

Thermal conductance of one-dimensional disordered harmonic chains

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We study heat conduction mediated by longitudinal phonons in one-dimensional disordered harmonic chains. Using scaling properties of the phonon density of states and localization in disordered systems, we find nontrivial scaling of the thermal conductance with the system size. Our findings are corroborated by extensive numerical analysis. We show that, surprisingly, the thermal conductance of a system with strong disorder, characterized by a “heavy-tailed” probability distribution, and with large impedance mismatch between the bath and the system, scales normally with the system size, i.e., in a manner consistent with Fourier’s law. We identify a dimensionless scaling parameter, related to the temperature scale and the localization length of the phonons, through which the thermal conductance for different models of disorder and different temperatures follows a universal behavior.

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Introduction. The study of heat transport via phonons in low-dimensional (spatial dimension $d < 3$) classical and quantum-mechanical systems has attracted considerable theoretical and experimental attention in recent years [1–13]. One of the main objectives of these studies is to understand the scaling of heat flux J which, according to Fourier’s law [4], should scale with the system size L as $J \propto L^{-1}$ (L is measured along the direction of heat propagation). But extensive numerical and analytical studies in the past few decades have revealed the possible violation of Fourier’s law for low-dimensional systems [10,14–18]. These studies show that $J \propto L^{(\gamma-1)}$ with $\gamma \neq 0$ which in turn implies L -dependent thermal conductivity, $\kappa = \lim_{L \rightarrow \infty} \lim_{\Delta T \rightarrow 0} \frac{JL}{\Delta T} \propto L^\gamma$ (ΔT being the temperature difference across the system) [4]. The violation of Fourier’s law in low-dimensional systems is also observed experimentally in the case of carbon nanotubes [19], nanowires [20], and graphene [21].

For systems of finite size, instead of thermal conductivity, κ , it is useful to study thermal conductance, $G = \kappa/L$, and we expect $G(L) \propto L^{-\beta}$, with $\beta (= 1 - \gamma) = 1$ for normal heat transport, while $\beta \neq 1$ implies anomalous heat transport.

Various aspects, such as disorder [14,22,23], phonon-phonon interaction [24,25], presence of pinning potential [26,27], nature of the heat baths [10], and the coupling between the system and the heat bath [23], have been shown to affect heat transport. Particularly, theoretical studies for one-dimensional isotopically (mass) disordered harmonic chains show that $J \propto L^{-1/2}$ with free boundary conditions [15] while $J \propto L^{-3/2}$ with a fixed boundary condition [14], implying that β can be $\frac{1}{2}$ or $\frac{3}{2}$. For this particular model, it was also shown that normal scaling (i.e., $\beta = 1$) can be observed only under specific choices of the thermal bath [10]. It was also argued, under free boundary conditions, that one-dimensional

harmonic chains with spatially *correlated* disorder may exhibit normal heat conduction asymptotically [22].

Can one have normal heat transport in one-dimensional disordered (uncorrelated) harmonic chains even within free boundary conditions? A recent theoretical study [23] predicts that for a *weakly* coupled disordered harmonic chain one may observe normal heat transport in the presence of *strong disorder*, when disorder is characterized by a heavy-tailed distribution. While it is important to verify this theoretical prediction, it is equally interesting to ask: How does thermal conductance scale with L if the coupling between the system and the heat bath is not weak? For a given coupling, how does β depend on the nature of the disorder? In this Rapid Communication, we address these questions by studying, analytically as well as numerically, the scaling of thermal conductance in one-dimensional disordered harmonic chains for different types of disorder and coupling between the system and the heat bath.

Heat conduction by phonons is similar to electrical conduction, but with a crucial difference: the presence of a localization threshold at zero frequency. This leads to a diverging localization length, $\xi(\omega)$, for $\omega \rightarrow 0$ [28,29] and has strong consequences on the scaling of thermal conductance. Specifically, for a given L and disorder strength, one can define a cut-off frequency ω_L , for which $\xi(\omega_L) = L$. All phonons with $\omega \leq \omega_L$ are effectively delocalized, i.e., $\xi(\omega) \geq L$, and contribute to the heat transport.

