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Anomalous heat conduction in a 2d Frenkel-Kontorova lattice

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Abstract. We show that in contrast to the 1d Frenkel-Kontorova (FK) chain known to obey the Fourier law of heat conduction and several 2d models which show logarithmic dependence of conductivity on system size, a scalar 2d FK lattice with commensurate structure exhibits anomalous heat conduction, whose thermal conductivity displays a power law behavior. The dependence of thermal gradient on bulk temperature and noise correlation is critically analyzed. A dynamical contribution to conductivity when the system attains a nonequilibrium steady state of thermal conduction has been identified.

PACS. 44.10.+i Heat conduction – 05.60.-k Transport processes – 05.70.Ln Nonequilibrium and irreversible thermodynamics

1 Introduction

Understanding heat conduction in low dimensional systems [1–19] from a microscopic point of view has been the subject of renewed current interest. A major focus of these studies is the recovery of century-old classical Fourier heat law. It has been shown that the model systems like the ding-a-dong model [4], a one dimensional chain comprised of fixed equidistant harmonic oscillators and intervening free particles arranged between the fixed particles, and its variant, ding-dong model [5] obey the Fourier law, i.e., conductivity remains independent of the system size. It has been argued that this behavior owes its origin to the non-integrability of the models. This assertion, however, is not sufficient for a number of other models, e.g., Fermi-Pasta-Ulam [6] or Toda chains [7]. The role of various periodic potentials has been studied quite extensively [20] in the context of ratchets recently. The studies show that the periodic potential has significant effect on transport properties. Based on the study of a number of one dimensional chains with on-site potentials [9–11] it has been demonstrated that lattice-phonon interaction serves as a main ingredient for the applicability of the Fourier Law of thermal conductivity. For example, a harmonically coupled chain with on-site cosine potential — the Frenkel-Kontorova (FK) model exhibits conductivity which is independent of system size — the hallmark of Fourier law. An important question is what happens when we go from 1d to 2d systems? Keeping in mind that the lattice-phonon interaction in addition to the nature of the on-site potential depends on bulk temperature of the lattice [11], even for a given small temperature difference at the boundaries of the lattice, the nature of thermal conductivity and any associated anomalous behavior is expected to depend crucially on the bulk temperature of the lattice itself. In the present article we explore this dependence in a scalar FK model [21] where each potential minimum of the on-site potential is occupied by one lattice atom i.e. the commensurate case in two dimensions, the first example of this kind, in the context of anomalous conduction. Specifically our object is threefold; (i) to what extent the thermal gradient along the direction of heat flow as well as the thermal conductivity depends on bulk temperature of the medium; (ii) to understand the nature of the divergence of thermal conductivity with the system size for a range of bulk temperatures; (iii) to identify the specific nature of nonequilibrium or dynamical contributions to the conductivity over and above its thermodynamic counterpart, by exploring the role of dissipation when the system attains a nonequilibrium steady state of thermal conduction.

In what follows we show that unlike its 1d counterpart, the 2d FK model does not obey the Fourier law. Depending on bulk temperature the conductivity displays power law behavior with system size in contrast to logarithmic divergence as observed in several other 2d models [16,17]. The identification of the dynamical contribution to conductivity enables us to distinguish between the energy diffusion and spatial diffusion limited regimes in the mechanism of thermal conduction.

2 2d Frenkel-Kontorova lattice

We consider a 2d lattice made of $N_x \times N_y$ equal mass (assumed to be unity) particles coupled harmonically with nearest neighbor interaction of unit force constant. The lattice particles are also subjected to an on-site potential

