Heat Conduction in 1D Monoatomic Chains

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Based on the following communication

1. Size dependent heat conduction in one dimensional lattices
   Tejal N. Shah, Shreya Shah and P. N. Gajjar
   - communicated

2. Anharmonicity dependent heat conduction in one dimensional lattices
   Shreya Shah, Tejal N. Shah and P. N. Gajjar
   - communicated

3. Computer simulation study of thermal conduction in 1D chains of anharmonic oscillators
   Tejal N. Shah and P. N. Gajjar
   - communicated

4. Heat conduction in one dimensional chains of anharmonic oscillators
   Tejal N. Shah and P. N. Gajjar
   - to be communicated


2.1 Introduction

Even though Fourier’s law of heat conduction has received great achievement in describing macroscopic thermal transport in the past two decades, its validity in low dimensional systems is still an open question. To understand the mechanism of the Fourier’s law of heat conduction at low dimensions, many attempts have been made in the past and a variety of features of thermal transport in one-dimensional (1D) system are observed [2.1-2.12]. These features are very vital and significant in the applications of nano-device, nanotube, nanowire, nanohorn. It is known that in a one-dimensional (1D) integrable system, like homogeneous harmonic chain [2.13] and the monoatomic Toda chain [2.5], the thermal conductivity diverges in the thermodynamic limit and no temperature gradient is formed, since the dominating energy carriers are not scattered and they propagate ballistically. On the other side, in some of the one-dimensional (1D) nonintegrable systems such as the ding-a-ling model [2.14], the Frenkel - Kontorova (FK) chain [2.4], and the discrete $\varphi^4$ model [2.15], the temperature gradient is uniform, and the heat conductivity $\kappa$ is a constant, being independent of system size. It means these one-dimensional (1D) systems [2.14, 2.15] obey Fourier’s law of heat conduction. Apart from these, in some anharmonic one-dimensional (1D) systems, like the Fermi - Pasta - Ulam (FPU) - $\beta$ - model [2.4, 2.16], the diatomic Toda chain [2.17], the temperature gradient is formed as $dT/dx \sim N^{-1}$, the total heat flux along the chains is proportional to $N^\alpha$, where $N$ is the system size and $0 < \alpha < 1$. They exhibit anomalous heat conduction.
behaviours. Computer simulation experiment show that anharmonicity is a necessary ingredient for the formation of the temperature gradient but it is not sufficient condition for normal conductivity. Because of very limited study, still heat transfer mechanism in solids at low dimensions is not understand clearly as electric current in semiconductor in circuits. Hence there is enough scope to take revisit on the problem of heat conduction in one-dimension (1D). The outcome and previous rigorous results motivated us to study the problem of heat conduction in one-dimensional (1D) monoatomic chains of non linear oscillators. As described in the first chapter, we report the study of heat conduction in one-dimensional (1D) monoatomic chains in this chapter 2 of the thesis. The size / chain length dependency and model parameter dependency of the heat conductivity has been investigated and reported over here.

2.2 Method of Simulation

In this section, simulation technique to study thermal properties of one-dimensional (1D) harmonic / anharmonic lattices without and with on-site potential is discussed. Due to the milestone work by Fermi, Pasta and Ulam, the FPU model has received huge attraction in understanding non linear statistical mechanics. To study the effect of non linearity on heat transport FPU model is one of the simplest lattice models. It played an important role in the development of computational physics and non linear dynamics. The Fermi - Pasta - Ulam (FPU) - β model [2.18] is used to explain the interaction between the oscillators. The Frenkel -
Kontorova (FK) model [2.19] is used to express on-site potential for substrate interaction. Despite its simple form, the Frenkel-Kontorova (FK) model exhibits very rich and complex behaviours. Recent years have witnessed an increasing interest in the study of heat conduction with these two models in low dimensional systems.