Model and background. We consider a one-dimensional disordered system consisting of N particles, each of mass M , connected by harmonic springs with spring constants K_i ($i = 1, 2, \dots, N - 1$), chosen randomly from a given distribution (cf. Fig. 1). K_i is the spring constant of the spring connecting particles i and $i + 1$ in the disordered chain. The two ends ($i = 1$ and $i = N$) of the chain of length L are coupled to two heat baths at temperatures T_1 (left bath) and T_2 ($< T_1$; right bath), respectively. Here, $L = (N - 1)r_0$ with r_0 being the average interparticle distance. Heat baths are modeled as ordered

*Deceased.

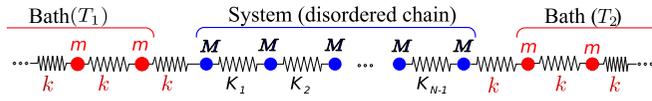


FIG. 1. Schematic illustration of a one-dimensional disordered harmonic chain. All particles and springs in the heat baths are identical, with mass m and spring constant k . Particles in the system all have mass M , and particles i and $(i + 1)$ are connected by a spring with stiffness K_i . The masses at the two ends of the disordered chain, $i = 1$ and $i = N$, are connected to heat baths through a spring of stiffness k .

harmonic chains consisting of an infinite number of equal masses (m), and connected by identical springs (k). The system is coupled to two heat baths via two springs each having spring constant k . If k is much smaller (larger) compared to the typical spring constant in the disordered chain, we refer to the system as weakly (strongly) coupled to the reservoir. Our setup corresponds to the case of “free boundary condition” [10,15] with no local pinning potential which has been shown to affect the scaling of heat flux [12,26]. Below we work in units where the mass M of the system’s particles, the natural frequency of the bath $\omega_0 = \sqrt{k/m}$, and Boltzmann’s constant are all set to unity. We express the stiffness of the springs in units of $M\omega_0^2 = 1$. For a fixed disorder strength, when we vary k to study the effect of coupling strength, we also vary m with it to maintain $\omega_0 = 1$.

In the current study, we consider two models of disorder: (1) Uniform distribution: $K_i = (1 + R_i)$ where R_i follows a uniform distribution of width W , i.e., $R_i \in [-W/2, W/2]$. Large values of W correspond to stronger disorder and $W = 2$ is the strongest possible disorder strength. (2) Power-law distribution: K_i follow a power-law probability distribution, $P(K) \propto K^{\epsilon-1}$, where $0 < K \leq 1$ and disorder strength is quantified by the dimensionless parameter $\epsilon (> 0)$ [30]. This situation arises naturally if K decays exponentially with inter-particle separation which follows a Poisson process [31,32]. The effective spring constant of the chain is the inverse of the sum of $1/K_i$, hence the compressibility Z is related to $\langle 1/K \rangle$. For $\epsilon = 1$, the behavior of Z changes drastically as the mean of the distribution $P(Z = K^{-1}) \propto Z^{-(\epsilon+1)}$ diverges at this point. We identify $\epsilon \leq 1$ as the strong disorder regime within this model. A smaller value of $\epsilon (< 1)$ implies a spring distribution with a power-law tail characterizing a “heavy-tailed” distribution [23].

As noted above, transport is mediated by effectively delocalized low-frequency phonons. Thus, it will be crucial to understand the scaling behavior of the localization length, $\xi(\omega)$, and density of states (DOS), $\rho(\omega)$, in the limit $\omega \rightarrow 0$ [33]. Earlier theoretical predictions related to these scaling behaviors are summarized in Table I and numerically demonstrated in Figs. 2(a), 2(b) and 3.