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$U(q_{ij})$. The Hamiltonian of the 2d lattice is given by

$$H = \sum_{i=1,j=1}^{N_x,N_y} \frac{p_{ij}^2}{2} + \sum_{i=1,j=1}^{N_x,N_y} \Big[\frac{1}{2}\{(q_{ij}-q_{i-1j})^2+(q_{ij}-q_{i+1j})^2 + (q_{ij}-q_{ij-1})^2 + (q_{ij}-q_{ij+1})^2\} + U(q_{ij})\Big] \quad (1)$$

where q_{ij} and p_{ij} are the displacement from the equilibrium position and momentum of (ij) particle, respectively. The on-site potential exerts a pinning force on the particles due to which the lattice becomes stabilized. For the present study we have considered $U(q_{ij}) = \cos(q_{ij})$ as the on-site potential. The 2d harmonic lattice in the presence of this potential is the 2d version of the FK lattice. For the purpose of heat conduction two Langevin heat baths having different temperatures are connected to the left and the right sides of the lattice. In the reduced description the particles of the lattice connected to the heat baths contain, in addition to the usual force terms due to nearest-neighbor interaction potential and on-site potential, a dissipation and a random force due to heat baths. The properties of the heat baths are characterized defining the characteristics of the fluctuation/noise sources due to heat baths. We consider here two different types of noise correlations.

Case I: White noise

The Langevin force of the left and right baths, η^L and η^R are characterized by the well-known fluctuation-dissipation relation. In case of white noise the noise terms are instantaneously correlated to each other and are given by

$$\langle \eta_j^L \rangle = 0 = \langle \eta_j^R \rangle \quad (2)$$

$$\langle \eta_i^L(t)\eta_j^L(t')\rangle = 2\Gamma k_B T_L \delta(t-t')\delta_{ij} \quad (3)$$

$$\langle \eta_i^R(t)\eta_j^R(t')\rangle = 2\Gamma k_B T_R \delta(t-t')\delta_{ij} \quad (4)$$

where T_L and T_R are the temperatures corresponding to left and right heat baths. Γ and k_B are the usual Markovian dissipation and Boltzmann constant, respectively.

Case II: Colored noise

We consider Gaussian distribution of exponentially correlated noise due to the bath, in which case the fluctuation-dissipation relations are given by

$$\langle \eta_i^L(t)\eta_j^L(t')\rangle = \frac{\Gamma k_B T_L}{\tau_c} e^{-|t-t'|/\tau_c}\delta_{ij} \quad (5)$$

$$\langle \eta_i^R(t)\eta_j^R(t')\rangle = \frac{\Gamma k_B T_R}{\tau_c} e^{-|t-t'|/\tau_c}\delta_{ij} \quad (6)$$

τ_c is the correlation time of the noise. For numerical solution of the Langevin equations arising due to coupling of the particle with heat bath we have employed the standard procedure [19,26]. We have used fixed boundary condition $q_{0j} = 0 = q_{N_x+1j}$ and $q_{i0} = 0 = q_{iN_y+1}$. Depending on the situation we have used the time step of integration as $\Delta t = 0.001$–0.01 and the time for integration $t = 5\times10^5$–2×10^6. We take care of the required inequality $\Delta t \ll \tau_c$. In addition long time integration is necessary for appropriate equilibration of the system. The local temperature of the lattice, the equilibrium time average of the kinetic energy of the (ij) particle, is defined as $T_{ij} = \langle p_{ij}^2\rangle$. Since there is no heat bath at the upper and lower sides of the lattice there is no thermal gradient along the y direction and the temperature of the ith layer is given by averaging along this direction as $T_i = \frac{1}{N_y}\sum_{j=1}^{N_y} T_{ij}$. The local heat flux along x direction from the particle (ij) to $(i+1j)$ is defined as $J_{ij} = \frac{1}{2}\langle (q_{i+1j}-q_{ij})(\dot{q}_{ij}-\dot{q}_{i+1j})\rangle$. Heat flux in the ith layer is further given by $J_i = \frac{1}{2N_y}\left\langle \sum_{j=1}^{N_y}(q_{i+1j}-q_{ij})(\dot{q}_{ij}-\dot{q}_{i+1j})\right\rangle$. At equilibrium the local heat flux must be independent of site (i). The global thermal conductivity of the lattice is then given as

