Review Article

Landauer-Datta-Lundstrom Generalized Transport Model for Nanoelectronics

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The Landauer-Datta-Lundstrom electron transport model is briefly summarized. If a band structure is given, the number of conduction modes can be evaluated and if a model for a mean-free-path for backscattering can be established, then the near-equilibrium thermoelectric transport coefficients can be calculated using the final expressions listed below for 1D, 2D, and 3D resistors in ballistic, quasiballistic, and diffusive linear response regimes when there are differences in both voltage and temperature across the device. The final expressions of thermoelectric transport coefficients through the Fermi-Dirac integrals are collected for 1D, 2D, and 3D semiconductors with parabolic band structure and for 2D graphene linear dispersion in ballistic and diffusive regimes with the power law scattering.

1. Introduction

The objectives of this short review is to give a condensed summary of Landauer-Datta-Lundstrom (LDL) electron transport model [1–5] which works at the nanoscale as well as at the macroscale for 1D, 2D, and 3D resistors in ballistic, quasiballistic, and diffusive linear response regimes when there are differences in both voltage and temperature across the device.

Appendices list final expressions of thermoelectric transport coefficients through the Fermi-Dirac integrals for 1D, 2D, and 3D semiconductors with parabolic band structure and for 2D graphene linear dispersion in ballistic and diffusive regimes with the power law scattering.

2. Generalized Model for Current

The generalized model for current can be written in two equivalent forms:

$$I = \frac{2q}{h} \int \gamma(E) \pi \frac{D(E)}{2} (f_1 - f_2) dE, \quad (1a)$$

$$I = \frac{2q}{h} \int T(E) M(E) (f_1 - f_2) dE, \quad (1b)$$

where “broadening” $\gamma(E)$ relates to transit time for electrons to cross the resistor channel:

$$\gamma(E) \equiv \frac{\hbar}{\tau(E)}; \quad (2)$$

density of states $D(E)$ with the spin degeneracy factor $g_s = 2$ is included; $M(E)$ is the integer number of modes of conductivity at energy E ; the transmission

$$T(E) = \frac{\lambda(E)}{\lambda(E) + L}, \quad (3)$$

where $\lambda(E)$ is the mean-free-path for backscattering and L is the length of the conductor; Fermi function

$$f(E) = \frac{1}{e^{(E-E_F)/kT} + 1} \quad (4)$$

is indexed with the resistor contact numbers 1 and 2; E_F is the Fermi energy which as well as temperature T may be different at both contacts.

Equation (3) can be derived with relatively few assumptions and it is valid not only in the ballistic and diffusion limits, but in between as well:

$$\begin{aligned} \text{Diffusive: } L &\gg \lambda; \quad T = \frac{\lambda}{L} \ll 1, \\ \text{Ballistic: } L &\ll \lambda; \quad T \rightarrow 1, \\ \text{Quasi-ballistic: } L &\approx \lambda; \quad T < 1. \end{aligned} \quad (5)$$

The LDL transport model can be used to describe all three regimes.

It is now clearly established that the resistance of a ballistic conductor can be written in the form

$$R^{\text{ball}} = \frac{h}{q^2} \frac{1}{M(E)}, \quad (6)$$

where h/q^2 is fundamental Klitzing constant and number of modes $M(E)$ represents the number of effective parallel channels available for conduction.

This result is now fairly well known, but the common belief is that it applies only to short resistors and belongs to a course on special topics like mesoscopic physics or nanoelectronics. What is not well known is that the resistance for both long and short conductors can be written in the form

$$R(E) = \frac{h}{q^2} \frac{1}{M(E)} \left(1 + \frac{L}{\lambda(E)} \right). \quad (7)$$

Ballistic and diffusive conductors are not two different worlds, but rather a continuum as the length L is increasing. Ballistic limit is obvious for $L \ll \lambda$, while for $L \gg \lambda$ it reduces into standard Ohm's law:

$$R \equiv \frac{V}{I} = \rho \frac{L}{A}. \quad (8)$$

Indeed we could rewrite $R(E)$ above as

$$R(E) = \frac{\rho(E)}{A} [L + \lambda(E)] \quad (9)$$

with a new expression for specific resistivity:

$$\rho(E) = \frac{h}{q^2} \left(\frac{1}{M(E)/A} \right) \frac{1}{\lambda(E)}, \quad (10)$$

which provides a different view of resistivity in terms of the number of modes per unit area and the mean-free-path.

Number of modes

$$M(E) = M_{1D}(E) = \frac{h}{4} \langle v_x^+(E) \rangle D_{1D}(E), \quad (11a)$$

$$M(E) = WM_{2D}(E) = W \frac{h}{4} \langle v_x^+(E) \rangle D_{2D}(E), \quad (11b)$$

$$M(E) = AM_{3D}(E) = A \frac{h}{4} \langle v_x^+(E) \rangle D_{3D}(E) \quad (11c)$$

is proportional to the width W of the resistor in 2D and to the cross-sectional area A in 3D; $\langle v_x^+(E) \rangle$ is the average velocity in the $+x$ direction from contact 1 to contact 2.

For parabolic energy bands

$$E(k) = E_C + \frac{\hbar^2 k^2}{2m^*} \quad (12)$$

the 1D, 2D, and 3D densities of states are given by

$$D(E) = D_{1D}(E) L = \frac{L}{\pi \hbar} \sqrt{\frac{2m^*}{E - E_C}} H(E - E_C), \quad (13a)$$

$$D(E) = D_{2D}(E) A = A \frac{m^*}{\pi \hbar^2} H(E - E_C), \quad (13b)$$

$$D(E) = D_{3D}(E) \Omega = \Omega \frac{m^* \sqrt{2m^* (E - E_C)}}{\pi^2 \hbar^3} H(E - E_C), \quad (13c)$$

where A is the area of the 2D resistor, Ω is the volume of the 3D resistor, and $H(E - E_C)$ is the Heaviside step function. Then number of modes is

$$M(E) = M_{1D}(E) = H(E - E_C), \quad (14a)$$

$$M(E) = WM_{2D}(E) = W g_v \frac{\sqrt{2m^* (E - E_C)}}{\pi \hbar} H(E - E_C), \quad (14b)$$

$$M(E) = AM_{3D}(E) = A g_v \frac{m^* (E - E_C)}{2\pi \hbar^2} H(E - E_C), \quad (14c)$$

where g_v is the valley degeneracy.

Figure 1 shows qualitative behavior of the density of states and number of modes for resistors with parabolic band structure.

For linear dispersion in graphene,

$$E(k) = \pm \hbar v_F k, \quad (15)$$

where $+$ sign corresponds to conductivity band with $E_F > 0$ (n -type graphene) and $-$ sign corresponds to valence band with $E_F < 0$ (p -type graphene),

$$v(k) = \frac{1}{\hbar} \frac{\partial E}{\partial k} \equiv v_F \approx 1 \times 10^8 \text{ cm/s}. \quad (16)$$

Density of states in graphene is

$$D(E) = \frac{2|E|}{\pi \hbar^2 v_F^2} \quad (17)$$

and number of modes is

$$M(E) = W \frac{2|E|}{\pi \hbar v_F}. \quad (18)$$

Two equivalent expressions for specific conductivity deserve attention, one as a product of $D(E)$ and the diffusion coefficient $\bar{D}(E)$:

$$\sigma(E) = q^2 \bar{D}(E) \frac{D(E)}{L} \left\{ 1, \frac{1}{W}, \frac{1}{A} \right\}, \quad (19a)$$

FIGURE 1: Comparison of the density of states $D(E)$ and number of modes $M(E)$ for 1D, 2D, and 3D resistors with parabolic dispersion.

where

$$\bar{D}(E) = \langle v_x^2 \tau \rangle = v^2 \tau(E) \left\{ 1, \frac{1}{2}, \frac{1}{3} \right\} \quad (*)$$

with $\tau(E)$ being the mean free time after which an electron gets scattered, and the other as a product of $M(E)$ and $\lambda(E)$:

$$\sigma(E) = \frac{q^2}{h} M(E) \lambda(E) \left\{ 1, \frac{1}{W}, \frac{1}{A} \right\}, \quad (19b)$$

where the three items in parenthesis correspond to 1D, 2D, and 3D resistors.