![Diagram](image)

**Figure 2.1:** Schematic 1-D chain having mutually coupled oscillator in contact with two thermal reservoirs working at different temperatures, (a) Model without on-site potential and (b) model with on-site potential.

The system, illustrated in Figure 2.1, consists one-dimensional (1D) chain having mutually coupled
oscillators, coupled with two thermal reservoirs working at different temperatures. The study is carried out by considering only the interatomic interaction as well as with substrate interaction i.e. (a) without and (b) with on-site potential.

We consider a chain of N monoatomic oscillators. It is assumed that all oscillators are of equal mass m. Hence the central Hamiltonian of the one-dimensional (1D) chain is written as

\[ H = \sum \left[ \frac{p_i^2}{2m_i} + V(x_{i-1}, x_i) + U(x_i) \right] \]  \hspace{1cm} (2.1)

Here \( x_i \) is the displacement of \( i^{th} \) particle from its equilibrium position and \( p_i \) is the momentum of \( i^{th} \) particle. \( V(x_{i-1}, x_i) \) is the interaction potential between nearest neighbours and \( U(x_i) \) is the on-site potential representing the interaction with the substrate.

The well known FPU - \( \beta \) model is used to explain the interatomic interaction \( V(x_{i-1}, x_i) \). The non linearity or anharmonicity is introduce through the FPU - \( \beta \) model of the form

\[ V = \frac{(x_i - x_{i-1} - a)^2}{2} + \frac{\beta (x_i - x_{i-1} - a)^4}{4} \]  \hspace{1cm} (2.2)

For on-site potential the FK Model used to describe substrate interaction is of the form
where $K$ be the strength of the on-site potential and $b$ be the period of the on-site potential.

Now in equation (2.1) when $\beta = 0$ and $U = 0$, the chain reduces to harmonic chain without on-site potential. When $\beta = 0$ and $U \neq 0$, the chain is known as harmonic chain with on-site potential. When $\beta \neq 0$ and $U = 0$, the chain is referred as anharmonic chain without on-site potential. When $\beta \neq 0$ and $U \neq 0$, the chain is referred as the anharmonic chain with on-site potential.

Hamiltonian for each of these cases is

i) Harmonic chain without on-site potential

\[
H = \sum \left[ \frac{p_i^2}{2m} + \frac{(x_i - x_{i-1} - a)^2}{2} \right]
\]

(2.4)

ii) Harmonic chain with on-site potential

\[
H = \sum \left[ \frac{p_i^2}{2m} + \frac{(x_i - x_{i-1} - a)^2}{2} + \frac{K}{(2\pi)^2} \cos \left( \frac{2\pi x}{b} \right) \right]
\]

(2.5)

iii) Anharmonic chain without on-site potential

\[
H = \sum \left[ \frac{p_i^2}{2m} + V = \frac{(x_i - x_{i-1} - a)^2}{2} + \frac{\beta(x_i - x_{i-1} - a)^4}{4} \right]
\]

(2.6)
iv) Anharmonic chain with on-site potential

\[
H = \sum \left[ \frac{p_i^2}{2m_i} + \frac{(x_i - x_{i-1} - a)^2}{2} + \beta(x_i - x_{i-1} - a)^4 + \frac{K}{(2\pi)^2} \cos \left( \frac{2\pi}{b} x_i \right) \right]
\]  

(2.7)

In the present work we have considered lattice constant \(a = 1.0\) and mass of the oscillator \(m = 1\) throughout this chapter. Moreover, at the ends of the chain we impose two heat reservoirs with temperature \(T_L\) and \(T_R\), respectively that is, particle 1 is in contact with a heat reservoir at temperature \(T_L = 1.1\) and particle \(N\) is in contact with another heat reservoir at temperature \(T_R = 0.9\). In the present experiments of simulations, we use Langevin heat reservoirs \([2.2]\). In the Langevin thermostats, random forces and dissipation terms are introduced into the equations of motion. Namely, the equations of motion of the first and the last particles are

\[
\ddot{x}_1 = F_1 - F_2 - (\xi_L - \lambda_L \dot{x}_1)
\]

