Finite Heat conduction in 2D Lattices

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This paper gives a 2D harmonic lattices model with missing bond defects, when the capacity ratio of defects is enough large, the temperature gradient can be formed and the finite heat conduction is found in the model. The defects in the 2D harmonic lattices impede the energy carriers free propagation, by another words, the mean free paths of the energy carrier are relatively short. The microscopic dynamics leads to the finite conduction in the model.

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The study of heat conduction in models of insulating solids is a rather old and debated problem, and the more general problem is one of understanding the nonequilibrium energy current carrying state of a many body system. The most of the work on heat conduction investigated the process of heat transport in 1D lattices. The different models have been studied for obtaining Fourier’s law, several kinds of factors have been taken into account in the models, such as the nonlinearity, on-site potentials, mass disorder and etc. Then the typical 1D lattices Hamiltonian is

\[ H = \sum_{i=1}^{N} \left[ \frac{p_{i}^2}{2m_i} + V(q_{i+1} - q_i) + U(q_i) \right], \]

where \( m_i \) represents the mass of the \( i \)th particle, \( V \) is the potential energy of internal forces, and \( U \) is an on-site potential. Based on these studies, several sufficient or necessary conditions of the normal thermal conductivity in a 1D lattices are suggested, such as “nonintegrability is not sufficient to guarantee the normal thermal conductivity in a 1D lattice”, “in the Fourier law the phonon-lattice interaction is the key factor in 1D on-site potential or mass disorder lattice”, and recently Ref \[4\] and Ref \[5\] proved rigorously that the conductivity as given by the Green-Kubo formula always diverges in one dimensional momentum conserving systems, Ref \[3\] and Ref \[8\] give 1D models where momentum is conserved and yet the conductivity is finite.

Several models have been studied on 2D lattices heat conduction, for instance, in Ref \[6\] a 2D Lorentz gas, which describes a gas of non-interacting point particles moving in a box, is presented, in Ref \[7\] numerical simulations are performed for the 2D Toda-lattice. And the divergence of the heat conductivity in the thermodynamic limit is investigated in 2D lattices models of anharmonic solids with nearest-neighbor interaction from single-well potentials by A.Lippi and R.Livi \[8\].

Since, investigating the property of thermal conductivity is in order to understand that the macroscopic phenomena and their statistical properties are in terms of deterministic microscopic dynamics. We can roughly classify the 1D lattices model in to two categories. The first category includes homogeneous hamonic chains \[1\], Toda lattices \[2\] (in the models no temperature gradient can be formed), FPU lattices \[1\] (the thermal conductivity \( k \sim N^\alpha \) is divergent as one goes to the thermodynamic limit \( N\to\)unlimit, and \( \alpha \) is different in Toda lattices and FPU lattices) and etc. The character of these models is that the freely propagating energy carriers (particles, phonons or excitations) exists, then the finite heat conduction do not exist in these models. The second category includes other models, in which the free propagation energy carriers (particles, phonons or excitations) can not be found, such as the ding-a-ling model \[9\] (where a set of particles harmonically anchored to an external periodic lattices alternated with free particles), the ding-dong model \[10\] (a modification of the pervious system), the Frenkel-Kontorova model \[11\] (where on-site potential is introduced), the 1D mass disordered FPU lattices at low temperature \[11\] and the models in Ref \[4\] \[5\] \[8\]. Then the finite heat conduction can be found in the models.

In solids, the local theory and the nonlocal theory \[12\] of thermal conductivity have been addressed for different systems. Undoubtedly, the local theory has worked well in many applications, and nonlocal theory is able to give explain some experiments \[13\] where the local theory do not work. Which theory should be adopted in a special system, it depends on the mean free path of the heat carriers, since energy is transported by different kinds of heat carriers in the different systems. A local theory is adequate when the mean free paths are relatively short, the Fourier’s thermal conductivity has always been described using a local theory. When the mean free paths are relatively long, nonlocal heat conductivity gives a better describes. For example, the sample size is smaller than the mean free path, which corresponding to ballistic transport \[14\], a nonlocal theory is adequate.

In this paper we discuss heat conduction in a 2D harmonic lattices. In Ref \[15\], rigorous studies have shown that the thermal conductivity \( \kappa \) diverges in 1D pure harmonic lattices. Afterwards, it was expected that phonon waves should be damped by the scattering processes due to impurity defects (disorder), thus the finite heat conduction should
be obtained. Unfortunately, it was found that isotopic disorder in a harmonic chain yields a diverging conductivity \[14\]. These results suggest that Fourier law cannot be obtained with 1D harmonic chains. Then, how are about 2D harmonic lattices? The present paper deals with a 2D harmonic lattice with the missing bond defects, which is an other kinds important defects and different form impurity defects (disorder), such as in solid \( H_2O \), there are the L defect (a missing hydrogen bond), which play also an important role in the ice properties related to transport and relaxation \[17\].

