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Influence of heat bath on the heat conductivity in disordered anharmonic chain

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Abstract. We study heat conduction in a one-dimensional disordered anharmonic chain with arbitrary heat bath by using extended Ford, Kac and Mazur (FKM) formulation, which satisfy the fluctuation-dissipation theorem. A simple formal expression for the heat conductivity κ is obtained, from which the asymptotic system-size (N) dependence is extracted. It shows $\kappa \sim N^{\alpha}$. As a special case we give the expression that $\kappa \sim N^{1/2}$ for free boundaries, and $\kappa \sim N^{-1/2}$ for fixed boundaries, from which we can get the conclusion that the momentum conservation is a key factor of the anomalous heat conduction. Comparing with different ∇T, the heat conductivity shows large difference between the linear system and the nonlinear system.

PACS. 44.10.+i Heat conduction – 05.70.Ln Nonequilibrium and irreversible thermodynamics – 05.60.Gg Quantum transport – 05.45.Ac Low-dimensional chaos

The problem of heat conduction in one dimensional system is an interesting one in the context of nonlinear dynamics and nonequilibrium statistical physics, which has attracted more attention in the past two decades due to the dramatic achievement in the application of miniaturized devices [1–3]. More and more numerical calculations are focused on the dependence of the heat current J on system size N. According to the Fourier's law one expects $J \sim 1/N$, and many works about this have been done, in their works many different heat baths [4] were arbitrarily adopted, since these researchers believed that the heat conduction is only the characteristic of the system itself, and it should be independent of the boundary conditions. But a large number of studies suggest that in one dimensional chain it may not always be true, and suppose that $J \sim 1/N^{\alpha}$, where N is the length of the lattice. One of the earliest modes investigated was the disordered harmonic chain (DHC). Thus the problem is analytically tractable to a large extent and the exponent α has been obtained analytically, though in a semirigorous way. It is found that α depends on boundary conditions, for the fixed boundary conditions $\alpha = 1/2$ and for free boundary conditions $\alpha = 3/2$. Later on, in order to show that exponential instability is a necessary condition, Alonso et al. [5–9] studied the heat conduction in a Lorentz gas channel and a quasi-1D billiard with circular scatterers, systems with linear instability, and found that heat conduction obeys the Fourier law. However, the dependence of heat conduction on boundary condition has not been studied in a precise way.

In this paper, we revisit this problem. We take a general formulation of the problem for a disordered anharmonic chain (FPU chain) which can let us view the two different boundary conditions as two special cases of a range of possible thermal reservoirs satisfying the fluctuation dissipation theorem. The method is based on the formalism which was first developed by Ford, Kac, and Mazur (FKM), They dealt with the reservoirs as an infinite noninteracting system in their works [10–12]. Initially, it was used to study Brownian motion in coupled oscillators and was later inducted to a general study with the problem of quantum particles coupled to the quantum mechanical heat reservoir [13,14]. In the approach reservoirs are assumed to be a collection of oscillators which are initially in equilibrium. The reservoirs degrees of freedom are then eliminated, and the system can use quantum Landauer equation to study it. Thus the reservoirs can be viewed as a source of noise and dissipation to the system. Our work presents the formalism for bosons, which is applied to the thermal conductance. The heat conductivity is investigated when the chain connects to two different model heat baths separately. It can be found that the heat conductivity κ depends on not only the properties of the disordered chain itself but also the spectral properties of the heat baths, and the dependence of heat conductivity on the heat temperature is also our interest. Furthermore, the effect of system itself on heat current is investigated for the special case.

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We consider heat conduction through a one-dimensional disordered anharmonic chain. Particles $i = 1, 2, ..., N$ with random masses are connected by equal spring constants. The general 1D many-body Hamiltonian of the system can be written as

$$H_0 = \sum_{l=1}^{N} \frac{p_l^2}{2m_l} + \sum_{l=1}^{N-1} \frac{(x_l - x_{l+1})^2}{2} + \frac{(x_1^2 + x_N^2)}{2} + \lambda \sum_{l=1}^{N-1} \frac{(x_l - x_{l+1})^4}{4} \quad (1)$$

where x_l are the displacements of the particles about their equilibrium positions; p_l are their momenta; m_l are the random masses. The particles in the bulk evolve through the Heisenberg equations of motion while the boundary particles 1 and N are coupled to the reservoirs. Furthermore, the coupling to heat baths is effected by including dissipative and noise terms in the equations of motion of the end particles.