Analytical results. To study the heat transport we follow the Landauer scattering approach in which propagation of a phonon of given frequency ω through the disordered chain is characterized by a transmission coefficient, $\tau(\omega)$. For a one-dimensional system the thermal conductance $G(L, T)$ is [34]

$$G(L, T) \approx \int_0^\infty \frac{d\omega}{(2\pi)^2} \hbar \omega \frac{\partial f_T(\omega)}{\partial T} \tau(\omega), \quad (1)$$

TABLE I. Summary of the scaling behavior for thermal conductance, G (from this work), density of states (DOS), ρ , and localization length, ξ (from Refs. [28,29,32,36,37]) under different impedance mismatch (coupling k) and disorder strengths.

Disorder	Localization	DOS	Impedance mismatch	Conductance
Uniform	$\xi \sim \omega^{-2}$	$\rho \sim 1$	Any	$G \sim L^{-1/2}$
Power law, $\epsilon \geq 2$ (weak)	$\xi \sim \omega^{-2}$	$\rho \sim 1$	Any	$G \sim L^{-1/2}$
Power law, $1 \leq \epsilon \leq 2$	$\xi \sim \omega^{-\epsilon}$	$\rho \sim 1$	Any	$G \sim L^{-1/\epsilon}$
Power law, $\epsilon \leq 1$ (strong)	$\xi \sim \omega^{-2\epsilon/(\epsilon+1)}$	$\rho \sim \omega^{\epsilon/(\epsilon+1)}$	Low High	$G \sim L^{-(1+\epsilon)/2\epsilon}$ $G \sim L^{-1}$

where f_T is the Bose-Einstein distribution function and we also assume $\Delta T = T_1 - T_2 \ll T = \frac{T_1 + T_2}{2}$.

The system features two competing frequency scales: the disorder-related ω_L and the thermal frequency $\omega_T = T/\hbar$. Phonons with $\omega > \omega_L$ do not contribute to conductance because they are localized. Phonons with $\omega > \omega_T$ do not contribute because they are not populated. Therefore, the integral in Eq. (1) is better represented in terms of the nondimensional frequency $x = \omega/\omega_T$,

$$G(L, T) = \frac{3g_{qm}}{\pi^2} \int_0^\infty dx \frac{x^2 e^x}{(e^x - 1)^2} \tau(x \omega_T). \quad (2)$$

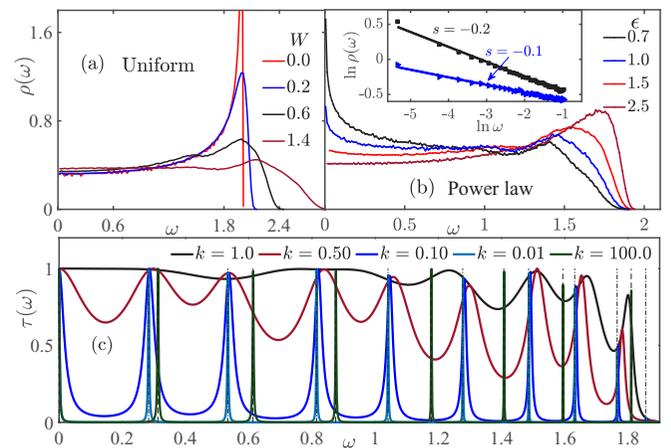


FIG. 2. Density of states, $\rho(\omega)$, as a function of phonon frequency ω for different disorder strengths for a one-dimensional harmonic chain with (a) uniform disorder and (b) power-law disorder and $N = 2000$. (a) For $W = 0$, $\rho(\omega)$ diverges when $\omega \rightarrow 2$ and vanishes for $\omega > 2$. The presence of disorder ($W > 0$) smears out the divergence at $\omega = 2$ and gives rise to finite $\rho(\omega)$ for $\omega > 2$. For $\omega \rightarrow 0$, $\rho(\omega)$ approaches a constant for all disorder strengths. (b) For power-law disorder, $\rho(\omega)$ diverges at $\omega \rightarrow 0$ in the strong disorder regime and approaches a constant in the intermediate and weak regimes (inset). (c) The transmission coefficient $\tau(\omega)$ for various coupling strengths (k) and a given realization of disorder (uniform disorder with $W = 0.5$ and $N = 11$). For $k = 1.0$, transmission is roughly constant up to a cutoff frequency ω_L . For $k \ll 1$ or $k \gg 1$, τ is sharply peaked around the eigenfrequencies of the disordered chain.

