Annexure - IX

UNIVERSITY GRANTS COMMISSION
BAHADUR SHAH ZAFAR MARG
NEW DELHI – 110 002

PROFORMA FOR SUBMISSION OF INFORMATION AT THE TIME OF SENDING THE FINAL REPORT OF THE WORK DONE ON THE PROJECT

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3. UGC Approval No. and Date

F. No. 43-256/2014(Sr) dated 23.07.2015

4. Date of Implementation

01.07.2015 to 30.06.2018

5. Tenure of the Project

Three years (01.07.2015 to 30.06.2018)

6. Total Grant Allocated

Rs. 5,59,500/-

7. Total Grant Received

Rs. 5,32,000/-

8. Final Expenditure

Rs. 5,19,897/-

9. Title of the Project

Theoretical and Computational Investigation of Heat Conduction in Low Dimension Lattice: 2D and 3D systems

10. Objectives of the project

The objectives of the project were following:

I. Analytical and numerical investigations of heat conduction in 1d and 2d systems with

various nonlinear potentials with special emphasis on long range interactions to make general conclusions on the role of nonlinearity and long-range interactions on the thermal energy propagation.

II. Numerical investigations of thermal energy transport in 3d nonlinear lattices. Special emphasis will be put on the aspect ratio of the lattice to find out its effect on thermal conduction.

III. Investigation on role of the dissipation constant of the thermal bath in the heat conduction. Close similarity of dissipation constant dependence of thermally activated rate processes and thermal conductivity will be explored further.

IV. The behavior of the thermal conductance with temperature will be examined closely, keeping in mind that recently temperature dependence of thermal conductivity individual silicon nanowires has been made.

V. Effect of noise correlation of the stochastic thermal bath on the thermal conductivity.

VI. Role of impurities in the lattice on thermal conductivity in the 3d systems will be explored numerically.

11. Whether objectives were achieved

Some of the key objectives of the project has been achieved. Particularly we have investigated the role of interaction potential, temperature and dissipation constant on the thermal conductivity in one-dimensional lattice model. We also have investigated heat conduction in the two-dimensional lattice model with nearest neighbor interaction potential of Fermi-Pasta-Ulam (FPU) FPU-β potential. Both in the one- and two-dimensional lattice models, we determined the scaling laws of thermal conductivity with the size of the system. In the case of one-dimensional lattice, the thermal conductivity shows a power-law scaling, on the contrary in the two-dimensional lattice it shows logarithmic divergence. Therefore, compared to one-dimensional lattice the divergence of the thermal conductivity with the system size is slower. Furthermore, we showed that the scaling coefficient of the power-law divergence in one-dimensional lattice is temperature dependent. In the low and high temperature regimes the scaling coefficients are different. The scaling coefficients are ~0.5 and ~0.33 in the low and high temperature regimes, respectively. The details of the work is described below.

We have considered a one-dimensional lattice model with a nearest-neighbor interaction potential. The classical Hamiltonian for the model can be represented as

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i=1}^{N-1} V(x_i - x_{i-1}) \qquad (1)$$

Where x_i and p_i are the displacement from equilibrium position and momentum of the i-th particle, respectively. The mass and the total number of particles on the chain are given by m and N, respectively. The nearest-neighbor interaction potential between the particle i and (i-1) is given by $V(x_i - x_{i-1})$. As we have not considered any external potential, our lattice model becomes a momentum conserving chain. We fixed m=1 for our calculations throughout. We have chosen the asymmetric double well nearest-neighbor interaction potential of the form given by

$$V(x) = -\frac{1}{2}k_1x^2 + \frac{1}{3}k_3x^3 + \frac{1}{4}k_4x^4 \qquad (2)$$

where k_2, k_3 and k_4 are three positive constants. This potential belongs to the general class of FPU-$\alpha\beta$ potential and due to the cubic nonlinearity the potential becomes asymmetric ($V(x) \neq V(-x)$). The asymmetric nature of double well potential is determined by the cubic nonlinear parameter k_3. In order to study the thermal conduction through the nonlinear chain using nonequilibrium simulation method, both the ends of lattice are connected to Langevin heat baths having different temperatures. The equation of motion of the i-th particle in the chain is given by