$$\kappa = \sum_{i=1}^{N_x} \frac{J_i}{(T_L - T_R)}. \quad (7)$$

3 Results and discussions

Having defined several quantifiers associated with heat conduction we first represent the local temperature profile at different bulk temperatures $[T = \frac{1}{2}(T_L + T_R)]$ keeping the temperature difference between the baths $\Delta T = 1$. Figures 1a–1c represent the local temperature profile at several values of bulk temperatures $T = 0.6$, $T = 3.0$ and $T = 9.5$ for a fixed system size $N_x = 40, N_y = 40$. It is evident that at low bulk temperatures, e.g. at $T = 0.6$ (Fig. 1a) no thermal gradient occurs along the bulk. At higher bulk temperature the profile shows a finite thermal gradient. In the 2d FK lattice heat is transmitted due to the interaction of phonons with the lattice (on-site potential). At low bulk temperature the lattice-phonon interaction is very weak and the lattice effectively behaves as a harmonic lattice resulting in no thermal gradient along the bulk [3]. With increase of bulk temperature as shown in Figures 1b, 1c phonon-lattice interactions become more prominent which cause thermal gradient along the bulk of the lattice. The results shown in Figures 1a–1c have been simulated in the Markovian limit with $\Gamma = 1.0$. We have checked that the presence of noise correlation does not change the above findings. Figures 1a–1c indicates that the temperature distribution along the chain is discontinuous at the boundary of the lattice. This discontinuity results from the strong boundary resistance, known as Kapitza resistance, across the interface. The temperature discontinuity appears at the boundary of two dissimilar substances. The mismatch of phonon modes, due to the dissimilarity of the substances, results in boundary resistance [22]. We have checked that the appearance of boundary jump is not due to the fixed boundary condition used in the simulation. Using both fixed boundary conditions in x and y directions, and open boundary conditions in x and periodic boundary conditions in y we find similar boundary jump of temperature (see Fig. 2).

It is interesting to note that a 1d FK lattice obeys [9,11] the Fourier law of heat conduction depending

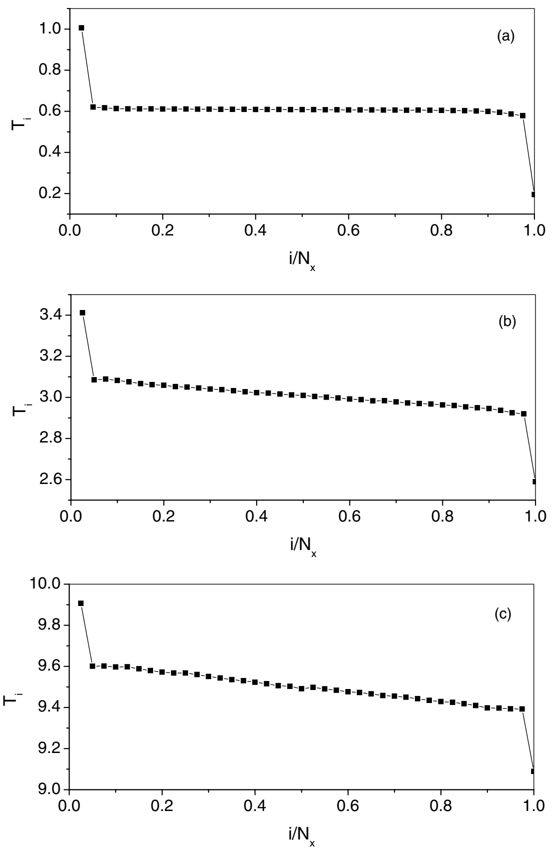

Fig. 1. Local temperature profile for 2d FK lattice at three different bulk temperatures (a) $T = 0.6$, (b) $T = 3.0$, and (c) $T = 9.5$ with $\Delta T = 1.0$, $\Gamma = 1.0$ and $N_x = N_y = 40$ in the Markovian limit (units arbitrary).

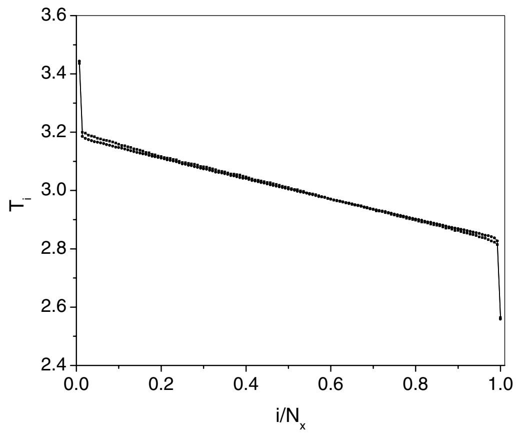

Fig. 2. Comparison of T_i vs. i/N_x profiles using two different boundary conditions, circles represent open boundary conditions in the x direction and periodic boundary conditions in the y direction, and boxes represent fixed boundary conditions in both directions using $N_x = N_y = 140$ and $\Gamma = 1.0$.