Although (19b) is not well known, the equivalent version in (19a) is a standard result that is derived in textbooks. Both (19a) and (19b) are far more generally applicable compared with traditional Drude model. For example, these equations give sensible answers even for materials like graphene whose nonparabolic bands make the meaning of electron mass somewhat unclear, causing considerable confusion when using Drude model. In general we must really use (19a) and (19b) and not Drude model to shape our thinking about conductivity.

These conceptual equations are generally applicable even to amorphous materials and molecular resistors. Irrespective of the specific $E(p)$ relation at any energy, the density of states $D(E)$, velocity $v(E)$, and momentum $p(E)$ are related to the total number of states $N(E)$ with energy less than E by the fundamental relation

$$D(E) v(E) p(E) = N(E) \cdot d, \quad (**)$$

where d is the number of dimensions. Being combined with (19a), it gives one more fundamental equation for conductivity:

$$\sigma(E) = \frac{q^2 \tau(E)}{m(E)} \left\{ \frac{N(E)}{L}, \frac{N(E)}{LW}, \frac{N(E)}{LA} \right\}, \quad (19c)$$

where electron mass is defined as

$$m(E) = \frac{p(E)}{v(E)}. \quad (20)$$

For parabolic $E(p)$ relations, the mass is independent of energy, but in general it could be energy-dependent as, for example, in graphene the effective mass

$$m^* = \frac{E_F}{v_F^2}. \quad (21)$$

2.1. Linear Response Regime. Near-equilibrium transport or low field linear response regime corresponds to $\lim(dI/dV)_{V \rightarrow 0}$. There are several reasons to develop low field transport model. First, near-equilibrium transport is the foundation for understanding transport in general. Concepts introduced in the study of near-equilibrium regime are often extended to treat more complicated situations, and near-equilibrium regime provides a reference point when we analyze transport in more complex conditions. Second, near-equilibrium transport measurements are widely used to characterize electronic materials and to understand the properties of new materials. And finally, near-equilibrium transport strongly influences and controls the performance of most electronic devices.

Under the low field condition let

$$f_0(E) \approx f_1(E) > f_2(E), \quad (22)$$

where $f_0(E)$ is the equilibrium Fermi function, and an applied bias

$$V = \frac{\Delta E_F}{q} = \frac{(E_{F1} - E_{F2})}{q} \quad (23)$$

is small enough. Using Taylor expansion under constant temperature condition

$$f_2 = f_1 + \frac{\partial f_1}{\partial E_F} \Delta E_F = f_1 + \frac{\partial f_1}{\partial E_F} qV \quad (24)$$

and property of the Fermi function

$$+\frac{\partial f}{\partial E_F} = -\frac{\partial f}{\partial E}, \quad (25)$$

one finds

$$f_1 - f_2 = \left(-\frac{\partial f_0}{\partial E} \right) qV. \quad (26)$$

The derivative of the Fermi function multiplied by kT to make it dimensionless

$$F_T(E, E_F) = kT \left(-\frac{\partial f}{\partial E} \right) \quad (27)$$

is known as thermal broadening function and shown in Figure 2.

FIGURE 2: Fermi function and the dimensionless normalized thermal broadening function.

If one integrates F_T over all energy range, the total area

$$\int_{-\infty}^{+\infty} dE F_T(E, E_F) = kT, \quad (28)$$

so that we can approximately visualize F_T as a rectangular pulse centered around $E = E_F$ with a peak value of $1/4$ and a width of $\sim 4kT$.

The derivative $(-\partial f_0 / \partial E)$ is known as the Fermi conduction window function. Whether a conductor is good or bad is determined by the availability of the conductor energy states in an energy window $\sim \pm 2kT$ around the electrochemical potential E_{F0} , which can vary widely from one material to another. Current is driven by the difference $f_1 - f_2$ in the “agenda” of the two contacts which for low bias is proportional to the derivative of the equilibrium Fermi function (26). With this near-equilibrium assumption for current (1b), we have

$$I = \left[\frac{2q^2}{h} \int T(E) M(E) \left(-\frac{\partial f_0}{\partial E} \right) dE \right] V = GV, \quad (29)$$

with conductivity

$$G = \frac{2q^2}{h} \int T(E) M(E) \left(-\frac{\partial f_0}{\partial E} \right) dE, \quad (30)$$

known as the Landauer expression which is valid in 1D, 2D, and 3D resistors, if we use the appropriate expressions for $M(E)$.

For ballistic limit $T(E) = 1$. For diffusive transport $T(E)$ is given by (3). For a conductor much longer than a mean-free-path the current density equation for diffusive transport is

$$J_x = \frac{\sigma}{q} \frac{d(E_F)}{dx}, \quad (31)$$

where the electrochemical potential E_F is also known as the quasi-Fermi level.

For a 2D conductor the surface specific conductivity is

$$\sigma_s = \frac{2q^2}{h} \int M_{2D}(E) \lambda(E) \left(-\frac{\partial f_0}{\partial E} \right) dE \quad (32)$$

or in a different form

$$\sigma_s = \int \sigma'_s(E) dE, \quad (33a)$$

where differential specific conductivity

$$\sigma'_s(E) = \frac{2q^2}{h} M_{2D}(E) \lambda(E) \left(-\frac{\partial f_0}{\partial E} \right). \quad (33b)$$

Similar expressions can be written for 1D and 3D resistors.

Another way to write the conductance is the product of the quantum of conductance, times the average transmission, times the number of modes in the Fermi windows:

$$G = \frac{2q^2}{h} \langle \langle T \rangle \rangle \langle M \rangle, \quad (34a)$$

$$\langle M \rangle = \int M(E) \left(-\frac{\partial f_0}{\partial E} \right) dE, \quad (34b)$$

$$\langle \langle T \rangle \rangle = \frac{\int T(E) M(E) \left(-\partial f_0 / \partial E \right) dE}{\int M(E) \left(-\partial f_0 / \partial E \right) dE} = \frac{\langle MT \rangle}{\langle M \rangle}. \quad (34c)$$

Yet another way to write the conductance is in terms of the differential conductance $G'(E)$ as

$$G = \int G'(E) dE, \quad [S] \quad (35a)$$

$$G'(E) = \frac{2q^2}{h} M(E) T(E) \left(-\frac{\partial f_0}{\partial E} \right). \quad (35b)$$

2.2. Thermocurrent and Thermoelectric Coefficients. Electrons carry both charge and heat. The charge current is given by (1a) and (1b). To get the equation for the heat current, one notes that electrons in the contacts flow at an energy $E \approx E_F$. To enter a mode $M(E)$ in the resistor electrons must absorb (if $E > E_F$) or emit (if $E < E_F$) a thermal energy $E - E_F$. We conclude that to get the heat current equation we should insert $(E - E_F)/q$ inside the integral. The resulting thermocurrent

$$I_Q = \frac{2}{h} \int (E - E_F) T(E) M(E) (f_1 - f_2) dE. \quad (36)$$

It is important from practical point of view that both expressions—for the electric current (1a) and (1b) and thermocurrent (36)—are suitable for analysis of conductivity of any materials from metals to semiconductors up to modern nanocomposites.

