Phonon-mediated thermal conductance of mesoscopic wires with rough edges

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We present an analysis of acoustic-phonon propagation through long, free-standing, insulating wires with rough surfaces. Owing to a crossover from ballistic propagation of the lowest-frequency phonon mode at \( \omega < \omega_1 = \pi c / W \) to a diffusive (or even localized) behavior upon the increase of phonon frequency, followed by reentrance into the quasi-ballistic regime, the heat conductance of a wire acquires an intermediate tendency to saturate within the temperature range \( T \sim \hbar \omega_1 / k_B \).

During recent years, low-temperature heat transport experiments on electrical insulators have been extended to mesoscopic systems, where the wavelength of thermal phonons can be comparable to the geometrical size of the device. In this regime, phonon transport through a thermal conductor such as an electrically insulating solid wire, formed from an undoped semiconductor may exhibit ballistic waveguide propagation. This possibility has stimulated interest in the guided-wave, phonon-mediated heat conductance, \( \kappa(T) \) of ballistic wires (with a width \( W \) much smaller than the length \( L \)) connecting a heat reservoir to a thermal bath.\[1\]

In the present paper, we analyse the low-temperature heat transport \((k_B T \sim \hbar \pi / W\), where \( c \) is the sound velocity) heat transport in relatively long \((L/W \sim 100)\) free-standing insulating wires by taking into account the effect of surface roughness. The idea behind this analysis is based on the assumption that, in a long wire, the wire edge or surface roughness may result in strong scattering, and even in the localization of acoustic waves in the intermediate-frequency range, whereas the low-frequency part of the phonon spectrum would always have ballistic properties due to the specifics of sound waves. In the high-frequency part of the spectrum, phonons would have quasiballistic properties, too. This may result in a non-monotonic temperature dependence of the thermal conductance of such a system.

To verify the possibility of the existence of such a regime, in principle, we investigate the dependence on frequency \( \omega \) of the transmission coefficient \( I(\omega) \) using a simplified model of a solid waveguide which has been chosen to reflect two features of this problem: the influence of roughness on the propagation of vibrations and the suppression of scattering on the roughness upon the decrease of the excitation frequency. We approach the problem numerically, by studying the transmission coefficient averaged over many realizations of a wire characterized by a given distribution of length scales in the surface roughness, and using this to find the heat conductance, \( \kappa(T) \). Phonon-mediated heat transport in quasi-one-dimensional systems can be studied using the same theoretical techniques as electron transport.\[2,3\] However, in contrast to electrical conductance, which at low temperatures is determined by transport properties of electron waves at the Fermi energy, the thermal conductance of a phonon waveguide is determined by all phonon energies \( \omega \) up to \( \hbar \omega \sim k_B T \). This smears out effects of confinement in the transverse direction in the temperature dependence of \( \kappa(T) \) in ballistic systems,\[4\] but results in a pronounced feature in \( \kappa(T) \) for strongly disordered free-standing wires. The latter has the form of an intermediate saturation regime in \( \kappa(T) \) following a linear \( T \) dependence at the lowest temperatures, with an anomalous length dependence of the saturation value, that scales as \( \kappa_{sat} \propto L^{-1/2} \) for wires with a white-noise spectrum of roughness.

**Transmission coefficient analysis and localization of acoustic modes.** Below, we classify phonon modes in a wire by the number \( n \) of nodes in the displacement amplitude. The \( n = 0 \) lowest-frequency vibrational mode \((\omega < \omega_1 = c \pi / W\), where \( c \) is the velocity of sound) corresponds to equal displacements over the cross section of a free-standing wire and has a linear dispersion; others have frequency gaps, \( \omega_n(q) = \sqrt{(cq)^2 + (\pi nc / W)^2} \).