on the values of different parameters such as bulk temperature, coverage parameter, winding number etc. Whether 2d FK model exhibits similar behavior requires a closer look into the dependence of thermal conductance with

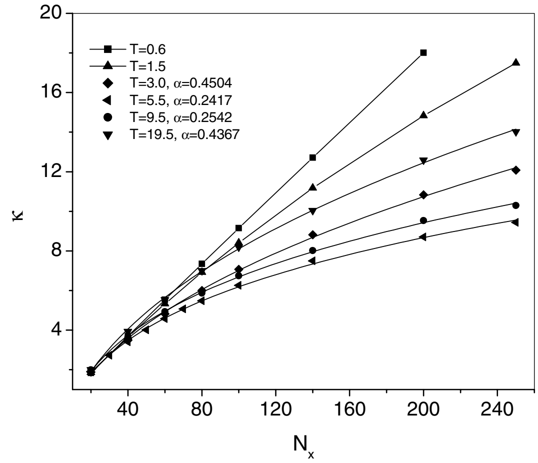

Fig. 3. Dependence of κ on system size (N_x) for 2d FK lattice at different T with $\Delta T = 1.0$ and $\Gamma = 1$ in the Markovian limit (solid line-fitted curve) (units arbitrary).

the system size and also the role of temperature on the system size dependence of thermal conductivity. To this end in Figure 3 we have plotted thermal conductivity, κ, of the lattice at different bulk temperatures, T, keeping $\Delta T = 1.0$ and for $\Gamma = 1.0$ in the Markovian limit. At very low bulk temperature $T = 0.6\,(T_L = 1.1, T_R = 0.1)$ κ diverges linearly with the system size. With increase of temperature $T = 1.5\,(T_L = 2.0, T_R = 1.0)$ the κ vs. N_x profile diverges slightly from linearity. In the intermediate to very high temperature regime ($T = 3.0, T = 5.5, T = 6.0, T = 9.5, T = 19.5$) κ, in general, obeys power law divergence $\kappa \propto N_x^{\alpha}$ with $0.3 < \alpha < 0.5$. At very low temperature as mentioned earlier the system behaves as a 2d harmonic lattice with no thermal gradient along the bulk of the lattice displaying linear divergence of κ. With increase of bulk temperature of the lattice the lattice-phonon interactions responsible for energy transfer set in in the system. This power law dependence of κ is in contrast to what has been observed in a wide class of 2d systems, e.g., harmonic lattice with disorder [18,19], Fermi-Pasta-Ulam β model [16,17] etc. In order to check the dependence of divergence of thermal conductivity with system size on boundary conditions we have carried out the simulation with open boundary condition in x and periodic boundary condition in y. Figure 4 shows the comparative profiles of κ vs. N_x for fixed boundary condition in both directions and open boundary condition in x and periodic boundary condition in y for the parameter set $T_L = 3.5$, $T_R = 2.5$, $\Gamma = 1.0$. It is clear from the figure that the overall qualitative nature of the curves does not change with the boundary conditions. The thermal conductivity still shows power law divergence with system size. Why the 2d scalar FK model shows power law divergence of thermal conductivity still remains an open problem. The preliminary findings of Li et al. [23] suggest that systems exhibiting normal diffusion follow the Fourier law of heat conduction whereas systems exhibiting anomalous diffusion do not obey the Fourier law. In view of their results there may be anomalous diffusion operating in the