When there are differences in both voltage and temperature across the resistor, then we must the Fermi difference $(f_1 - f_2)$ expands to Taylor series in both voltage and temperature and get

$$f_1 - f_2 \approx \left(-\frac{\partial f_0}{\partial E} \right) q \Delta V - \left(-\frac{\partial f_0}{\partial E} \right) \frac{E - E_F}{T} \Delta T, \quad (37)$$

where $\Delta V = V_2 - V_1$, $\Delta T = T_2 - T_1$, and $T = (T_1 + T_2)/2$.

Deriving a general near-equilibrium current equation is now straightforward. The total current is the sum of the contributions from each energy mode:

$$I = \int I'(E) dE, \quad (38a)$$

where the differential current is

$$I'(E) = \frac{2q}{h} T(E) M(E) (f_1 - f_2). \quad (38b)$$

Using (37) we obtain

$$I'(E) = G'(E) \Delta V + S'_T(E) \Delta T, \quad (39a)$$

where

$$G'(E) = \frac{2q^2}{h} T(E) M(E) \left(-\frac{\partial f_0}{\partial E} \right) \quad (39b)$$

is the differential conductance and

$$\begin{aligned} S'_T(E) &= -\frac{2q^2}{h} T(E) M(E) \left(\frac{E - E_F}{qT} \right) \left(-\frac{\partial f_0}{\partial E} \right) \\ &= -\frac{k}{q} \left(\frac{E - E_F}{kT} \right) G'(E) \end{aligned} \quad (39c)$$

is the Soret coefficient for electrothermal diffusion in differential form. Note that $S'_T(E)$ is negative for modes with energy above E_F (n -resistors) and positive for modes with energy below E_F (p -resistors).

Now we integrate (39a) over all energy modes and find

$$I = G\Delta V + S_T\Delta T, \quad [A], \quad (40a)$$

$$I_Q = -TS_T\Delta V - K_0\Delta T, \quad [W] \quad (40b)$$

with three transport coefficients, namely: conductivity given by (35a) and (35b); the Soret electrothermal diffusion coefficient

$$S_T = \int S'_T(E) dE = -\frac{k}{q} \int \left(\frac{E - E_F}{kT} \right) G'(E) dE, \quad [A/K] \quad (40c)$$

and the electronic heat conductance under the short circuit conditions ($\Delta V = 0$)

$$K_0 = T \left(\frac{k}{q} \right)^2 \int \left(\frac{E - E_F}{kT} \right)^2 G'(E) dE, \quad [W/K], \quad (40d)$$

where current I is defined to be positive when it flows in conductor from contact 2 to contact 1 with electrons flowing in opposite direction. The heat current I_Q is positive when it flows in the $+x$ direction out of contact 2.

Equations (40a), (40b), (40c), and (40d) for long diffusive resistors can be written in the common form used to describe bulk transport as

$$J_x = \sigma \frac{d(E_F/q)}{dx} - s_T \frac{dT}{dx}, \quad [A/m^2], \quad (41a)$$

$$J_{Qx} = TS_T \frac{d(E_F/q)}{dx} - \kappa_0 \frac{dT}{dx} \quad [W/m^2] \quad (41b)$$

with three specific transport coefficients

$$\sigma = \int \sigma'(E) dE,$$

$$\sigma'(E) = \frac{2q^2}{h} M_{3D}(E) \lambda(E) \left(-\frac{\partial f_0}{\partial E} \right), \quad [1/\Omega \cdot m \cdot J], \quad (41c)$$

$$s_T = -\frac{k}{q} \int \left(\frac{E - E_F}{kT} \right) \sigma'(E) dE, \quad [A/m \cdot K], \quad (41d)$$

$$\kappa_0 = \left(\frac{k}{q} \right)^2 \int \left(\frac{E - E_F}{kT} \right)^2 \sigma'(E) dE, \quad [W/m \cdot K]. \quad (41e)$$

These equations have the same form for 1D and 2D resistors, but the units of the various terms differ.

The inverted form of (40a), (40b), (40c), and (40d) is often preferred in practice, namely:

$$\Delta V = RI - S\Delta T, \quad (42a)$$

$$I_Q = -\Pi I - K\Delta T, \quad (42b)$$

where

$$S = \frac{S_T}{G}, \quad (42c)$$

$$\Pi = TS, \quad (42d)$$

$$K = K_0 - \Pi SG. \quad (42e)$$

In this form of the equations, the contributions from each energy mode are not added; for example, $R \neq \int R(E) dE$.

Similarly, the inverted form of the bulk transport equations (41a), (41b), (41c), (41d), and (41e) becomes

$$\frac{d(E_F/q)}{dx} = \rho J_x + S \frac{dT}{dx}, \quad (43a)$$

$$J_{Qx} = TSJ_x - \kappa \frac{dT}{dx} \quad (43b)$$

with transport coefficients

$$\rho = \frac{1}{\sigma}, \quad (43c)$$

$$S = \frac{S_T}{\sigma}, \quad (43d)$$

$$\kappa = \kappa_0 - S^2 \sigma T. \quad (43e)$$

In summary, when a band structure is given, number of modes can be evaluated from (11a), (11b), and (11c) and if a model for the mean-free-path for backscattering $\lambda(E)$ can be chosen, then the near-equilibrium transport coefficients can be evaluated using the expressions listed above.

2.3. Bipolar Conduction. Let us consider a 3D semiconductor with parabolic dispersion. For the conduction band

$$M_{3D}(E) = g_v \frac{m^*}{2\pi\hbar^2} (E - E_C) \quad (E \geq E_C) \quad (44a)$$

and for the valence band

$$M_{3D}^{(v)}(E) = g_v \frac{m_p^*}{2\pi\hbar^2} (E_V - E) \quad (E \leq E_V). \quad (44b)$$

The conductivity is provided with two contributions: for the conduction band

$$\sigma = \frac{q^2}{h} \int_{E_C}^{\infty} M_{3D}(E) \lambda(E) \left(-\frac{\partial f_0}{\partial E} \right) dE \quad (45a)$$

and for the valence band

$$\sigma_p = \frac{q^2}{h} \int_{-\infty}^{E_V} M_{3D}^{(v)}(E) \lambda_p(E) \left(-\frac{\partial f_0}{\partial E} \right) dE. \quad (45b)$$

The Seebeck coefficient for electrons in the conduction band follows from (41a), (41b), (41c), (41d), and (41e):

$$\sigma = \int_{E_C}^{\infty} \sigma'(E) dE, \quad (46a)$$

$$\sigma'(E) = \frac{2q^2}{h} M_{3D}(E - E_C) \lambda(E) \left(-\frac{\partial f_0}{\partial E} \right), \quad (46b)$$

$$s_T = -\frac{k}{q} \int_{E_C}^{\infty} \left(\frac{E - E_F}{kT} \right) \sigma'(E) dE, \quad (46c)$$

$$S = \frac{s_T}{\sigma}. \quad (46d)$$

Similarly, for electrons in the valence band we have

$$\sigma_p = \int_{-\infty}^{E_V} \sigma'_p(E) dE, \quad (47a)$$

$$\sigma'_p(E) = \frac{2q^2}{h} M_{3D}^{(v)}(E_V - E) \lambda_p(E) \left(-\frac{\partial f_0}{\partial E} \right), \quad (47b)$$

$$s_T^{(v)} = -\frac{k}{q} \int_{-\infty}^{E_V} \left(\frac{E - E_F}{kT} \right) \sigma'_p(E) dE, \quad (47c)$$

$$S_p = \frac{s_T^{(v)}}{\sigma_p}, \quad (47d)$$

but the sign of S_p will be positive.

