

Nonunique steady states in the disordered harmonic chain

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The heat transport in disordered harmonic chains (DHCs) with arbitrary heat baths is studied, based on a general formulation developed by Dhar [Phys. Rev. Lett. **86**, 5882 (2001)]. The obtained temperature profile of a steady state is very unusual for any heat bath: (i) it is not unique, but dependent on the initial condition; (ii) it may be highly nonlinear, even though the temperature difference of the two ends of the system is in zero limit, and the temperature gradient ∇T is not inversely proportional to the system size; and (iii) when a DHC is coupled to two thermostats with the same temperature, the temperature of the system is still not uniform. The localized higher frequency normal modes induced by the mass disorders are responsible for these strange properties.

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The study of heat conduction in one dimensional systems is an interesting problem in the context of both nonlinear dynamics and nonequilibrium statistical physics, which has attracted a lot of attention in recent years [1]. Many authors had investigated the heat conduction of some classical Hamiltonian systems for the purpose of finding the macroscopic Fourier law, $J = -K(T)\nabla T$, in these model systems, where J is the heat current, ∇T is the local temperature gradient, and K is the heat conduction. As a general conclusion, a system size (N) dependence of J , $J \sim 1/N^\alpha$ has been confirmed, at least in the thermodynamic limit. Usually, people believe that the temperature profile of the system is linear (at least while the difference of temperatures of two ends ΔT is small), so $\nabla T \sim 1/N$, hence heat conduction $K \sim N^{1-\alpha}$. For $\alpha = 1$, K is independent of N , we say that the heat conduction of the system is normal or the system obeys Fourier's law; otherwise, we say that K is abnormal. Up to now, a variety of results have been reported in many systems [1–5]. But since most works are limited to numerical simulations of some nonlinear systems, it is very difficult to get definite conclusions. Some authors have shown qualms about the simulations [6–10].

In these previous studies about heat conduction, many different heat baths [1] were arbitrarily adopted, since these researchers believed that the heat conduction is the property of the system itself, it should be independent of the boundary conditions, although some earlier studies revealed that the size dependence of J (exponent α) is different for two particular heat baths [2,3] in a disordered harmonic chain (DHC). Recently, Dhar [6] restudied heat conduction in a DHC with arbitrary heat baths, he found that α is usually dependent on the choice of heat baths. By supposing $\nabla T \sim 1/N$, he concluded that the heat conduction depends on the heat baths in the DHC. But is ∇T truly proportional to $1/N$ in a DHC? As we know, boundary conditions may lead to jumps in temperatures, hence correct the gradient of temperature [11,12] but usually the correction is small and disappears in the thermodynamic limit. However, if the temperature profile of the system is nonlinear and its drop mainly occurs at the boundary zone [13], ∇T may be not proportional to $1/N$. Another relative question is about the

temperature profile of a DHC. Very recently, in a DHC, Hu *et al.* [8,14] found numerically that the stationary temperature is not unique, but Dhar [15] thought that the results may be due to the insufficient equilibration times in simulation or by using a particular heat bath. Whether the unique steady state exists in a DHC is still not very clear. For general heat baths or Hamiltonians, it is very difficult to mathematically prove the existence and uniqueness of a steady state [1].

In this paper, we try to study these questions in a DHC with arbitrary heat baths, based on a general formulation developed by Dhar [6]. We found some interesting results: (1) the temperature profile of the DHC is highly nonlinear; (2) the local temperature gradient in the middle zone of the chain is proportional to $N^{-3/2}$ rather than N^{-1} , but it is still independent of the heat baths, the main drop of temperature only occurs at the boundary zone; (3) even DHC is coupled to two thermostats with the same temperature, the temperature of the system is still inhomogeneous, it means that the energy cannot transport very well to the system from thermostats, so the system cannot be driven to an equilibrium state by the thermostats; and (4) a logical conclusion is that the initial energies of particles in the middle zone of chain cannot be dissipated very well, then their stationary temperatures are dependent on their initial value. Hence we prove generally that the unique steady state in a DHC does not exist. By analyzing the normal modes localized at the middle zone of the DHC, we explained the nonuniqueness of steady state.