We consider the following equations of motion [15],

$$\begin{aligned} m_1 \ddot{x}_1 =& -(2x_1 - x_2) + \lambda(x_2 - x_1)^3 \\ &+ \gamma \int_{-\infty}^{t} dt' A_L(t - t') \times x_1(t') + \eta_L(t) \\ m_l \ddot{x}_l =& -(-x_{l-1} + 2x_l - x_{l+1}) \\ &- \lambda[(x_l - x_{l-1})^3 - (x_{l+1} - x_l)^3] \\ m_N \ddot{x}_N =& -(2x_N - x_{N-1}) - \lambda(x_N - x_{N-1})^3 \\ &+ \gamma' \int_{-\infty}^{t} dt' A_R(t - t') \times x_N(t') + \eta_R(t) \end{aligned} \quad (2)$$

where the terms $A_{L,R}(t)$ and $\eta_{L,R}(t)$ describe the dissipation and noise. The characteristics of these terms will be specified soon. At time $t = -\infty$, the reservoirs are in thermal equilibrium. To obtain the particular solution to this set of equations we define the Fourier transforms:

$$\begin{aligned} x_l(\omega) &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt x_l(t) e^{i\omega t}, \\ A^{+}_{L,R}(\omega) &= \int_{-\infty}^{+\infty} dt A_{L,R}(t) e^{i\omega t}, \\ \eta(\omega) &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} \eta_l(t) e^{i\omega t}. \end{aligned} \quad (3)$$

We can get the following particular solution through the Fourier transformation:

$$\begin{aligned} x_l(t) &= \int_{-\infty}^{+\infty} d\omega \hat{Z}^{-1}_{lm}(\omega) \eta_m(\omega) e^{-i\omega t}, \\ \hat{Z}_{lm} &= \hat{\phi}_{lm} - \hat{A}_{lm} \end{aligned} \quad (4)$$

with

$$\begin{aligned} \hat{\phi}_{lm} &= -(\delta_{l,m+1} + \delta_{l,m-1}) + (2 - m_l \omega^2)\delta_{l,m}, \\ \hat{A}_{lm} &= \delta_{l,m}[\gamma^2 A_L(\omega)\delta_{l,1} + \gamma'^2 A_R(\omega)\delta_{l,N}], \\ \eta_l(\omega) &= \gamma \eta_L(\omega)\delta_{l,1} + \gamma' \eta_R(\omega)\delta_{l,N} + \lambda[F_l - F_{l+1}]. \end{aligned} \quad (5)$$

The full of solution at time t would be the sum of this particular solution and a general solution of the homogeneous equation, which would depend on the initial conditions. There we are only interested in the non-equilibrium steady state properties, so we will not consider the general solution here. The function $F_{l,l+1}$ give a rise to nonlinear effects characterized by

$$\begin{aligned} F_l = (x_l(\omega) - x_{l-1}(\omega)) \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} d\omega' d\omega'' \\ \times (x_l(\omega') - x_{l-1}(\omega'))(x_l(\omega'') - x_{l-1}(\omega'')). \end{aligned} \quad (6)$$

For the properties of the dissipation and noise we will give a simple explanation. Let us consider the system driven by a noise $\eta(\omega)$ with the following correlation [14]

$$\langle \eta_L(\omega) \eta_R(\omega') \rangle = I(\omega) \delta(\omega + \omega') \quad (7)$$

where

$$I(\omega) = f(\omega) b(\omega)/\pi \quad (8)$$

$\eta(\omega)$ and $\eta'(\omega')$ are independent, so $\langle \eta(\omega) \eta'(\omega') \rangle = 0$. When the dissipation is given by $A(\omega) = a(\omega) - ib(\omega)$, $a(\omega)$ and $b(\omega)$ are real. We turn to calculate the steady-state heat current and average kinetic energy. According to the current conservation $\partial \hat{u}/\partial t + \partial \hat{J}/\partial x = 0$, we arrive at

$$\hat{J} = (\dot{x}_{l-1} x_l - \dot{x}_l x_{l-1})/2. \quad (9)$$

By using equation (4) and its solution, we can get

$$\begin{aligned} \langle J \rangle = \int_{-\infty}^{+\infty} d\omega (i\omega) [\gamma^2 \hat{Z}^{-1}_{l,1}(\omega) \hat{Z}^{-1}_{l-1,1}(-\omega) I(\omega) \\ + \gamma'^2 \hat{Z}^{-1}_{l,N}(\omega) \hat{Z}^{-1}_{l-1,N}(-\omega) I'(\omega)] + P_l. \end{aligned} \quad (10)$$

It's the nonlinear general solution of the disordered anharmonic oscillator chain. The P_l is just the result of the nonlinear interaction. If we ignore the item P_l, it will become the solution of DHC.