$$\ddot{x}_i = k_2(2x_i - x_{i+1} - x_{i-1}) - k_3[(x_i - x_{i-1})^2 - (x_{i+1} - x_i)^2] - k_4[(x_i - x_{i-1})^3 - (x_{i+1} - x_i)^3] - \gamma_i \dot{x}_i + \eta_i \quad (3)$$

where the fluctuation (η_i) and dissipation (γ_i) terms are defined as $\eta = \eta_L\delta_{i,1} + \eta_R\delta_{i,N}$ and $\gamma_i = \gamma(\delta_{i,1} + \delta_{i,N})$, respectively. The heat baths are characterized by the fluctuation-dissipation relations followed by the two Markovian heat baths, $\langle \eta_L(t)\eta_L(t')\rangle = 2\gamma k_B T_L \delta(t-t')$ and $\langle \eta_R(t)\eta_R(t')\rangle = 2\gamma k_B T_R \delta(t-t')$. The γ, k_B, T_L and T_R are the dissipation constant, Boltzmann constant, temperatures of left and right heat baths, respectively. The values of k_B and γ were chosen to be unity throughout. We varied the left and right bath temperatures T_L and T_R) to investigate the effect of temperature on the divergence behavior of thermal conductivity. In this context we defined two relevant quantities: the temperature difference, $\Delta T = T_L - T_R$ and the average temperature, $T = \frac{T_L+T_R}{2}$.

The instantaneous local heat current between i-th and (i+1)-th particle is defined by

$$j_i = \frac{1}{2}(\dot{x}_i + \dot{x}_{i+1})\frac{\partial H}{\partial x_i} \quad (4)$$

Defining the time-averaged local heat current as $J_i = \lim_{t\to\infty} \frac{1}{t}\int_0^t j_i(\tau)d\tau$, that reaches a nonequilibrum stationary state across the lattice after long time, the global heat current in the lattice is given by

$$J = \sum_{i=i}^{N-1} \frac{J_i}{N-1} \quad (5)$$

The thermal conductivity is related to the steady state global heat current as

$$\kappa = \frac{JN}{\Delta T} \quad (6)$$

In the thermodynamic limit (large N), in 1D momentum conserving systems J has been predicted to scale as $J \sim N^{\alpha-1}$. Thus κ becomes divergent with a power law scaling relation as $\kappa \sim N^{\alpha}$, where α is the scaling exponent.

In order to numerically integrate the dynamical equations (3), we used 4-th order Runge-Kutta method to achieve higher accuracy. In the interaction potential (2) we fixed $k_2 = 0.1$, $k_4 = 0.002$ and varied k_3 (0.003 or 0.006) in order to explored the effect of asymmetry on the nature of divergence in κ. Further to investigate the temperature dependence of divergence we chose various combination of T and ΔT. We used fixed boundary condition (BC), $x\_0 = x_{N+1} = 0$, in our calculations.

In Fig.1a we show the divergence of thermal conductivity for the asymmetric potential ($k_3 = 0.003$) with varying average heat bath temperatures keeping the ΔT fixed. For three different values of T the system exhibits power-law divergence of thermal conductivity with α ranging between 0.31-0.35. These α values are similar to the predicted $\alpha = \frac{1}{3}$ by renormalization group theory, mode coupling theory and many numerical simulations. We found similar divergence of κ for the same system with higher asymmetry ($k_3 = 0.006$) in the interaction potential (Fig.1b). One important aspect of these divergence behavior is that the average temperature of the system is large. Therefore at the high temperature limit the asymmetric-double well-momentum-conserving system behaves similar to the symmetric-FPU-$\alpha\beta$-momentum-conserving system.

