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Anomalous quantum heat transport in a one-dimensional harmonic chain with random couplings

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Abstract
We investigate quantum heat transport in a one-dimensional harmonic system with random couplings. In the presence of randomness, phonon modes may normally be classified as ballistic, diffusive or localized. We show that these modes can roughly be characterized by the local nearest-neighbor level spacing distribution, similarly to their electronic counterparts. We also show that the thermal conductance $G_{\rm th}$ through the system decays rapidly with the system size ($G_{\rm th} \sim L^{-\alpha}$). The exponent α strongly depends on the system size and can change from $\alpha < 1$ to $\alpha > 1$ with increasing system size, indicating that the system undergoes a transition from a heat conductor to a heat insulator. This result could be useful in thermal control of low-dimensional systems.

(Some figures may appear in colour only in the online journal)

1. Introduction

The derivation of Fourier's law of heat conduction from microscopic dynamics without any *ad hoc* statistical assumption is one of the great challenges in nonequilibrium statistical mechanics [1]. Even in the context of classical dynamical systems, the issue of heat transport, in spite of having a long history (recently reviewed in [2]), is not completely settled. Here, a central issue is to determine how the heat current (J) through the system depends on the system size (L). In a one-dimensional (1D) harmonic chain, no global thermal gradient occurs due to the lack of scattering between modes [3]; thus, one expects $J \propto L^0$. However, some classical nonlinear systems of interacting particles, especially those with nonlinear on-site potentials [4], typically exhibit a diffusive behavior above a critical interaction strength, which then leads to the onset of Fourier's law ($J = -\kappa \nabla T \propto L^{-1}$), relating the macroscopic heat flux to the temperature gradient. Further, a lot of studies have found that the heat transport is abnormal with $J \propto L^{-\alpha}$ in many other 1D systems [5–7], and the exponent α differs in a number of ways. In particular, it has been shown that in a classical mass-disordered harmonic chain the exponent α is $1/2$ when the baths are modeled by semi-infinite harmonic chains [8].

Even less is known about heat transport in quantum systems, such as spin chains [9–18] and quantum harmonic chains [19, 20], despite many studies. The main problem is that, unlike in classical systems, the time and space computer requirements for numerical simulations of quantum systems exponentially increase with the system size, especially in spin systems. As a result, investigations have been so far mainly focused on the linear response theory [9, 10], whose validity is questionable [21]. We recall that in integrable systems such as 1D spin-1/2 Heisenberg chains, due to the existence of nontrivial conservation laws, the current–current correlation functions typically do not decay to zero, thus implying ballistic transport [9, 22]. However, nonballistic heat transport has also been observed in spin systems [13–16]. In the 1D quantum harmonic chain with random couplings, it was shown recently that a finite temperature gradient can be created [19]. However, the dependence of the heat current on the system size remains unclear.

In this paper we report results for heat conduction in 1D harmonic lattices with random couplings by using the nonequilibrium Green's function method. We show that the phonon states, which can normally be classified as ballistic modes, diffusive modes, and localized modes, may be characterized by the local nearest-neighbor level spacing distribution $P(s)$. We also find that on the large length scale most eigen-modes are probably localized except those close to the zero frequency (due to translational invariance). Thus the heat current decays rapidly with the system size and the system becomes a heat insulator when the system size is large enough. This behavior of phonons is similar to the electron transport in 1D disordered systems, although electrons and phonons differ in that electron transport is dominated by electrons near the Fermi level (when the temperature is not high) whereas in the case of phonons nearly all frequencies participate in heat transport. The reason may be that phonons obey Bose–Einstein statistics while electrons obey Fermi–Dirac statistics.

2. Model and method

We consider heat conduction through a 1D disordered harmonic chain consisting of L particles. The particles have common mass m, while the couplings between the nearest-neighbor particles are random. Another type of disorder is mass disorder, and actually a mass-disordered system can be mapped to one with random couplings by a rescaling transformation. Thus we focus on systems with random couplings in the following. The Hamiltonian of the system is then

$$H_{\mathrm{s}} = \sum_{i=1}^{L} \frac{p_i^2}{2m} + \sum_{i=1}^{L-1} \frac{k_i}{2}(x_{i+1} - x_i)^2, \tag{1}$$

where x_i and p_i denote the coordinate and the momentum of the ith particle, and k_i is the random coupling. At the two ends the system is connected to two semi-infinite harmonic chains serving as leads, whose Hamiltonians read

$$H_\alpha = \sum_{i=1}^{\infty} \frac{p_{\alpha,i}^2}{2m} + \sum_{i=1}^{\infty} \frac{k}{2}(x_{\alpha,i+1} - x_{\alpha,i})^2, \tag{2}$$

where $\alpha = l, r$. The coupling between the leads and the system is

$$H_{\mathrm{c}} = \frac{k}{2}(x_{l,1} - x_1)^2 + \frac{k}{2}(x_{r,1} - x_{\mathrm{L}})^2. \tag{3}$$