The aforementioned feature originates from the fact that edge disorder suppresses the transmission of all coherent phonon modes at high frequencies, but has a little influence on the \( n = 0 \) mode at \( \omega \to 0 \), where \( \Gamma(\omega \to 0) \to 1 \). The transmission coefficient of this mode is mainly determined by direct backscattering, whose rate depends on the intensity of the surface roughness harmonic \( \langle \delta W_q^2 \rangle \) with wave number \( q \sim \omega / c \). According to Rayleigh scattering theory in one dimension, the mean free path of this mode diverges at \( \omega \to 0 \) as

\[
 I_0(\omega) \sim (\omega_1 / \omega)^2 \left( W^2 / \langle \delta W_q^2 \rangle \right) W, \quad (1)
\]

even if long-wavelength Fourier components \( \delta W_q \) are equally represented in the surface roughness \( \delta W(x) \). In an infinitely long wire with white-noise randomness on the surface, this results in a localization length \( L_\ast \) for the lowest phonon mode which diverges at \( \omega \to 0 \) as

\[
 L_\ast(\omega) \sim I_0(\omega) \propto \omega^{-2}. \quad (2)
\]

The latter statement is based on the equivalence between the localization problem for various types of waves. For a wire shorter than \( L_\ast \), scattering yields

\[
 1 - \langle \Gamma(\omega) \rangle = \alpha \omega^2 \text{ at } \omega < \omega_1. \quad (3)
\]
In contrast, at higher frequencies, all modes in a wire with a white-noise randomness backscatter (either via intra- or inter-mode process) typically at the length scale of $l \sim W/\langle (\delta W/W)^2 \rangle$. Hence, for frequencies $\omega > \omega_1$, the transmission coefficient tends to follow a linear frequency dependence, $\langle T(\omega) \rangle \sim (\omega W/c) (l/L) \ln(W/\omega/\epsilon)$, which is typical for diffusion in quasiballistic systems. The crossover from the low-frequency regime to the intermediate-frequency range in a long enough wire can, therefore, be nonmonotonic, with a pronounced fall towards zero at $\omega \lesssim \omega_1$, similar to that discussed by Blencowe in relation to the phonon propagation in thin films. As a result, an irregular wire may exhibit ballistic phonon propagation at low frequencies, whereas, at higher frequencies $\omega_1 \lesssim \omega$, surface roughness would yield diffusive phonon propagation, or even localization.

The numerical simulations reported below confirm the above naive expectations. In these simulations, we model the phonons in a crystalline wire cut from a thin film (with the thickness much less than the wire width) as longitudinal waves in a two-dimensional strip whose width $W(x)$ fluctuates with rms value $\langle (\delta W/W)^2 \rangle^{1/2} = 0.1$ on a length scale $\xi$ longer or of order $W$. The effect of the width fluctuations consists of the scattering of acoustic waves propagating along the wire. The model that we adopt here gives a very simplified representation of a real system, since we ignore the existence of torsional and transverse bending modes of the wire excitations, which are known to transfer heat in adiabatic ballistic constrictions. However, it takes into account two features of sound waves: their scattering and the possible localization by the surface roughness, and the almost ballistic properties at both ultra-low and high frequencies. In a continuum model, these lattice vibrations are described by a displacement field $u(x, y)$, which obeys 2D wave equation inside a wire

$$\omega^2 u + c^2 \nabla^2 u = 0,$$  

(4)

Displacements obey free boundary conditions $n \nabla u = 0$ at $y = \pm(W/2 + \delta W_s(x))$, where $s = 1, 2$ indicates the upper and lower edge of the wire, and $n$ stands for the local normal direction to the wire edge. In the simulations, we discretize Eq. (4) on a square lattice with about 200 sites across the wire cross section and, then, compute $\langle T(\omega) \rangle$ numerically using the transfer matrix method for 100 disorder realizations. Our numerical code overcomes problems of instability by QL factorising the transfer matrices at each step. Furthermore, at the end of each calculation, the S-matrix is checked for unitarity.

