Heat conduction in the disordered harmonic chain revisited

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A general formulation is developed to study heat conduction in disordered harmonic chains with arbitrary heat baths that satisfy the fluctuation-dissipation theorem. A simple formal expression for the heat current J is obtained, from which its asymptotic system-size (N) dependence is extracted. It is shown that the "thermal conductivity" depends not just on the system itself but also on the spectral properties of the fluctuation and noise used to model the heat baths. As special cases of our heat baths we recover earlier results which reported that for fixed boundaries $J \sim 1/N^{3/2}$, while for free boundaries $J \sim 1/N^{1/2}$. For other choices we find that one can get other power laws including the "Fourier behaviour" $J \sim 1/N$.

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The problem of heat conduction in one-dimensional classical systems of interacting particles has attracted a lot of attention in recent years [1]. A central issue here is determination of the dependence of the heat current J on system size N. According to Fourier's law one expects $J \sim 1/N$ but a large number of studies [1–5,8–13] suggest that in one dimensions this may not always be true. Instead one finds that $J \sim 1/N^{\alpha}$ where α is usually different from one. Some obviously interesting and important questions are: what are the necessary and sufficient conditions under which $\alpha = 1$?, what does α depend on and are there universality classes? One of the main problems in the field has been that most studies have been limited to numerical simulations of nonlinear systems and it has been difficult to arrive at definite conclusions from results of such studies. Thus, so far no clear understanding has emerged. We note that numerical simulations are problematic because: (i) accurate numerical solutions of nonlinear equations are very time consuming, (ii) equilibration times are typically very long and this limits one to small system sizes and (iii) dependence on boundary conditions not clearly understood.

One of the earliest models to be investigated was the disordered harmonic chain [2–5]. This problem is analytically tractable to a large extent and the exponent α has been obtained analytically, though in a semi-rigorous way. Surprisingly α seems to depend on boundary conditions: for fixed boundary conditions (the Lebowitz model [4]) $\alpha = 1/2$, while for free boundaries (the Rubin-Greer model [3]) $\alpha = 3/2$. This dependence on boundary conditions has not been understood in a precise way.

In this paper we revisit this problem. We present a general formulation of the problem which enables one to view the two different boundary conditions as two special cases of a range of possible thermal reservoirs satisfying the fluctuation dissipation theorem. An approximate scheme, based on results from the theory of product of random matrices, along with inputs from our numerical studies, enables us to obtain the asymptotic N-dependence of the current. We find the surprising result that *the exponent α depends not only on the properties of the disordered chain itself, but also on the spectral properties of the heat baths*. For special choices of baths one gets the "Fourier behaviour" $\alpha = 1$.

We consider heat conduction through a one-dimensional disordered harmonic chain. Particles $i = 1, 2...N$ with random masses are connected by harmonic springs with equal spring constants (set to the value 1). The Hamiltonian of the system is thus

$$H = \sum_{l=1}^{N} \frac{p_l^2}{2m_l} + \sum_{l=0}^{N} \frac{(x_l - x_{l+1})^2}{2} \qquad (1)$$

where $\{x_l\}$ are the displacements of the particles about their equilibrium positions, $\{p_l\}$ their momenta and $\{m_l\}$ are the random masses. We put the boundary conditions $x_0 = x_{N+1} = 0$. The particles in the bulk evolve through the classical equations of motion while the boundary particles, namely particles 1 and N are coupled to heat baths. The coupling to heat baths is effected by including dissipative and noise terms in the equations of motion of the end particles. The choice of the dissipative and fluctuating forces is not unique. Different forms can be chosen provided that they satisfy the fluctuation-dissipation theorem.

We consider the following equations of motion for the particles:

$$\begin{aligned} m_1 \ddot{x_1} &= -2x_1 + x_2 + \int_{-\infty}^{t} dt' A_L(t-t') x_1(t') + \eta_L(t) \\ m_l \ddot{x_l} &= -2x_l + x_{l-1} + x_{l+1} \qquad l = 2, 3...(N-1) \\ m_N \ddot{x_N} &= -2x_N + x_{N-1} + \int_{-\infty}^{t} dt' A_R(t-t') x_N(t') + \eta_R(t), \end{aligned} \qquad (2)$$