The total system is therefore $H = H_{\mathrm{s}} + H_{\mathrm{l,r}} + H_{\mathrm{c}}$. In the simulations, we keep $k_i = \alpha_i k$. Here the dimensionless quantity α_i is uniformly distributed in $[1 - W/2,\ 1 + W/2]$ with W controlling the strength of random couplings.

We calculate the heat current by using the standard nonequilibrium Green's function formalism [23, 24]. The left and the right leads are taken into account via the self-energies $\mathbf{\Sigma}^{\mathrm{r}}_{\mathrm{L,R}}(\omega)$, and the retarded Green's function for the system is calculated as

$$\mathbf{G}^{\mathrm{r}}(\omega) = [\mathbf{M}\omega^2 - \mathbf{K}_{\mathrm{s}} - \mathbf{\Sigma}^{\mathrm{r}}_{\mathrm{L}}(\omega) - \mathbf{\Sigma}^{\mathrm{r}}_{\mathrm{R}}(\omega)]^{-1}, \tag{4}$$

where $\mathbf{M}$ is a diagonal matrix with elements corresponding to the masses of the particles and $\mathbf{K}_{\mathrm{s}}$ is the dynamic matrix for the central system. The phonon transmission is then given by

$$\mathcal{T}(\omega) = \mathrm{Tr}[\mathbf{\Gamma}_{\mathrm{L}}(\omega)\mathbf{G}^{\mathrm{r}}(\omega)\mathbf{\Gamma}_{\mathrm{R}}(\omega)\mathbf{G}^{\mathrm{a}}(\omega)], \tag{5}$$

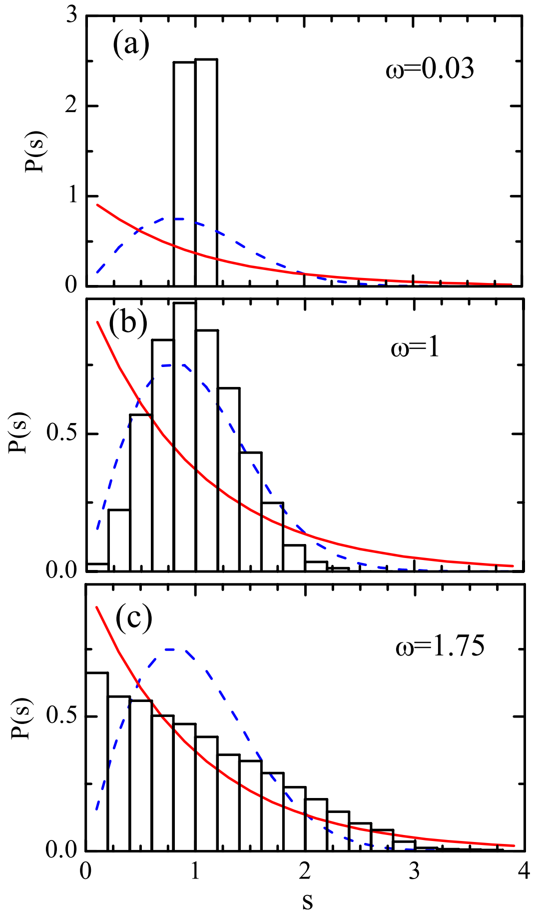

Figure 1. Level distributions around three typical frequencies. The random couplings are uniformly distributed in [0.9, 1.1], i.e., $W = 0.2$. The results are obtained by counting 40 levels around a frequency and then summarized over 100 disorder realizations. The length of the system is $L = 1000$. The Poisson distribution (full line) and the Wigner distribution (dashed line) are also shown for comparison. Here $m = k = 1$.

