Thermal conductivity in 1d: disorder-induced transition from anomalous to normal scaling

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It is well known that the contribution of harmonic phonons to the thermal conductivity of 1D systems diverges with the harmonic chain length \( L \) (explicitly, increases with \( L \) as a power-law with a positive power). Furthermore, within various one-dimensional models containing disorder it was shown that this divergence persists, with the thermal conductivity scaling as \( \sqrt{L} \) under certain boundary conditions, where \( L \) is the length of the harmonic chain. Here we show that when the chain is weakly coupled to the heat reservoirs and there is strong disorder this scaling can be violated. We find a weaker power-law dependence on \( L \), and show that for sufficiently strong disorder the thermal conductivity stops being anomalous – despite both density-of-states and the diverging localization length scaling anomalously. Surprisingly, in this strong disorder regime two anomalously scaling quantities cancel each other to recover Fourier’s law of heat transport.

Over the past decades, studying the thermal conduc-
tance of low-dimensional systems has generated much
interest both theoretically and experimentally, and both at
the classical and quantum level [1,8]. Intriguingly, the
thermal conductivity of an ordered lattice diverges, in
di.

The model.

Consider a chain of harmonic springs, con-
structed as follows. First, \( N \) points are chosen randomly
and uniformly in the interval \([0, L]\), and a mass \( M \)
is placed on each of them. Without loss of generality we
choose \( L = N – 1 \), such that the average nearest-neighbor
distance \( r_{nn} = 1 \). Next, the springs between nearest-
neighbor masses are chosen as:

\[
K = e^{-r/\xi},
\]

(1)

with \( r \) the distance and \( \xi \) a constant. The dimension-
less parameter \( \epsilon \equiv \xi/r_{nn} \) is a measure of the disorder,
where for \( \epsilon \to 0 \) the distribution of spring constants be-
comes very broad, corresponding to the case of strong
disorder. Since the nearest-neighbor distance follows a

Poisson process, we find that:

\[
P(K) \propto K^{\epsilon - 1}.
\]

(2)

The spectrum and localization properties of this model
were studied in Refs. [9,11], and are reviewed below.

Consider coupling the system now to two infinite, ther-
al baths, at temperatures \( T_1 \) and \( T_2 \). Within each of
the bath, phonons of all frequencies would be propagating
in both directions. The partitioning of phonon energies
is given by the Bose-Einstein distribution, and each of
them is transmitted through the disordered region with
some probability \( T(\omega) \) (depending on the properties of
the disordered region as well as its coupling to the baths).
Accounting for the density-of-states in the leads, the heat
flux going from left to right is found to be [3]:

\[
\dot{Q} = \frac{1}{2\pi} \int_0^\infty \omega N_{T_1}(\omega) h_\omega d\omega,
\]

(3)

where \( T(\omega) \) is the transmission probability of a phonon
with frequency \( \omega \) and \( N_{T_1} \) is the Bose-Einstein function.
By writing a similar expression for the right-to-left heat
flux and taking the limit \( T_1 - T_2 \to 0 \), we find that the
heat conductance \( G \) (distinct from the conductivity, \( \sigma \))
is:

\[
G = \frac{1}{2\pi} \int_0^\infty T(\omega) \frac{\partial N_{T_1}(\omega)}{\partial T} |_{T_1} h_\omega d\omega.
\]

(4)

Note that here \( T(\omega) \) is the frequency-dependent trans-
mission, while \( T \) is the temperature. Later we will see
that in the thermodynamic limit \( L \to \infty \) the dominant
contribution to this integral comes from low frequency
phonons, in which case we can approximate \( \frac{\partial N_{T_1}(\omega)}{\partial T} \approx \frac{k_B}{\hbar \omega} \). Therefore we find the conductance is given by:

\[
G = \frac{k_B}{2\pi} \int_0^\infty T(\omega) d\omega.
\]

(5)
A similar result is obtained in Ref. [4].