where the terms $A_{L,R}(t)$ and $\eta_{L,R}(t)$ describe dissipation and noise, and will be specified later. We assume, unlike [2], that the heat baths have been switched on at $t = -\infty$. To obtain the particular solution to these set of equations we define the Fourier transforms $x_l(\omega) = \int_{-\infty}^{\infty} x_l(t)e^{-i\omega t}$; $\eta_{L,R}(\omega) = \int_{-\infty}^{\infty} \eta_{L,R}(t)e^{-i\omega t}$; $A_{L,R}(\omega) = \int_0^{\infty} A_{L,R}(t)e^{-i\omega t}$. Plugging these into Eq. (2) leads to the following particular solution:

$$
\begin{aligned}
x_l(t) &= \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega \hat{Y}^{-1}_{lm}(\omega)\hat{\eta}_m(\omega)e^{i\omega t}, \qquad \text{where} \qquad (3)\\
\hat{Y} &= \hat{\Phi} - \omega^2\hat{M} - \hat{A}(w) \qquad \text{with}\\
\hat{\Phi}_{lm} &= -\delta_{l,m+1} + 2\delta_{l,m} - \delta_{l,m-1}\\
\hat{M}_{lm} &= m_l\delta_{l,m}; \qquad \hat{A}_{lm} = \delta_{l,m}(A_L(\omega)\delta_{l,1} + A_R(\omega)\delta_{l,N})\\
\hat{\eta}_l &= \eta_L(\omega)\delta_{l,1} + \eta_R(\omega)\delta_{l,N}.
\end{aligned}
$$

The full 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. Since we are interested in the steady state properties only, we will not require the general solution.

We now specify the properties of the dissipation and noise. Let us consider a system driven by a stationary noise $\eta(t)$ with the following correlator

$$\langle \eta(\omega)\eta(\omega')\rangle = 2\pi T I(\omega)\delta(\omega+\omega'). \qquad (4)$$

If the dissipation is given by $A(\omega) = a(\omega) - ib(\omega)$, where $a(\omega)$ and $b(\omega)$ are real, then it follows from the fluctuation dissipation theorem [6] that the choice

$$I(\omega) = 2b(\omega)/\omega \qquad (5)$$

ensures thermal equilibration of the system to the temperature T. We choose the same $I(\omega)$ and $A(\omega)$, satisfying Eq. (5), at both boundaries. The noise correlators given by Eq. (4) are made different by setting $T = T_L$ at the left end and $T = T_R$ at the right end. For thermal equilibration it is necessary that the range of frequencies, over which $I(\omega)$ is non-zero, includes the normal modes of the disordered chain, and we will only consider cases where this is true.

For any given disorder realization, the energy current in the steady state is given by

$$J = \langle [\int_{-\infty}^{t} dt' A_L(t-t')x_1(t') + \eta_L(t)]\dot{x}_1(t)\rangle, \qquad (6)$$

where $\langle ...\rangle$ denotes a noise average. Using Eqs. (3,4,5), and after some algebraic manipulations, this reduces to the following simple form:

$$
\begin{aligned}
J &= \frac{T_L - T_R}{4\pi}\int_{-\infty}^{\infty} d\omega t_N^2(\omega) \qquad \text{where} \qquad (7)\\
t_N^2(\omega) &= 4b^2(\omega)Y^{-1}_{1N}(\omega)Y^{-1}_{1N}(-\omega)
\end{aligned}
$$

We note that $t_N^2(\omega)$, which is like a transmission coefficient, depends both on the system and bath properties. We now proceed to write the current in a form where the separate effects of the bath and system are more explicit. We first note that

$$
\begin{aligned}
& Y^{-1}_{1N}(\omega)Y^{-1}_{1N}(-\omega) = |\Delta_N(\omega)|^{-2} \quad \text{with}\\
& \Delta_N(\omega) = Det[Y]\\
&= D_{1,N} - A(\omega)(D_{2,N} + D_{1,N-1}) + A^2(\omega)D_{2,N-1}\\
&= (1, \quad -A(\omega))\begin{pmatrix} D_{1,N} & -D_{1,N-1}\\ D_{2,N} & -D_{2,N-1}\end{pmatrix}\begin{pmatrix}1\\ A(\omega)\end{pmatrix}, \qquad (8)
\end{aligned}
$$

where $D_{l,m}$ is defined to be the determinant of the submatrix of $\hat{\Phi} - \omega^2\hat{M}$ beginning with the lth row and column and ending with the mth row and column. Clearly $D_{l,m}$ depends on the system alone while $A(\omega)$ depends on the bath. We further note the following result which is easy to prove:

$$
\begin{aligned}
&\begin{pmatrix} D_{1,N} & -D_{1,N-1}\\ D_{2,N} & -D_{2,N-1}\end{pmatrix} = T_1T_2....T_N \qquad \text{where} \qquad (9)\\
&T_l = \begin{pmatrix} (2 - m_l\omega^2 & -1\\ 1 & 0\end{pmatrix}
\end{aligned}
$$