where $\mathbf{\Gamma}_{\mathrm{L,R}} = \mathrm{i}[\mathbf{\Sigma}^{\mathrm{r}}_{\mathrm{L,R}}(\omega) - \mathbf{\Sigma}^{\mathrm{r},\dagger}_{\mathrm{L,R}}(\omega)]$ and $\mathbf{G}^{\mathrm{a}}(\omega) = \mathbf{G}^{\mathrm{r},\dagger}(\omega)$. The phonon thermal current can be calculated from the phonon transmission function $\mathcal{T}$ as

$$J_{\mathrm{ph}}(T) = \frac{\hbar}{2\pi}\int_0^\infty \mathrm{d}\omega\, \omega\, \mathcal{T}(\omega)\, [n_{\mathrm{B}}(T_{\mathrm{L}}) - n_{\mathrm{B}}(T_{\mathrm{R}})], \tag{6}$$

where $n_{\mathrm{B}}(T_{\mathrm{L,R}}) = (\mathrm{e}^{\hbar\omega/k_{\mathrm{B}}T_{\mathrm{L,R}}} - 1)^{-1}$ is the Bose–Einstein distribution and $T_{\mathrm{L,R}}$ is the left (right) bath temperature. In the linear response regime, the phonon thermal conductance is then

$$G_{\mathrm{ph}}(T) = \frac{\hbar^2}{2\pi k_{\mathrm{B}} T^2}\int_0^\infty \mathrm{d}\omega\, \omega^2\, \mathcal{T}(\omega)\, \frac{\mathrm{e}^{\hbar\omega/k_{\mathrm{B}}T}}{(\mathrm{e}^{\hbar\omega/k_{\mathrm{B}}T} - 1)^2}. \tag{7}$$

If Fourier's law is satisfied, one would expect $G_{\mathrm{ph}} \propto 1/L$.

3. Results

First, we consider the nearest-neighbor level spacing distribution. Similarly to the level distribution in the 1D tight binding Anderson model for electrons [25], we expect

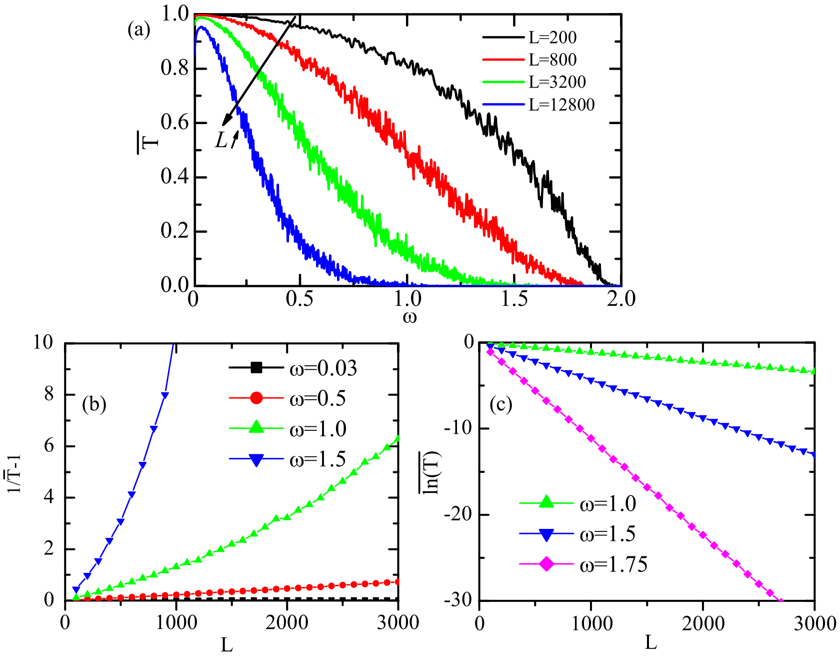

Figure 2. (a) Phonon transmission as a function of the frequency. The random couplings are uniformly distributed in [0.9, 1.1] (or $W = 0.2$). The results are obtained for 100 disorder realizations. (b) $1/\bar{\mathcal{T}} - 1$ as a function of the system length for several frequencies. (c) Averaged logarithm of transmission ($\overline{\ln \mathcal{T}}$) as a function of length for several frequencies. Here $m = k = 1$.