Consider now a model in which the bath consists of an infinite set of identical masses \( m \) and springs \( k \), with lattice constant \( a \). Masses in the disordered region will have indices of 1 to \( N \). Masses 1 and \( N \) will be connected to the bath via a spring of strength \( k \). The model is illustrated schematically in Fig. 1. We shall now show that the transmission through this chain is well approximated by a sum of narrow Lorentzians, with different widths and areas. Thus, they contribute non-uniformly to the integral of Eq. [5].

\[
\bar{x} = [A + M\omega^2 I]^{-1}\bar{b} = \sum_{\lambda} \frac{1}{\lambda + M\omega^2} \langle \langle \bar{b} | |v_{\lambda}\rangle \rangle |v_{\lambda}\rangle , \tag{9}
\]

where we are using the quantum-mechanical notation for convenience, and assumed that the eigenmodes are normalized. In the following we shall also assume that the eigenmodes entries are real, which we can assume without loss of generality since \( A \) is Hermitian.

If the springs in the ordered region are sufficiently small, the transmission will be negligible for nearly every frequency, except when \( \omega \) is close to an eigenfrequency of the chain (in which case the denominator vanishes). We will assume this to be the case, and later on we will establish the precise condition on \( k \) and \( m \) for this to hold (note that this is one particular way of realizing the thermal bath). When the driving frequency is close to this resonant frequency by a detuning \( \delta \lambda = M(\omega^2 - \omega_0^2) \), only this particular eigenmode \( |v\rangle \) will contribute to the sum of Eq. [9], leading to:

\[
\bar{x} \approx \frac{1}{\delta \lambda} \langle \langle \bar{b} | |v\rangle \rangle |v\rangle . \tag{10}
\]

These equations determine \( r \) and \( t \). Solving leads to:

\[
t = \frac{-kv_N v_N e^{-2i\lambda} (1 - e^{-2i\lambda})}{e^{2i\lambda} (e^{-i\lambda} + k |v_N|^2 + |v_1|^2)} . \tag{11}
\]

Note that, as expected, in order for the transmission to be non-negligible the eigenmode should have support both at the beginning and end of the disordered chain, i.e., only eigenmodes which have localization lengths comparable or larger to the length of the chain contribute to the transmission, and hence to the thermal conductance. Later we shall show that for \( L \to \infty \), only the low-lying modes will be delocalized, hence we can assume the frequency \( \omega \) and thus \( \chi \) to be small. Hence:

\[
T = |t|^2 \approx \frac{4k^2 \chi^2 (v_1 v_N)^2}{\chi^2 \delta \lambda^2 + (\delta \lambda + k |v_1|^2 + |v_N|^2)^2} , \tag{12}
\]

leading to:

\[
T \approx \frac{4k^2 \chi^2 (v_1 v_N)^2}{(\delta \lambda + S)^2 + \chi^2 S^2} , \tag{13}
\]

where \( S \approx k |v_1|^2 + |v_N|^2 \) and \( \delta \lambda = -M(\omega^2 - \omega_0^2) \). It is useful to replace \( \delta \lambda + S \) with \( -M(\omega^2 - \tilde{\omega}^2) \approx -2M\tilde{\omega}(\omega - \tilde{\omega}) \),
which shows that this form is approximately a Lorentzian in terms of $\omega$:

\[
T(\omega) \approx \frac{4k^2\chi^2(v_1v_N)^2}{2M\omega(\omega - \tilde{\omega})^2 + \chi^2S^2}. \tag{14}
\]

An example of this is shown in Fig. 2. The maximal transmission is governed by the asymmetry of the eigenmode, and is 1 for $v_1 = v_N$. The area associated with each Lorentzian is:

\[
\Sigma_\lambda = 2\pi k_B \frac{\sqrt{km}(v_1v_N)^2}{M} \frac{1}{v_1^2 + v_N^2}. \tag{15}
\]

