quad k_B=1.38\times 10^{-23}\ \text{J K}^{-1},$$

we have $T_r\sim(10^2-10^3)T$, which means that the room temperature corresponds to the dimensionless temperature T about the order of $0.1-1$. So, if T is very high such as to 10^2, then the actural temperature is about 10^4-10^5 K, at this temperature the displacment of the particle from its equilibrium can be up to the order of 10, which we think is unrealistic for physical systems. Therefore, like Casati *et al.* [1], we always keep T at very small values in our numerical simulations.

The Hamiltonian (2) is a very special case. In fact, we can write it into a general form,

$$H=\sum_i H_i, \quad H_i=\frac{p_i^2}{2}+V(x_{i-1},x_i)+U(x_i). \tag{4}$$

Here $V(x_{i-1},x_i)$ stands for the interaction potential of the nearest-neighbor particles; $U(x_i)$ is a periodic external potential, which is an analog of the lattice, and as we shall see later that it plays a crucial role in determining the behavior of the thermal conductivity. If $U(x_i)$ vanishes and $V(x_{i-1},x_i)$ takes the anharmornic form, Eq. (4) is then the FPU β model, which has been discussed by Lepri *et al.* [3]. Therefore, a variety of 1D models can be put into the framwork of Eq. (4). By changing the form $V(x_{i-1},x_i)$ and $U(x_i)$, we will obtain different thermal conductive behaviors.

To study the heat conduction in 1D model, we choose the same approach as that used by Lepri *et al.* [3], namely, two Nosé-Hoover thermostats [7] are put on the first and last particle, keeping the temperature at T_+ and T_-, respectively. The equations of motion of these two particles are determined by

$$\begin{aligned}
\ddot{x}_1&=-\zeta_+\dot{x}_1+f_1-f_2,\\
\ddot{x}_N&=-\zeta_-\dot{x}_N+f_N-f_{N+1},\\
\dot{\zeta}_+&=\dot{x}_1^2/T_+-1, \quad \dot{\zeta}_-=\dot{x}_N^2/T_--1.
\end{aligned} \tag{5}$$

The equation of motion for the central particles is

$$\ddot{x}_i=f_i-f_{i+1}, \quad i=2,\ldots,N-1, \tag{6}$$

where $f_i=-V'(x_{i-1}-x_i)-U'(x_i)$ is the force acting on the particle. $x_0=0$ and $x_{N+1}=0$.

We have carried out extensive numerical simulations with a large range of parameters of N, $T_\pm$, and K for a variety forms of $V(x_{i-1},i)$ and $U(x_i)$. We used the seventh-order and eighth-order Runge-Kutta algorithm, which provides very stable and more accurate results than those of the usual fifth-order Runge-Kutta method. The spatial temperature profile for the standard FK model is shown in Fig. 1. It is clear that although our FK model has an additional external potential, if its strength K is sufficiently large (compared with the temperature), we can obtain the same scaling relation as that obtained by Lepri *et al.*. This scaling indicates that the temperature gradient scales as N^{-1}. We have confirmed that this scaling relation is also true for many different modified FK models. For example, we have changed $V(x_{i-1},x_i)$ to the anharmonic case as discussed by Lepri *et al.* or changed the external potential $U(x_i)$ to one with a higher harmonic term, such as

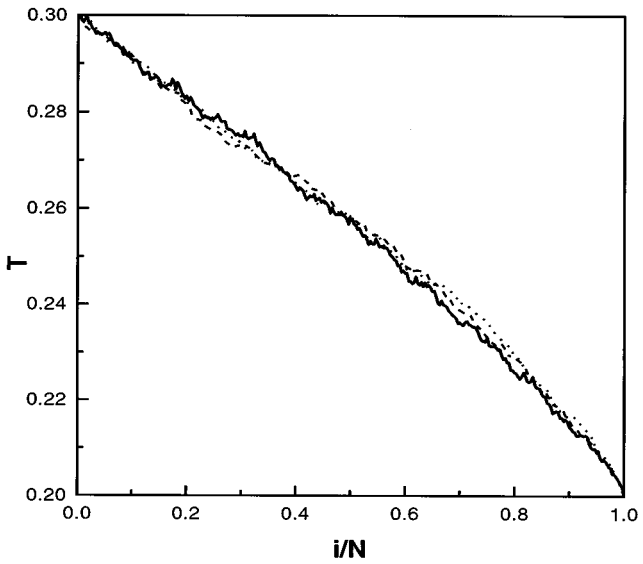

FIG. 1. Temperature profile for the FK model (2) with parameter $K=5$. $T_+=0.3$, $T_-=0.2$. The average is taken over the 10^6 interval after the transient time 10^4. The particle numbers are 300 (solid line), 200 (dashed line), and 100 (dotted line), respectively.