Fig. 1 shows the results of such simulations obtained for wires with a white-noise spectrum of roughness and an aspect ratio $L/W = 30$. Both the low- and high-frequency asymptotic behaviour of transmission coefficient confirm the expected non-monotonic dependence of $\langle T(\omega) \rangle$ for a wire of length $L \lesssim L_*$.
\[ \kappa = \int_0^\infty \frac{d\omega (\hbar \omega)^2}{2\pi k_B T^2} \frac{\exp(h\omega/k_BT)}{[\exp(h\omega/k_BT) - 1]^2} \langle \Gamma(\omega) \rangle \]  

(6)

For a wire with the transmission coefficient shown in Fig. 2(a), where \( \langle \Gamma(\omega) \rangle \approx 1 + \omega/\omega_1 \), \( \kappa(T) \) is plotted by the dashed-line (1) in Fig. 3, which shows the crossover from linear to quadratic temperature dependence (at \( T \sim \theta_1 = 6 \hbar \omega_1/k_B \pi^2 \)) discussed in Ref. 2.

\[ \kappa \approx (k_B^2 \pi/6h) T + (0.7k_B^2/h) T^2/\theta_1. \]  

(7)

The ballistic character of heat transport in Eq. (7) is reflected by the independence of \( \kappa \) on the sample length.

In a wire, where the transmission coefficient sufficiently drops at \( \omega \sim \omega_1 \), as in Fig. 1, we approximate the low-frequency behavior of the transmission coefficient by a step function, \( \langle \Gamma(\omega) \rangle = \theta(\omega_1 - \omega) \), which yields an intermediate saturation of the thermal conductance at the temperature \( T \sim \theta_1 \).

\[ \kappa(T) \approx \frac{k_B \omega_1}{2\pi} \left\{ \begin{array}{ll} 2T/\theta_1, & T < \theta_1; \\ 1, & \theta_1 < T < \theta_1L/W. \end{array} \right. \]  

(8)

The numerical result shown in Fig. 3 by a solid line is in a qualitative agreement with such an expectation. The horizontal arrow indicates the saturation value expected from equation (9). The upper limit in the saturation interval mentioned in Eq. (9) indicates the restoration of ballistic conditions for phonon propagation at wavelengths short enough to avoid wave diffraction at corrugated surfaces.

Theoretically, the intermediate saturation \( \kappa(T) \approx \kappa_{\text{sat}} \) at low temperatures is a more robust feature in longer wires of length \( L \gg l \sim W/\langle \delta W/W \rangle^2 \), where even the lowest mode, \( n = 0 \) is localized at frequencies \( \omega_n(L) < \omega < \omega_1 \). Here \( \omega_n(L) \sim \omega_1 \left( W^2/\langle \delta W/W \rangle^2 \right)^{1/2} \sqrt{W/L} \) is the frequency at which the localization length of \( n = 0 \) acoustic mode is comparable to the wire length. In this case, the saturation takes place at a lower temperature \( \theta_n \sim \hbar \omega_n/k_B \), and we find that the saturation value of the thermal conductance within temperature interval \( \theta_1 \leq T < \theta_1L/W \) has an anomalous dependence on the sample length,

\[ \kappa_{\text{sat}} \approx \int_0^\infty \frac{d\omega}{2\pi} \rho \left( \frac{\omega}{\omega_0} \right) \sim \frac{k_B \omega_1}{2\pi} \left( \frac{1}{L} \right)^{1/2}. \]  

(9)

This is an example of a more general scaling law for white-noise roughness; for a wire with a fractally rough edge, \( \langle \delta W_q \rangle^2 \propto q^z, L_q(\omega) \propto \omega^{-(2+z)} \).

In summary, our analysis of phonon propagation through long free-standing insulating wires with rough surfaces has highlighted a feature in the temperature dependence of the heat conductance \( \kappa(T) \), which results from the crossover from ballistic propagation of the lowest-frequency phonon mode at \( \omega \ll \omega_1 \) to diffusive (or even localized) behavior, with a re-entrance to the quasi-ballistic regime. Although the model used in this calculation has been restricted to only one (longitudinal) excitation branch in the wire spectrum, we believe that this feature persists also in more realistic multi-mode models (which take into account torsional modes and the wire vibrations of other polarizations), since all lowest sound modes are scattered by the surface roughness with the rate decreasing upon the decrease of the frequency. A drastic difference between phonon transport properties in different frequency intervals results in a tendency of the heat conductance of a wire to saturate provisionally at the temperature range of \( T \sim h\omega/k_B \). An intermediate saturation value of the wire heat conductance depends on the length of a wire, and, in wires with length larger than the scattering length of phonons with frequencies \( \omega \sim \omega_1 \) has an anomalous length dependence, \( \kappa_{\text{sat}} \propto L^{-1/2} \).

