Thermal conductance and giant fluctuations in one-dimensional disordered systems

R. Maynard and E. Akkermans
Centre de Recherches sur les Très Basses Températures et Université Scientifique et Médicale de Grenoble, Centre National de la Recherche Scientifique, Boîte Postale 166X, 38042 Grenoble Cedex, France
(Received 14 June 1985)

The thermal conductance for the energy transport through a disordered harmonic chain is calculated by a tunneling expression of the energy current. The dominant contribution comes from quasiballistic phonons for which the localization length is comparable to the size of the chain. A universal regime of conductance in $k_B^2T/\hbar$ is obtained at low temperature, while giant fluctuations are predicted at higher temperature. Analogies with electrical conductance are established and conditions for measurements are discussed.

It is well known that one-dimensional disordered systems can support only localized states. This has been established both for electrons and phonons, but the transport property of these disordered chains is a much more intricate problem. The difficulties arise from interference effects of the scattered waves which prevent the use of a quasiclassical approximation of the Boltzmann type. For electrons, an important theoretical effort[1–3] has led to a new formulation of the electrical conductance in terms of the transmission coefficient first proposed by Landauer.[1] In this way, a new temperature dependence of the electrical conductance has been recently proposed by Azbel.[4] The present paper is devoted to the calculation of the temperature T and size L dependence of the thermal conductance $G(L,T)$ of a disordered chain. It constitutes a counterpart of the phonon problem of the electrical conductance. The main difference between electrons and phonons is the existence of the thershold of localization at zero frequency. As a consequence, the localization length diverges strongly at low frequency,[5–9] as ω^{-2} for a weakly disordered medium. The main results are the following: There is a characteristic frequency ω^* (and corresponding temperature T^*) related to the disorder and the finite size of the chain which separates the phonon into two classes: ballistic and resonant. At low temperature the thermal conductance varies linearly in temperature in a universal non-Ohmic regime independent of disorder, sound velocity, and size. Above T^*, thermal conductance becomes independent of temperature on average, but for a given sample it has a nonmonotonic variation. The distribution of random conductances obeys a central limit theorem but with giant fluctuations decaying in size as $L^{-1/4}$. These results have been established in the elastic scattering approximation. Effects of anharmonicity[10] are expected at higher temperature and will be neglected.

Consider a chain of length L where the masses of the atoms are independent random variables with average $\overline{M}$ and variance σ_M^2. At both ends of this disordered chain an elastic continuum is matched which supports elastic waves of the same acoustic impedances as the average chain. A wave of frequency ω incident from the left is partially transmitted through the random isotopic chain. The transmission coefficient $\mathcal{T}(\omega,L)$ is defined as the ratio of the transmitted energy flow to the incident energy flow. O'Connor[11] has established that the random function $\ln\mathcal{T}(\omega,L)$ obeys the central limit theorem with mean value $-2L/\xi_0(\omega)$ and variance proportional to L. At low frequency the localization length $\xi_0(\omega)$ has been found[5–9] equal to

$$\xi(\omega)=\frac{8\omega_D^2}{\sigma_M^2\pi^2\omega^2}\ , \tag{1}$$

where ω_D is the Debye frequency.

This result is obtained by a perturbation expansion to lowest order in the fluctuation of masses and is of the order of the elastic mean free path. The relation $\xi(\omega^*)=L$ defines a cutoff frequency ω^* for a low-pass band filter by $\omega^*=(2\sqrt{2}\omega_D)/(\pi\sigma_M\sqrt{L}\,)$.