Consider a 2D lattices model as follow (Fig.1): the 2D square lattices is made of \( N_x \times N_y \) particles, the equilibrium positions of the particles labelled by the index \((i, j)\), every particle just interacts with the nearest neighbor particle by the harmonic restore-force, and some missing bond defects exist in the lattices, the vibration of every particle restricts in one dimension. The Hamiltonian of the 2D lattices model with defects is

\[
H = \sum_{i=1,j=1}^{N_x,N_y} \frac{p_{i,j}^2}{2m_{i,j}} + \sum_{i=1,j=1}^{N_x,N_y} \left[ \frac{1}{2} \alpha_{i,j} (q_{i,j+1} - q_{i,j})^2 + \frac{1}{2} \beta_{i,j} (q_{i+1,j} - q_{i,j})^2 \right].
\]  

(2)

where \( p_{i,j} \) is the momentum of the \((i, j)\) particle, \( q_{i,j} \) is the displacement from the equilibrium position. And \( \alpha_{i,j}, \beta_{i,j} \) are coefficients of the interactive force, here \( \alpha_{i,j} \) and \( \beta_{i,j} \) just take two kinds values 0 or 1, \( \alpha_{i,j} = 0, \beta_{i,j} = 0 \) means that a missing bond defect exists, here the capacity ratio of defects is order to \( \gamma \), \( \gamma = 0 \) means that the lattices is a pure harmonic lattices. Since the mass disorder do not be considered, the dimensionless mass \( m_{i,j} \) is unity for the lattices. For simpler expression, take \( N_x = N_y \) and \( N = N_xN_y \). The periodic boundary conditions are assumed in the left and right boundary. The particles \((1, j) \ j = 1, \ldots, N_y \) in the top boundary of the lattices contact with the high temperature heat bath \( T_1 \) and the particles \((N_x, j) \ j = 1, \ldots, N_y \) in the bottom boundary contact with the low temperature heat bath \( T_2 \). And the Nose-Hoover \[18\] heat bath act on the top line particles and the bottom line particles, keeping them at temperature \( T_1 \) and \( T_2 \), respectively. The equations of motion of these particles are determined by

\[
\begin{align*}
\dot{q}_{i,j} &= -\xi_{i,j} p_{i,j} + q_{2,j} + q_{1,j+1} + q_{1,j-1} - 4q_{i,j}, \\
\dot{\xi}_{i,j} &= \frac{p_{i,j}^2}{T_1} - 1; \\
\dot{q}_{N_x,j} &= -\xi_{N_x,j} p_{N_x,j} + q_{N_x-1,j} + q_{N_x,j+1} + q_{N_x,j-1} - 4q_{N_x,j}, \\
\dot{\xi}_{N_x,j} &= \frac{p_{N_x,j}^2}{T_1} - 1, \quad j = 1, \ldots, N_y; \quad \text{and} \quad j = 0 \iff j = N_y.
\end{align*}
\]  

(3)

Two physical observables, the dynamical temperature and the heat flux of the 2D lattices model need to be defined. The definition of the local temperature, which is same as the local temperature of 1D lattices system, is the time average of the kinetic energy of the particle

\[
T_{i,j} = \langle p_{i,j}^2 \rangle,
\]  

(4)

where \( \langle \cdot \rangle \) denotes time average. The components of the local heat flux vector \( \vec{J}_{i,j} \) is

\[
J_{i,j \rightarrow i,j+1} = \langle p_{i,j} f_{i,j+1} \rangle; \quad J_{i,j \rightarrow i+1,j} = \langle p_{i,j} f_{i+1,j} \rangle
\]  

(5)

where \( J_{i,j \rightarrow i,j+1} \) denoted to the flow of potential energy form the particle \((i, j)\) to the particle \((i, j + 1)\); \( J_{i,j \rightarrow i,j+1} \) denoted to the flow of potential energy form the particle \((i, j)\) to the particle \((i + 1, j)\). It is worth to define the total heat flux value of the lattices system,

\[
N_j |J_{i,j}| = \sum_{i=1,j=1}^{N_x,N_y} \left| \vec{J}_{i,j} \right| = \sum_{i=1,j=1}^{N_x,N_y} \sqrt{(J_{i,j \rightarrow i,j+1})^2 + (J_{i,j \rightarrow i+1,j})^2}
\]  

(6)

Then the time evolution of the displacement and the momentum of each lattices point is calculated in system (1). All values and processes were analyzed for time scales of \( 10^6 - 10^7 \). The 2D lattices has been simulated for the following capacity ratio of defects \( \gamma = 0.0, 0.006, 0.016, 0.026, 0.06, 0.16, 0.21, 0.26, 0.31, 0.36, 0.46 \) and for the following particle numbers \( N = 31^2, 41^2, 51^2, 61^2, 71^2 \) and \( 111^2 \). Additional numerical simulation shows the process of the wave propagation in the lattices.

The numerical simulation of the 2D lattices has demonstrated that the different value of \( \gamma \) leads to very different heat conductivity. When \( \gamma = 0 \), it means that the 2D model is pure harmonic lattices, and the 2D model provide similar results to 1D pure harmonic model, no temperature gradient can be formed. When \( \gamma \) is large enough, the temperature gradient can be formed in the 2D model. In Fig.2, the temperature profiles at \( \gamma = 0 \) is plotted and the results is expected, the slice of the figure at any fixed \( j \) shows that the temperature profiles is as same as 1D pure

2
harmonic model. Increasing the capacity ratio of defects in the lattices, the temperature gradient is formed. A typical example is shown in Fig.3. Next figure (Fig.4) shows the distribution of the heat flux at same parameters as Fig.3. It is obvious that the missing bond defects block the heat flux’s direct advance, and the heat flow is different at the every lattices position.