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ness through the factors $\beta^{j,i}$, which indicate the existence ($\beta^{j,i} = 1$) or absence ($\beta^{j,i} = 0$) of neighbouring sites. The width of each wire cross-section, $W_i = W + \delta W_1 + \delta W_2$ is randomly generated by introducing a random function $r_i = \sum_{i=1}^{N_{\text{max}}} a_m \sin \left(\frac{2\pi m}{L}\right)$, where $N_{\text{min}}$ and $N_{\text{max}}$ are chosen to yield the desired harmonic content, $a_m$ are randomly taken from the interval $[-w/2, w/2]$, and $i$ is the coordinate along the wire axis. Finally, we normalise the fluctuation of the width to a desired r.m.s. value, so that $\delta W_1(i) = \sqrt{\langle (\delta W_1)^2 \rangle / 2} (r^s(i) - < r^s(i) >) / \sqrt{< r^s(i) >}$.

One can also speak of a cooling time of an overheated specimen due to the phonon-mediated cooling through the wire into a bath, with $T_{\text{bath}} \ll T_0$. Then, the temporal evolution of the temperature can be described by equation $C(T)\frac{dT}{dt} = -\dot{Q}(T)dt$, where $C(T) = \frac{2}{T^3} \pi^3 \rho V k_B (\frac{T}{\Theta})^\beta$ is the Debye heat capacity of a specimen, and $V$ is its volume. The cooling time can be found by integrating this equation with respect to the temperature, which yields $\tau(T_0) = \int_{0}^{T_0} dTC(T)/\dot{Q}(T)$. We estimate $\tau(T_0)$ analytically in two limits: i) $\langle \Gamma(\omega) \rangle \approx a + b\omega$ (with $a \sim 1$, $b \sim \omega^{-1}$) and ii) $\langle \Gamma(\omega) \rangle \approx \theta(\omega_* - \omega)$ of a weakly disordered wire and a strongly disordered wire with the length $L \gg l$, respectively. In case i), we find approximately equal to

$$\tau(T_0) \approx 2\pi^6 V \rho \frac{h^2 \omega_1}{k_B T_0} \left(1 + \frac{0.7h\omega_1}{k_B T_0} \ln \frac{h\omega_1}{1.5k_B T_0 + h\omega_1}\right)$$

In case ii) of a long wire, we interpolate $\dot{Q}$ using $\int_{0}^{\infty} \frac{z^2}{\Gamma(k_B T z) [e^z - 1]^{-1}} dz \approx \frac{[T/\theta_*]^{1/2} (1 + T/\theta_*)} {\sqrt{2\pi}} T$, and arrive at $\tau(T_0) \approx 245V \rho \omega_{*}^{-1}(3\theta_* T_0^2 + 2T_0^3)/\theta^3$.

FIG. 1. Ensemble-average transmission coefficient for 100 samples versus frequency for white-noise roughness. Inset: the dependence of $(1 - \langle \Gamma \rangle)$ and inverse localization length on the frequency for $\omega \ll \omega_1$. Linear regression gave power dependence equal to 1.9 and 1.7, respectively. The arrows in the inset indicate which pair of axes corresponds to each curve.
FIG. 2. Transmission coefficient versus frequency for two coloured noise spectra of disorder described in the text. In (a) the dashed line represents the transmission coefficient for a perfect wire.

FIG. 3. Thermal conductance versus temperature for three different regimes of disorder. (1) corresponds to the quasi ballistic regime, (2) corresponds to the disorder regime of figure 2(b), and (3) to the white-noise regime. The horizontal arrow indicates the saturation value of $\kappa$. 