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SIZE DEPENDENT HEAT CONDUCTION IN ONE DIMENSIONAL LATTICES

Tejal N. Shah[1], Shreya Shah[2] and P. N. Gajjar[2]
[1]*Bhavan's Sheth R.A. College of Science, Khanpur, Ahmedabad 380 001, Gujarat, India*
[2]*Department of Physics, University School of Sciences, Gujarat University, Ahmedabad 380 009, Gujarat, India*

ABSTRACT

Computer experiments have been performed to study the size dependent thermal conductivity of 1D chains of anharmonic oscillators. In addition to the anharmonic interaction due to Fermi-Pasta-Ulam-β (FPU-β) model, an onsite potential due to Frenkel-Kontorova (FK) model (K/2 = 5) has been used. The size dependent temperature profile, thermal conductivity and heat flux are simulated for different chain lengths N = 8, 12, 20, 36 and 68. It is concluded that heat flux obeys $J = CN^{\beta}$. Relation between KN and N gives linear relation KN = aN.

Keywords: *Heat conduction; thermal conductivity; Anharmonic oscillator; Fermi – Pasta – Ulam model; Frenkel – Kontorova model.*

INTRODUCTION

Unlike electronic devices, the devices that seek to control the flow of heat pose difficulties since the carriers of heat viz., phonons are not point particles having definite mass and charge. Generally one-dimensional (1-D) lattice model has been used to get clear understanding of heat transfer at low dimensions. As considerable interest is growing in developing nanoscale devices, it becomes vital to study heat transport at this scale. Without a clear understanding on heat flow in nano-structures it will not be possible to pump-out radiant heat from the nano-devices which affects the device efficiency. It is extremely difficult to do experimental study of heat conduction at nanoscale, since the thermal contacts, thermal baths and thermal sensors are to be connected to nano – devices. Hence one has to prepare even smaller size gadgets for these. So in the absence of exhaustive experimental studies extensive theoretical and numerical experiments have been performed to investigate the phenomenon of heat transport at low dimensions. Based on earlier studies, it is well known that basic models without on-site potential like homogeneous harmonic chains [1], Toda lattices [2], Fermi-Pasta-Ulam lattices [3], etc. give a divergent thermal conductivity due to the existence of long wavelength modes [4]. By including special features such as periodic potential [5, 6], or on-site potentials like the ding-a-ling model [7], the ding-dong model [8], the Frenkel-Kontorova model [3], the discrete ϕ^4 model [9] etc., finite thermal conductivity can be obtained. Later on it is also observed that for inhomogeneous harmonic and anharmonic chain with FPU-β model temperature gradient is built up and thermal conductivity is finite [10,11]. In this paper we would like to study size dependent heat conduction in one dimensional lattices. The FPU-β model [12] is used to explain the interaction between the oscillators while FK Model [13] is used to express on-site potential for substrate interaction. The temperature profiles, characteristics of heat flux and thermal conductivity have been simulated as a function of the chain length of 1D chain of nonlinear oscillators. In the present study the number of oscillators are taken as N = 8, 12, 20, 36 and 68. The Langevin thermostat [14] is used to keep the constant temperature at the first and the last particle of the chain. In the reduced temperature unit, the first particle is kept at T_L = 0.3 while the last particle is kept at T_R = 0.2. Here T_L is the temperature of the left end of the chain and T_R is the temperature of the right end of the chain. We have used fixed boundary conduction in the present study.

*Corresponding author: *tejal.shah999@gmail.com*

METHOD OF COMPUTATION

The Hamiltonian for the considered 1-D chain of anharmonic oscillators is of the form

$$H = \sum_{i=1}^{N}\left[\frac{p_i^2}{2m_i} + V(x_{i-1}, x_i) + U(x_i)\right] \quad (1)$$

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 onsite potential representing the interaction with the substrate.

The nonlinearity or anharmonicity in the interparticle interaction is introduced through the FPU-β model [10]

$$V(x_{i-1}, x_i) = \frac{(x_{i-1} - x_i - a)^2}{2} + \frac{\beta (x_{i-1} - x_i - a)^4}{4} \quad (2)$$

Here β is the coupling constant and lattice constant a = 1.