(2.8)

\[
\ddot{x}_N = F_N - F_{N+1} - (\xi_R - \lambda_R \dot{x}_N)
\]

(2.9)

The equations of motion of the central, \(N-2\) particles have the form

\[
\ddot{x}_i = F_i - F_{i+1}, \quad \text{for } i = 2, \ldots, N-1
\]

(2.10)

where \(F_i = -V'(x_{i+1}, x_i) - U'(x_i)\) is the force acting on the \(i^{th}\) particle.

The equations of motion are integrated numerically by the fifth order Runge-Kutta integrator algorithm.
Extensive molecular dynamic simulations have been performed for $> 10^7$ time units so that system attends a stationary state and the local heat flux is constant along the chain. We have used fixed boundary condition.

$$J_i = x_i \frac{\partial V(x_{i+1}, x_i)}{\partial x_i}$$

(2.11)

After a long time simulation, when system reaches a non-equilibrium steady state, the time average $J = \langle J_i(t) \rangle$ is independent of the index $i$ and then the heat conductivity is computed by

$$\kappa = \frac{-J}{dT/dx}.$$ 

(2.12)

### 2.3 Results and Discussion

The temperature profiles, characteristics of heat flux ($J$) and thermal conductivity ($\kappa$) have been simulated as a function of the chain length. The dependence of heat conductivity on non-linearity coefficient as well as on the strength of the periodic on-site potential is also predicted. In the present study the number of oscillators are taken as $N = 100, 200, 400, 800$ and $1600$.

First we have carried out the simulation with the harmonic lattice by taking $\beta = 0$ in FPU - $\beta$ model and $K/2\pi = 0$ in FK model. It is well known that in one-dimensional (1D) homogenous harmonic lattice temperature gradient can not be formed and thus thermal conductivity cannot be defined.
Figure 2.2: Temperature profile for $N = 200$ with $T_L = 1.1$ and $T_R = 0.9$ for harmonic chain without on-site potential.

Figure 2.2 shows the temperature profile of one-dimensional (1D) harmonic lattice for $N = 200$ particles. The analysis of heat conduction in the harmonic lattice is very simple. Here energy is equally distributed among every normal modes. Every normal mode carries the same amount of heat energy and transfers it from the hot end to the cold end without any dissipation due to the non interaction between the normal modes. Hence we found that there is no well defined temperature gradient in the stationary state, because temperature inside the chain equals to the average of two heat baths. Here kinetic temperature is plotted against the normalized particle's coordinate ($i/N$).
We also study the effect of on-site potential on thermal properties of one-dimensional (1D) harmonic lattices. For on-site potential we use FK model with $K = 5/2n$.

Figure 2.3: Temperature profile for $N = 200$ with $T_L = 1.1$ and $T_R = 0.9$ for harmonic chain with on-site potential.

Figure 2.3 shows the temperature profile of one-dimensional (1D) harmonic lattice ($\beta = 0$) with on-site potential ($U \neq 0$) for $N = 200$ particles. In the harmonic chain with on-site potential, the temperature gradient is built up but even after $10^7$ time units steady state is not achieved and kurtosis are seen. The temperature gradient in this case is because of the interaction of phonons with substrate.
Figure 2.4: Temperature profile for $N = 200$ with $T_L = 1.1$ and $T_R = 0.9$ for anharmonic chain without on-site potential.

Figure 2.4 shows the temperature profile of one-dimensional (1D) anharmonic lattice ($\beta = 1$) without on-site potential ($U = 0$) for $N = 200$ particles. Here it is clearly seen that temperature gradient is formed. It is also interesting to note that there exists a boundary jump in the temperature profile for the FPU - $\beta$ model nearer to the heat baths. The FPU - $\beta$ model demonstrate that nearly constant temperature gradient do not imply Fourier's heat flow.
Figure 2.5: Temperature profile for $N = 200$ with $T_L = 1.1$ and $T_R = 0.9$ for anharmonic chain with on-site potential.