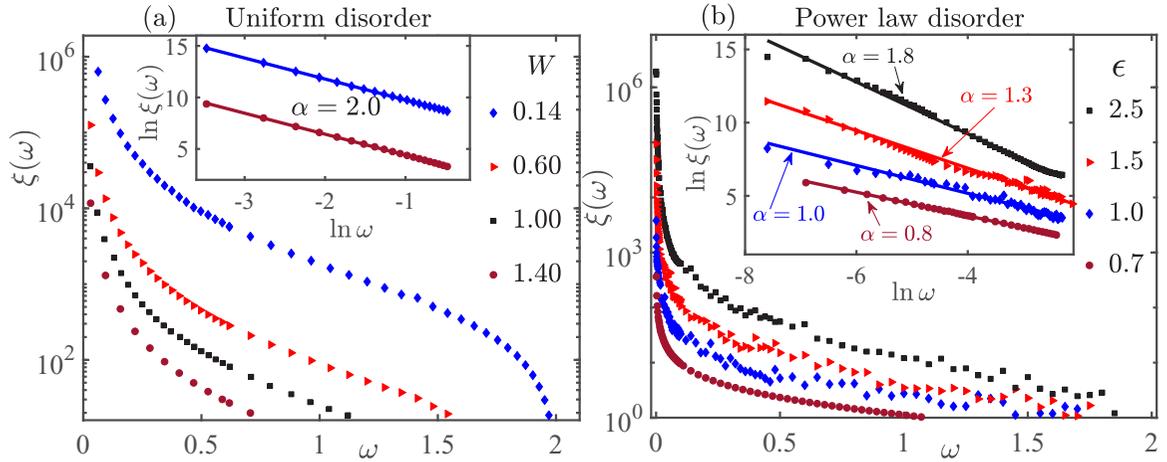


FIG. 3. The dependence of localization length, $\xi(\omega)$, on the frequency ω of the phonons for different strengths of disorder (y axis in logarithmic scale) for (a) uniform disorder and (b) power-law disorder. For small frequencies ($\omega \rightarrow 0$), $\xi(\omega)$ diverges as $\omega^{-\alpha}$ where α depends on disorder strength. (a) For uniform disorder, $\alpha = 2$ in weak as well as strong disorder regimes. (b) For power-law disorder, $\alpha \approx 2$ for weak disorder ($\epsilon > 2$) while for intermediate disorder ($1 < \epsilon \leq 2$), $\alpha \approx \epsilon$ and in the strong disorder regime ($\epsilon \leq 1$), $\alpha \approx \frac{2\epsilon}{1+\epsilon}$ (inset).

Here $g_{qm} = \pi^2 T / (3h)$ is the quantum of thermal conductance [34,35], which is the universal value of $G(L, T)$ in the limit $T \rightarrow 0$. To see this, note that $\tau(\omega) \rightarrow 1$ for $\omega \rightarrow 0$ due to the existence of a Goldstone mode, related to the translational invariance of the system. Using this fact, it is straightforward to show that for a given L Eq. (2) yields $G(L, T) \rightarrow g_{qm}$ for very small T ($\omega_T \ll \omega_L$), regardless of any other property of $\tau(\omega)$. g_{qm} is thus the natural unit of conductance for our system and below we express all results in these units by defining $G_{qm}(L, T) = G(L, T) / g_{qm}$.

Of course, the limit of $L \rightarrow \infty$ and finite T is of more interest, but an exact evaluation of the integral in the general case is not feasible. Nonetheless, much insight can still be gained in some interesting cases.

