The origin of normal heat conduction in one-dimensional classics system

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We propose a new one-dimensional lattice model with strong asymmetric interaction potential and investigate heat conduction in this model numerically. We find that Fourier law is obeyed. Based on the phonon theory, we find a new scattering mechanism of phonon because of the breaking of the lattice segment. It is shown that in most of scattering process in this model momentum is destroyed as well as the Umklapp phonon-phonon scattering process which leads to the normal heat conduction. At last, we extend our analysis to the same class model with asymmetry interaction potential and get a general conclusion.

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The heat conduction in one-dimensional classic system is a long debated problem in statistical physics. Although Peierls’s theory [1] shows that the Umklapp phonon scattering process can lead to the normal heat conduction in lattice system, but it is not definitely clear in one-dimensional system what is the sufficient and necessary condition for the valid of Fourier law. This problem has been attracting much attention in these two decades [2]. It is previously believed that the break of momentum conservation may be the reason for the normal heat conduction. The numerical studies [3-5] showed that in one-dimensional system subjected to on-site potential heat conductivity is independent on system size, which indicates the valid of Fourier law. The momentum is not conserved in these models because of external potential. However, such external potential is not nature in real material, just in some treatment of many-body system the mean field theory can produce this potential. On the other hand, it has been suggested analytically that the conservation of momentum is the key for the anomalous conductivity in low dimension [6]. One can consider one-dimensional model with the mentum conservation without external potential such as Fermi-Pasta-Ulam (FPU) model. The interaction between phonons will arise because of nonlinear term in interaction between particles and it was expected there should be a finite heat conductivity. However, the numerical results showed that the heat conductivity \( \kappa \) is size-dependent [7] and divergent versus the system size as \( \kappa \sim L^\alpha \), which was also confirmed by the mode-coupling theory [8], kinetic theory [9] and fluid hydrodynamic theory [10]. The studies on one-dimensional hard-point model also showed the divergent of heat conductivity and it is believed that in this momentum conserved model heat conduction is anomalous and \( \alpha \) is common universal of this kind of model [11, 12]. However, there are few results which are not in agreement with this belief. One-dimensional rotor model was showed to have a finite heat conductivity [13, 14]. Recently, one-dimensional lattice system with asymmetric interaction potential was studied numerically and found to have a finite heat conductivity [12].

In this paper, our goal is to find the origin of normal heat conduction in one-dimensional system without introducing a external potential, We investigate the heat conduction in a new proposed one-dimensional lattice model using molecule simulation and find Fourier law is obeyed. Using the phonon theory, we find a new scattering process which does not occurs in one-dimensional lattice with symmetric interaction. It will destroy the momentum conservation of phonon and leads to the normal heat conduction.

We consider a new one-dimensional lattice system with Hamiltonian

\[
H = \sum_n \frac{p_i^2}{2} + V(x_i - x_{i-1} - a)
\]

where \( x_i \) and \( p_i \) are the position and momentum of \( i \)th particle respectively and \( V \) is the interaction potential energy. \( a \) is the lattice constant which is the equilibrium distance between pairs particles. We take a special form of the interaction potential. We assume the interaction between pairs particles is still spring like. However, when the distance between neighbor particles is smaller than the lattice constant, there is interaction between them. If the distance is larger than lattice constant, the interaction vanish. Hence, this interaction potential is

\[
V(x) = \begin{cases} 
\frac{1}{2}x^2, & x < 0 \\
0, & x \geq 0
\end{cases}
\]

In Fig.1, we give a schematic picture of the interaction potential. We can find this model has not only the properties of lattice, but also of the gas model.

To investigate the heat conduction using the computer simulation, the model should be connected with heat bath. We adapt Noose-Hoover [16] heat bath on the ends of the present model. By setting the temperature difference, we can calculate the heat current in this model after the thermal steady state is approached.

We find that in this model temperature gradient can be well formed along the chain if the simulation time is sufficiently large.
FIG. 1: The schematic of the interaction potential energy.

long enough, which indicates the local thermal equilibrium state can be reached. In Fig. 2, we plot the heat conductivity $\kappa$ as the function of the system size $L$, we note that when the system size is small, the heat conductivity is divergent. However, when the system size is larger than 2000, $\kappa$ become divergent slowly and comes into a saturate value which mean we can expect a normal heat conduction. This result shows that even in a momentum conservation one-dimensional system, a finite heat conduction can be found.

Comparing the interaction potential used here with the interaction potential used in ref. [15], we can see although they have different form, but they both have asymmetric properties. And, the asymmetry in our model is much stronger than others and heat conductivity in our model is easy to converge. So a question arises, is the asymmetry of interaction lead to normal heat conduction? If so, what is the underlying mechanism. In the following, we will investigate these problems.