The results of [2,4] follow from the following choices of heat baths:

$$
\begin{aligned}
&\text{(i) Lebowitz model}: A(\omega) = -i\gamma\omega;\ I(\omega) = 2\gamma, \qquad (10)\\
&\text{(ii) Rubin} - \text{Greer model}:\\
&A(\omega) = 1 - \frac{\omega^2}{2} - i\frac{\omega}{2}(4-\omega^2)^{1/2};\ I(\omega) = (4-\omega^2)^{1/2} \quad |\omega| < 2\\
&A(\omega) = 1 - \frac{\omega^2}{2} + \frac{\omega}{2}(4-\omega^2)^{1/2};\ I(\omega) = 0 \quad |\omega| > 2 \qquad (11)
\end{aligned}
$$

Using these in Eq. (7) we get the heat currents, J_L and J_{RG}, for the two models respectively as:

$$
\begin{aligned}
&J_L = \pi^{-1}(T_L - T_R)\gamma^2\int_{-\infty}^{\infty} d\omega\omega^2 j_N(\omega)\\
&j_N(\omega) = \{2\gamma^2\omega^2\\
&+D^2_{1,N} + \gamma^2\omega^2(D^2_{1,N-1} + D^2_{2,N}) + \gamma^4\omega^4D^2_{2,N-1}\}^{-1} \qquad (12)\\
&J_{RG} = (4\pi)^{-1}(T_L - T_R)\int_{-2}^{2} d\omega\omega^2(4-\omega^2)j_N(\omega)\\
&j_N(\omega) = \{D^2_{1,N} + D^2_{2,N-1} + (D_{1,N-1} + D_{2,N})^2\\
&\qquad + 2[2(1-\omega^2/2)^2 - 1]D_{1,N}D_{2,N-1}\\
&-2(1-\omega^2/2)(D_{1,N} + D_{2,N-1})(D_{1,N-1} + D_{2,N})\}^{-1}, \qquad (13)
\end{aligned}
$$

which are the same as in [2,4] (the differences are due to a slightly different convention used by us). Semi-rigorous arguments [2,3,5] indicate that $\langle J_L\rangle \sim 1/N^{3/2}$ while $\langle J_{RG}\rangle \sim 1/N^{1/2}$, where the angular brackets now denote a disorder average. For finite chains it is straightforward to numerically compute the integrals appearing in Eqs. (12,13) for given realizations of disorder and then perform disorder averages to obtain $\langle J_L\rangle$ and $\langle J_{RG}\rangle$. We show the results in Fig. (1) for the case where the masses are chosen from a uniform distribution between $1-\delta m$ to $1+\delta m$. We do get the expected power-law behaviours.

We now present a scheme which allows us to determine the N-dependence of the current for arbitrary choices of heat baths. This is based on the following observations:

(i) The first observation follows from the Furstenberg theorem on the limiting form of product of random non-commuting variables. For the case considered here, the theorem states that, for almost any choice of the sequence of random masses $\{m_l\}$,

$$\lim_{N\to\infty} \frac{1}{N} \log |T_1 T_2 .... T_N u| = \gamma(\omega) > 0 \qquad (14)$$

for any non-zero vector u, with fluctuations of order $1/\sqrt{N}$. Further it can be shown that [2,5] in the limit $\omega \to 0^+$,

$$\gamma(\omega) \to (< m^2 > - < m >^2) w^2 / (8 < m >). \qquad (15)$$

This means [from Eq. (9)] that the $D_{l,m}$, which occur in the denominator of the integrand in Eq. (7), diverge exponentially with N, and hence the only significant contribution to the current comes from low frequency components of order $\lesssim 1/N^{1/2}$. We note that the fact that low frequency modes are extended follows from the translational invariance of the random-mass model.