For low-frequency phonons $\omega\leq\omega^*$ the transparency is nearly perfect. They propagate ballistically through the chain as through a periodic chain. At higher frequency no analytical expression of $\mathcal{T}(\omega,L)$ is available. By numerical simulations of this model, Azbel[12] has observed resonance tunneling modes at discrete values of frequency ω_ν emerging from a background of exponentially damped transmission coefficients. Moreover, these resonant eigenstates are not perfectly sharp, but their widths are exponentially small. For electrons, Azbel[13] has quantified these numerical results by a very simple expression of the product of the resonant transmission coefficient $\mathcal{T}_\nu$ by the width

$$\mathcal{T}_\nu\delta\epsilon_\nu\simeq\exp[-(L+2\Lambda_\nu)/\xi_0]\ ,$$

where Λ_ν is the distance between the maximum of this localized mode ν and the center of the sample. Λ_ν are assumed independent random variables uniformly distributed between 0 and $L/2$, an hypothesis supported by the recent work of Gor'kov *et al.*[14] This gives rise to very large fluctuations of the transmission coefficient which will provide sharp structure of thermal conductance. Such fluctuations cannot be smoothed by thermal broadening. We propose to use Azbel's approximation for the transmission coefficient $\mathcal{T}_\nu$ and to assume, in addition, a uniform separation of the modes: $\delta\omega_\nu=2\pi v/L$, where v is the sound velocity:

$$\mathcal{T}_\nu\delta\omega_\nu=\frac{2\pi v}{L}\exp\left[-\frac{L+2\Lambda_\nu}{\xi_0(\omega_\nu)}\right]\ . \tag{2}$$

Since the contribution of the high frequencies is exponentially small—an exact result first established by O'Connor[11]—we will use the expression (1) of $\xi_0(\omega_\nu)$ in (2). The random character of this transmission coefficient is now contained in the uniformly distributed random variable Λ_ν. This does not violate the central limit theorem,[11] since the probability of occurrence of these resonant tunneling modes is vanishingly small for L large. Moreover, at low frequency the extrapolated $\mathcal{T}_\nu$ from (2) has the correct functional dependence on L and ω.

The problem of heat transfer can be simply formulated in terms of the transmission coefficient in a way similar to that for conduction through a tunnel junction.

Let us consider the left-hand side of the random chain a blackbody source of phonons at temperature $T+dT$, while the right-hand side of the chain is in contact with a blackbody source at temperature T. The contribution to the thermal current for the phonons ω carrying energy from the left to the right is given by

$$I=\tfrac{1}{2}\hbar\omega v g_1(\omega)n(\omega,T+dT)\mathcal{T}(\omega,L) \;,$$

where $g_1(\omega)=(\pi v)^{-1}$ is the one-dimensional density of states per unit length, and $n(\omega,T)$ the Planck distribution. By subtracting the thermal current from the right, one obtains the expression for thermal conductance:

$$G(T,L)=\frac{k_B}{2\pi}\int_0^\infty d\omega\, E\left[\frac{\hbar\omega}{k_BT}\right]\mathcal{T}(\omega,L) \;, \tag{3}$$

where $E(x)=x^2e^x(e^x-1)^{-2}$ is the Einstein specific-heat function. The expression (3) can be analyzed at two levels of approximation. At the simplest level we suppose that only the ballistic phonons $(\omega<\omega^*)$ can carry heat $(\mathcal{T}=1)$ and neglect the other contributions $(\mathcal{T}=0)$. Then,

$$G^{(0)}(T,L)\simeq k_B\int_0^{\omega^*}\frac{d\omega}{2\pi}E\left[\frac{\hbar\omega}{k_BT}\right] \;, \tag{4}$$

which provides two asymptotic regimes:

$$G^{(0)}(T,L)=\begin{cases}\dfrac{\pi^2}{3}\dfrac{k_B^2T}{\hbar}, & T<T^*\\[2mm] \alpha\dfrac{k_B^2T^*}{2\pi\hbar}, & T>T^*\end{cases} \tag{5}$$

where $T^*=\hbar\omega^*/k_B$, $\alpha=1$.

It is remarkable that the low-temperature contribution (5) is a universal function of T which depends neither on disorder nor on the elastic constant of the chain. This can also be understood from the classical kinetic formula. At one dimension $G=K/L$, where K is the thermal conductivity given by $K\approx C_1vl$, where C_1 is the specific heat per unit length and l the elastic mean free path. Since $C_1\simeq v^{-1}$ and $l\simeq L$ for ballistic phonons, the thermal conductance becomes a universal function of T. It is also surprising that at low temperature G is size independent, while at the plateau it depends on $L^{-1/2}$ through T^*. In neither regime does it obey Ohm's law.