Figure 2.5 show, the temperature profile for chain of anharmonic oscillator with on-site potential. It is observed that introduction of the FK model in the FPU - $\beta$ model, boundary jump in the temperature profile disappears. This leads us to conclude that the presence of the on-site potential is responsible for the diminishes of the thermal boundary resistance, although the precise mechanism responsible for such behaviour remains hitherto unclear and a better understanding is definitely desirable [2.20 - 2.22].
Figure 2.6: The comparison of temperature profiles of various monoatomic chain for $N = 200$ with $T_L = 1.1$ and $T_R = 0.9$.

In Figure 2.6, all the temperature profiles for 4 models are shown for common comparison and justify the importance of harmonicity, anharmonicity and on-site potential.
The present study is extended reasonably for five one-dimensional (1D) chains of non linear oscillators. The number of oscillators are taken as $N = 100, 200, 400, 800$ and $1600$. As the temperature profile gives the characteristic between lattice position and temperature. In Figures 2.7 and 2.8 we plot the temperature profile of anharmonic chain without on-site potential and with on-site potential for different system size. The temperature profile indicates that the temperature gradient can be formed in both cases i.e. without on-site potential and with on-site potential. It is clear evidence from present study that shape of the profile becomes non linear on increasing the chain length. This nontrivial temperature profile obeys a simple scaling relation for increasing the number of nonlinear oscillators. This indicants that for these models temperature gradient scales as $1/N$. 
Figure 2.7: Temperature profile for $N = 100, 200, 400, 800$ and $1600$ with $T_L = 1.1$ and $T_R = 0.9$ for anharmonic chain without on-site potential.
Figure 2.8: Temperature profile for $N = 1600$, 800, 400, 200 and 100 with $T_L = 1.1$ and $T_R = 0.9$ for anharmonic chain with on-site potential.
The behaviour of heat current $J$ as a function of chain length $N$ for monoatomic anharmonic chain without and with on-site potential is plotted in Figures 2.9 and 2.10 respectively. Figure 2.9 reveals the relation $J = 0.1989N^{-0.4886}$ with $R^2 = 0.998$ whereas Figure 2.10 reveals the relation $J = 0.1804N^{-1}$ with $R^2 = 0.9948$.

The behaviour of heat current $J$ as an inverse function of chain length $1/N$ is also plotted in Figures 2.11 and 2.12 for anharmonic chain without and with on-site potential respectively. This study conclude that $J = 2.4121/N$ with $R^2 = 0.4985$ for without on-site potential and $J = 0.1765/N$ with $R^2 = 0.9979$ for with on-site potential. As the model with FPU - $\beta$ + FK produces the better goodness of fit in comparison with only FPU - $\beta$ model.

![Graph](image)

**Figure 2.9:** Heat current $J$ as a function of chain length $N$ with $N = 100, 200, 400, 800$ and $1600$ with $T_L = 1.1$ and $T_R = 0.9$ for FPU-$\beta$ model.
Figure 2.10: Heat current $J$ as a function of chain length $N$ with $N = 100, 200, 400, 800$ and $1600$ with $T_L = 1.1$ and $T_R = 0.9$ for FPU-$\beta$ + FK model.

Figure 2.11: Heat current as $J$ a function of inverse of chain length $1/N$ with $N = 100, 200, 400, 800$ and $1600$ with $T_L = 1.1$ and $T_R = 0.9$ for FPU-$\beta$ model.
Figure 2.12: Heat current $J$ as a function of inverse of chain length $1/N$ with $N = 100, 200, 400, 800$ and $1600$ with $T_L = 1.1$ and $T_R = 0.9$ for FPU-$\beta + FK$ model.