What is going on when both the conduction and valence bands contribute to conduction? This can happen for narrow bandgap conductors or at high temperatures. In such a case, we have to simply integrate over all the modes and will find

$$\sigma^{\text{tot}} \equiv \sigma + \sigma_p = \frac{q^2}{h} \int_{E_1}^{E_2} M_{3D}^{\text{tot}}(E) \lambda(E) \left(-\frac{\partial f_0}{\partial E} \right) dE, \quad (48a)$$

$$M_{3D}^{\text{tot}}(E) = M_{3D}(E) + M_{3D}^{(v)}(E); \quad (48b)$$

moreover, we do not have to be worried about integrating to the top of the conduction band or from the bottom of the valence band because the Fermi function ensures that the integrand falls exponentially to zero away from the band edge. What is important is that in both cases we integrate the same expression with the appropriate $M_{3D}(E)$ and $\lambda(E)$

over the relevant energy difference $E_2 - E_1$. Electrons carry current in both bands. Our general expression is the same for the conduction and valence bands. There is no need to change signs for the valence band or to replace $f_0(E)$ with $1 - f_0(E)$.

To calculate the Seebeck coefficient when both bands contribute let us be reminded that in the first direct form of the transport coefficients (41a), (41b), (41c), (41d), and (41e) the contributions from each mode are added in parallel so the total specific Soret coefficient

$$s_T^{\text{tot}} = -\frac{k}{q} \int_{-\infty}^{+\infty} \left(\frac{E - E_F}{kT} \right) \sigma'(E) dE = S\sigma + S_p\sigma_p; \quad (49a)$$

then, the Seebeck coefficient for bipolar conduction

$$S^{\text{tot}} = \frac{S\sigma + S_p\sigma_p}{\sigma + \sigma_p}. \quad (49b)$$

Since the Seebeck coefficients for the conduction and valence bands have opposite signs, the total Seebeck coefficient just drops for high temperatures and the performance of a thermoelectrical device falls down.

In summary, given a band structure dispersion, the number of modes can be evaluated and if a model for a mean-free-path for backscattering can be established, then the near-equilibrium transport coefficients can be calculated using final expressions listed above.

3. Heat Transfer by Phonons

Electrons transfer both charge and heat. Electrons carry most of the heat in metals. In semiconductors electrons carry only a part of the heat but most of the heat is carried by phonons.

The phonon heat flux is proportional to the temperature gradient

$$J_{Qx}^{\text{ph}} = -\kappa_L \frac{dT}{dx} \quad [\text{W/m}^2] \quad (50)$$

with coefficient κ_L known as the specific lattice thermal conductivity. Such an exceptional thermal conductor like diamond has $\kappa_L \approx 2 \cdot 10^3 \text{ W/m} \cdot \text{K}$ while such a poor thermal conductor like glass has $\kappa_L \approx 1 \text{ W/m} \cdot \text{K}$. Note that electrical conductivities of solids vary over more than 20 orders of magnitude, but thermal conductivities of solids vary over a range of only 3-4 orders of magnitude. We will see that the same methodology used to describe electron transport can be also used for phonon transport. We will also discuss the differences between electron and phonon transport. For a thorough introduction to phonons use classical books [6–9].

To describe the phonon current we need an expression like for the electron current (1b) written now as

$$I = \frac{2q}{h} \int T_{\text{el}}(E) M_{\text{el}}(E) (f_1 - f_2) dE. \quad (51)$$

For electrons the states in the contacts were filled according to the equilibrium Fermi functions, but phonons obey Bose statistics; thus, the phonon states in the contacts are filled according to the equilibrium Bose-Einstein distribution

$$n_0(\hbar\omega) = \frac{1}{e^{\hbar\omega/kT} - 1}. \quad (52)$$

Let temperature for the left and the right contacts be T_1 and T_2 . As for the electrons, both contacts are assumed ideal. Thus the phonons that enter a contact are not able to reflect back, and transmission coefficient $T_{\text{ph}}(E)$ describes the phonon transmission across the entire channel.

It is easy now to rewrite (51) to the phonon heat current. Electron energy E we replace by the phonon energy $\hbar\omega$. In the electron current we have charge q moving in the channel; in case of the phonon current the quantum of energy $\hbar\omega$ is moving instead; thus, we replace q in (51) with $\hbar\omega$ and move it inside the integral. The coefficient 2 in (51) reflects the spin degeneracy of an electron. In case of the phonons we remove this coefficient, and instead the number of the phonon polarization states that contribute to the heat flow lets us include to the number of the phonon modes $M_{\text{ph}}(\hbar\omega)$. Finally, the heat current due to phonons is

$$Q = \frac{1}{h} \int (\hbar\omega) T_{\text{ph}}(\hbar\omega) M_{\text{ph}}(\hbar\omega) (n_1 - n_2) d(\hbar\omega), \quad [\text{W}]. \quad (53)$$

In the linear response regime by analogy with (26),

$$n_1 - n_2 \approx -\frac{\partial n_0}{\partial T} \Delta T, \quad (54)$$

where the derivative according to (52) is

$$\frac{\partial n_0}{\partial T} = \frac{\hbar\omega}{T} \left(-\frac{\partial n_0}{\partial(\hbar\omega)} \right), \quad (55)$$

with

$$\frac{\partial n_0}{\partial(\hbar\omega)} = \left(-\frac{1}{kT} \right) \frac{e^{\hbar\omega/kT}}{(e^{\hbar\omega/kT} - 1)^2}. \quad (56)$$

Now (53) for small differences in temperature becomes

$$Q = -K_L \Delta T, \quad (57)$$

where the thermal conductance

$$K_L = \frac{k^2 T}{h} \int T_{\text{ph}}(\hbar\omega) M_{\text{ph}}(\hbar\omega) \times \left[\left(\frac{\hbar\omega}{kT} \right)^2 \left(-\frac{\partial n_0}{\partial(\hbar\omega)} \right) \right] d(\hbar\omega), \quad [\text{W/K}]. \quad (58)$$

Equation (57) is simply Fourier's law stating that heat flows down to a temperature gradient. It is also useful to note that the thermal conductance (58) displays certain similarities with the electrical conductance

$$G = \frac{2q^2}{h} \int T_{\text{el}}(E) M_{\text{el}}(E) \left(-\frac{\partial f_0}{\partial E} \right) dE. \quad (59)$$

The derivative

$$W_{\text{el}}(E) \equiv \left(-\frac{\partial f_0}{\partial E} \right) \quad (60)$$

known as the Fermi window function that picks out those conduction modes which only contribute to the electric current. The electron windows function is normalized:

$$\int_{-\infty}^{+\infty} \left(-\frac{\partial f_0}{\partial E} \right) dE = 1. \quad (61)$$

In case of phonons the term in square brackets of (58) acts as a window function to specify which modes carry the heat current. After normalization,

$$W_{\text{ph}}(\hbar\omega) = \frac{3}{\pi^2} \left(\frac{\hbar\omega}{kT} \right) \left(\frac{\partial n_0}{\partial(\hbar\omega)} \right); \quad (62)$$

thus finally

$$K_L = \frac{\pi^2 k^2 T}{3h} \int T_{\text{ph}}(\hbar\omega) M_{\text{ph}}(\hbar\omega) W_{\text{ph}}(\hbar\omega) d(\hbar\omega) \quad (63)$$

with

$$g_0 \equiv \frac{\pi^2 k^2 T}{3h} \approx (9.456 \times 10^{-13} \text{ W/K}^2) T, \quad (64)$$

known as the quantum of thermal conductance experimentally observed first in 2000 [10].

Comparing (59) and (63) one can see that the electrical and thermal conductances are similar in structure: both are proportional to corresponding quantum of conductance times an integral over the transmission times the number of modes times a window function.