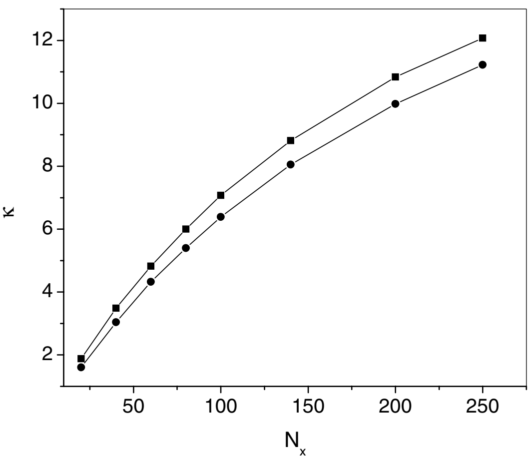

Fig. 4. κ vs. N_x for with two different types of boundary conditions, upper line using fixed boundary conditions in both directions and lower line using open boundary conditions in the x direction and periodic boundary conditions in the y direction with the parameter set $T_L = 3.5$, $T_R = 2.5$ and $\Gamma = 1.0$.

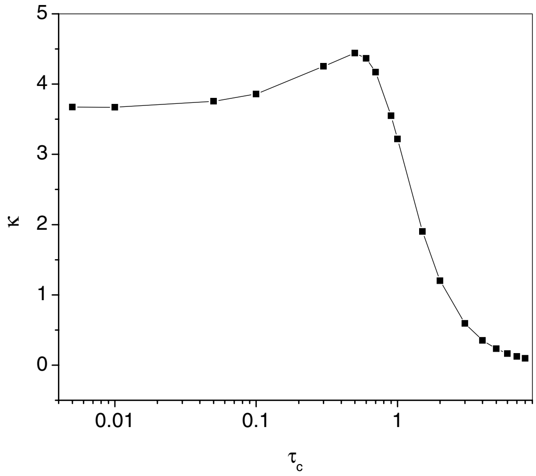

Fig. 5. Dependence of κ with correlation time (non-Markovian bath) τ_c.

2d scalar FK model resulting in the anomalous behavior of heat conductivity and power law dependence of thermal conductivity.

The effect of spectral properties of the heat bath has been considered earlier in the heat conduction problem for 1d FPU-β [24], disordered harmonic chain [25] etc. In the context of heat conduction in a 2d lattice we now study the effect of memory of heat bath. Figure 5 describes the effect of correlation time of noise (τ_c) of the heat bath on thermal conductivity for a lattice with size $N_x = 40$, $N_y = 40$, $T_L = 2.0$, $T_R = 1.0$ and $\Gamma = 1.0$. In the limit of small τ_c thermal conductivity is nearly independent of τ_c suggesting the Markovian nature of the heat bath. With the increase of τ_c, conductivity first increases followed by a sharp decrease which tends towards a stationary value of thermal conductivity. In the very short memory time regime the bath essentially behaves as a Markovian bath so that in this regime thermal conductivity is insensitive to

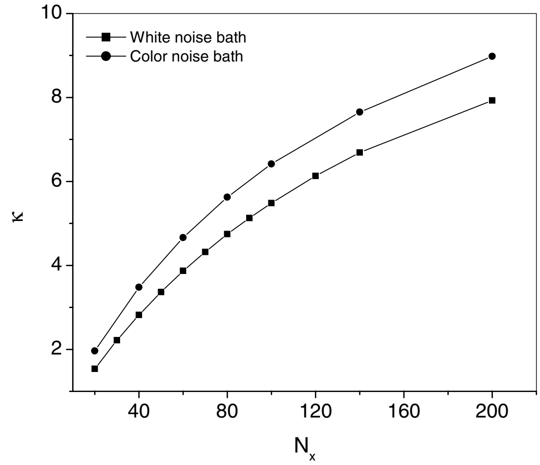

Fig. 6. Plot of thermal conductivity κ vs. system size N_x for two different heat baths, Markovian (circle) and no-Markovian baths ($\tau_c = 1.0$) (square).

response time of the heat bath. At the very high τ_c limit the large correlation of the thermal fluctuations puts a delay in the equilibration of system and thereby restricts the system to transport energy from one lattice site to another. To study the effect of correlation time of the bath on divergence profile of the thermal conductivity with system size we plot in Figure 6 κ vs. N_x for Markovian and non-Markovian heat baths. It is clear for the plot that there is no qualitative change in nature of divergence of κ with the system size suggesting that the non-Markovian effect does not play any significant role in the mechanism of energy transport along the lattice.

