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.

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

The first convincing result of the Fourier heat law in a classical system was given by Casati et al. They studied the so-called ding-a-ling model, which is a 1-D chain consists of the fixed equidistant hard-point particle harmonic oscillators, and inbetween 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 have 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 inbetween. Furthermore, they have studied the temperature dependence of the thermal conductivity and found that it increases monotonically with the temperature.

Most recently, Lepri et al. have studied the Fermi-Pasta-Ulam (FPU) $\beta$ model. This model represents the simplest anharmonic approximation of a monoatomic solid. They put the Nosé-Hoover thermostats act on the first and the last particle keeping constant temperature $T_+$ and $T_-$, respectively. They shown 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 question: under what condition the heat conduction of a 1-D many-body Hamiltonian system having the Fourier heat law. To this end, we shall consider different models, such as the Frenkel Kontorova (FK) model and the harmonic dissipative model etc. 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. — Either the ding-a-ling or the ding-dong model is more or less an artificial model. We would like to turn to a more realistic model, which is close to true physical system, i.e. the Frenkel Kontorova 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 and absorbed epitaxial monolayers etc. in condensed matter physics. This model displays very rich interesting phenomena. However, we shall not discuss in detail all this properties in this paper, for more details please see Refs. Our attentions are focused on the thermal conductivity in this paper.

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

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

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

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

By doing this, we have a new effective dimensionless temperature $T_r$. The real temperature $T_r$ is related to $T$ through the following relation,
\[ T_r = \frac{m\omega_0^2b^2}{k_B}T \]  

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

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

\[ b \sim 10^{-10} \text{cm}, \quad m \sim 10^{-26} - 10^{-27} \text{kg}, \quad k_B = 1.38 \times 10^{-23} \text{JK}^{-1}, \]

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 \( 10^9 \), then the actual temperature is about \( 10^9 \) degree, at this temperature the displacement 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 \([3]\) is a very special case. In fact, we can write it into a general form,

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

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 anharmonic form, Eq. \([4]\) is then FPU \( \beta \) model which has been discussed by Lepri et al \([3]\). Therefore, a variety of 1-D models can be put into the framework 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 1-D model, we choose the same approach as that used by Lepri et al \([3]\), namely, two Nosé-Hoover thermostats \([3]\) 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,

\[ \ddot{x}_1 = -\zeta_+ \dot{x}_1 + f_1 - f_2, \]
\[ \ddot{x}_N = -\zeta_- \dot{x}_N + f_N - f_{N+1}, \]
\[ \zeta_+ = \frac{\omega_0^2}{T_+} - 1, \quad \zeta_- = \frac{\omega_0^2}{T_-} - 1. \]  

The equation of motion for the central particles is,

\[ \ddot{x}_i = f_i - f_{i+1}, \quad i = 2, \ldots, N-1, \]

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

![FIG. 1. Temperature profile for the FK model \([3]\) with parameter \( K = 5 \), \( T_+ = 0.3 \), \( T_- = 0.2 \). The average is taken over \( 10^6 \) interval after the transient time \( 10^5 \). The particle numbers are 300 (solid line), 200 (dashed line) and 100 (dotted line), respectively.](image)

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 us much stable and more accurate results than that from the usual fifth-order Runge-Kutta method. The spatial temperature profile for 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 sufficient large (compared with the temperature), we can obtain the same scaling relation as that obtained by Lepri et al \([3]\). 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 \([3]\), or changed the external potential \( U(x_i) \) to that one with higher harmonic term, such as,

\[ U(x_i) = -\frac{K_1}{(2\pi)^2} \cos(2\pi x_i) - \frac{K_2}{(4\pi)^2} \cos(4\pi x_i). \]  

The derivation of the heat flux of the \( i \)th particle differs slightly from that of Lepri et al \([3]\). The local heat flux \( J(x, t) \), which is defined by the continuity equation. Taking the volume integration on both sides of this equation, we can obtain
\[ J_i - J_{i-1} = \dot{x}_i \frac{\partial V}{\partial x_i}(x_i, x_{i+1}) - \dot{x}_{i-1} \frac{\partial V}{\partial x_{i-1}}(x_{i-1}, x_i). \]  
(8)

Thus the heat flux is defined by

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

Numerically, the time average \( J \) is independent of the index \( i \) for long enough time.

The \( N \) dependence of \( J \times N \) is plotted in Fig. 2 for different models. As is easily seen that 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 non-zero and at sufficient lower temperature, \( J \times N \) is a constant implying \( 1/J \) diverges with \( N \). Since the temperature gradient vanishes as \( N^{-1} \) as is shown in Fig. 1, thus the Fourier heat law is justified.

**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 \( \beta \) model discussed by Lepri et al. Our results for FPU \( \beta \) model at very low temperature shown in Fig. 3 also demonstrate that \( J \times N \) 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.

Based on the above results, we are convinced to conclude 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 finite as was 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 have no lattice. This is because the dissipation, the heat radiates during the transport. Our numerical results have verified this. But we will discuss this more in detail in another paper [3].)

In the case of having 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 results in the thermal resistance, eventually leads to the Fourier heat law. In the ding-a-ling model and the ding-dong models 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 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, thus the increment of the thermal conductivity. Whereas in the absence of lattice, increase temperature will produce more phonons, which in turn reduce the phonons’ mean free path, consequently decreases the heat flux. Therefore, the temperature dependence behaviour of 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 of the thermal conductivity \( \kappa \). For the FPU \( \beta \) model (\( \beta = 0.9 \), solid circle), the heat flux decreases monotonically with temperature, whereas in the standard FK model with \( (K = 5 \), solid triangle) increases with temperature.
Another very important thing deserves noting is the case in which the anharmonicity and the external potential coexists. 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. At 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 that case of the standard FK model (solid triangle) due to the anharmonicity which produces more phonons to transfer heat. The anharmonicity becomes more and more important when the temperature is increased, this is why at higher temperature region, a relative flat region shows up in Fig. 3. Furthermore, it must be noted that our numerical results shown that for FK model shown in Fig. 3 the Fourier heat law is valid only at lower temperature region \( T < 1 \), at higher temperature the Fourier heat law broken down due to the reason mentioned before.

\[
V = x^2/2 + \beta x^4/4 \quad \text{and} \quad U = -K \cos(2\pi x)/(2\pi)^2
\]

![Fig. 3](image-url)

**FIG. 3.** The temperature dependence of heat flux \( J \) for the FPU \( \beta \) model (\( \beta = 0.9 \), solid circle), the standard FK model Eq. (4) (\( K=5 \), 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 draw just for guiding the eyes.

From many experimental results (see e.g. the book of Srivastava [9] or other textbooks of solid state physics, such as that of Kittel [10]), we observe that the thermal conductivity increases with temperature at 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 1-D particle chain, we understood 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 for 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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