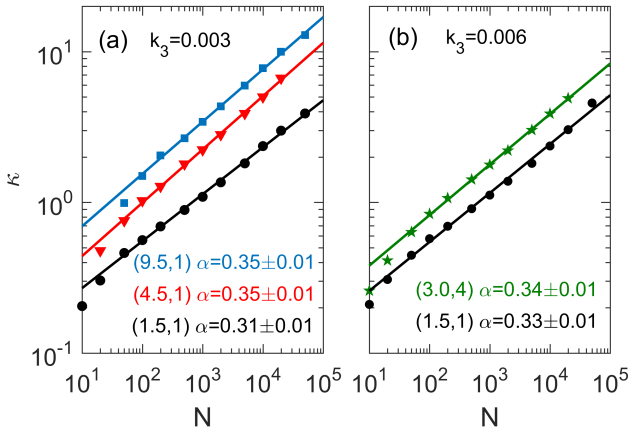

Fig.1: Divergence of κ as a function of chain length, *N*. Different colored symbols represent simulations with different average bath temperatures with fixed temperature difference, $(T, \Delta T)$; circle: (1.5,1), triangle: (4.5,1), square: (9.5,1) and star: (3.0,4). Solid lines are from power law fitting ($\kappa \sim N^{\alpha}$). The values of α are indicated inside the plots for (a) $k_3 = 0.003$ and (b) $k_3 = 0.006$.

We next investigated the divergence behavior of κ for a range of average temperature values in the intermediate to low T limits again by varying the heat bath temperatures. Particularly we aimed to determine the nature of divergence in the intermediate and low temperature regimes. In Fig.2 we show the divergence of κ in different average temperatures of the system with $k\_3 = 0.003$. Fig.2 indicates that the qualitative nature of divergence changes depending on the average temperature of the heat bath. The conductivity diverged sharply with $\alpha = 0.49$ at very low temperature. With increase of temperature the divergence becomes shallow with $\alpha = 0.18$. Further increase of temperature the conductivity appears to saturate with N with $\alpha = 0.07$. At high temperature κ shows its usual divergence behavior with $\alpha = 0.31$. The striking feature of the temperature dependent thermal conductivity here is that two different types of scaling behaviors of κ at very low ($\alpha = 0.49$) and very high ($\alpha = 0.31$) temperatures. Repeating calculations with higher asymmetry of the potential ($k_3 = 0.006$) also resulted similar observations as in $k_3 = 0.003$ (Fig.3). Thus our simulation results indicate that the values of α depends on the temperature of the system in asymmetric interaction potential.

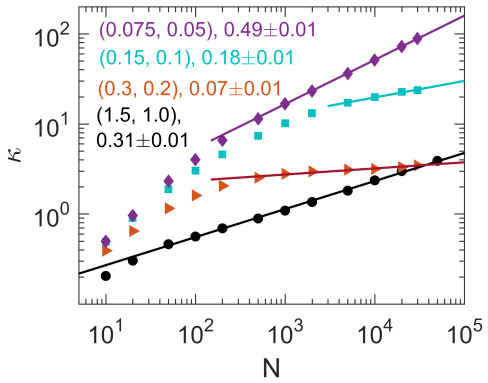

Fig.2: Divergence of κ as a function of N for different average T and ΔT; circle: (1.5,1), triangle: (0.3,0.2), square: (0.15,0.1) and diamond: (0.075,0.05). The asymmetric parameter k_3 was 0.003. The α values are indicated inside the plot.

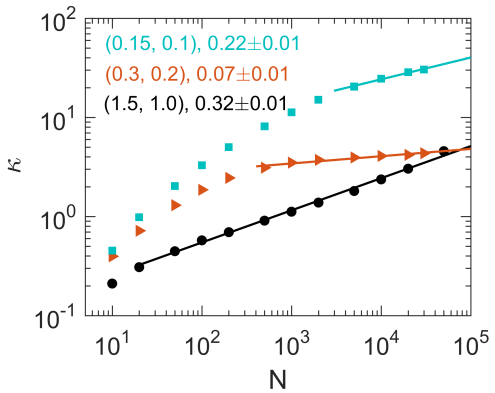

Fig.3: Divergence of κ with N at different temperatures with asymmetric parameter $k_3 = 0.006$.