(ii) The result Eq. (15) has been obtained in the strict limit of $N \to \infty$ when the ratio of successive particle displacements reaches a stationary state. For finite N, we find from our numerical studies that this result is true only for $\omega \gtrsim 1/N^{1/2}$. In Fig. (2) we have plotted $\langle |D_{1,N}| \rangle$ as a function of frequency. We find that the exponential growth predicted by Eq. (15) does not occur at $\omega \lesssim 1/N^{1/2}$. In this range we find instead [see Fig. (3)] that $D_{1,N}$ is very accurately given by its form for the ordered case with masses all equal to $< m >= 1$. Thus over the range $\omega \lesssim 1/N^{1/2}$, we shall approximate $j(\omega)$ in Eq. (7) by its form for the ordered chain. We expect this approximation to be good as long as we are interested only in the asymptotic N-dependence.

For the equal mass case one has $D_{1,N} = \sin[k(N+1)]/\sin(k)$ where $\omega = 2\sin(k/2)$. Hence within our approximate scheme we then get the following expression for the disorder-averaged current:

$$\langle J \rangle \sim (T_L - T_R) \int_0^{1/N^{1/2}} f(k) dk \qquad (16)$$
$$f(k) = b^2(\omega) \sin^2(k) \cos(k/2) \times \{ |\sin[k(N+1)] - 2A(\omega)\sin(kN) + A^2(\omega)\sin[k(N-1)]| \}^{-2}.$$

It is clear that the form of $A(\omega)$ at low frequencies will determine the asymptotic N-dependence of the current. For the Lebowitz model $A(\omega) = -i\gamma\omega$ while for the Rubin-Greer model $A(\omega) \sim 1 - i\omega$ and Eq. (16) does give the expected $1/N^{3/2}$ and $1/N^{1/2}$ behaviour for the two cases respectively. In general we find that $J \sim \frac{1}{N^\alpha}$ where the exponent α depends on the low-frequency behaviour of $A(\omega)$. Some special cases are:
(i) $A(\omega) \sim -isgn(\omega)\omega^s$: Eq. (16) then gives $\alpha = s/2 + 1$ for $s > 0$.
(ii) $A(\omega) \sim 1 - isgn(\omega)\omega^s$: in this case we get $\alpha = 1 - s/2$ for $0 < s < 1$ and $\alpha = s/2$ for $s \geq 1$. Note that the case $s = 2$ gives $\alpha = 1$ that is, a Fourier-like behaviour. We verify this by a numerical evaluation of the integral in Eq. (7) for chains of finite length and given disorder, and then averaging of the current over many disorder realizations. The result is shown in Fig. (1).

One simple way of generating thermal sources with different spectral properties is to couple the disordered chain to an infinite set of oscillators in thermal equilibrium. The distribution of oscillator frequencies can be arbitrary except that it should include the range of the disordered chain frequencies. In this case it can be shown that the equations of motion are of the general form Eq. (2) with $A(t) = \int_0^\infty G(\omega_q) \sin(\omega_q t) d\omega_q$ where $G(\omega_q)$ depends on the choice of oscillator frequencies. The Rubin-Greer model, where the bath is simply an infinite ordered chain, corresponds to the choice $G(\omega_q) = \frac{1}{\pi}\omega_q(4 - \omega_q^2)^{1/2}$ for $\omega_q \leq 2$ and zero elsewhere.

Finally, we have also studied the effect of introducing a quadratic external potential, in addition to the mass disorder. In this case, the low frequency current-carrying modes are suppressed and we find that the current decays exponentially with system-size.

In summary we have studied the nonequilibrium steady state of a mass disordered harmonic chain coupled to heat baths at different temperature. We have shown that the system size dependence of the energy current, given by $J \sim 1/N^\alpha$, is determined not just by the properties of the system itself but also by those of the heat baths. One gets a continuous set of exponents α depending on the low frequency spectral properties of the bath. This seems contrary to the general belief in nonequilibrium statistical mechanics that the steady state of a close-to-equilibrium system will not depend on the details of the boundary conditions sustaining the steady state. We explain this by arguing as follows: the integrability of the harmonic system prevents local thermal equilibrium from being established and so the system is really far-from-equilibrium. Each of the noninteracting modes independently carries some energy current and the total current depends on how exactly the heat baths distribute energy among the various modes. For non-integrable systems, we expect that there should be transfer of energy amongst various modes leading to a state of local thermal equilibrium. Hence energy transport should be independent of boundary conditions. However careful studies are needed to verify that this is actually true, especially for systems which may be close to integrable ones. Indeed the possibility of boundary condition dependence is suggested from the results of some studies on nonlinear models [9,10]. These have often been attributed to the fact that some boundary conditions lead to jumps in the temperatures at the boundaries which in turn makes it difficult to extract the correct system-size dependence of current. However our study shows the possibility of boundary-condition dependence even in the absence of such jumps.