We consider the DHC system,

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

where x_l are the displacements of the particles around their equilibrium positions, p_l are their momenta, and m_l are the random masses. Here, the particles 1 and N are coupled to heat baths including dissipative and noise terms, which satisfy the fluctuation dissipation theorem (FDT). The equations of motion are

$$\begin{aligned}
 m_1 \ddot{x}_1 &= -2x_1 + x_2 + \int_{-\infty}^t dt' A_L(t-t')x_1(t') + \eta_L(t), \\
 m_l \ddot{x}_l &= -2x_l + x_{l-1} + x_{l+1}, \\
 l &= 2, 3, \dots, (N-1),
 \end{aligned} \tag{2}$$

$$m_N \ddot{x}_N = -2x_N + x_{N-1} + \int_{-\infty}^t dt' A_R(t-t')x_1(t') + \eta_R(t),$$

where $A_{L,R}(t)$ and $\eta_{L,R}(t)$ describe dissipation and noise. We have a particular solution of Eq. (2),

$$x_i(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \hat{Y}_{lm}^{-1}(\omega) \hat{\eta}_m(\omega) e^{i\omega t},$$

where

$$\begin{aligned}
 \hat{Y}(\omega) &= \hat{\Phi}(\omega) - \hat{A}(\omega), \\
 \hat{\Phi}_{l,m} &= -\delta_{l,m+1} + (2 - m_l \omega^2) \delta_{l,m} - \delta_{l,m-1}, \\
 \hat{A}_{l,m} &= \delta_{l,m} [A_L(\omega) \delta_{l,1} + A_R(\omega) \delta_{l,N}], \\
 \hat{\eta}_l &= \eta_L(\omega) \delta_{l,1} + \eta_R(\omega) \delta_{l,N}.
 \end{aligned} \tag{3}$$

Here the function of frequency $f(\omega)$ is the Fourier transform of the function $f(t)$. The noise $\eta(t)$ is considered with the correlator [6], $\langle \eta(\omega) \eta(\omega') \rangle = 2\pi T I(\omega) \delta(\omega + \omega')$, where for the left and right heat sources, the temperatures are T_L and T_R , respectively. The dissipation term $A(\omega) = a(\omega) - ib(\omega)$. From the FDT, we have $I(\omega) = 2b(\omega)/\omega$. In this paper, we choose the same $A(\omega)$ at both boundaries.

The heat current can be written as

$$\begin{aligned}
 J &= \left\langle \left[\int_{-\infty}^t dt' A_L(t-t')x_1(t') + \eta_L(t) \right] \dot{x}_1(t) \right\rangle \\
 &= \frac{(T_L - T_R)}{4\pi} \int_{-\infty}^{\infty} d\omega j(\omega),
 \end{aligned} \tag{4}$$

and the temperature of the i th particle is

$$T_i = \langle m_i \dot{x}_i^2(t) \rangle = \frac{T_L}{2\pi} \int_{-\infty}^{\infty} d\omega a_i(\omega) + \frac{T_R}{2\pi} \int_{-\infty}^{\infty} d\omega b_i(\omega), \tag{5}$$

where $\langle \dots \rangle$ denotes the noise average. $j(\omega)$, $a_i(\omega)$, and $b_i(\omega)$ are independent of the thermostats temperatures T_L and T_R , we have

$$j(\omega) = 4b^2(\omega) / |DY_{1,N}|^2,$$

$$a_i(\omega) = m_i 2b(\omega) \omega |DY_{i+1,N}|^2 / |DY_{1,N}|^2,$$

$$b_i(\omega) = m_i 2b(\omega) \omega |DY_{1,i-1}|^2 / |DY_{1,N}|^2,$$

where

$$DY_{1,N} = [1, -A(\omega)] \begin{pmatrix} D_{1,N} & -D_{1,N-1} \\ D_{2,N} & -D_{2,N-1} \end{pmatrix} [1, A(\omega)]^T, \tag{6}$$