Therefore it depends on the product $\frac{(v_1v_N)^2}{v_1^2 + v_N^2}$ but not explicitly on the frequency. Specifically, the contribution of all delocalized modes to the conductance is constant. For a purely delocalized mode (on the scale of the disordered region, $L$) we have $v_1 = v_N = \frac{1}{\sqrt{N}}$ and thus the contribution to the thermal conductance is $\Sigma_\lambda = \frac{2\pi k_B \sqrt{km}}{M N}$. Note that this constant is different than the “quantum of thermal conductance” [3], and depends on the properties of the bath (through $k$ and $m$). Next, we will consider how the disorder affects the scaling of the thermal conductance, by summing over the contribution of all modes which are effectively delocalized.

\[
FIG. 2. \text{ Numerical simulation of a weakly disordered chain of length } N = 50. \text{ The red vertical lines show the eigenfrequencies of the disordered region, which nearly coincide with the Lorentzian peaks in the transmission. The area under each Lorentzian is determined by the product of the amplitudes of the right and left masses, and increases with the degree of \textquote{delocalization} of the mode. The red dashed lines indicate the eigenfrequencies of the disordered chain, and their height corresponds to the numerator of Eq. (11).}
\]

Application to disordered chain. Within the aforementioned model, in the thermodynamic limit phonons of all frequencies are localized, with a diverging length scale at $\omega \to 0$. As noted above, for a finite system of size $L$, according to Eq. (13) only phonons will localization length of order or larger than $L$ will contribute to the thermal conductance, with each mode contributing a constant amount independent of frequency. Thus we can write:

\[
G \approx \int_0^{\omega_c} \nu(\omega)d\omega, \tag{16}
\]

where $\nu(\omega)$ is the density-of-states (DOS) of the phonons in the disordered region and the localization length at $\omega_c$ equals $L$. (Note that the DOS is proportional to $N$).

According to Ref. [10], for disorder below a critical strength ($\epsilon \geq 1$ in our above definitions) we have Debye DOS (constant in 1d) and for $\epsilon \leq 2$ the localization length diverges as [12]:

\[
l_{loc}(\omega) \propto 1/\omega^2. \tag{17}
\]

This result – corresponding to Rayleigh scattering in one dimension – has been also derived in Refs. [13] [14] for low-lying acoustic modes with weak disorder of a different type. Moreover, since in one-dimensional systems the localization length equals the mean free path [15], this result reflects the Rayleigh-like nature of scattering in the weakly disordered regime.

Plugging this into Eq. (16) we find:

\[
G(L) \propto 1/\sqrt{L}. \tag{18}
\]

This implies that the thermal conductivity $\sigma$ diverges as $\sqrt{L}$, a result obtained in the context of several other related disordered models [11] [16] [17].

Intriguingly, this result changes when we consider strong disorder. For $1 \leq \epsilon \leq 2$, the DOS follows a Debye spectrum, while the localization length diverges more slowly in this regime [10]:

\[
l_{loc}(\omega) \propto 1/\omega^{\epsilon}. \tag{19}
\]

Note that it is precisely at the point $\epsilon = 2$ that the variance in the compressibility of the system becomes ill-defined: the effective spring constant is the sum of $1/K$, hence the compressibility is related to $1/K$. The distribution of $z = 1/K$ follows $p(z) \propto 1/z^{1+\zeta}$, hence it becomes heavy-tailed at the point $\zeta = 2$. Similarly, at the point $\zeta = 1$ the mean of this distribution diverges making the compressibility ill-defined in the continuum limit – as we shall now see, the behavior will again dramatically change at this point. This is reminiscent of the qualitative change in the diffusion properties in the
context of anomalous diffusion [16] as well as the emergence of aging in Bouchaud’s trap model when the mean trapping time diverges [17].