For on-site potential, the FK Model used to describe substrate interaction is of the form

$$U(x_i) = -\frac{K}{(2\pi)^2}\cos\left(\frac{2\pi x_i}{b}\right) \quad (3)$$

In the present simulation work, mass M = 1 unit, spring constant K = 0.5 and the period of on-site potential b = 1. The local temperature is define as

$$T = \left\langle \frac{\sum_{i=1}^{N} p_i^2}{Nm} \right\rangle_{\mu} \quad (5)$$

Or

$$T = \left\langle \frac{p_i^2}{m} \right\rangle_{\mu} \tag{6}$$

Langevin heat baths are put on the first and last oscillators, keeping them at $T_L = 0.3$ and $T_R = 0.2$, respectively. Hence the equations of motion are

$$\ddot{x}_1 = f_1 - f_2 - (\xi_L \dot{x}_1 - \lambda_L x_1) \tag{7}$$

$$\ddot{x}_N = f_N - f_{N+1} - (\xi_R \dot{x}_N - \lambda_R x_N) \tag{8}$$

$$\ddot{x}_i = f_i - f_{i+1} \quad \text{fori} = 2, \ldots\ldots, \text{N-1} \tag{9}$$

where $f_i = -V'(x_{i-1}, x_i) - U'(x_i)$ is the force acting on the i^{th} particles, ξ is an independent Wiener process with zero mean, and variance parameter λ = 1. The ξ and λ which models the microscopic action of the thermostats and implement the interaction of the first and last particles with the heat reservoirs by introducing random forces and dissipation.

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 i.e. the first and last particles are fixed with heat bath. The local heat flux is determined by

$$J_i = \dot{x}_i \frac{\partial V(x_{i-1}, x_i)}{\partial x_i} \tag{10}$$

After a long time simulation, when system reaches a non-equilibrium steady state, the time average J=<Ji(t)> is independent of the index i and then the heat conductivity κ is computed by

$$\kappa = \frac{-J}{dT/dx} \tag{11}$$

RESULTS AND DISCUSSION

The present study is carried out for five different 1D chains of non linear oscillators. The sizes of oscillators are taken as N = 8, 12, 20, 36 and 68 ($N=2^n+4$). As the temperature profile gives the characteristic between lattice position and temperature, in Fig. 1, the temperature profiles for N = 68 coupled oscillators in the absence of anharmonicity coefficient is shown. 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,

$$\frac{T_L + T_R}{2} = \frac{0.3 + 0.2}{2} = 0.25.$$

Now we have introduced the anharmonicity in FPU - β model via $\beta = 1$. Figure 2 shows the temperature profile for different system size. The temperature profiles indicate that the temperature gradient is formed. It is clear evidence from this that the shape of the profile becomes nonlinear on increasing the chain length. This nontrivial temperature profile obeys a simple scaling relation for increasing the number of nonlinear oscillators and shows that the temperature gradient scales as $dT/dx \sim N^{-1}$.

The behaviour of heat current J as a function of chain length N for three different values of anharmonicity parameter β are plotted in Fig. 3, which reveals the relation $J = CN^P$ having P = -1.02, -1.02, -0.93 and R^2 = 0.998, 0.999, 0.999 for β = 0.1, 0.5 and 1, respectively. Here R^2 is the statistical parameter to judge the goodness of best fit. From this graph we conclude that heat flux J is inversely proportional to N and the heat flux diverges with system size. Presently obtained results for the thermal conductivity as a function of system size are also plotted in Fig. 4, which revels the power law, $J = CN^P$.

Relation between κN and N is shown in Fig. 5. Which gives linear relation κN = 0.027N, κN = 0.036N and κN = 0.044 for β = 0.1, 0.5 and 1 respectively. From that we conclude that as system size increases, thermal conductivity κ increases.

CONCLUSION

We have confirmed that the system size plays an important role in 1D chain for anharmonic oscillators. As the system size increases the shape of the profile becomes nonlinear. It is also concluded that as nonlinearity coefficient β increases, flux J also increases for the same system size and for constant strength of the on-site potential $K/2\pi$ i.e. the heat flow is affected not only by the phonon-lattice interaction of FK model, but also by the phonon-phonon interaction of FPU-β model. Such simulation results will be very important while studying the heat conduction at nano scale. This study helps us in using the nano – wire, nano – tubes of different length scale for specific thermal conduction.

ACKNOWLEDGEMENT

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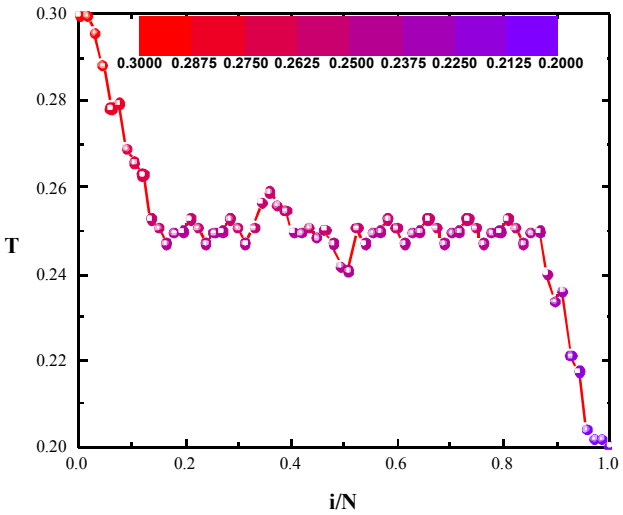

Figure 1: Temperature profile for 1D harmonic lattice with chain length N=68 (anharmonicity parameter $\beta = 0$).