Large numbers of past numerical simulations of the non-integrable system had been verified that we can use the Fourier law to study it [16–18],

$$\langle J \rangle = -\kappa \nabla T. \quad (11)$$

Here, κ is the transport coefficient of thermal conductivity.

In the literature the dependence of κ on the size of system N has been used to characterize the anomalous conductor. The work of Hatano about heat conduction had proved that no gap existed in the temperature profile. So we can safely define the thermal conductivity as

$$\kappa = \frac{\langle J \rangle N}{T_L - T_R} \quad (12)$$

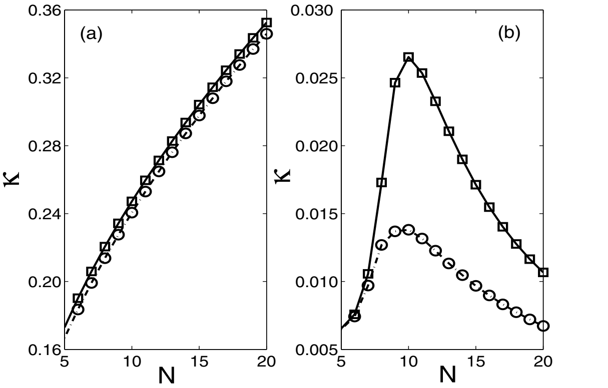

Fig. 1. System size (N from 5 to 20) dependence of the heat conductivity with considering different heat bath. Squares correspond to the FPU model with $\lambda = 1$. Circles represent the DHC model with $\lambda = 0$. Here $T_L = 1.0$ and $T_R = 0.2$, (a) we consider $A(\omega) = 1 - i\omega$; (b) we take $A(\omega) = -ir\omega$.

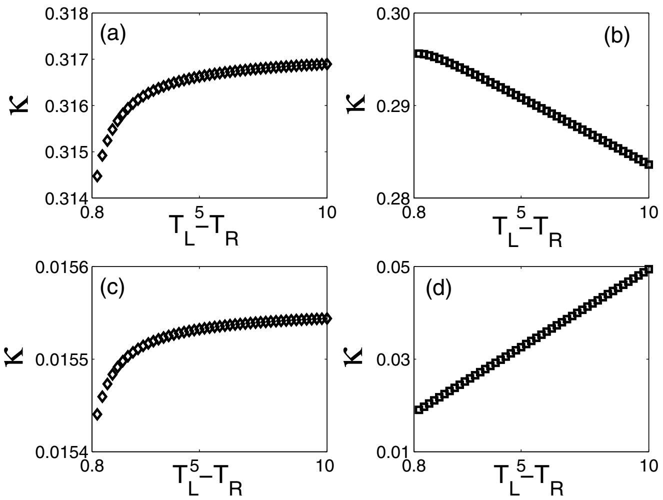

Fig. 2. ΔT (it's defined as $T_L - T_R$) dependence of κ, (a) and (c) represents the result of the DHC model; (b) and (d) correspond to the FPU-β model ($\lambda = 0.5$). ΔT from 0.8 to 10.0

where $\langle J \rangle$ is defined by equation (10). The system size dependence of the thermal conductivity is shown in Figure 1. We can get

$$\kappa \sim N^{\alpha}. \tag{13}$$

When we take into consideration the heat bath with the condition of Rubin-Greer model, we can see $\kappa \sim N^{\frac{1}{2}}$ in Figure 1a clearly. To the Lebowitz model, when the size of system is $N \leq 9$, the heat conductivity κ increases along with the N, and when the size is $N > 9$ we can find $\kappa \sim N^{-\frac{1}{2}}$. For finite N, we find from our numerical studies that low frequency modes largely reflects the translational invariance of the model and the only significant contribution to the κ comes from low components of order $\omega \leq 1/N^{1/2}$.