$$DY_{1,i-1} = [D_{1,i-1}, -D_{2,i-1}] [1, A(\omega)]^T,$$

$$DY_{i+1,N} = [D_{i+1,N}, -D_{i+1,N-1}] [1, A(\omega)]^T.$$

Here $D_{l,m}$ and $DY_{l,m}$ are the determinants of the submatrix of $\hat{\Phi}$ and \hat{Y} beginning with the l th row and column and ending with the m th row and column, respectively. For a DHC, we calculate the current and temperature for given realizations of disorder and then perform disorder averages. In this paper, the masses of particles are a uniform distribution from $1 - \delta m$ to $1 + \delta m$ and $\delta m = 0.22$. Considering the symmetry of the system, we have

$$\langle a_i(\omega) \rangle = \langle b_{N+1-i}(\omega) \rangle. \tag{7}$$

From there, we note $\langle \dots \rangle$ as a disorder sample average. So, we can rewrite the local temperature as

$$T_i = T_L t_j + T_R t_i, \tag{8}$$

where $j = N + 1 - i$ and $t_i = 1/2\pi \int b_i(\omega) d\omega$ is the normalized temperature. The local temperature gradient $\nabla T \approx (T_j - T_i)/(j - i)$. In the middle zone of the chain, if we choose $j = N + 1 - i$, then

$$\nabla T \approx (T_R - T_L) \frac{t_j - t_i}{j - i} \approx (T_R - T_L) \nabla t. \tag{9}$$

For a DHC, using the transport matrix T_i , we have [2,6]

$$\begin{aligned}
 \begin{pmatrix} D_{1,N} & -D_{1,N-1} \\ D_{2,N} & -D_{2,N-1} \end{pmatrix} &= T_1 T_2 \cdots T_N, \\
 (D_{1,i-1}, -D_{2,i-1}) &= u T_{i-1} T_{i-2} \cdots T_1, \\
 (D_{i+1,N}, -D_{i+1,N-1}) &= u T_{i+1} T_{i+2} \cdots T_N,
 \end{aligned} \tag{10}$$

where

$$T_i = \begin{pmatrix} 2 - m_l \omega^2 & -1 \\ 1 & 0 \end{pmatrix} \text{ and } u = (1, 0).$$

From the Furstenberg theorem [6,16,17] on the limiting form of the product of random noncommuting variables, for almost any choice of the sequence of random masses $\{m_i\}$, we have

$$\lim_{n \rightarrow \infty} \frac{1}{n} \ln |T_{i+1} T_{i+2} \cdots T_{i+n} v| = \gamma(\omega) > 0 \tag{11}$$

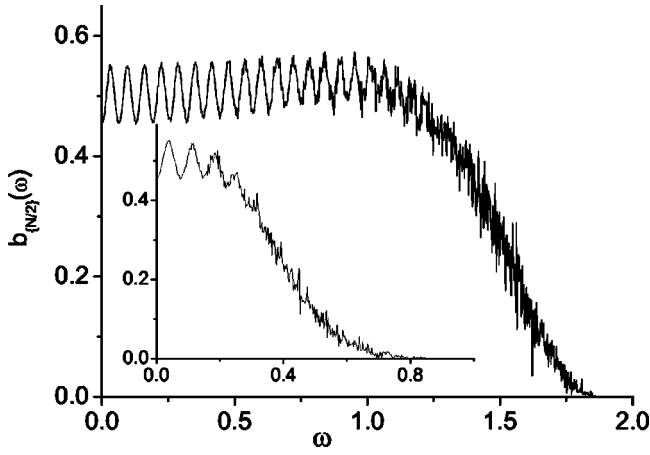


FIG. 1. Frequency dependence of normalized temperature of the $(N/2)$ th particle $b_{N/2}$ for $N=100$ and $N=2500$ (inset) in a DHC with a particular heat bath. We find that $b_{N/2}$ decreases fast when $\omega > a/\sqrt{N}$, $a \sim 10$. There are similar results for other heat baths.

for almost any nonzero vector v , in the limit $\omega \rightarrow 0^+$. For finite n , Dhar [6] found numerically that this result was true only for $\omega > 1/n^{1/2}$.