We first consider the situation where the stiffness of the coupling spring k is comparable to that of the chain, i.e., $k \approx 1$. In this case there is relatively little impedance mismatch between the chain and the bath, implying less reflectance of the incident phonons from the bath-system boundary. In this situation, phonons get transmitted even when their frequency is not close to an eigenfrequency of the chain. Therefore, from a scaling perspective we can approximate that $\tau(\omega) = 1$ for all phonons with $\omega \leq \omega_L$ and zero otherwise. A numerical calculation of $\tau(\omega)$, shown in Fig. 2(c), demonstrates that this approximation is crude but reasonable. As shown below, it quantitatively captures the scaling behavior.

With this approximation, Eq. (1) depends only on the dimensionless combination ω_L / ω_T (which is the upper integration limit) implying that thermal conductance for $k \approx 1$ should follow a universal curve, independent of temperature and disorder, when expressed in terms of ω_L / ω_T . In fact the integral can be carried out in closed form, and for large L (or large T , i.e., $\omega_T \gg \omega_L$) it reads

$$G_{qm}(L, T) \approx \frac{3}{\pi^2} \left(\frac{\omega_L}{\omega_T} \right) + O\left(\frac{\omega_L}{\omega_T} \right)^2. \quad (3)$$

In order to get the explicit dependence on system size in this limit, we use the known scaling $\xi(\omega) \propto \omega^{-\alpha}$ (see [23]

and Fig. 3). Straightforward manipulation shows that this implies $G_{qm} \propto L^{-1/\alpha} T^{-1}$, that is, $\beta = \alpha^{-1}$ in this limit of small impedance mismatch and large L . Also, for a given L , $G(T) \propto T$ for small T and $G(T) \sim \text{const}$ (saturates) for high T [33].

For uniform disorder, theory predicts $\alpha = 2$ implying $G(L) \propto L^{-1/2}$, in accord with previously reported results for a mass-disordered chain under free boundary condition [10,15]. For power-law disorder, as α depends on disorder strength ϵ , β also depends on ϵ with $G \propto L^{-1/2}$, $L^{-1/\epsilon}$, and $L^{-[(1+\epsilon)/2\epsilon]}$ in the weak, intermediate, and strong disorder regimes, respectively. These results are summarized in Table I.

This concludes the case of $k \approx 1$, where transmission is approximately constant for all ω below a certain cutoff. How does the picture change in the case of strong impedance mismatch, $k \gg 1$ or $k \ll 1$? In this case transmission is negligible for almost all frequencies, except those which are close to an eigenfrequency of the disordered chain. In previous work [23], it was shown that in the weak-coupling limit, $k \ll 1$, τ has a structure of nonoverlapping Lorentzians for phonons with $\omega < \omega_L$ [cf. Fig. 2(c)]. Each Lorentzian is centered around an eigenfrequency of the disordered chain and the area of each Lorentzian, i.e., its integrated contribution to the thermal conductance, was shown to be ω independent for the delocalized modes [23]. Calculating the integral in general for any ω_L / ω_T is difficult, but if we are only interested in the scaling behavior for large L , the integral essentially counts the number of eigenmodes of the disordered chain within the frequency range $0 < \omega \leq \omega_L$ [38]:

$$G(L) \approx \Sigma \int_0^{\omega_L} d\omega \rho(\omega), \quad (4)$$

where Σ is the area of each Lorentzian. Considering $\rho(\omega) = D\omega^s$ [see [23] and Figs. 2(a) and 2(b)], where D depends on disorder, for large L we get