First we consider one-dimensional harmonic chain of particle each of them has mass $m$ and is coupled each other by the interaction $V(x) = \frac{\omega_0^2}{2} x^2$. With the period boundary condition a set of normal mode coordinates are given by

$$Q_k = \frac{1}{\sqrt{N}} \sum_{l=1}^{N} x_l \exp(i k l),$$
$$P_k = \frac{1}{\sqrt{N}} \sum_{l=1}^{N} p_l \exp(i k l),$$

where $k$ is the wave vector and given by $k = \frac{2\pi j}{N}$ and $j$ is a integer chosen so that $k$ is in the Brillouin zone ($-\pi, \pi$). In quantum mechanic, one can use the annihilation and creation operators $a_k$ and $a_k^\dagger$, and $a_k$ is defined as

$$a_k = \sqrt{\frac{m \Omega_k}{2\hbar}} (Q_k + \frac{i P_k}{m \Omega_k}),$$

where $\Omega_k$ are the normal mode frequencies given by

$$\Omega_k = 2 \omega_0 | \sin \frac{k}{2} | = \omega_o |\omega_k|,$$

the Hamiltonian is diagonalized as

$$H = \sum_k \omega_k \left( \frac{1}{2} + a_k^\dagger a_k \right).$$

The quantum of vibrational energy is called a phonon. In the Peierls theory of solid, the heat conduction is carried by phonons, if there is no scattering between phonons, the mean free path will become infinite and temperature gradient can’t formed. By introducing the nonlinear interaction between particles, it is shown that there exists collisions between phonons. If the momentum of phonons is conserved during the collision, this process is called normal process and if the momentum is not conserved it is called Umklapp process. Only the later will contribute to the normal heat conduction because in which the heat resistance can be formed. In the previous works on this subject, the main aim was to find a scattering mechanism to cause normal heat conduction. The external potential is believed to be a key to answer this question. In real space the momentum conservation is destroyed by the external potential, so it is suggested that it is true for phonon.

Let’s consider our model which has the features of both the lattice model and gas model. We can not apply phonon theory to it directly because pair particles have no interaction if the distance between them is larger than

FIG. 2: The heat conductivity $\kappa$ as the function the system size. The temperature at two heat bath are $T_+ = 0.3$ and $T_- = 0.2$ respectively.


\[ k_1 = \frac{2\pi}{L_1} j_1, \]

where \( j \) is an integer and takes the values from 1 to \( N_1 - 1 \).

In the subsequent evolution of model, it is expected that at certain time, there will be a breaking in this segment that one particle will move far away one of its neighbor and their distance is larger than \( a \). As a result, the original segment now splits into two segments as shown in Fig.3. Assuming the number of particles in these two segment are \( N_2 \) and \( N_3 \) and the lengths of them are \( L_2 \) and \( L_3 \) respectively. Hence, the wave vectors of phonons in these two new lattice segments are

\[ k_2 = \frac{2\pi}{L_2} j_2, \]
\[ k_3 = \frac{2\pi}{L_3} j_3, \]

where \( j_2 \) and \( j_3 \) are also positive integers and their maximal values are \( N_2 - 1 \) and \( N_3 - 1 \). As \( L_1 = L_2 + L_3 \), it is easy to see

\[ k_2 > k_1, k_3 > k_1. \]

After the breaking of segment phonons are changed. That is to say that the breaking of segment is a mechanism that causes the change, namely scattering, of phonon. Let's consider the one in original segment with the wave vector \( k'_1 = 2\pi/L_1 \) and its quasi-momenta is \( \hbar k'_1 \). In the breaking of segment, it will split into many phonons. The wave vectors of new generated phonons take the values in equation (8). Consider a simple three phonons process that one phonon splits into two phonons, we denote their momenta as \( \hbar k''_2 \) and \( \hbar k'''_3 \), it is easy to find that the momentum is not conserved that

\[ \hbar k'_1 \neq \hbar k''_2 + \hbar k'''_3, \]

due to the equation (9). \( k''_2 \) and \( k'''_3 \) are larger than \( k'_1 \). To make the equivalent of both sides of above equation, one should add another momenta into left side. We denote its wave vector by \( G \) and get a equation as following

\[ \hbar k'_1 + \hbar G = \hbar k''_2 + \hbar k'''_3. \]