To determine the temperature dependence of α, we plotted it as a function of T for two different values of asymmetric parameter k_3 (Fig.4). With increase in T, α decreases sharply and passing through a minimum it increases to saturate with $\alpha = 0.35$ at high T. The weakest divergence of κ occurs at the intermediate T both for low and high asymmetries of the potential. The comparison of α vs. T for low and high k_3 indicates that the divergence behaviors of thermal conductivity for different asymmetry values are identical. If the saturation of κ in this system was an asymmetry induced effect then there must have been a shift in α vs. T plots for the two different values of k_3. However the two curves overlap with each other. Further for the same reason, expectedly higher asymmetry would have resulted saturation of κ at lower N as compared to lower asymmetry. The comparison of κ vs. N profiles for higher and lower asymmetry at different T (Fig.5) do not indicate any such asymmetry induced early saturation of κ. These results and analyses point out that the saturation of κ may be a finite length effect occurs only at intermediate T. However our results does point out that the nature of divergence is indeed temperature dependent.

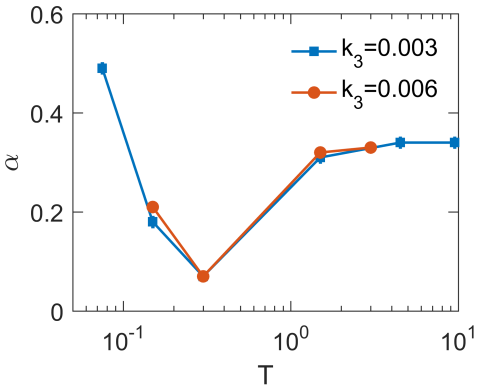

Fig.4: Temperature dependence of α for two different values of asymmetric parameters k_3. The sizes of error bars on α are nearly same as the sizes of the markers.

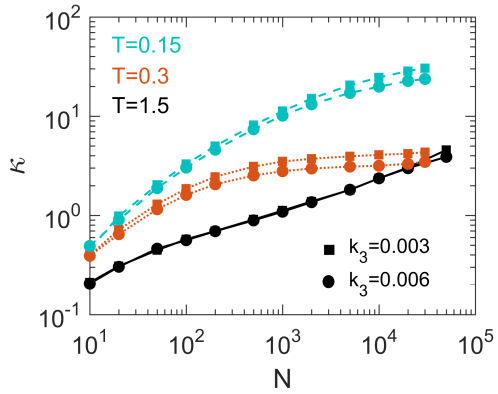

Fig.5: Comparison of divergence of κ with N for different values of asymmetric parameter k_3 at various average bath temperatures, T.

In order to determine the finite-size effect on α we calculated the local divergence coefficient, α_N, by determining the local slope in κ vs. N line. In Fig.6 we present the α_N as a function of N estimated at various T for two different values of asymmetry parameter. At high T the well-known thermodynamic limit of 0.33 is achieved at the shorter length of the chain. On the other hand, at very low T, α appeared to settle at $\alpha \sim 0.5$ value, indicating the different scaling behavior of the system depending on the temperature of the system. However at the intermediate T with increasing N, α_N decreases below the thermodynamic limit ($\alpha = 0.33$, dashed line in Fig.6) and passing through a minimum it shows an increasing trend for both the values of asymmetry parameters. Similar trend was seen for $T = 0.15$ although without the minimum as probably the minimum is located at larger N. As at these two temperatures the local α does not settle to a particular value, it may be concluded that the value of α at the intermediate T are not from the thermodynamic limit of the system.

The presence of two wells separated by a barrier in double well interaction potential makes the lattice system somewhat different as compared to usual FPU class of single-well interaction potentials. At high T regime, due to the increased thermal noise from the heat baths the system will be able to transition between the two wells. However, at low T regime the system will be trapped in one of wells depending on the initial state of the system. In order to assess the temperature dependent dynamic nature of the system, we calculated order parameter, $\frac{1}{N-1}\sum_{i=1}^{N-1}|\langle x_{i+1} - x_i\rangle|$, at various T for two different values of asymmetry parameter k_3 (Fig.7a). This order parameter essentially reflects the equilibrium average of absolute displacement from the adjacent particle. We find that the value of the order parameter saturates to two distinct regimes at low and high T indicating temperature dependent disparate nature of the system. The two different types of divergence exponents of thermal conductivity ($\alpha \sim 0.5$ and $\alpha \sim 0.033$)

in the low and high T thus correlate with the order parameter of the system. The qualitative nature of the order parameter does not depend on the asymmetry parameter k_3. Further we plotted the ensemble averaged displacement with the adjacent particle, $\langle x_{i+1} - x_i \rangle$, of a chain with $N = 500$ at high and low (Fig.7b-c) temperatures and these two plots suggest the dichotomous dynamical behavior of the lattice with double well potential. Particularly the confinement of the system in the two wells is evident at the low T. Whereas at high T the fluctuations are more or less homogeneous. Therefore our estimated temperature dependent divergence characteristics of thermal conductivity is due to the distinct qualitative nature of the system at low and high T.