$$G \propto \omega_L^{s+1} \propto L^{-[(s+1)/\alpha]}. \quad (5)$$

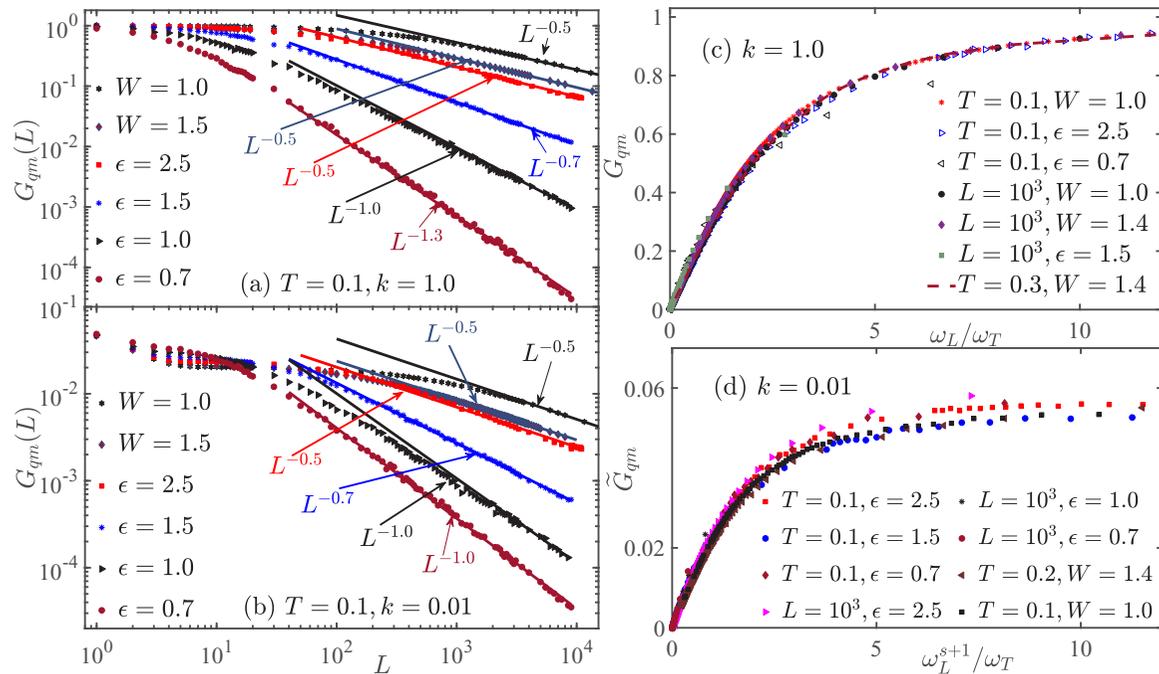


FIG. 4. Dependence of the thermal conductance $G_{qm}(L)$ on the length L of the disordered chain for uniform (disorder strength W) and power-law (disorder strength ϵ) disorder in a log-log plot with (a) $k = 1.0$ and (b) $k = 0.01$. The mean temperature is fixed at $T = 0.10$. For $k = 1.0$, $G_{qm}(L) \approx 1$ for very small L , while $G_{qm}(L) \propto L^{-\beta}$ for large L . $\beta \neq 1$ for $k = 1.0$ except for $\epsilon = 1$. For $k = 0.01$, $\beta = 1.0$ in the strong disorder regime ($\epsilon \leq 1.0$) while in all other cases $G_{qm}(L)$ scales anomalously. Unified description of thermal conductance for one-dimensional disordered harmonic chains with different models of disorder in terms of the variable (c) ω_L/ω_T (for $k = 1.0$) and (d) ω_L^{s+1}/ω_T (for $k = 0.01$). Here, $\tilde{G}_{qm} = \frac{(s+1)G_{qm}}{D}$ (see text for details).

Thus, in the weak-coupling regime $G_{qm} \propto L^{-(s+1)/\alpha} T^{-1}$ for a fixed T . For uniform disorder, as well as power-law disorder with $\epsilon > 1$ (i.e., the weak and intermediate regimes), we have $s = 0$ and thus the scaling of thermal conductance with L remains the same as in the case of an impedance-matched bath $k \approx 1$. Interestingly, for strong disorder, $\epsilon < 1$, we have $s = \frac{\epsilon-1}{\epsilon+1}$ and $\alpha = \frac{2\epsilon}{1+\epsilon}$, which together cancel out exactly to yield normal Fourier-like heat conduction $\beta = 1$. Also, note that, when expressed in terms of ω_L^{s+1}/ω_T , thermal conductance should follow a universal curve in the weak-coupling regime and the large L limit.