$$U(x_i)=-\frac{K_1}{(2\pi)^2}\cos(2\pi x_i)-\frac{K_2}{(4\pi)^2}\cos(4\pi x_i). \tag{7}$$

The derivation of the heat flux of the ith particle differs slightly from that of Lepri *et al.*. The local heat flux $J(x,t)$ is defined by the continuity equation. Taking the volume integration on both sides of this equation, we can obtain

$$J_i-J_{i-1}=\dot{x}_i\frac{\partial V}{\partial x_i}(x_i,x_{i+1})-\dot{x}_{i-1}\frac{\partial V}{\partial x_{i-1}}(x_{i-1},x_i). \tag{8}$$

Thus the heat flux is defined by

$$J_i=\dot{x}_i\frac{\partial V}{\partial x_i}(x_i,x_{i+1}). \tag{9}$$

Numerically, the time average $J=\langle J_i(t)\rangle$ is independent of the index i for long enough time.

The N dependence of JN is plotted in Fig. 2 for different models. As is easily seen for different FK models [with different $V(x_{i-1},x_i)$ and/or different $U(x_i)$], as long as $U(x_i)$ is nonzero and at sufficiently lower temperature, JN is a constant, implying that $1/J$ diverges with N. Since the temperature gradient vanishes as N^{-1} as shown in Fig. 1, the Fourier heat law is justified.

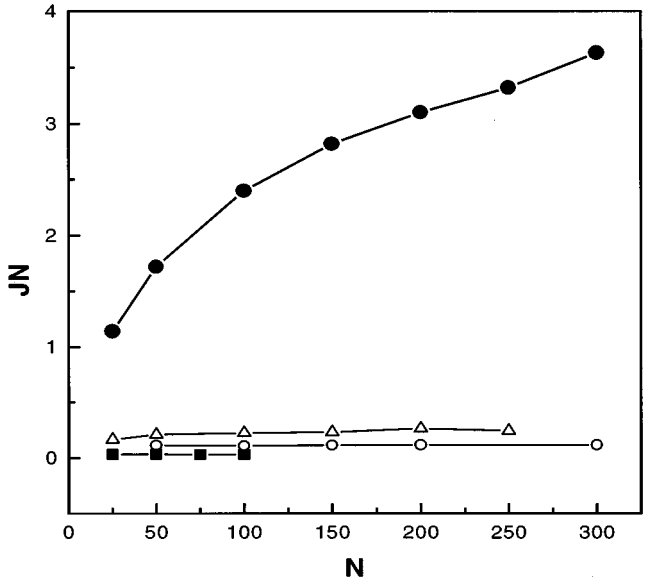

FIG. 2. JN vs the number of particles N for different models. $T_+=0.3$ and $T_-=0.2$ for all cases. The solid circle represents the results of the FPU β model ($\beta=0.5$). The open circle is the result of the FK model given by Eq. (2) with $K=5$; the solid square is for the FK model with an external potential (7), with $K_1=5$ and $K_2=15$; and the open triangle is for the FK model with $V=x^2/2+\beta x^4/4$, $U=-K\cos(2\pi x)/(2\pi)^2$, $\beta=0.9$, $K=5$. The lines are drawn to guide the eyes.

Abnormal thermal conductivity. Things become very different if $U(x_i)$ vanishes. In this case, the heat conduction does not obey the Fourier heat law neither for the harmonic form $V(x_{i-1},x_i)$ nor for the anharmonic form such as the FPU β model discussed by Lepri *et al.* Our results for the FPU β model at very low temperature shown in Fig. 3 also demonstrate that JN diverges as approximately $N^{1/2}$, which means that the thermal conductivity diverges as $N^{1/2}$. This agrees with that of Lepri *et al.* at much higher temperature.

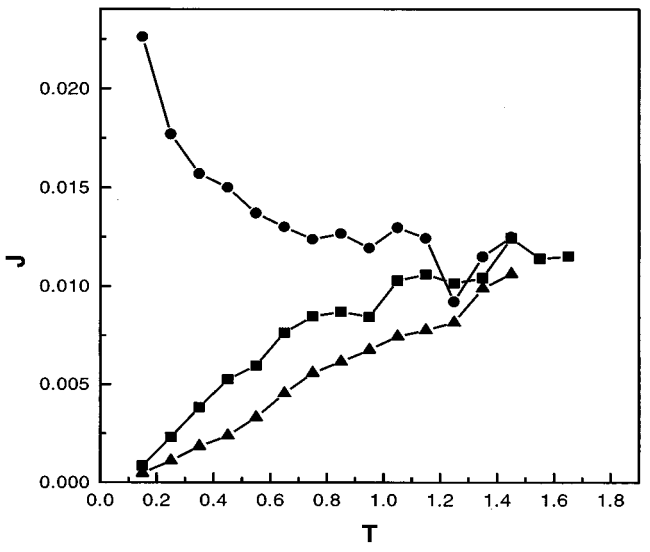

FIG. 3. The temperature dependence of heat flux J for the FPU β model ($\beta=0.9$, solid circle), the standard FK model Eq. (2) ($K=5$, solid triangle), and the FK models with an anharmonic interparticle potential $V(x)=x^2/2+\beta x^4/4$ and external potential $K\cos(2\pi x)/(2\pi)^2$ at $\beta=0.9$, $K=5$ (solid square). The line is drawn to guide the eyes.