that the distribution $P(s)$ in this harmonic system may be used to measure the chaotic behavior of phonons. We shall look at the local frequency spectra around some typical frequencies. Without disorder the phonon spectrum is $\omega_q = \sqrt{4k/m}\sin(q/2)$, where q is the wavevector. The local frequency spectrum, excluding frequencies around $\omega \sim \sqrt{4k/m}$, is quasi-equidistant, so that the eigenstates are extended and regular and we thus expect a Delta-type distribution, $P_\delta(s) = \delta(s-1)$. In the presence of disorder, phonons may be scattered differently. Specifically, close to the zero frequency ($\omega \sim 0$), where phonon modes have long wavelengths and thus are less affected by the disorder, we then expect a Delta-type distribution $P_\delta(s)$. However, in the high frequency region, where phonon modes are strongly affected by the disorder, the eigenstates may be effectively localized on the scale of the sample length, thus resulting in a Poisson distribution, $P_\mathrm{P}(s) = \exp(-s)$. In between these regions, one may expect that the eigenstates are delocalized and chaotic, which means that the eigenstates are uncorrelated with the distribution close to Wigner type, $P_\mathrm{W}(s) = (\pi s/2)\exp(-\pi s^2/4)$. Figure 1 shows the level distributions around three typical frequencies. The results are obtained by counting 40 levels around a frequency and then summarized over 100 disorder realizations. As expected, the three level distributions at $\omega = 0.03$, $\omega = 1$, and $\omega = 1.75$ are very close to $P_\delta(s)$, $P_\mathrm{W}(s)$, and $P_\mathrm{P}(s)$, respectively. In fact, these three distributions may be used to identify the ballistic, diffusive, and localized transport regimes as discussed below.

Figure 2(a) shows how the averaged transmission depends on the frequency for different sample lengths L with disorder strength $W = 0.2$. For a pure harmonic chain the transmission is unity. In the presence of disorder, the transmission normally decreases with increasing length L. However, the transmission at low frequencies (e.g., $\omega = 0.03$) weakly varies with the length, which is a characteristic of the ballistic transport regime with the level distribution being of Delta-type as shown in figure 1(a). For slightly higher frequencies, scattering events start to dominate the transport as L increases and a crossover from the ballistic to the diffusive regime occurs. In this regime, the transmission can be described by the sum of the ballistic and diffusive contributions, $\bar{\mathcal{T}}(\omega) = 1/(1 + L/l_e(\omega))$, where $l_e(\omega)$ is the mean free path [26]. In figure 2(b), we can clearly see that the dependence of the transmission on the length at $\omega = 0.03$ and 0.5 is well described by $\bar{\mathcal{T}}(\omega) = 1/(1 + L/l_e)$. At $\omega = 1$, the transmission may be also described by this relation on the length scale $L \sim 1000$, where the level spacing is close to the Wigner distribution as shown in figure 1(b). However, on a larger length scale $L > 2000$, deviation appears as the mode at $\omega = 1$ begins to be localized.

For even higher frequencies, disorder induced scattering effects become increasingly important as L increases. As a result, the localization regime is established. This regime is characterized by an exponential decrease of the transmission with the length, i.e., $\overline{\ln \mathcal{T}} = -L/\xi(\omega)$, where $\xi(\omega)$ is the localization length [26]. From figure 2(c), we can see that the transmission at $\omega = 1.75$ is well described by this localization scaling law with the level spacing being described by the Poisson distribution.

Next, we consider the heat transport through the system. Figure 3 shows the heat conductance as a function of length for different disorder strengths. To be more realistic, here we keep $\omega_{\max} \equiv 2\sqrt{k/m} = 300$ THz. For the strong disorder $W = 1$ we can clearly observe a transition from abnormal transport

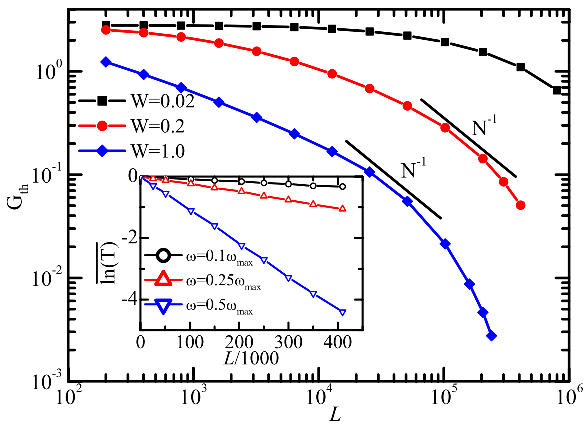

Figure 3. The phonon thermal conductance versus the sample length for different disorder strengths W. Here we keep $\omega_{\max} \equiv 2\sqrt{k/m} = 300$ THz, and G_{th} is thus in units of 10^{-10} W K^{-1}. The temperature is $T = 300$ K. The inset shows $\overline{\ln \mathcal{T}}$ as a function of length for three frequencies when the disorder strength is $W = 0.02$.