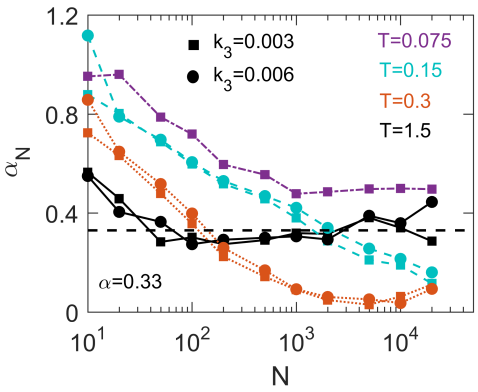

Fig.6: Plot of local divergence coefficient α_N with N for different values of asymmetric parameter k_3 and at different average bath temperature, T. α_N was estimated by calculating the local slope of κ vs. N plots given in Fig.2 and Fig.3. The horizontal dashed line represents $\alpha = 0.33$.

In order to ensure that the contributions from the cubic and quartic terms in the potential are not negligible, we calculated ensemble average of second, third and fourth order terms in the potential (Fig.8) at different temperatures. Our calculations indicate that the contributions from the cubic and the quartic terms are not negligible as compared to the quadratic term. Further the values of these terms show a non-monotonous temperature dependence that is in consistent with the temperature dependent scaling of thermal conductivity. Based on the used values k_2, k_3 and k_4, the absolute values of the coefficients in the potential (2) were 0.05, 0.001/0.002 and 0.0005. The progressively decreasing values of these coefficients further justifies the truncation of the polynomial beyond fourth order in Taylor expansion.

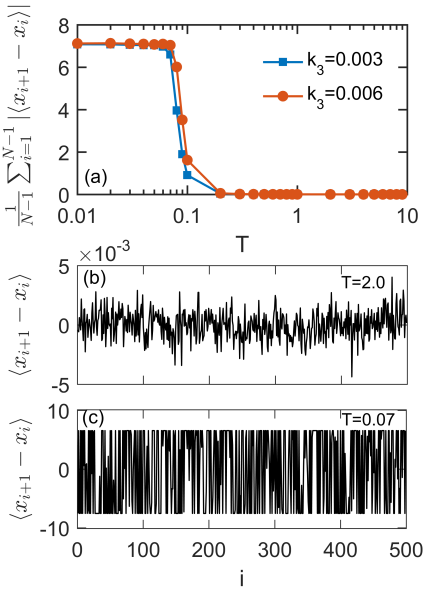

Fig.7: a) Temperature dependence of the order parameter for a chain with $N = 500$. The average displacement from the adjacent particle along the chain at $T = 2.0$ (b) and $T = 0.07$ (c).

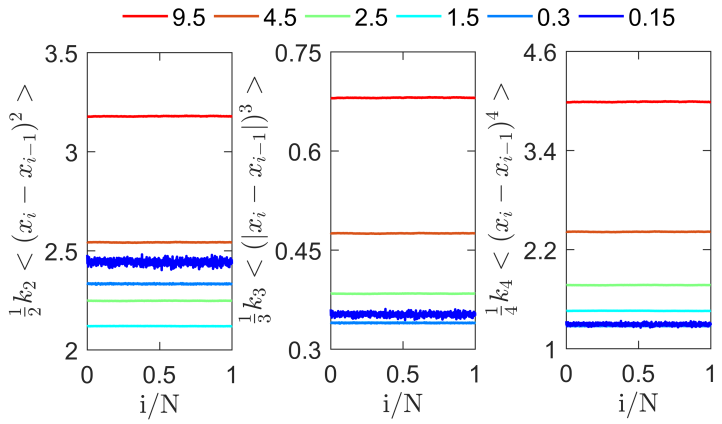

Fig.8: Absolute average contributions of second, third and fourth order terms in the potential for a chain with $N = 1000$ and $k_3 = 0.003$. The values of temperature are indicated at the top of the figure.