Now the total particles number $N$ dependence of the total heat flux value $N |J_{i,j}|$ is shown in Fig.5. The total heat flux value increase with particles number increase becomes slow, when increase the capacity ratio of defects in the lattices. When $\gamma > 0.26$, the total heat flux value nearly is a constant with particles number increase. And we calculate the larger lattices $N = 111^2$, the numerical results suggest that the finite heat conduction exists in the model.

Finally, the process of the wave propagation in the model is checked at $\gamma = 0$ and $\gamma = 0.26$. At time $t = 0$, we give a excitations on the boundary of the lattices(Fig.6), then the snapshot at some time $t$ is recorded. Fig.7 records the results of $\gamma = 0$ (the pure harmonic lattices), Fig.8 records the results of $\gamma = 0.26$ (the finite conduction lattices). Fig.7 shows that in the pure harmonic 2D lattices the freely propagating energy carriers exists or the mean free paths are relatively long. Fig.7 shows that in the harmonic 2D lattices with defects the freely propagating energy carriers do not be found or the mean free paths are relatively short. So, the harmonic 2D lattices with defects($\gamma = 0.26$) exhibits the finite conduction.

Hence, the above results allow one to conclude: when $\gamma = 0$, it means that the 2D lattices is a pure harmonic lattices. The microscopic dynamics shows that the freely propagating energy carriers exists or the mean free paths are relatively long. The macroscopic phenomena is that the temperature gradient can not be formed and the total heat flux value increase with particles number increase. The 2D lattices lead to a infinite heat conduction; when $\gamma > 0.26$, it means that defects exist in the 2D harmonic lattices. The microscopic dynamics shows that the freely propagating energy carriers not be found or the mean free paths are relatively short. The macroscopic phenomena is that the temperature gradient can be formed and the total heat flux value do not change with particles number increase. Then the 2D lattices lead to a finite heat conduction. In summary, this paper give a hamonic model with missing bond defects, when the capacity ratio of defects is enough large, the temperature gradient can be formed and a finite heat conduction is found in this model.

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Figure Caption

Fig.1. The 2D harmonic lattices model with missing bond defects is shown.
Fig.2. Temperature profile for the 2D pure hamonic model. The x axis and y axis are the site index $(i,j)$ of the particle, the z axis is the dynamical temperature $T_{i,j}$. The values of the parameters are as follow: $\gamma = 0.0$, the temperature of heat baths $T_1 = 16$, $T_2 = 4$ and system size $N = 51^2$. The data are taken after the $10^6$ time interval.
Fig. 3. Temperature profile for the 2D harmonic lattices with missing bond defects. The x axis and y axis are the site index \((i, j)\) of the particle, the z axis is the dynamical temperature \(T_{i,j}\). The values of the parameters are as follow: \(\gamma = 0.06\), the temperature of heat baths \(T_1 = 16, T_2 = 4\) and system size \(N = 51^2\). The data are taken after the \(10^6\) time interval.

Fig. 4. The stationary distribution of the heat flux vector \(\vec{J}_{i,j}\) for the harmonic model with missing bond defects. The x axis and y axis are the site index \((i, j)\) of the particle. The values of the parameters are as follow: \(\gamma = 0.06\), the temperature of heat baths \(T_1 = 16, T_2 = 4\) and system size \(N = 51^2\). The data are taken after the \(10^6\) time interval.

Fig. 5. The total heat flux value vs the particles number at the same heat baths temperature. The x axis is the particles number \(N\), the y axis is total heat flux value \(N |J_{i,j}|\). The sub-figure magnifies a part of the Fig.5 in the box of the red edge line, where \(\gamma = 0.21, 0.26, 0.31, 0.36, 0.46\) and a additional particles number \(N = 111^2\).

Fig. 6. Input pulse. The x axis and y axis are the site index \((i, j)\) of the particle, the z axis is the energy \(E\) of every particle. The system size is \(N = 111^2\). The figure plots the input pulse on the boundary.

Fig. 7. Response to input pulse in the pure harmonic model. The x axis and y axis are the site index \((i, j)\) of the particle, the z axis is the energy \(E\) of every particle. The values of the parameters are as follow: \(\gamma = 0.0\), system size \(N = 111^2\). The figure shows the snapshot at \(t = 40\).

Fig. 8. Response to input pulse in the harmonic model with defects. The x axis and y axis are the site index \((i, j)\) of the particle, the z axis is the energy \(E\) of every particle. The values of the parameters are as follow: \(\gamma = 0.26\), system size \(N = 111^2\). The figure shows the snapshot at \(t = 40\).
Top Heat Bath: $T_1$

Bottom Heat Bath: $T_2$

Fig. 1.
Fig. 3.