The effect of bulk temperature of the lattice on thermal conductivity is shown in Figure 7. The behavior of thermal conductivity with bulk temperature is a reflection of the lattice-phonon interaction at different temperatures. In the low temperature regime the nonlinearity due to the on-site cosine potential is insignificant. With increasing temperature the mean free paths of phonons are considerably reduced which leads to decrease in heat transport. At higher temperatures the lattice-phonon interactions set in and increase of temperature results in an increase of more active phonon modes leading to increase of heat transport. It is evident that above the crossover temperature (around $T \sim 5.0$ in Fig. 7) thermal conductivity follows the traditional Arrhenius behavior. This enables one to identify the thermal activation of each phase $(q_{i+1j} - q_{ij})$ or $(q_{ij+1} - q_{ij})$ over a barrier with a probability given by the Boltzmann factor $\exp(-E/k_BT)$ where E ($E \gg k_BT$) is the energy of activation, typically the height of potential energy barrier. The Arrhenius behavior of κ is the reflection of equilibrium thermal Boltzmann distribution function $\exp(-E/k_BT)$. But in the low temperature regime the equilibrium Boltzmann distribution is not a valid distribution function [26] for description of thermalization, so at low temperature κ does not show Arrhenius behavior. The low temperature behavior of the thermal conductivity can be accounted if the Boltzmann distribution $\exp(-E/k_BT)$ is

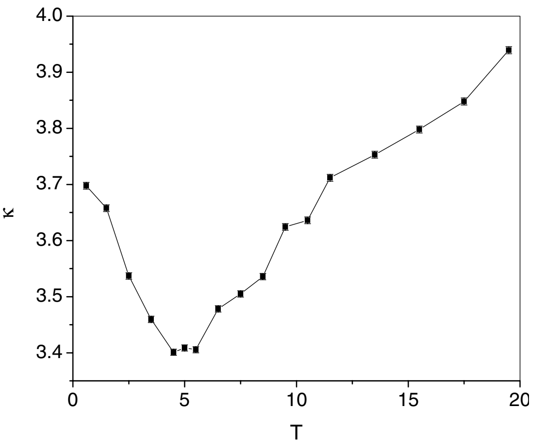

Fig. 7. Dependence of κ with T for the system size $N_x = N_y = 40$ keeping $\Delta T = 1.0$ with $\Gamma = 1.0$ in the Markovian limit (units arbitrary).

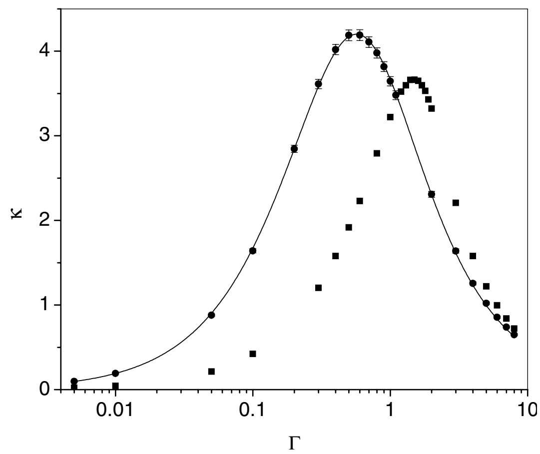

Fig. 8. Kramers' turnover for thermal conductivity: the variation of κ with Γ for Markovian bath (circle) and non-Markovian bath ($\tau_c = 1.0$) (square) with $T_L = 2$, $T_R = 1$ and $N_x = N_y = 40$. Solid lines are the fitted curves with interpolation formula as given in the text.

replaced by the Wigner canonical thermal distribution [27] $\exp(-E/\hbar\omega_0(\bar{n}(\omega_0) + 1/2))$ where ω_0 is the characteristic frequency of the system and $\bar{n}(\omega_0)$ refers to Bose-Einstein distribution of the form $\bar{n}(\omega_0) = [\exp(\hbar\omega_0/k_BT) - 1]^{-1}$, $\hbar$ is the Planck's constant. $\hbar\omega_0[\bar{n}(\omega_0) + 1/2]$ refers to the characteristic dispersion of energy, which goes over to k_BT in the classical limit $k_BT \gg \hbar\omega_0$, so that Wigner distribution reduces to Boltzmann distribution. On the other hand in the vacuum limit ($\bar{n} = 0$) this assumes the form of zero point energy $\hbar\omega_0/2$. Thus an interesting feature of this canonical thermal distribution is that it remains a valid pure state nonsingular distribution function even at absolute zero. The special advantage of this distribution has been exploited recently in developing a quantum Langevin equation [26] where the harmonic oscillator thermal bath is described by this canonical distribution function.