Beyond this crude approximation of ballistic phonons, one can retain, following Azbel,[13] the contribution of the resonant tunneling modes to the thermal conductance. The discrete version of (3) can be written as

$$G(T,L)=\frac{k_B}{2\pi}\sum_\nu\frac{1}{Lg_1(\omega_\nu)}E\left[\frac{\hbar\omega_\nu}{k_BT}\right]\exp\left[-\frac{L+2\Lambda_\nu}{\xi(\omega_\nu)}\right] \;, \tag{6}$$

where the random transmission coefficient $\mathcal{T}_\nu$ from (2) has been used. Now G is a random function defined by a sum of random variables independent but nonidentically distributed. The number of terms in the sum (6) is limited by the temperature through the Einstein function. More quantitatively, since the average separation of the modes is $2\pi v/L=\pi\omega_M/L$, this number is $LT/2\Theta_D$. Therefore, for $T>>\Theta_D/L$ we are justified in applying the central limit theorem for the thermal conductance. This is a fundamental property for the conductance *at finite temperature*. By direct application of the Lindeberg version[15] of the central limit theorem, we established that G obeys a normal law centered at the average conductance $\overline{G}$ and with a variance σ_G^2 given by the sum of the variances of each term. The average conductance is straightforwardly obtained from (6):

$$\overline{G}(T,L)=\frac{k_B}{2\pi}\int_0^{\omega_D}d\omega\, E\left[\frac{\hbar\omega}{k_BT}\right]\frac{\xi(\omega)}{L}e^{-L/\xi(\omega)} \times(1-e^{-L/\xi(\omega)}) \;, \tag{7}$$

which produces again the two regimes of conductance of the ballistic approximation with a minor correction for the numerical prefactor: $\alpha=(\sqrt{\pi}/3)(\sqrt{2}-1)$. The variance of the transmission coefficient for the resonant mode ν is

$$\sigma_\nu^2=\frac{\xi(\omega_\nu)}{2L}\exp\left[-\frac{2L}{\xi(\omega_\nu)}\right]\left[1-\exp\left[-\frac{2L}{\xi(\omega_\nu)}\right]\right] \times\left[1-\frac{\tanh[L/2\xi(\omega_\nu)]}{L/2\xi(\omega_\nu)}\right] \;, \tag{8}$$

and the variance of the thermal conductance σ_G^2 is obtained by an integral over the continuous variable ω; one obtains

$$\sigma_G^2=\left[\frac{k_B}{2\pi}\right]^2\int d\omega\,[Lg_1(\omega)]^{-1}E^2\left[\frac{\hbar\omega}{k_BT}\right]\sigma^2(\omega) \;. \tag{9}$$

From (8), σ_ν^2 has a maximum around ω^*: Below ω^* it increases as $(\omega/\omega^*)^4$, but above ω^* it decreases as $\omega^{-2}\exp[-2(\omega/\omega^*)^2]$. The Einstein function determines the relevant range of variation of the frequencies up to $k_BT/\hbar$ in (9). Then σ_G^2 is given by the integrated variance σ_ν^2 from 0 to $k_BT/\hbar$. At low temperature $T<T^*$, it is easy to obtain the relative fluctuations of the thermal conductance $\sigma_G/\overline{G}$, proportional to $\Theta_D^{1/2}T^{3/2}L^{-1/2}(T^*)^{-2}$ (Θ_D is the Debye temperature). When T increases to be of the order of or greater than T^*, the relative fluctuations become temperature-independent and proportional to $(\Theta_D/T^*)^{1/2}\times L^{-1/2}$. Since $T^*\simeq\Theta_D\sigma_M^{-1}L^{-1/2}$, the relative fluctuations of the thermal conductance are proportional to $\sigma^{1/2}L^{-1/4}$: These are *giant fluctuations*, because they decay as $L^{-1/4}$ rather than as $L^{-1/2}$ for standard fluctuations. The origin of this unusual result must be sought in the exponentiation of the uniformly distributed variables Λ_ν. This provides $\sigma_G\simeq\Theta_D^{1/2}(\overline{G}/L)^{1/2}$, and $\overline{G}$ varies as $L^{-1/2}$ in this plateau regime. It must be noticed that it is the quasiballistic modes, $\omega\lesssim\omega^*$, which give the dominant contribution to $\overline{G}$ or σ_G^2. This justifies the approximation of the low-frequency localization length in Eq. (1) in the general expressions given by Eqs. (6) and (9).