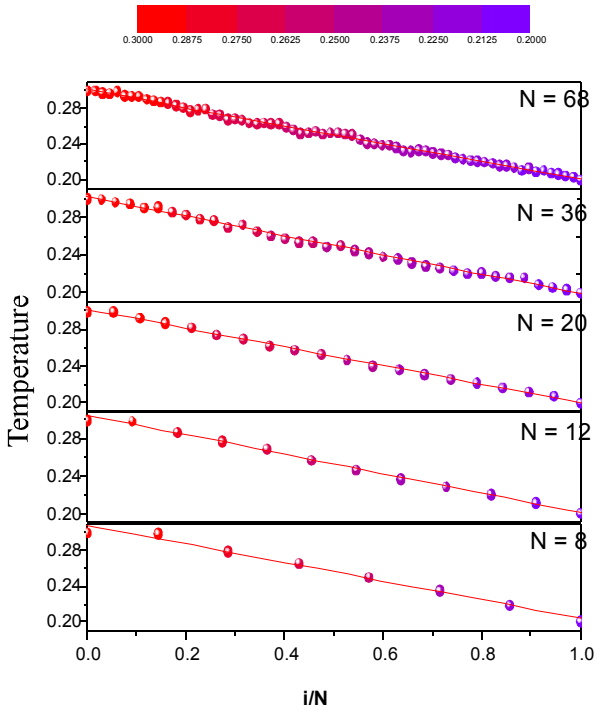

Figure 2: Temperature profile for N = 8, 12, 20, 36 and 68 with $T_L = 0.3$ and $T_R = 0.2$ under fixed boundary condition.

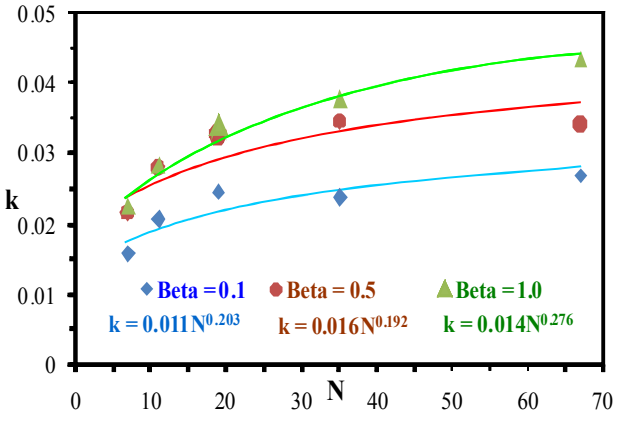

Figure 4: *Thermal conductivity of 1D – chain of anharmonic oscillators as a function of system size.*

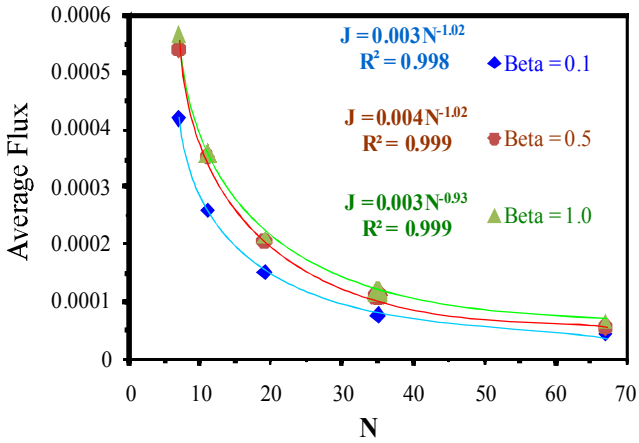

Figure 3: *Average Heat flux J versus N for β =0.1, 0.5 and 1* under fixed boundary condition.

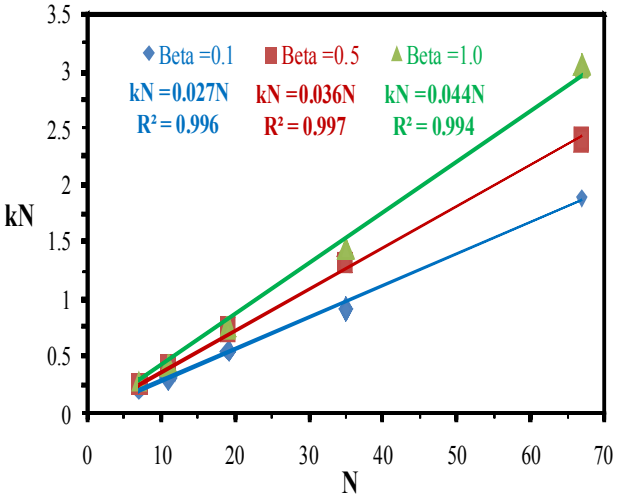

Figure 5: *Relation* of thermal conductivity with system size of 1D chain of anharmonic oscillators *for β =0.1, 0.5 and 1* under fixed boundary condition.

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