While the Boltzmann factor pertains to an equilibrium situation, it is also interesting to extract out the dynamical contribution over and above the thermodynamic contribution to thermal conductivity under nonequilibrium steady state conditions. To this end we have plotted the variation of κ with dissipation constant Γ in Figure 8. The conductivity first increases linearly with Γ in the low dissipation regime followed by a decrease as Γ^{-1} in the high dissipation regime after passing through a maximum and thus exhibiting a bell-shaped curve. It is easy to understand that this variation remains outside the purview of the theory of activation which is essentially thermodynamic in its content. A clue in understanding this variation lies in the resemblance of this turnover of κ as a Kramers turnover of rate constant. If we take care of nonequilibrium contributions [28] to κ as $\kappa = \kappa_{thermodynamic} \times f_{nonequilibrium}$. In view of the strong similarity between thermal conductivity and the Kramers' rate constant associated with the activated barrier crossing, we mean by 'thermodynamic contribution' the contribution due to the Arrhenius factor of the rate constant while 'dynamical contribution' corresponds to the factor which appears due to the nonequilibrium steady state dynamics of the system which can be identified as the pre-exponential factor of the rate constant. When $f_{nonequilibrium} = \omega_b^{-1}(-\Gamma/2 + \sqrt{(\Gamma/2)^2 + \omega_b^2})$ in the intermediate to strong dissipation regime and $f_{nonequilibrium} = \Gamma A$ in the low dissipation regime where ω_b and A are appropriately chosen constants it is possible to account for the turnover by a fitted curve as shown by the solid line in Figure 8, at two different baths (Markovian and non-Markovian) with the help of an interpolation formula [28] of the form $\kappa^{-1} = \kappa_{IH}^{-1} + \kappa_W^{-1}$. Here the IH and W refer to intermediate to high and weak damping, respectively. Figure 8 in contrast to Figure 7 therefore extracts out the nonequilibrium steady state contribution over and above the thermodynamic contribution to thermal conductivity and we may infer that both spatial diffusion as well as energy diffusion are integral parts of the mechanism of heat conduction in high and low dissipation regimes. In Kramers' theory it is possible to calculate explicitly the constants A and ω. In the context of heat conduction we believe that it is possible to calculate these constants starting from a microscopic approach of the problem. The calculation of explicit analytic expression of thermal conductivity still remains to be addressed. Keeping in mind the resemblance with the Kramers's rate constant the model parameters should be dependent on T and τ_c.

4 Conclusion

To summarize we have considered anomalous heat conduction in a scalar 2d FK model with commensurate structure. It has been shown that the occurrence of a thermal gradient depends crucially on the bulk temperature. In turn, the nature of the thermal gradient determines the behavior of thermal conductivity as a function of system size. While in the harmonic limit achievable at very low temperature of the bulk the conductivity diverges linearly, one observes power law divergence at some intermediate range of temperatures. This is markedly different from what has been found earlier in a class of 2d lattices (e.g. Fermi-Pasta-Ulam β lattice [16] etc.) exhibiting logarithmic dependence of κ on the system size. This puts a question mark on the conjecture that logarithmic divergence in 2d systems is fairly universal. We have also explored the effect of response time of Langevin heat baths on the thermal conductivity and also on the divergence profile of the thermal conductivity with lattice size. The study shows that the effect of heat bath response time is very weak on the divergence profile. The study of the dependence of κ on dissipation enables us to identify the regimes of spatial diffusion or energy diffusion as a part of nonequilibrium dynamical contribution to thermal conductivity beyond its thermodynamic content.

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