Eq. (19) implies that:

\[ G(L) \propto 1/L^{1/\epsilon}. \] (20)

Thus, the thermal conductance becomes normal (i.e., obeying Fourier’s law) as opposed to anomalous at the point \( \epsilon = 1 \).

Finally, for even stronger disorder, \( \epsilon \leq 1 \), we have [10]:

\[ \nu(\omega) \propto \omega^{\frac{-1}{\epsilon}}, \] (21)

Thus, for strong disorder the DOS develops a strong singularity at the origin approximately diverging as \( 1/\omega \). This “boson-peak” like behavior as well as the localization length scaling in this regime were derived using a strong-disorder renormalization group procedure in Ref. [11]. The localization length in this case scales as:

\[ l_{loc}(\omega) \sim 1/\omega^{\frac{1}{2\epsilon}}. \] (22)

This implies that:

\[ G(L) \propto 1/L. \] (23)

Thus, for disorder above a critical threshold the divergence of the thermal conductivity is remedied, and the thermal conductivity \( \sigma \) becomes independent of system size. These results are summarized in Fig. 3 and in Table 1, which constitute our main results.

We may now revisit our previous assumption – that a single eigenmode contributes to each transmission peak. This is equivalent to demanding that the Lorentzians are well separated. The width of each of the delocalized modes can be readily identified from Eq. (14) to be \( \sqrt{\epsilon m N/M} \) (for all disorder regimes). Their separation is the inverse of the local DOS. For the weak disorder regime, the DOS is constant and scales as \( \frac{1}{L^{1/\epsilon}} \), where \( K = 1 \) is the strongest possible spring within the model. Hence the condition for the applicability of the approximation is \( k/K \ll M/m \). The same is true in the intermediate disorder, since the DOS is still constant. However for the strong disorder regime \( \epsilon < 1 \) the DOS is given by Eq. (21), hence the condition becomes \( \sqrt{\epsilon m N/M} \ll \omega \frac{1}{2\epsilon} \sqrt{K/M} \). This condition has to be fulfilled for the typical delocalized frequency \( \omega_c \sim N^{-1/\epsilon} \), giving a more stringent (N-dependent) condition for the ratio \( \frac{K}{M} \).

To summarize, we have studied a simple model of phonon conduction in 1D harmonic chain, and found intriguing behavior of the thermal conductivity. While for weak disorder we reproduce the known \( \sqrt{L} \) scaling of the conductivity with system size, we found that for “heavy-tailed” disorder this scaling changes, with a scaling exponent that changes smoothly until the disorder power-law reaches a critical threshold at which the Fourier law is recovered – despite density-of-states and localization length both scaling differently than in the weak disorder regimes (i.e., they do not follow the Debye and Rayleigh laws). Further work will establish what physical system are described by a weak coupling to the thermal bath as studied here, and what happens in the case of stronger coupling, where interference between the different eigenmodes is significant, potentially via the use of numerical simulations. Furthermore, in the future it would be interesting to study how strong disorder affects the phonon thermal conductivity in higher dimensions, and what the fate of Fourier’s law is in that scenario.

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TABLE I. Summary of expected exponents for thermal conductance (from this work), DOS and localization length (from Ref. [10]).

| Disorder strength | DOS exponent $\propto \omega^\alpha$ | Localization length exponent $\propto 1/\omega^\beta$ | Thermal conductivity exponent $\propto L^\theta$ |
|------------------|-----------------------------------|---------------------------------|-------------------------------|
| $\epsilon > 2$ (weak disorder) | 0 (Debye) | 2 (Rayleigh) | 1/2 (anomalous) |
| $1 < \epsilon \leq 2$ (intermediate disorder) | 0 (Debye) | $\epsilon$ | $1 - 1/\epsilon$ (anomalous) |
| $\epsilon \leq 1$ (strong disorder) | $i\frac{1}{\epsilon}$ | $\frac{2\epsilon}{1+\epsilon}$ | 0 (normal) |

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