Understanding the divergent nature of thermal conductivity in low dimensional systems has been a long-standing problem. A large number of theoretical and numerical calculations on 1-D momentum conserving systems concluded power-law divergence of thermal conductivity with the length of lattice. In this study we used nonequilibrium simulation method to show that the divergent nature of κ in 1-D asymmetric lattice depends on the temperature of the heat baths. In the thermodynamic limit, the system exhibits $\alpha \sim 0.5$ and $\alpha \sim 0.33$ at low and high T respectively. Therefore, our calculations point out two different scaling behavior of the same system depending on the temperature of the system. We emphasize that our finding of temperature dependent divergence of thermal conductivity in asymmetric double well interaction potential may as well be obtained in case of symmetric double well potential as there is no significant dependence of asymmetry on the divergence behavior.

We investigated the two-dimensional momentum conserving lattice next to determine the scaling law of thermal conductivity with the size of the lattice. Here we have used FPU-β potential to model the nearest-neighbor interaction between the particles. The form of the potential is $V(x) = \frac{1}{2}k_1x^2 + \frac{1}{4}k_4x^4$. In the 2-D lattice each particle interacts with four neighboring particles. The classical Hamiltonian representing the nonlinear 2-D lattice is given as

$$H = \sum_{j=1}^{N_y}\sum_{i=1}^{N_x}\frac{p_{ij}^2}{2m} + \sum_{j=1}^{N_y-1}\sum_{i=1}^{N_x-1}\left[V\left(x_{ij} - x_{i-1,j}\right) + V\left(x_{ij} - x_{i,j-1}\right)\right] \tag{7}$$

Where N_x and N_y are the length of the lattice in the x and y directions. The two sides of the lattice are connected to Langevin heat baths with different temperatures, T_L and T_R. The properties of the heat baths are same as in the case of 1-D lattice. Following the similar method as in the 1-D lattice the steady state heat flux along the i-th layer in 2-D lattice is given as

$$j_i = \frac{1}{2N_y}\langle\sum_{j=1}^{N_y}\left(x_{i+1,j} - x_{i,j}\right)\left(\dot{x}_{i,j} + \dot{x}_{i+1,j}\right)\rangle \tag{8}$$

The thermal conductivity in the 2-D lattice is defined as

$$\kappa = \sum_{i=i}^{N_x}\frac{j_i}{T_R - T_L} \tag{9}$$

We calculated the local temperature along the 2-D lattice and in Fig.9 we present it for lattice of different

dimensions. These plots indicate that a temperature gradient is established in the lattice due to the nonlinear nearest-neighbor interaction potential.

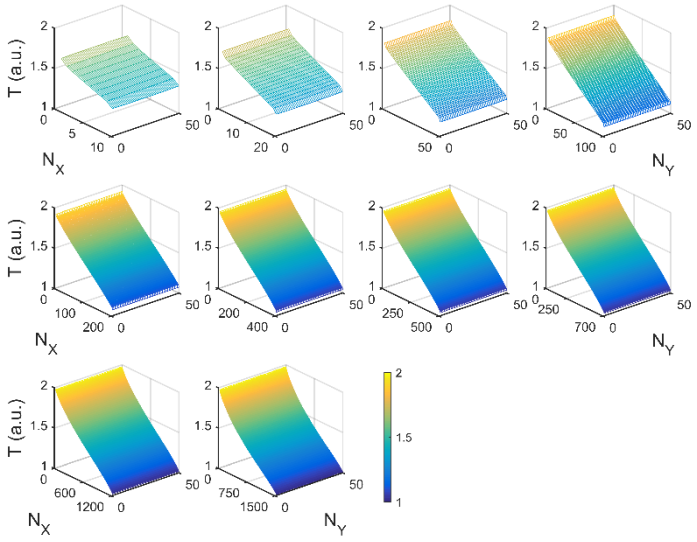

Fig.9: Local temperature profiles in 2-D lattice of different sizes with $T_L = 2$ and $T_R = 1$.