The thermal broadening functions for electrons and phonons have similar shapes and each has a width of a few kT . In case of electrons this function is given by (27) or

$$F_T(x) \equiv \frac{e^x}{(e^x + 1)^2} \quad (65)$$

with $x \equiv (E - E_F)/kT$ and is shown on Figure 2. This function for phonons is given by (62) or

$$F_T^{\text{ph}}(x) \equiv \frac{3}{\pi^2} \frac{x^2 e^x}{(e^x - 1)^2} \quad (66)$$

with $x \equiv \hbar\omega/kT$. Both functions are normalized to a unity and shown together on Figure 3.

Along with the number of modes determined by the dispersion relation, these two window functions play a key role in determining the electrical and thermal conductances.

3.1. Thermal Conductivity of the Bulk Conductors. The thermal conductivity of a large diffusive resistor is a key material property that controls performance of any electronic devices. By analogy with the transmission coefficient (3) for electron transport, the phonon transmission

$$T_{\text{ph}}(\hbar\omega) = \frac{\lambda_{\text{ph}}(\hbar\omega)}{\lambda_{\text{ph}}(\hbar\omega) + L} \Big|_{L \gg \lambda_{\text{ph}}} \longrightarrow \frac{\lambda_{\text{ph}}(\hbar\omega)}{L}. \quad (67)$$

It is also obvious that for large 3D conductors the number of phonon modes is proportional to the cross-sectional area of the sample:

$$M_{\text{ph}}(\hbar\omega) \propto A. \quad (68)$$

FIGURE 3: Broadening function for phonons compared to that of electrons.

Now let us return to (57) dividing and multiplying it by A/L , which immediately gives (50) for the phonon heat flux postulated above:

$$\frac{Q}{A} \equiv J_{Qx}^{\text{ph}} = -\kappa_L \frac{dT}{dx} \quad (69)$$

with specific lattice thermal conductivity

$$\kappa_L = K_L \frac{L}{A}, \quad (70)$$

or substituting (67) into (63), one for the lattice thermal conductivity finally obtains

$$\kappa_L = \frac{\pi^2 k^2 T}{3h} \int \frac{M_{\text{ph}}(\hbar\omega)}{A} \lambda_{\text{ph}}(\hbar\omega) W_{\text{ph}}(\hbar\omega) d(\hbar\omega). \quad (71)$$

It is useful now to define the average number of phonon modes per cross-sectional area of the conductor that participate in the heat transport:

$$\left\langle \frac{M_{\text{ph}}}{A} \right\rangle \equiv \int \frac{M_{\text{ph}}(\hbar\omega)}{A} W_{\text{ph}}(\hbar\omega) d(\hbar\omega). \quad (72)$$

Then

$$\kappa_L = \frac{\pi^2 k^2 T}{3h} \left\langle \frac{M_{\text{ph}}}{A} \right\rangle \langle \langle \lambda_{\text{ph}} \rangle \rangle, \quad (73)$$

where the average mean-free-path is defined now as

$$\langle \langle \lambda_{\text{ph}} \rangle \rangle = \frac{\int (M_{\text{ph}}(\hbar\omega)/A) \lambda_{\text{ph}}(\hbar\omega) W_{\text{ph}}(\hbar\omega) d(\hbar\omega)}{\int (M_{\text{ph}}(\hbar\omega)/A) W_{\text{ph}}(\hbar\omega) d(\hbar\omega)}. \quad (74)$$

Thus, the couple of the phonon transport equations (69) and (73) corresponds to similar electron transport equations:

$$J_x = \frac{\sigma}{q} \frac{d(E_F)}{dx}, \quad (75)$$

$$\sigma = \frac{2q^2}{h} \left\langle \frac{M_{\text{el}}}{A} \right\rangle \langle \langle \lambda_{\text{el}} \rangle \rangle. \quad (76)$$

The thermal conductivity (73) and the electrical conductivity (76) have the same structure. It is always a product of the corresponding quantum of conductance times the number of modes that participate in transport, times the average mean-free-path. These three quantities for phonons will be discussed later.

3.2. Specific Heat versus Thermal Conductivity. The connection between the lattice specific thermal conductivity and the lattice specific heat at constant volume is well known [6–9]. We will show now that corresponding proportionality coefficient is a product of an appropriately-defined mean-free-path $\langle \langle \Lambda_{\text{ph}} \rangle \rangle$ and an average phonon velocity $\langle v_{\text{ph}} \rangle$, namely:

$$\kappa_L = \frac{1}{3} \langle \langle \Lambda_{\text{ph}} \rangle \rangle \langle v_{\text{ph}} \rangle C_V. \quad (77)$$

The total phonon energy per unit volume

$$E_{\text{ph}} = \int_0^\infty (\hbar\omega) D_{\text{ph}}(\hbar\omega) n_0(\hbar\omega) d(\hbar\omega), \quad (78)$$

where $D_{\text{ph}}(\hbar\omega)$ is the phonon density of states. By definition,

$$\begin{aligned} C_V &\equiv \frac{\partial E_{\text{ph}}}{\partial T} = \frac{\partial}{\partial T} \int_0^\infty (\hbar\omega) D_{\text{ph}}(\hbar\omega) n_0(\hbar\omega) d(\hbar\omega) \\ &= \int_0^\infty (\hbar\omega) D_{\text{ph}}(\hbar\omega) \left(\frac{\partial n_0(\hbar\omega)}{\partial T} \right) d(\hbar\omega) \\ &= \frac{\pi^2 k^2 T}{3} \int_0^\infty D_{\text{ph}}(\hbar\omega) W_{\text{ph}}(\hbar\omega) d(\hbar\omega), \end{aligned} \quad (79)$$

where (55) and (62) were used. Next, multiply and divide (71) by (79) and obtain the proportionality we are looking for:

$$\begin{aligned} \kappa_L &= \left[\frac{(1/h) \int_0^\infty (M_{\text{ph}}(\hbar\omega)/A) \lambda_{\text{ph}}(\hbar\omega) W_{\text{ph}}(\hbar\omega) d(\hbar\omega)}{\int_0^\infty D_{\text{ph}}(\hbar\omega) W_{\text{ph}}(\hbar\omega) d(\hbar\omega)} \right] C_V. \end{aligned} \quad (80)$$

To obtain final expression (77) and correct interpretation of the proportionality coefficient we need to return to (67). This expression can be easily derived for 1D conductor with several simplifying assumptions. Nevertheless it works very well in practice for a conductor of any dimension. Derivation of (67) is based on the interpretation of the mean-free-path $\lambda(E)$ or $\lambda(\hbar\omega)$ as that its inverse value is the probability per unit length that a positive flux is converted to a negative flux. This is why λ is often called a mean-free-path for backscattering. Let us relate it to the scattering time τ . The distinction between mean-free-path and mean-free-path for backscattering is easiest to see for 1D conductor. Let an electron undergo a scattering event. For isotropic scattering the electron can forward scatter or backscatter. Only backscattering is relevant for the mean-free-path for scattering, so the time between backscattering events is 2τ . Thus the mean-free-path for backscattering is twice the mean-free-path for scattering:

$$\lambda_{1D}(E) = 2\Lambda(E) = 2v(E)\tau(E). \quad (81a)$$

It was shown that the proper definition of the mean-free-path for backscattering for a conductor of any dimension [11] is

$$\lambda(E) = 2 \frac{\langle v_x^2 \tau \rangle}{\langle |v_x| \rangle}, \quad (***)$$

where averaging is performed over angles. For isotropic bands,

$$\lambda_{2D}(E) = \frac{\pi}{2} v(E) \tau(E), \quad (81b)$$

$$\lambda_{3D}(E) = \frac{4}{3} v(E) \tau(E). \quad (81c)$$

The scattering time is often approximately written as the power law scattering:

$$\tau(E) = \tau_0 \left(\frac{E - E_C}{kT} \right)^s, \quad (82)$$

where exponent s describes the specific scattering mechanism: for acoustic phonon scattering in 3D conductor with parabolic dispersion $s = -1/2$ and for ionized impurity scattering $s = +3/2$ [12].