We first choose $T_L = T_R = T$, usually, a uniform temperature profile is expected, hence $T_i = T$ for any i . Since the normalized temperature t_i is independent of the T_L and T_R , from Eq. (8), we know that t_i should be symmetric about $(N/2, 1/2)$, in other words, $t_{N/2+i} + t_{N/2-i} = 1$. But from Eq. (11) and the numerical results shown in Fig. 1, we find that the $b_{N/2}(\omega)$ exponentially decreases as frequency increases unless $\omega < a/\sqrt{N}$, where $a \sim 10$, is a constant. So $t_{N/2}$ is zero rather than the expected $1/2$ in the thermodynamic limit ($N \rightarrow \infty$). Then we obtain the first surprising result, *the system cannot be driven to the equilibrium state by thermostats with the same temperature*. In Fig. (2), t_i is shown as a function of position in the DHC ($N=1000$) with three different heat baths, which are the Lebowitz model $A(\omega) \sim -i\gamma\omega$, the Rubin-Greer model $A(\omega) \sim 1 - i\omega$, and the Fourier model $A(\omega) \sim 1 - i\omega^2$, respectively [6]. The obtained t_i is very small except $i \sim N$, *the temperature is highly nonlinear; and it has a finite value only while $i \sim N$* . A noted fact is that $t_i \approx 0.5$, except for $i=1$ or N in an ordered harmonic chain (OHC), since the dissipation-term-satisfied the FDT, can ensure thermal equilibration of the system. The real temperature distribution of the DHC is also shown in the left-lower inset of Fig. 2, where $T_L = T_R = 1$, the temperature of the middle zone is far lower than the temperature of the boundary zone. It means that the temperature distribution is inhomogeneous in the DHC, even though the heat flow is zero. In the right-upper inset of Fig. 2, the approximate linear tem-

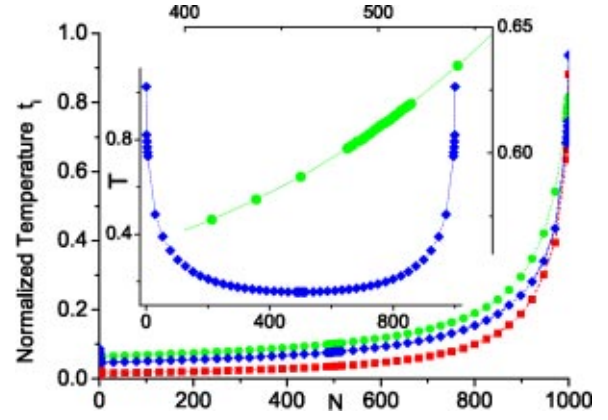


FIG. 2. The normalized temperature distribution t_i in the DHC with three different heat baths, the system size $N=1000$. In the left lower inset, the inhomogeneous temperature profile is shown when $T_L = T_R = 1$, where T_L and T_R are the temperatures of two thermostats. In the right-upper inset, $T_L = 1$ and $T_R = 5$, the temperatures of the middle zone are shown. We only show the result of one heat bath in the inset, the results of other heat baths are similar.

perature profile in the middle zone is shown, where $T_L = 1$ and $T_R = 5$, but in the left boundary zone, the temperature gradient is negative (not shown). We numerically calculated the heat current J , the results were in agreement with that of Dhar [6]. Moreover, we also calculated the temperature $t_{N/2}$ and the temperature gradient $\nabla t_{N/2}$, which are shown in Fig. 3. We found that $t_{N/2}$ decreases to zero as N increases. $t_{N/2} \sim N^{-w}$ as N is large, in which w is dependent on the heat baths. It means that the motion states of particles in the middle zone of the DHC are independent of the temperature of thermostats in the thermodynamic limit.