Some other interesting questions are: (1) are the peculiarities of the harmonic chain generic to any integrable system, (2) are these results also true for harmonic systems in higher dimensions and (3) can the present formalism be extended to the quantum-mechanical case. The answers to these questions may have implications for understanding experiments on heat conduction in systems such as insulating nanowires, where similar boundary related effects could lead to modification of Landauer-type formulas for thermal conductivity [14].

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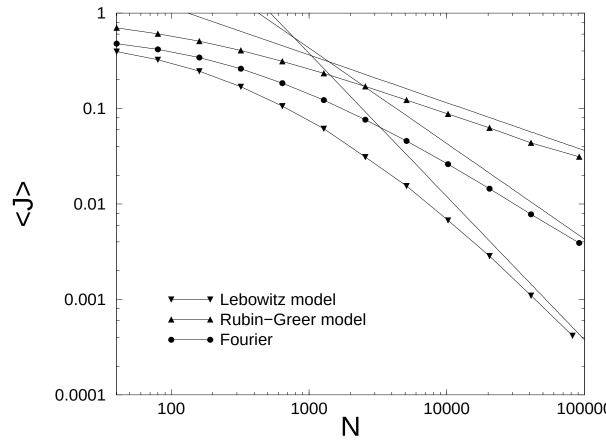

FIG. 1. System size dependence of the disorder averaged steady state current for three different models of heat baths. The straight lines shown have slopes 1/2, 1 and 3/2. In all cases the disorder strength $\delta m = 0.2$. The error in the measurements is of the order of the size of the points.

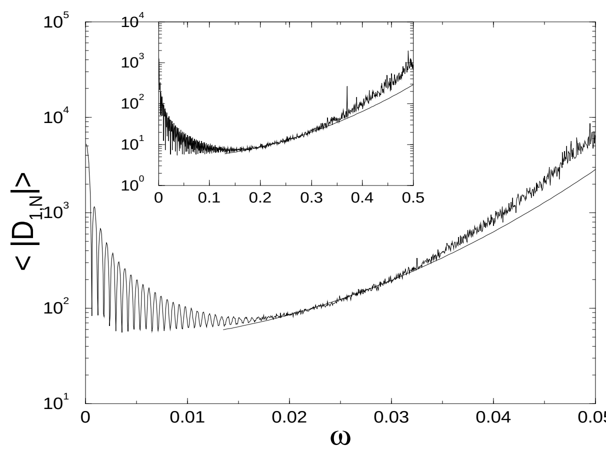

FIG. 2. Growth of solutions in a random harmonic chain for $N = 10^6$ and $N = 10^4$ (inset). The disorder strength was taken to be $\delta m = 0.2$. Note that the exponential growth starts from $\omega \approx c/\sqrt{N}$ (with $c \approx 13$). The smooth solid curves correspond to the exponential growth predicted by Eq. (15).

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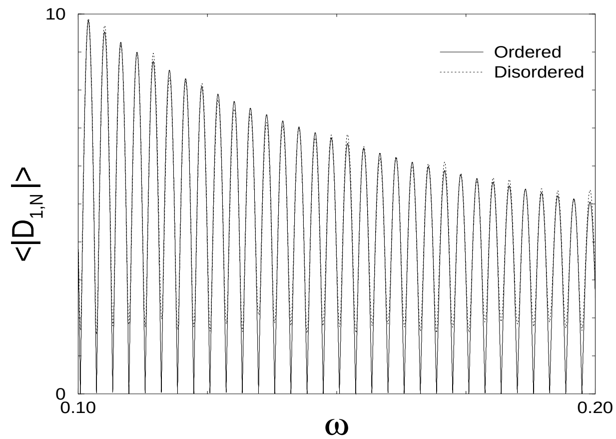

FIG. 3. Frequency dependence of $\langle|D_{1,N}|\rangle$ at small w for $\delta m = 0.2$ and $N = 10^4$ is compared with $|D_{1,N}|$ for the ordered chain.