Analogous power law is often used for mean-free-path:

$$\lambda(E) = \lambda_0 \left(\frac{E - E_C}{kT} \right)^r. \quad (83)$$

For parabolic zone structure $v(E) \propto E^{1/2}$; thus $r = s + 1/2$ with $r = 0$ for acoustic phonon scattering, and $r = 2$ for ionized impurity scattering.

Coming back to our initial task to derive (77) from (80) for 3D conductor according to (81c) we have

$$\lambda_{ph}(\hbar\omega) = \frac{4}{3} v_{ph}(\hbar\omega) \tau_{ph}(\hbar\omega), \quad (84)$$

where, according to (81a),

$$v_{ph}(\hbar\omega) \tau_{ph}(\hbar\omega) = \Lambda_{ph}(\hbar\omega), \quad (85)$$

and finally

$$\lambda_{ph}(\hbar\omega) = \frac{4}{3} \Lambda_{ph}(\hbar\omega). \quad (86)$$

It was stated above in (11c) that the density of states and number of modes for electrons in 3D are

$$M_{el}(E) = AM_{3D}(E) = A \frac{\hbar}{4} \langle v_x^+(E) \rangle D_{3D}(E). \quad (87)$$

Let us rewrite this formula for phonons. Note that the spin degeneracy for electrons $g_s = 2$ is included with the density of states:

$$D_{3D}(E) = 2D'_{3D}(E), \quad (88)$$

and for spherical bands in 3D conductor,

$$\langle v_x^+(E) \rangle = \frac{v_{el}(E)}{2}. \quad (89)$$

Collecting (87) up to (89) all together in case of phonons, we have

$$\begin{aligned} M_{ph}(\hbar\omega) &= A \frac{\hbar}{2} \left(\frac{v_{ph}(\hbar\omega)}{2} \right) 2D_{ph}(\hbar\omega) \\ &= A \frac{\hbar}{4} v_{ph}(\hbar\omega) D_{ph}(\hbar\omega). \end{aligned} \quad (90)$$

Substituting (86) and (90) into (80), we obtain

$$\begin{aligned} \kappa_L &= \left[\frac{(1/3) \int_0^\infty \Lambda_{ph}(\hbar\omega) v_{ph}(\hbar\omega) D_{ph}(\hbar\omega) W_{ph}(\hbar\omega) d(\hbar\omega)}{\int_0^\infty D_{ph}(\hbar\omega) W_{ph}(\hbar\omega) d(\hbar\omega)} \right] C_V. \end{aligned} \quad (91)$$

Multiplying and dividing (91) by

$$\int_0^\infty v_{ph}(\hbar\omega) D_{ph}(\hbar\omega) W_{ph}(\hbar\omega) d(\hbar\omega), \quad (92)$$

we finally get (77) with proportionality coefficient between κ_L and C_V as the product of an average mean-free-path as

$$\begin{aligned} \langle \langle \Lambda_{ph} \rangle \rangle &\equiv \frac{\int_0^\infty \Lambda_{ph}(\hbar\omega) v_{ph}(\hbar\omega) D_{ph}(\hbar\omega) W_{ph}(\hbar\omega) d(\hbar\omega)}{\int_0^\infty v_{ph}(\hbar\omega) D_{ph}(\hbar\omega) W_{ph}(\hbar\omega) d(\hbar\omega)} \end{aligned} \quad (93)$$

and an average velocity as

$$\langle v_{ph} \rangle \equiv \frac{\int_0^\infty v_{ph}(\hbar\omega) D_{ph}(\hbar\omega) W_{ph}(\hbar\omega) d(\hbar\omega)}{\int_0^\infty D_{ph}(\hbar\omega) W_{ph}(\hbar\omega) d(\hbar\omega)}, \quad (94)$$

with the appropriate averaging.

Equation (77) is often used to estimate the average mean-free-path from the measured κ_L and C_V , if we know the average velocity, which is frequently assumed to be the longitudinal sound velocity. The derivation above has identified the precise definitions of the $\langle \langle \Lambda_{ph} \rangle \rangle$ and $\langle v_{ph} \rangle$. If a phonon dispersion is chosen one can always compute the average velocity according to (94), and it is typically very different from the longitudinal sound velocity. Thus, estimates of the average mean-free-path can be quite wrong if one assumes the longitudinal sound velocity [13].

3.3. Debye Model. For 3D conductors there are three polarization states for lattice vibrations: one for atoms displaced in the direction of propagation (longitudinal/ L) and two for atoms displaced orthogonally to the direction of propagation (transverse/ T). The low energy modes are called acoustic modes/ A : one LA mode analogous to sound waves propagating in air and two TA modes. Near $q \rightarrow 0$ dispersion of acoustic modes is linear:

$$\hbar\omega = \hbar v_D q, \quad (95)$$

and is known as Debye approximation. The Debye velocity v_D is an average velocity of the L and T acoustic modes. In case of LA mode v_D is simply the sound velocity $v_s \propto m^{-1/2}$ with m being an effective mass of vibrating atom. Typically, $v_s \approx 5 \times 10^3$ m/s, about 20 times slower than the velocity of a typical electron.

The bandwidth of the electronic dispersion is typically $BW \gg kT$, so only states near the bottom of the conduction band where the effective mass model is reasonably accurate

are occupied. For phonons the situation is much different; the bandwidth $BW \approx kT$, so states across the entire Brillouin zone are occupied. The widely used Debye approximation (95) fits the acoustic branches as long as q is not too far from the center of the Brillouin zone.

With the Debye approximation (95) it is easy to find the density of the phonon states:

$$D_{\text{ph}}(\hbar\omega) = \frac{3(\hbar\omega)^2}{2\pi^2(\hbar v_D)^3}, \quad [\text{J}^{-1} \cdot \text{m}^{-3}], \quad (96)$$

where the factor of three is for the three polarizations. Then one can obtain the number of phonon modes per cross-sectional area from (90):

$$M_{\text{ph}}(\hbar\omega) = \frac{3(\hbar\omega)^2}{4\pi(\hbar v_D)^2}. \quad (97)$$

Since all the states in the Brillouin zone tend to be occupied at moderate temperatures, we are to be sure that we account for the correct number of states. For a crystal there are $3N/\Omega$ states per unit volume. To find the total number of states we have to integrate the density of states:

$$\int_0^{\hbar\omega_D} D_{\text{ph}}(\hbar\omega) d(\hbar\omega), \quad (98)$$

with the upper limit as $\hbar$ times the so-called Debye frequency to produce the correct number of states, namely:

$$\hbar\omega_D = \hbar v_D \left(\frac{6\pi^2 N}{\Omega} \right)^{1/3} \equiv kT_D. \quad (99)$$

The Debye frequency defines a cutoff frequency above which no states are accounted for. This restriction can also be expressed via a cutoff wave vector q_D or as a Debye temperature:

$$T_D = \frac{\hbar\omega}{k}. \quad (100)$$

For $T \ll T_D$, only states with $q \rightarrow 0$ for which the Debye approximation is accurate are occupied.

Now we can calculate the lattice thermal conductivity by integrating (71) to the Debye cutoff energy

$$\kappa_L = \frac{\pi^2 k^2 T}{3h} \int_0^{\hbar\omega_D} \frac{M_{\text{ph}}(\hbar\omega)}{A} \lambda_{\text{ph}}(\hbar\omega) W_{\text{ph}}(\hbar\omega) d(\hbar\omega) \quad (101)$$

and estimate $M_{\text{ph}}(\hbar\omega)$ according to (71). The integral can be taken numerically or analytically if appropriate expression for the mean-free-path is used. This is how the lattice thermal conductivities were first calculated [14, 15]. The theory and computational procedures for the thermoelectric transport coefficients were developed further in [11, 13, 16].