It is conclusive that for understanding the heat flow and for validity of Fourier's heat conduction law for monoatomic chains, both the anharmonicity and on-site interaction are essential. These observations are in confirmation to that the heat current $J$ diverges with the chain length $N$ in the one-dimensional (1D) anharmonic chain.

In Figure 2.13 we plot the $N$ dependence of $J_N$ for FPU - $\beta$ and FPU - $\beta + FK$ models. It can be observed that for FPU - $\beta$ model, $J_N$ diverges with system size $N$ and hence Fourier' heat law is not justified for this model, but for FPU - $\beta + FK$ model $J_N$ is constant, implying that
1/J diverges with N. Our result is similar to previous study [2.4, 2.23].

Figure 2.13: The comparison of JN as a function of chain length N with N = 100, 200, 400, 800 and 1600 with TL = 1.1 and TR = 0.9.

The behaviour of thermal conductivity κ as a function of chain length N for anharmonic chain with and without on-site potential is plotted in Figure 2.14. The result shows a typical character of one-dimensional (1D) non linear lattices having divergent thermal conductivity. Thermal conductivity converges to a constant value for anharmonic chain with on-site potential.
The size effect of thermal conductivity for anharmonic lattice is also investigated in both two cases. Figure 2.15 shows the N dependence of $kN$ for anharmonic chain without on-site potential and Figure 2.16 is for with on-site potential. It is found that $kN$ increases with the N. For anharmonic lattice without on-site potential thermal conductivity is abnormal while for with on-site potential normal thermal conductivity is obtained. The best fit relation with $R^2 = 0.9818$ is obtained from the relation $kN = 0.8805N$ for anharmonic chain with on-site potential.
Figure 2.15: Dependence of thermal conductivity $\kappa$ with chain length $N$ for anharmonic chain without on-site potential.

Figure 2.16: Dependence of thermal conductivity $\kappa$ with chain length $N$ for anharmonic chain with on-site potential
Investigations are also carried out for heat current (J) and thermal conductivity (κ) by varying strength of the non linearity / anharmonicity β in FPU - β model and by varying the strength of the on-site periodic potential K in FK model.

To investigate the dependence of the thermal conductivity of one-dimensional (1D) chain on non linearity parameter β, the computed result are shown in Figure 2.17.

![Figure 2.17: Thermal conductivity κ as a function of β with N = 200, Te = 1.1 and TR = 0.9 and K/2π=5.](image)

Here we have kept K/2π = 5 and N = 200. In the absence of lattice, if the interparticle potential is harmonic (β = 0), then no phonon-phonon interaction exist and the heat transfer takes place at the speed of sound which results to the infinite thermal conductivity. In
the present case, due to the presence of lattice, even for harmonic model the thermal conductivity remains finite. It is seen from the present study that thermal conductivity increases linearly as \( k = 0.133 + 0.804\beta \). The non linearity coefficient makes phonons to interact among themselves and soliton transforms the heat along the chain. This agrees with the previous observations [2.4, 2.6, 2.9, 2.10].

The behaviour of the heat current \( J \rightarrow K/2\pi \) and the thermal conductivity \( k \rightarrow K/2\pi \) are shown in Figure 2.18 and Figure 2.19, respectively.

It is known that if the substrate interaction \( U(x_i) \) is absent, the heat conduction does not obey the Fourier's heat conduction law neither for harmonic form nor for the anharmonic form of \( V(x_{i-1}, x_i) \). In the presence of anharmonic interparticle potential and harmonic lattice potential, it is seen that the heat current and thermal conductivity decreases exponentially with increase in the strength of the periodic on-site potential \( K \) of Frenkel - Kontorova (FK) model. This shows that as the strength \( K \) increase the phonons travelling from hot-end to cold-end suffer strong interaction with lattice and phonons will be scattered by it which results in thermal resistance. Hence as long as the lattice exists phonons experience resistance resulting to the Fourier's heat conduction law. This reduces the conductivity of one-dimensional (1D) chain of anharmonic oscillators. This is very important result implies that the system tends to a thermal insulator for high value of strength of the periodic on-site potential \( K \).
Figure 2.18: Heat current $J$ as a function of $K/2\pi$ with $N = 200$, $T_L = 1.1$ and $T_R = 0.9$ and $\beta = 1$.