This is a Umklapp process. In fact, in the breaking of segment, the phonon \( k'_1 \) should split into many new phonons in two new segments. The wave vector of each new phonon is larger than the old one. So, it is also showed that such multi-phonon process should satisfy equation as

\[ \hbar k'_1 + \hbar G = \sum_{i=1}^{m_1} \hbar k''_i + \sum_{j=1}^{m_2} \hbar k'''_j, \]

where \( m_1 \) and \( m_2 \) are the numbers of phonons involved in this process in the two new segments. \( G \) is an additional term to fulfill the equality of equation. This process is also a kind of Umklapp process. For other phonons in initial segment, it can also be showed in this way that in most scattering processes the momentum conservation are destroyed, although for the phonons with larger wave vector in segment before breaking, there will be few processes that satisfies momentum conservation. On the other hand, as is well known, only the phonon with low wave vector contribute to the heat conduction. In term of our illustration, the scattering processes of phonons with small wave vectors are almost Umklapp process. Hence, we can conclude that the breaking of lattice segment in this model is a scattering mechanism of phonons which destroys the momentum conservation. As a result we can expect the normal heat conduction in this model confirmed by the numerical result in Fig.2.

As our model has the asymmetric interaction which cause the breaking in the evolution of model, next, we extend our analysis to the models with other asymmetric interaction, such as Lennard-Jones potential written as

\[ V(r) = \varepsilon \left[ \left( \frac{r_m}{r} \right)^{12} - 2 \left( \frac{r_m}{r} \right)^6 \right], \]

where \( r \) is the distance between pairs particles. For one-dimensional lattice, \( r = x_i - x_{i-1} \). \( r_m \) is the distance at which potential has the minimum. \( \varepsilon \) is the depth of potential well. As well known, Lennard-Jones potential is
asymmetric around the minimum. To show the asymmetric more clearly, we calculate the differential of potential around the the minimum of potential and define a rate as

\[ \gamma = \frac{dV(r)}{dr} \bigg|_{r = r_m + \Delta r} - \frac{dV(r)}{dr} \bigg|_{r = r_m - \Delta r} \]  (14)

where \( \Delta r \) is the relative displacement of particle from its equilibrium position. Some results are illustrated in Fig.4, we can find that for fixed parameters of potential the differential of potential at the same displacement on the two sides of minimum become more different when the displacement \( \Delta r \) becomes large, which shows the asymmetric of interaction potential. And, we find that \( r_m \) determines the degree of asymmetry of potential. When \( r_m \) becomes small, the differential of potential, namely, the force acted on pairs particles becomes much smaller when the two particles leave apart than the case when two particles move close to each other.

To use phonon theory, the general treatment of nonlinear potential is to approximate it by expanding it around the minimum and just take the second order term as the first order term is zero. However, as the expansion coefficient of second term, \( dV/dr \) is taken at the minimum no matter what sigh of \( \Delta r \). Hence, the asymmetry is lost in the approximation.

To involve the asymmetry in the linear approximation, we expand the potential along the trajectory. We can get the function of linear term. For simplicity, we use the average linear term function. And the form of it on the left side and right side of minimum denoted by \( k_l \) and \( k_r \) are defined as following

\[ k_l = \frac{1}{r_m - r_l} \int_{r_l}^{r_m} \frac{dV(r)}{dr} \, dr = \frac{V(r_m) - V(r_l)}{r_m - r_l} \]
\[ k_r = \frac{1}{r_r - r_m} \int_{r_m}^{r_r} \frac{dV(r)}{dr} \, dr = \frac{V(r_r) - V(r_m)}{r_r - r_m} \]  (15)

Considering the case \( r_m - r_l = r_r - r_m \), it is easy to conclude from Fig.4 that \( k_l \) is larger than \( k_r \), showing the asymmetry. Thus, we can consider the evolution of this model in linear approximation. The coupling constant between pairs particles are dependent on distance, taking value \( k_l \) or \( k_r \). In other words, it is time-dependent. In the evolution, with the change of distance of pairs particles, there will be a crossover at which the coupling constant will switch between \( k_l \) and \( k_r \), then the phonon spectrum will change. It is a scattering mechanic of phonons. Consider the small \( r_m \), it can be expected that \( k_l \gg k_r \), we can ignore \( k_r \) and only \( k_l \) exists, then the model with Lennard-Jones potential is reduced to our model. Hence our finding of the scatting of phonon can be applied to such model and the same conclusion is obtained.

In conclusion, we found normal heat conduction in our one-dimensional lattice model with asymmetric interaction, that provides another example which obey Fourier law with momentum conserved. It is to say that the momentum conservation is not the necessary condition for normal heat conduction. Furthermore, we found in our model, due to the asymmetric interaction potential, there is a scattering mechanism caused by the breaking of the segment, which leads to the normal heat conduction. That is to say the phonon spectrum is time-dependent. We can apply our analysis to other model with asymmetric interaction. As is well known, the asymmetric interaction potential is the reason for the expansion of solid density [17]. Our finding indicates that it can account for the normal heat conduction.

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