3.4. Phonon Scattering. Phonons can scatter from defects, impurity atoms, isotopes, surfaces and boundaries, and electrons and from other phonons. Phonon-phonon scattering

occurs because the potential energy of the bonds in the crystal is not exactly harmonic. All higher order terms are treated as a scattering potential. Two types of phonon scattering are considered. In the normal process two phonons interact and create a third phonon with energy and momentum being conserved:

$$\begin{aligned} \hbar\vec{q}_1 + \hbar\vec{q}_2 &= \hbar\vec{q}_3, \\ \hbar\vec{\omega}_1 + \hbar\vec{\omega}_2 &= \hbar\vec{\omega}_3. \end{aligned} \quad (102)$$

The total momentum of the phonon ensemble is conserved; thus this type of scattering has little effect on the heat flux.

In a second type of scattering, umklapp/ U -scattering, the two initial phonons have larger momentum; thus the resulting phonon would have a momentum outside the Brillouin zone due to unharmonic phonon-phonon as well as electron-phonon interactions. The U -scatterings are the basic processes in the heat transport especially at high temperatures. Scattering on defects/ D and on boundaries/ B is also important. Scattering rates are additive; thus the total phonon scattering rate is

$$\frac{1}{\tau_{\text{ph}}(\hbar\omega)} = \frac{1}{\tau_U(\hbar\omega)} + \frac{1}{\tau_D(\hbar\omega)} + \frac{1}{\tau_B(\hbar\omega)} \quad (103)$$

or alternatively, in terms of the mean-free-path (84),

$$\frac{1}{\lambda_{\text{ph}}(\hbar\omega)} = \frac{1}{\lambda_U(\hbar\omega)} + \frac{1}{\lambda_D(\hbar\omega)} + \frac{1}{\lambda_B(\hbar\omega)}. \quad (104)$$

Expressions for each of the scattering rates are developed [17]. For scattering from point defects,

$$\frac{1}{\tau_D(\hbar\omega)} \propto \omega^4, \quad (105)$$

known as the Rayleigh scattering which is like the scattering of light from the dust.

For boundaries and surfaces,

$$\frac{1}{\tau_B(\hbar\omega)} \propto \frac{v_{\text{ph}}(\hbar\omega)}{L}, \quad (106)$$

where L is the shortest dimension of the sample.

A commonly used expression for U -scattering is

$$\frac{1}{\tau_U(\hbar\omega)} \propto T^3 \omega^2 e^{-T_D/bT}. \quad (107)$$

With this background we are now able to understand the temperature dependence of the lattice thermal conductivity.

3.5. Lattice Thermal Conductivity versus Temperature. The temperature dependence of the lattice thermal conductivity κ_L is illustrated for bulk Si on Figure 4.

According to (73) κ_L is proportional to the number of the phonon modes that are occupied $\langle M_{\text{ph}}/A \rangle$ and to the average value of the phonon mean-free-path $\langle \lambda_{\text{ph}} \rangle$. The curve $\kappa_L(T)$ can be explained by understanding how $\langle M_{\text{ph}} \rangle$ and $\langle \lambda_{\text{ph}} \rangle$ vary with temperature.

FIGURE 4: The experimental [18] and calculated [13] thermal conductivity of bulk Si as a function of temperature.

It can be shown using (72) that, at low temperatures,

$$\langle M_{\text{ph}} \rangle \propto T^3, \quad (T \rightarrow 0) \quad (108)$$

so the initial rise in thermal conductivity is due to the fact that the number of populated modes rises quickly with temperature. At low temperatures boundary scattering is important. As the temperature increases more short-wavelength phonons are produced. These phonons scatter from point defects, so defect scattering becomes more and more important. As the temperature approaches the T_D , all of the phonon modes are populated and further increases in temperature do not change $\langle M_{\text{ph}} \rangle$. Instead, the higher temperatures increase the phonon scattering by U -processes, and the thermal conductivity drops with increasing temperatures.

3.6. Difference between Lattice Thermal and Electrical Conductivities. We have already noted the similarity between phonon transport equations (69) and (73) and electron transport equations (75) and (76). The average electron and phonon mean-free-paths are of the same order of magnitude. Why then does the electrical conductance vary over many more orders of magnitude while the lattice thermal conductance varies only over a few? The answer lies in the corresponding windows functions (60) and (62). For both electrons and phonons, higher temperatures broaden the window function and increase the population of states. For electrons, however, the position of the Fermi level has a dramatic effect on the magnitude of the window function. By controlling the position of the Fermi level, the electrical conductivity can be varied over many orders of magnitude. For the phonons the width of the window function is determined by temperature only.

Another key difference between electrons and phonons relates to how the states are populated. For a thermoelectric device $E_F \approx E_C$, and the electron and phonon window

functions are quite similar. However, for electrons the BW of the dispersion is very large, so only a few states near the bottom of the conduction band are populated: the effective mass approximation works well for these states, and it is easy to obtain analytical solutions. For phonons, the BW of the dispersion is small. At moderate temperatures states all across the entire Brillouin zone are occupied: simple analytical approximations do not work, and it is hard to get analytical solutions for the lattice thermal conductivity.

3.7. Lattice Thermal Conductivity Quantization. By analogy with the electronic conduction quantization,

$$G^{\text{ball}} = \frac{2q^2}{h} M(E_F), \quad (109)$$

over 30 years ago Pendry [19] stated the existence of the quantum limits to the heat flow. In fact, if $T \rightarrow 0$ in (63), then the phonon window $W_{\text{ph}}(\hbar\omega)$ is sharply peaked near $\hbar\omega = 0$:

$$K_L = \frac{\pi^2 k^2 T}{3h} T_{\text{ph}}(0) M_{\text{ph}}(0). \quad (110)$$

For a bulk conductor $M_{\text{ph}}(\hbar\omega) \rightarrow 0$ as $\hbar\omega \rightarrow 0$, but for nanoresistors like a nanowire or nanoribbon one can have a finite number of phonon modes. For ballistic phonon transport, $T_{\text{ph}} = 1$ and one can expect that

$$K_L = \frac{\pi^2 k^2 T}{3h} M_{\text{ph}}. \quad (111)$$

Exactly this result was proved experimentally using 4-mode resistor at $T < 0.8$ K [10]; thermoconductivity measurements agree with the predictions for 1D ballistic resistors [20–22].

The quantum of thermal conductance

$$g_0 \equiv \frac{\pi^2 k^2 T}{3h} \quad (112)$$

represents the maximum possible value of energy transported per phonon mode. Surprisingly, it does not depend on particle statistics: the quantum of thermal conductance is universal for fermions, bosons, and anyons [23–25].

4. Conclusions

In summary, we see that the LDL concept used to describe electron transport can be generalized for phonons. In both cases the Landauer approach generalized and extended by Datta and Lundstrom gives correct quantitative description of transport processes for resistors of any nature and any dimension and size in ballistic, quasiballistic, and diffusive linear response regimes when there are differences in both voltage and temperature across the device. We saw that the lattice thermal conductivity can be written in a form that is very similar to the electrical conductivity, but there are two important differences.

The first difference between electrons and phonons is the difference in bandwidths of their dispersions. For electrons,

the dispersion $BW \gg kT$ at room temperature, so only low energy states are occupied. For phonons, $BW \approx kT$, so at room temperature all of the acoustic modes across the entire Brillouin zone are occupied. As a result, the simple Debye approximation to the acoustic phonon dispersion does not work nearly as well as the simple effective mass approximation to the electron dispersion.