Figure 2.19: Thermal conductivity $\kappa$ as a function of $K/2\pi$ with $T_L = 1.1$ and $T_R = 0.9$ and $\beta = 1$. 
We have also studied the reverse linear chain. Hence we have reversed the position of heat baths and simulated the temperature profiles, heat current and thermal conductivity for the reverse monoatomic anharmonic lattice with on-site potential.

Figure 2.20: Temperature profile for reverse anharmonic chain with on-site potential \( (T_L = 0.9 \text{ and } T_R = 1.1) \) and anharmonic chain with on-site potential \( (T_L = 1.1 \text{ and } T_R = 0.9) \).

Figure 2.20 shows the result of temperature profiles for reverse case of linear monoatomic anharmonic lattice with on-site potential for \( N = 200 \) with \( T_L = 0.9 \) and \( T_R = 1.1 \) along with the result due to \( T_L = 1.1 \) and \( T_R = 0.9 \). It is seen that the reverse and forward temperature profiles are almost identical and no thermal rectification is predicted.
2.4 Flag Points

In the summary, following are the important conclusions of the present study.

❖ Our computer simulation study of thermal conduction in one-dimensional (1D) monoatomic chain as well as others such reports provide the better understanding of heat conduction mechanism for monoatomic materials.

❖ The present study reports the results where the anharmonicity and external potential coexist, this situation is more closer to the real physical system and we conclude that the heat flow is affected not only by the phonon-phonon interaction but also affected by the phonon-lattice interactions. It is also noted by Li and Wang [2.24] that the subdiffusion process has been observed in many real physical systems such as highly ramified media in porous systems, percolation clusters, fractals, charge carrier transport in amorphous semiconductors.

❖ Such simulation results will be very important while studying the heat conduction at nano-scale, designing for thermal devices. No thermal rectification is seen in monoatomic one-dimensional (1D) non linear lattices. This study will also be helpful in understanding the thermal conductivity mechanism in polymers, fibers, bio-mass, DNA / RNA Chains.
Chapter 2

References

[2.1] Joseoph Ford

[2.2] Stefano Lepri, Roberto Livi, and Antonio Politi

[2.3] Abhishek Dhar

[2.4] Bambi Hu, Baowen Li, and Hong Zhao

[2.5] Bambi Hu, Baowen Li, and Hong Zhao

[2.6] Stefano Lepri, Roberto Livi and Antonio Politi

[2.7] Nianbei Li and Baowen Li

[2.8] Trieu Mai, Abhishek Dhar, and Onuttom Narayan

[2.9] C. Giardin'a, R. Livi, A. Politi, and M.
Vassalli,

[2.10] Santhosh G. and Deepak Kumar

[2.11] O. V. Gendelman and A. V. Savin

[2.12] Zhao Yuan, Xue Bao-Xue, Wang Yan-Mei, and Yi Lin

[2.13] Z. Rieder, J. L. Lebowitz and E. Lieb


[2.16] Stefano Lepri, Roberto Livi, and Antonio Politi

[2.17] Takahiro Hatano

[2.18] E. Fermi, J. Pasta and S. Ulam


[2.20] K. Aoki and D. Kusnezor

[2.21] C. Alabiso, M. Casartelli, and P. Mavenzoni

[2.22] Alexander Fillipov, Bambi Hu, Baowen Li, and
Alexander Zeltser

[2.23] Lo Wei Chung
“Simulation study on a microscopic model for
thermal transistor”
Ph.D. Thesis, National University of Singapore,
(2007).

[2.24] Baowen Li and Jiao Wang