The previous analysis applies to the electrical conductance problem with only a few modifications. Following Azbel and Di Vincenzo,[16] the energies of the resonant tunneling states ϵ_ν replace ω_ν, the derivative of the Fermi function $(-\partial f/\partial\epsilon)_{\epsilon=\epsilon_\nu}$ replaces the Einstein function, while the localization length ξ_0 is assumed to be energy independent and shorter than L. Instead of Eq. (6), the electrical conductance $G_e(T,L)$ can be written

$$G_e(T,L)=\frac{e^2}{2\pi\hbar}\sum_\nu [L\rho_1(\epsilon_\nu)]^{-1}\left(-\frac{\partial f}{\partial \epsilon}\right)_{\epsilon=\epsilon_\nu}\exp\left(-\frac{L+2\Lambda_\nu}{\xi_0}\right), \tag{10}$$

where $\rho_1(\epsilon)$ is the density of states per unit length. As for the phonons, if T is sufficiently high ($T >> T_F/L$, where T_F is the Fermi temperature), the random electrical conductance G_e obeys the central limit theorem with mean value $\overline{G}_e$ and variance $\sigma^2_{G_e}$.

The mean value $\overline{G}_e$ is obtained directly from (10) by averaging the transmission coefficient, which gives, for $\xi_0 << L$,

$$\overline{G}_e \simeq \frac{e^2}{2\pi\hbar}\frac{\xi_0}{L}e^{-L/\xi_0} \ .$$

It must be emphasized that the T independence of $\overline{G}_e$ comes both from the double averaging procedure (sampling and thermal) and the non-energy dependence of the localization length while the non-sampling averaged G_e is found to be temperature dependent in Refs. (13) and (16). The variance $\sigma^2_{G_e}$ is simply obtained from the same variance σ^2_ν of the transmission coefficient as given by (8), but with σ^2_ν independent of ν:

$$\sigma^2_{G_e}=\left(\frac{e^2}{2\pi\hbar}\right)^2\sigma^2_\nu\int d\epsilon\,[L\rho_1(\epsilon)]^{-1}\left(-\frac{\partial f}{\partial\epsilon}\right)^2 \ . \tag{11}$$

Since the integral over ϵ in (11) gives a term proportional to $T_F/(TL)$ and $\sigma^2_\nu \simeq (\xi_0/2L)\exp(-2L/\xi_0)$, we obtain finally for the relative fluctuations of the electrical conductance $\sigma_{G_e}/\overline{G}_e \simeq (T_F/T\xi_0)^{1/2}$.

These giant fluctuations do not depend on the size L, while for standard fluctuations one would expect an $L^{-1/2}$ attenuation. The main difference with phonons is that no states of electrons are ballistic: They are assumed to be restricted to the vicinity of the Fermi energy. These fluctuations established for sample averaging can be measured by varying the chemical potential μ of the electron gas. Simply, changing μ shifts the derivative of the Fermi distribution $(-\partial f/\partial E)$ along the spectrum of the resonant tunneling modes. We can then calculate the reduced correlation function of the conductance:

$$C(\Delta\mu)=\frac{\langle\delta G(\mu+\Delta\mu)\delta G(\mu)\rangle_{\text{av}}}{\langle\delta G^2(\mu)\rangle_{\text{av}}}=\frac{3}{\sinh^2 x}(x\coth x-1) \tag{12}$$

where $x=\Delta\mu/2T$. $C(\Delta\mu)$ decreases for high $\Delta\mu$ as $(\Delta\mu/T)\exp(-\Delta\mu/T)$, and then T appears as the correlation energy for these fluctuations when $\Delta\mu$ varies. We advance this as a possible explanation of the nonmonotonicity in electrical conductance with changing the chemical potential as observed recently in inversion layers.[17,18]