In Figure 2, we plot the ΔT dependence of κ. The particle number is kept at $N = 16$. From (a) and (c), we can see that the result of κ is driving to a constant as the size increase. For the nonlinear system, it appears to be a linear behavior. No matter what models heat bath are adopted by us, the result shows $\kappa \sim 1/T$ in Figures 2b and 2d. It's demonstrated that (b) and (d) obey the Fourier law if the system is a momentum conservation system, and in the case of anharmonic interparticle potential $V(x_{l-1}, x_l)$ such as our studied FPU model, the phonon-phonon interaction is produced due to the anharmonicity. Although the temperature gradient can be formed, the results are shown that the thermal conductivity diverges in the works of Hu et al. [19] at low temperature as well as ours at high temperature. As long as the lattice exists, the phonons will be scattered by it and those results in thermal resistance, eventually leading to the Fourier law, and we believe that it might be a general rule that if the phonon-lattice interaction is dominant, the heat conduction will obey the Fourier law, no matter the system is a harmonic or anharmonic one.

In order to investigate the contribution of the system to the current, we take into account $\lambda = 0$, using equations (2, 7) and after some algebraic manipulation, equa-

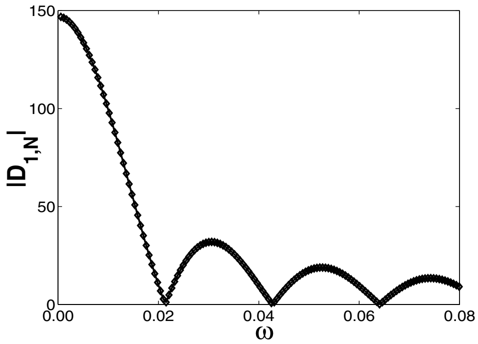

Fig. 3. Frequency dependence of $|D_{1,N}|$ at low frequency ω for $\delta m = 0$ and $N = 148$.

tion (9) is reduced to the following simple form

$$\langle J \rangle = \int_{-\infty}^{+\infty} d\omega t_N^2(\omega)(f - f'). \tag{14}$$

We note that

$$t_N^2(\omega) = \gamma^2 \gamma'^2 \omega b(\omega) b'(\omega) \Big/ (\pi \left| Y_{1,N} \right|^2), \tag{15}$$

which is like a transmission coefficient, depends on both system and bath properties. We write the $\mathrm{Det}[Y_{1,N}] = D_{1,N} - A(\omega)(\gamma^2 D_{2,N} + \gamma'^2 D_{1,N-1}) + \gamma^2\gamma'^2 A^2(\omega) D_{2,N-1}$, where $D_{l,m}$ denotes determinant of the submatrix formed from ϕ. Clearly, $D_{l,m}$ depends on the system alone while $A(\omega)$ depends on the bath. We can see that the $\omega \longrightarrow 0$ give the main effect on the current in Figure 3. At the mean time, the effects of the ω display some periodic properties with the amplitude decreased.

In summary, We start with the Heisenberg's equation of motion and have studied the nonequilibrium steady state of a one-dimensional disordered chain coupling to heat bath at different temperatures. We find that the size dependence, $\kappa \sim N^{\alpha}$, is determined not just by the properties of the system; the exponent α depends on the low-frequency spectral properties of the bath. Dhar's work has mentioned (i) $A(\omega) \sim -i\mathrm{sgn}(\omega)\omega^s$, there $\alpha = -s/2$ for $s > 0$; (ii) $A(\omega) \sim 1 - \mathrm{sgn}(\omega)\omega^s$, then $\alpha = s/2$ for $0 < s < 1$ and $\alpha = 1 - s/2$ for $s \geq 1$ [15,20]. It seems to be conflicting with the general viewpoint of nonequilibrium statistical mechanics that the steady state of a close-to-equilibrium system will not depend on details of the boundary conditions to sustain the steady state. In our work, we find the anomalous heat conductivity as a simple consequence of the total momentum conservation and the result consistent with the conclusions of Prosen [21].

We have established a connection between normal heat conduction and anomalous heat conduction in 1D system. Equation (13) includes all possible results which are observed in different heat bath models. We have given a comparison between the harmonic conditions and the anharmonic conditions and found some similar properties to each other which have shown in our conclusions and pictures. At the same time many diversities are found, to which more attentions have been paid. It's obvious that the temperature dependence of heat conductivity is nonlinear character for the harmonic chain, while linear for the anharmonic chain. At the end of the paper, the effects of different ω on the current at low frequency are discussed and some interesting phenomena are discovered. The conclusions which we have gotten from the above may have a great help for us to investigate the heat conduction of nanophase materials, the single walled carbon nanotubes, nanowires and so on [22,23].

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