In the low frequency range, the numerical results of Dhar [6] indicate that the determinant $\langle |D_{1,N}| \rangle$ in the DHC equals approximately to the value in the OHC, and since the $j(\omega)$ and $b_i(\omega)$ (when i is not near N) exponentially decrease in the higher frequency zone, we can approximately calculate the heat current J and the normalized temperature t_i by integrating $j(\omega)$ and $b_i(\omega)$ in low frequency zone. In the OHC, $D_{1,N}(\omega) = \sin[k(N+1)]/\sin(k)$, where $\omega = 2\sin(k/2)$. Using the approximation in the formula of $j(\omega)$, Dhar gave the value of α in a DHC with any heat bath. For t_i , if $i \ll N$ and N is a large number, we approximately have $N-i \sim N$, the upper limit of the integral is $\sim 1/\sqrt{N}$. We have

$$t_j - t_i \sim \int_0^{1/\sqrt{N}} 2b(\omega)\omega \cos(k/2) \sin[(j-i)k] f(k) dk, \quad (12)$$

where

$$f(k) = \frac{\sin[k(N+1)] + |A(\omega)|^2 \sin[k(N-1)] - 2\text{Re}A(\omega) \sin(kN)}{|\sin[k(N+1)] - 2A(\omega) \sin(kN) + A^2(\omega) \sin[k(N-1)]|^2}.$$

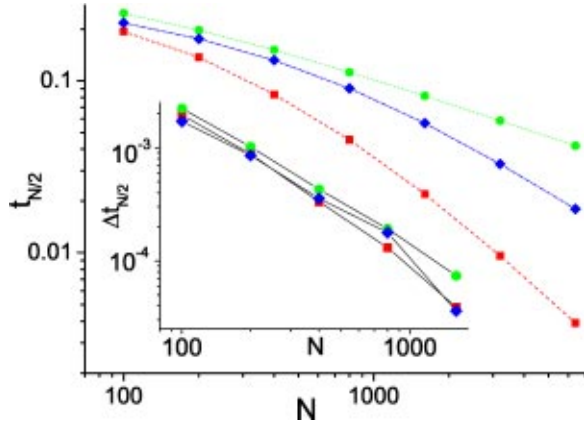


FIG. 3. The temperature of the $(N/2)$ th particle as a function of the system size N for three different heat baths. Inset, the gradient of temperature in the middle zone of the DHC as a function of N .

Here i and j are at the middle of the chain, satisfying $i \ll N$, $j \ll N$, and $i + j = N + 1$.

From Eq. (12), we find that the gradient of temperature $\nabla t \approx (t_j - t_i)/(j - i)$ is proportional to N^β and the obtained β is $-3/2$ for very general heat baths, which include $A(\omega) \sim -i \operatorname{sgn}(\omega) \omega^5$ and $A(\omega) \sim 1 - i \operatorname{sgn}(\omega) \omega^5$. The result has been tested by numerical calculations on the Lebowitz model, Rubin-Greer model, and the Fourier model, which are shown in inset of Fig. 3. As we know, ∇T is usually supposed as $(T_R - T_L)/N$. But in the DHC, the local temperature gradient is dependent on the position of the chain, moreover, it is negative in the left boundary zone (the middle temperature is very low). For the strange temperature profile, the usually defined local thermal conductivity K is negative in some positions, which can not be due to the temperature dependence of K . However, except for the boundary zones, K can be locally defined, $K \sim J/\nabla T$, and in the middle zone of the chain, $\nabla T \sim N^{-3/2}$.

These surprising results can be understood from the frequency distribution of heat current and temperature (kinetic energies). Due to the mass disorders, the higher frequency normal modes are localized in the DHC. These localized modes cannot transport very well thermal energy through the whole system, so the temperature in the middle zone is independent of the thermostats. Similarly, the energy in the middle zone of the chain also cannot transport very well to the ends of the chain, which are coupled with the thermostats, so it is not dissipated, hence we conclude that the temperature profile of a DHC should be dependent on the initial condition.