There are several conditions for experimental observation that must be discussed. First, for realistic values of $L=1$ cm, $\Theta_D=300$ K and $\sigma_M=10^{-2}$ one finds $T^*=5$ K. Moreover, the value of the mean thermal conductance G at the plateau is equal to 10^{-12} W K^{-1}. This value is small but measurable: It is equivalent to a thermal conductivity $K \simeq 10^{-2}$ $\text{W m}^{-1}\text{K}^{-1}$ of a thin wire of cross section 1 μm^2 and of 1 cm length.

The condition of one dimensionality for a thin fiber must be formulated in the following way. First, the reflection of phonons on boundaries must be specular and not diffuse. This is usually the case at low temperatures $T \leqslant 1$ K, where the wavelength of the dominant phonons (typically 1 μm) is longer than the scale of the roughness of the surface. Secondly, for a section of diameter d of a fiber one expects dimensional crossover of the density of states over a range of temperature of Θ_D/d. For observing the universal regime this implies very thin fibers $d \leqslant \Theta_D/T^*$, which, for the typical material considered previously, limits d to 10^2 atomic distances. Another aspect of the one-dimensional nature is the localization length $\xi(\omega)$ longer than d. Actually, this condition is fulfilled since the quasiballistic phonons which provide all the present features have a localization length comparable to L.

[1] R. Landauer, Philos. Mag. **21**, 863 (1970).
[2] P. W. Anderson, D. J. Thouless, E. Abrahams, and D. S. Fisher, Phys. Rev. B **22**, 3519 (1980).
[3] P. W. Anderson, Phys. Rev. B **23**, 4828 (1981).
[4] M. Ya. Azbel, A. Hartstein, D. P. Di Vincenzo, Phys. Rev. Lett. **52**, 1641 (1984).
[5] M. Ya. Azbel, Phys. Rev. B **28**, 4106 (1983).
[6] O. N. Dorokhov, Solid State Commun. **41**, 431 (1982).
[7] O. N. Dorokhov, Zh. Eksp. Teor. Phys. **83**, 234 (1982) [Sov. Phys. JETP **56**, 128 (1982)].
[8] K. Ishii, Prog. Theor. Phys. Suppl. **53**, 77 (1973).
[9] E. Akkermans and R. Maynard, J. Phys. **45**, 1549 (1984).
[10] J. Jackle, Solid State Commun. **39**, 1261 (1981).
[11] A. J. O'Connor, Commun. Math. Phys. **45**, 63 (1975).
[12] M. Ya Azbel, Phys. Rev. B **27**, 3901 (1983).
[13] M. Ya. Azbel, Solid State Commun. **45**, 527 (1983).
[14] L. P. Gor'kov, O. N. Dorokhov, and F. V. Prigara, Zh. Eksp. Teor. Fiz. **84**, 1440 (1983) [Sov. Phys. JETP **57**, 838 (1983)].
[15] W. Feller, *An Introduction to Probability Theory and its Applications*, 2nd ed., Wiley Series in Probability and Mathematical Statistics (Wiley, New York, 1971), p. 262.
[16] M. Ya. Azbel and D. P. Di Vincenzo, Solid State Commun. **49**, 949 (1984).
[17] R. K. Kwasnick, M. A. Kastner, J. Melngailis, and P. A. Lee, Phys. Rev. Lett. **52**, 224 (1984).
[18] N. R. Couch and M. Pepper, J. Phys. C **17**, L985 (1984).