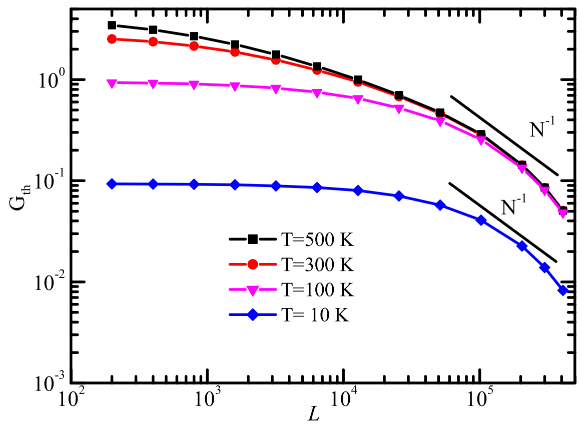

Figure 4. The phonon thermal conductance versus the sample length for different temperatures; $W = 0.2$. Here we keep $\omega_{\max} \equiv 2\sqrt{k/m} = 300$ THz, and G_{th} is in units of 10^{-10} W K^{-1}.

($\alpha < 1$) to heat insulator ($\alpha > 1$), occurring at around $L = 3 \times 10^4$. As the strength of the disorder becomes less, the transition takes place on a larger length scale. For $W = 0.2$ the transition takes place at around $L = 10^5$. For an even weaker disorder strength ($W = 0.02$) the behavior at $L > 10^6$ is not displayed in figure 3 due to limited computation ability. However, we may expect that the transition would happen on a length scale of $\sim 10^6$. This may also be understood from the averaged logarithm of transmission for $W = 0.02$ (see the inset). In fact, except for the phonon modes around $\omega = 0$, where the transmission would always be close to unity due to the translational invariance, most phonon modes become localized with increasing system length as shown in the inset, thus leading to a rapid decay of thermal conductance on the large length scale. Further, it is noteworthy that in our case the exponent α increases with increasing sample length, in contrast to the previously reported classical results [8], where α converges to a constant with the length.

In figure 4, we plot the thermal conductance versus the length at different temperatures. At low temperature, only low frequency modes contribute to the heat conductance, and the transmission at these frequencies changes little when the sample length is small. Thus, the thermal conductance changes slowly on the small length scale. At around $L = 10^5$ the transition from abnormal transport to heat insulator occurs and the thermal conductance begins to decay rapidly, indicating that even the low frequency modes begin to become localized. For high temperatures the thermal conductances converge to almost the same value on the large length scale. This is because at high temperatures ($k_B T \gg \hbar\omega$) only the transmissions at low frequencies take appreciable values, and equation (7) thus reduces to $G_{\text{th}} = \frac{k_B}{2\pi} \int_0^\infty \mathrm{d}\omega \mathcal{T}(\omega)$, implying that the thermal conductance becomes temperature-independent. At high temperatures we can also observe a transition from abnormal transport to heat insulator at around $L = 10^5$.

4. Summary

We have studied the quantum heat transport in a 1D disordered harmonic system in the nonequilibrium Green's function formalism. Generally, the phonon states in such a system can be classified as ballistic modes, diffusive modes, and localized modes. We have shown that these three kinds of phonon mode can be characterized by the local nearest-neighbor level spacing distribution $P(s)$. Further, we have found that as the system length increases, the system undergoes a transition from a heat conductor ($\alpha < 1$) to a heat insulator ($\alpha > 1$), regardless of the temperature. In our case, the exponent α in $J \propto L^{-\alpha}$ varies over the whole range of the sample length. As the strength of the disorder becomes less, the length scale on which the transition occurs becomes larger. These results could be useful in thermal control of low-dimensional systems. For example, by doping the system could be tuned into a heat insulator. Indeed, a recent work shows that the thermal conductivity of silicon nanowires can be reduced exponentially by isotopic disorder [27].

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