Next, we calculate the thermal conductivity for each lattice using the equations (8) and (9). A plot of thermal conductivity with the size of the lattice (Fig.10) indicates that in the macroscopic limit of the large lattice size, 2-D nonlinear lattice shows logarithmic divergence of thermal conductivity with the dimension of the lattice ($\kappa \sim \ln N_x$). It is important to note that the divergence does not depend on the length of the lattice in the direction in which there is no flow of heat. These results show that the divergence of the thermal conductivity with the size of the lattice is slow in the 2-D lattice as compared to the 1-D lattice that we shows a power-law divergence.

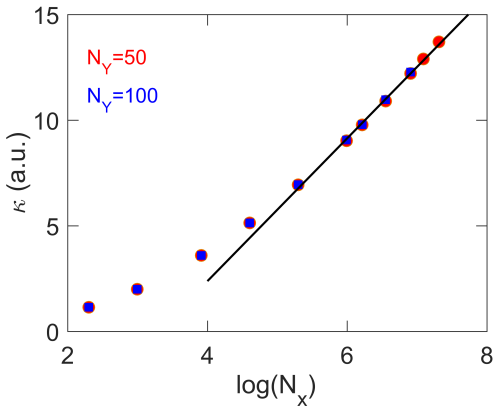

Fig.10: The logarithmic divergence of the κ with the length of the lattice in the x direction (N_x) for a fixed length of lattice in y direction (N_y). The solid line represents the fitted line. The logarithmic divergence remains unaltered for different values of N_y.

12. Achievements from the project

Understanding the heat conduction in finite dimensional insulator systems has been a long standing and much debated problem for some time. Particularly a major focus has been establishing Fourier's law of heat conduction in low dimensional systems. In one dimension it has been established that the thermal conductivity diverges with a power law scaling with the system size. However, establishing the exact value of the divergence exponent has been controversial and varied from one calculation to another. Here we investigated thermal conduction in one dimensional lattice model with asymmetric double-well nearest-neighbor interaction potential using nonequilibrium simulation method. We showed that in the high and

low temperature regimes the divergence exponent, in the power-law divergence of the thermal conductivity, is different. In the high and low temperature regimes the exponent is ~0.5 and ~0.33, respectively. The temperature dependence of the exponent is a new finding and it settles the debate on the variation of the exponent from one study to another. Our calculations show that such variation is indeed due to the variation temperature used from one study to another. More importantly, it underscores that the exponent is a temperature dependent quantity. In can of 2-D lattice we showed that nonlinear lattice with FPU-β potential show a mush slower divergence in the form of logarithmic divergence.

13. Summary of the findings

We investigated thermal conduction in one dimensional lattice model with asymmetric double-well nearest-neighbor interaction potential using nonequilibrium simulation method. Our primary aim in this study was to investigate the nature of power law divergence in different regimes of average temperature of the system. Our major findings in this study are:

- In all the temperature regimes the thermal conductivity exhibits power-law divergence with the length of the chain.
- The system exhibits two distinctly different scaling exponents in the low and high temperature regimes. Therefore, the same system exhibits two different scaling depending on the temperature of the system.
- In the intermediate temperature the system exhibits a very weak divergence of thermal conductivity with the length of the chain. However further analysis shows that this weak divergence is a finite size effect of the system.

Our calculations, for the first time, shows that the scaling exponent in the power law divergence becomes temperature dependent. It also provided an explanation on the question of variation of the value of the exponent from one study to another.

In the case of two-dimensional lattice, we showed that temperature gradient is established along the lattice in presence of nonlinear nearest-neighbor interaction potential and 2-D lattice exhibits logarithmic divergence of the thermal conductivity with the length of the lattice in the direction of heat flow. Such divergence is not dependent on the length of the other direction in which there is not any flow of heat current. Furthermore, it shows that divergence of thermal conductivity in 2-D is slower ($\kappa \sim \ln N$) than the divergence in 1-D ($\kappa \sim N^{\alpha}$) insulator lattice.

14. Contribution to the society

Not applicable

15. Whether any Ph.D. enrolled/produced out of the project

None

16. Number of publications out of the project:

One (1)

1. Archana G R, D **Barik***, Temperature dependent divergence of thermal conductivity in momentum conserving 1D lattice with asymmetric potential, *Physical Review E*, **99,** 022103, 2019

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