Lastly, we deal with the case of very large k , i.e., the strong-coupling regime. A careful analysis, presented fully in the Supplemental Material [33], shows that this limit is equivalent to a system with the first and last particles excluded, i.e., effectively a system of $(N - 2)$ particles. Therefore, like in the case of weak coupling, $\tau(\omega)$ is composed of nonoverlapping peaks with an ω -independent area (cf. Fig. 2). Since $\rho(\omega)$ and $\xi(\omega)$ are independent of the coupling k , all our predictions for $k \ll 1$ hold also for $k \gg 1$. That is, the same scaling exponents emerge in the case of strong impedance mismatch, regardless of whether k is very small or very large. All our theoretical predictions for different disorder types and coupling strengths are summarized in Table I.

Numerical results. We test our theoretical predictions by numerically computing thermal conductance and other properties, such as density of states and localization lengths, for all cases considered above. The density of states, $\rho(\omega)$, for

different disorder strengths is shown in Figs. 2(a) and 2(b) for the uniform and power-law disorder, respectively, with $N = 2000$ [33]. For uniform disorder, $\rho(\omega)$ approaches a constant as $\omega \rightarrow 0$, that is, $s = 0$. For power-law disorder, $\rho(\omega)$ diverges with an exponent consistent with the theoretical prediction, $s = \frac{\epsilon-1}{\epsilon+1}$. For weak and intermediate disorder theory predicts $s = 0$ but a weak divergence is observed for $\epsilon = 1$, the origin of which is not clear to us at present.

To calculate G , we compute $\tau(\omega)$ directly for different k and disorder types using a transfer matrix method [33]. For a single realization of the disorder, the dependence of $\tau(\omega)$ on k is shown in Fig. 2(c) (with $W = 0.50$ and $N = 11$).

For a given disorder and a fixed ω , we find that $\tau(\omega)$ decays exponentially with L [33]. This defines a length scale which we interpret as the localization length ξ , i.e., $\tau(\omega, L) \propto \exp[-L/\xi(\omega)]$ [33]. We find that ξ diverges like $\xi(\omega) \propto \omega^{-\alpha}$, consistent with theoretical predictions (see Fig. 3).

Finally, we compute G for different L , T , disorder types, and coupling strengths, using Eq. (1), by considering $\omega \in (0, 2\omega_0)$. This is presented in Figs. 4(a) (for $k = 1.0$) and 4(b) (for $k = 0.01$), which shows that the numerical results for all cases agree with the theoretical predictions (for $k = 100$, see Supplemental Material [33]). Heat transport is anomalous ($\beta \neq 1$) for all cases except for the power-law disorder in the weak-/strong-coupling regime and also when $\epsilon = 1$ [Fig. 4(b)]. In addition, panels (c) and (d) demonstrate that when expressed in terms of ω_L/ω_T (for $k = 1$) and ω_L^{s+1}/ω_T (for $k = 0.01$), respectively, all data collapse on a single curve, following Eqs. (3) and (5).

Conclusions. In this Rapid Communication, we studied the nontrivial scaling behavior of thermal conductance, G , which depends both on the nature of disorder and the coupling between the system and the heat baths, in one-dimensional disordered harmonic chains. We found that G features anomalous scaling with L for uniform disorder and for weak and intermediate power-law disorder (i.e., with a well-defined mean). Interestingly, for strong power-law disorder and strong impedance mismatch, $k \ll 1$ or $k \gg 1$, normal scaling $G \propto L^{-1}$ is observed. For strong disorder and low impedance mismatch, i.e., $k \approx 1$, the scaling exponent β can be greater than unity. We also identified the dimensionless scaling parameter with which one has a unified description for all temperatures

and system sizes. It is worth noting that although G —a global measure of transport—features normal scaling in the strong disorder regime, we cannot conclude that heat transport is indeed normal, in the sense that local dynamics follow Fourier’s law. Thus, it remains to be explored how heat energy spreads in the system in the strong disorder regime.

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