Based on the above results, we are convinced that the key point of the normal thermal conductivity is the *periodic* external potential, which is analogous to the lattice.

If the lattice is absent, and the interparticle potential is harmonic, then no phonon-phonon interaction exists; thus the heat transfer would take place at the speed of sound and the thermal conductivity would be infinite, as pointed out by Debye in 1914. (However, if we add a dissipative term to the harmonic oscillator chain, then we could obtain the Fourier heat law, even though we do not have a lattice. This is because with dissipation the heat radiates during the transport. Our numerical results have verified this. But we will discuss this in more detail in another paper [8].)

In the case of an anharmonic interparticle potential $V(x_{i-1},x_i)$ such as that in the FPU model, the phonon-phonon interaction is produced due to the anharmonicity. Although the temperature gradient can be formed, nevertheless, as is shown by the work of Lepri *et al.* at high temperature as well as ours at low temperature, the thermal conductivity diverges.

As long as the lattice exists, the phonons will be scattered by it and this results in thermal resistance, eventually leading to the Fourier heat law. In the ding-a-ling model and the ding-dong model the fixed harmonic oscillator plays the role of the lattice, whereas in the FK model it is the periodic external potential. In these three cases the Fourier heat law is justified numerically. Thus we believe that it might be a general rule that if the phonon-lattice interaction is dominant, the heat conduction will obey the Fourier heat law, no matter whether the interparticle interaction is harmonic or anharmonic.

Temperature dependence of J. As discussed above, the crucial point of the Fourier heat law is the phonon-lattice interaction. The mean free path of the phonons is determined by the density of the lattice and does not change with the temperature. By increasing the temperature, more and more high energy phonons are excited, which results in the growth of the heat flux, and thus the increment of the thermal conductivity. Whereas in the absence of the lattice, increasing temperature will produce more phonons, which in turn reduces the phonons' mean free path, consequently decreasing the heat flux. Therefore, the temperature dependence behavior for normal and abnormal thermal conductivity should be very different. Our numerical calculations exactly demonstrate this point.

In Fig. 3, we plot the temperature dependence of heat flux for different models. The particle number is kept at $N=100$, and in all cases the temperature difference is fixed at $\Delta T=T_+-T_-=0.1$, thus J has the same behavior as the thermal conductivity κ. For the FPU β model ($\beta=0.9$, solid circle), the heat flux decreases monotonically with temperature, whereas in the standard FK model ($K=5$, solid triangle) it increases with temperature.

Another very important thing worth noting is the case in which the anharmonicity and the external potential coexist. It seems that this case is closer to the real physical system than others. We have performed the numerical simulation by using $V=x^2/2+\beta x^4/4$ and $U=-K\cos(2\pi x)/(2\pi)^2$ in Eq. (4).

The temperature dependence of J is shown in Fig. 3 (solid square). The heat flow is affected not only by the phonon-lattice interaction, but also by the phonon-phonon interaction. In the low-temperature region, the factor determining the heat conduction is the phonon-lattice interaction, therefore, the heat conduction obeys the Fourier heat law, but the heat flux is bigger than in the standard FK model (solid triangle) due to the anharmoncity, which produces more phonons to transfer heat. The anharmonicity becomes more and more important when the temperature is increased; this is why in the higher-temperature region a relative flat region shows up in Fig. 3. Furthermore, it must be noted that our numerical results show that for the FK model shown in Fig. 3 the Fourier heat law is valid only at the lower-temperature region $T<1$, at higher temperature the Fourier heat law broke down for the reason mentioned above.

From many experimental results (see, e.g., Srivastava [9] or other textbooks of solid state physics, such as that of Kittel [10]), we observe that the thermal conductivity increases with temperature in the lower-temperature region, whereas it decreases at high temperature. This can be understood well from the mechanism discussed in this paper.

In summary, by studying the dynamical equations of the 1D particle chain, we came to understand more about the heat conduction mechanism. Our numerical results as well as others up to date confirm our conjecture that the phonon-lattice interaction is the key factor in the Fourier heat law. Only the phonon-phonon interaction cannot give rise to the Fourier heat law; instead we will have the abnormal thermal conductivity, i.e., the thermal conductivity diverges as the particle's number. In the former case, the thermal conductivity grows with the temperature monotonically, whereas in the latter case it decreases.

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