We can more clearly understand the dependence of the initial condition. For the motion equation [Eq. (2)], its solu-

tion is the sum of the particular solution shown in Eq. (3) and the general solutions of equation $\hat{Y}\hat{x}=0$, which are

$$x_l = \sum_n c_n u_n^l \exp(i\omega_n t). \quad (13)$$

Here c_n are constant numbers, which are dependent on the initial condition of the system, u_n^l is the l th element of eigenvector \hat{u}_n , the corresponding eigenvalue is ω_n , which is usually a complex number. Before coupling with thermostats, the normal modes of the system are $\{\hat{u}_{0n}\}$ (the solution of equation $\hat{\Phi}\hat{u}=0$). After coupling with thermostats, these modes will transfer to the normal modes of the coupled system $\{\hat{u}_n\}$, this is a process of energy dissipation. In DHC, due to the mass disorder, the higher frequency modes of the system are localized. Supposing a mode \hat{u}_{0m} (the corresponding frequency is ω_{0m}) is localized in the middle zone of the chain [17], hence $u_{0m}^1 \approx u_{0m}^N \approx 0$ [18], then $\hat{Y}(\omega_{0m})\hat{u}_{0m}=0$ is also true, it means that the mode almost does not directly couple with the thermostats, and since there are no interactions between the different normal modes, the energy of the mode is not lost after the system is coupled to thermostats. From these discussions, we conclude that the steady state's temperature in the middle zone of the DHC mainly depends on the distribution of their initial motion among the localized modes. Very recently, using a particular heat bath, considering a harmonic chain, consisting of two types of particles (a segment of light particles is embedded in the middle of the other two segments of heavy particles), Hu *et al.* [8] numerically found that the steady states are dependent on the initial condition. They also found that the steady state is unique when adding a very small fraction of anharmonicity in the DHC. But in a comment of Dhar [15], the numerical result is doubted. Our results generally verify the nonuniqueness of a steady state in a DHC and show that the existence of noninteracting, localizing normal modes is responsible for these abnormal properties. Similarly, the heat baths' dependence of heat conduction found by Dhar in DHCs [6] is due to the same reason. These abnormal properties may not be true in other systems without the noninteracting localized normal modes.

In summary, we conclude that there are some very special thermal properties in a DHC, such as the inhomogeneous temperature distribution when the heat flow is zero, the nonunique steady states, the strange temperature profile, and so on. The reason of these properties is due to the existence of noninteracting localizing normal modes in the DHC.

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- [1] F. Bonetto, J.L. Lebowitz, and L. Rey-Bellet, e-print math-ph/0002052.
 [2] Z. Rieder, J.L. Lebowitz, and E. Lieb, *J. Math. Phys.* **8**, 1073 (1967).
 [3] R. Rubin and W. Greer, *J. Math. Phys.* **12**, 1686 (1971); A.

- Casher and J.L. Lebowitz, *ibid.* **12**, 1701 (1971).
 [4] G. Casati *et al.*, *Phys. Rev. Lett.* **52**, 1861 (1984).
 [5] B. Hu, B. Li, and H. Zhao, *Phys. Rev. E* **57**, 2992 (1998).
 [6] A. Dhar, *Phys. Rev. Lett.* **86**, 5882 (2001).
 [7] A. Dhar, *Phys. Rev. Lett.* **86**, 3554 (2001).

- [8] B. Li, H. Zhao, and B. Hu, Phys. Rev. Lett. **86**, 63 (2001).
[9] K. Aoki and D. Kusnezov, Phys. Rev. Lett. **86**, 4029 (2001).
[10] Lei Yang, Phys. Rev. Lett. **88**, 094301 (2002).
[11] S. Lepri, R. Livi, and A. Politi, Phys. Rev. Lett. **78**, 1896 (1997).
[12] T. Hatano, Phys. Rev. E **59**, R1 (1999).
[13] O.V. Gendelman and A.V. Savin, Phys. Rev. Lett. **84**, 2381 (2000).
[14] B. Li, H. Zhao, and B. Hu, Phys. Rev. Lett. **87**, 069402 (2001).
[15] A. Dhar, Phys. Rev. Lett. **87**, 069401 (2001).
[16] H. Furstenberg, Trans. Am. Math. Soc. **108**, 377 (1963).
[17] H. Matsuda and K. Ishii, Suppl. Prog. Theor. Phys. **45**, 56 (1970). The existence of the localized mode in a DHC has been proved in this reference.
[18] u_n^1 and u_n^N of the localized model exponentially decrease as N increases in the DHC.