The second difference between electrons and phonons is that for electrons the mode populations are controlled by the window function which depends on the position of the Fermi level and the temperature. For phonons, the window function depends only on the temperature. The result is that electrical conductivities vary over many orders of magnitude as the position of the Fermi level varies, while lattice conductivities vary over only a few orders of magnitude.

Finally, we also collect below the thermoelectric coefficients for parabolic band semiconductors and for graphene [5, 26].

Appendices

A. Thermoelectric Coefficients for 1D, 2D, and 3D Semiconductors with Parabolic Dispersion for Ballistic and Diffusive Regimes

Thermoelectric coefficients are expressed through the Fermi-Dirac integral of order j defined as

$$\mathfrak{F}_j(\eta_F) = \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{\eta^j}{\exp(\eta - \eta_F) + 1} d\eta, \quad (\text{A.1})$$

where the location of the Fermi level E_F relative to the conduction band edge E_C is given by the dimensionless parameter

$$\eta_F = \frac{E_F - E_C}{kT}. \quad (\text{A.2})$$

In expressions below thermoelectric coefficients (40a), (40b), (40c), (40d), (42a), (42b), (42c), (42d), and (42e) for diffusive regime were calculated with the power law scattering:

$$\lambda(E) = \lambda_0 \left(\frac{E}{kT} \right)^r. \quad (\text{A.3})$$

Thermoelectric coefficients for 1D ballistic resistors are:

$$\begin{aligned} G &= \frac{2q^2}{h} \mathfrak{F}_{-1}(\eta_F), \\ S_T &= -\frac{k}{q} \frac{2q^2}{h} [\mathfrak{F}_0(\eta_F) - \eta_F \mathfrak{F}_{-1}(\eta_F)], \\ S &= -\frac{k}{q} \left[\frac{\mathfrak{F}_0(\eta_F)}{\mathfrak{F}_{-1}(\eta_F)} - \eta_F \right], \end{aligned}$$

$$\begin{aligned} K_0 &= T \left(\frac{k}{q} \right)^2 \frac{2q^2}{h} [2\mathfrak{F}_1(\eta_F) - 2\eta_F \mathfrak{F}_0(\eta_F) + \eta_F^2 \mathfrak{F}_{-1}(\eta_F)], \\ K &= T \left(\frac{k}{q} \right)^2 \frac{2q^2}{h} \left[2\mathfrak{F}_1(\eta_F) - \frac{\mathfrak{F}_0^2(\eta_F)}{\mathfrak{F}_{-1}(\eta_F)} \right]. \end{aligned} \quad (\text{A.4})$$

Thermoelectric coefficients for 1D diffusive resistors are:

$$\begin{aligned} G &= \frac{2q^2}{h} \left(\frac{\lambda_0}{L} \right) \Gamma(r+1) \mathfrak{F}_{r-1}(\eta_F), \\ S_T &= -\frac{k}{q} \frac{2q^2}{h} \left(\frac{\lambda_0}{L} \right) \Gamma(r+1) \\ &\quad \times [(r+1) \mathfrak{F}_r(\eta_F) - \eta_F \mathfrak{F}_{r-1}(\eta_F)], \\ S &= -\frac{k}{q} \left[\frac{(r+1) \mathfrak{F}_r(\eta_F)}{\mathfrak{F}_{r-1}(\eta_F)} - \eta_F \right], \\ K_0 &= T \left(\frac{k}{q} \right)^2 \frac{2q^2}{h} \left(\frac{\lambda_0}{L} \right) \\ &\quad \times [\Gamma(r+3) \mathfrak{F}_{r+1}(\eta_F) - 2\eta_F \Gamma(r+2) \\ &\quad \times \mathfrak{F}_r(\eta_F) + \eta_F^2 \Gamma(r+1) \mathfrak{F}_{r-1}(\eta_F)], \\ K &= T \left(\frac{k}{q} \right)^2 \frac{2q^2}{h} \left(\frac{\lambda_0}{L} \right) \Gamma(r+2) \\ &\quad \times \left[(r+2) \mathfrak{F}_{r+1}(\eta_F) - \frac{(r+1) \mathfrak{F}_r^2(\eta_F)}{\mathfrak{F}_{r-1}(\eta_F)} \right]. \end{aligned} \quad (\text{A.5})$$

Conductivity $G = \sigma_{1D}/L$ is given in *Siemens*: $[\sigma_{1D}] = 1 \text{ S} \cdot \text{m}$. Similarly for other specific coefficients: $s_T = S_T L$; $\kappa_0 = K_0 L$; $\kappa = KL$.

Thermoelectric coefficients for 2D ballistic resistors are:

$$\begin{aligned} G &= W \frac{2q^2}{h} \frac{\sqrt{2\pi m^* kT}}{h} \mathfrak{F}_{-1/2}(\eta_F), \\ S_T &= -W \frac{k}{q} \frac{2q^2}{h} \frac{\sqrt{2\pi m^* kT}}{h} \\ &\quad \times \left[\frac{3}{2} \mathfrak{F}_{1/2}(\eta_F) - \eta_F \mathfrak{F}_{-1/2}(\eta_F) \right], \\ S &= -\frac{k}{q} \left[\frac{3 \mathfrak{F}_{1/2}(\eta_F)}{2 \mathfrak{F}_{-1/2}(\eta_F)} - \eta_F \right], \\ K_0 &= WT \left(\frac{k}{q} \right)^2 \frac{2q^2}{h} \frac{\sqrt{2\pi m^* kT}}{h} \\ &\quad \times \left[\frac{15}{4} \mathfrak{F}_{3/2}(\eta_F) - 3\eta_F \mathfrak{F}_{1/2}(\eta_F) + \eta_F^2 \mathfrak{F}_{-1/2}(\eta_F) \right], \\ K &= WT \left(\frac{k}{q} \right)^2 \frac{2q^2}{h} \frac{\sqrt{2\pi m^* kT}}{h} \\ &\quad \times \left[\frac{15}{4} \mathfrak{F}_{3/2}(\eta_F) - \frac{9 \mathfrak{F}_{1/2}^2(\eta_F)}{4 \mathfrak{F}_{-1/2}(\eta_F)} \right]. \end{aligned} \quad (\text{A.6})$$

Thermoelectric coefficients for 2D diffusive resistors are:

$$\begin{aligned}
 G &= W \frac{2q^2}{h} \left(\frac{\lambda_0}{L} \right) \frac{\sqrt{2m^*kT}}{\pi h} \Gamma \left(r + \frac{3}{2} \right) \mathfrak{F}_{r-1/2}(\eta_F), \\
 S &= -\frac{k}{q} \left[\frac{(r+3/2) \mathfrak{F}_{r+1/2}(\eta_F)}{\mathfrak{F}_{r-1/2}(\eta_F)} - \eta_F \right], \\
 S_T &= -W \frac{k}{q} \frac{2q^2}{h} \left(\frac{\lambda_0}{L} \right) \frac{\sqrt{2m^*kT}}{\pi h} \\
 &\quad \times \left[\Gamma \left(r + \frac{5}{2} \right) \mathfrak{F}_{r+1/2}(\eta_F) - \eta_F \Gamma \left(r + \frac{3}{2} \right) \mathfrak{F}_{r-1/2}(\eta_F) \right], \\
 K_0 &= WT \left(\frac{k}{q} \right)^2 \frac{2q^2}{h} \left(\frac{\lambda_0}{L} \right) \frac{\sqrt{2m^*kT}}{\pi h} \\
 &\quad \times \left[\Gamma \left(r + \frac{7}{2} \right) \mathfrak{F}_{r+3/2}(\eta_F) - 2\eta_F \Gamma \left(r + \frac{5}{2} \right) \right. \\
 &\quad \times \mathfrak{F}_{r+1/2}(\eta_F) + \eta_F^2 \Gamma \left(r + \frac{3}{2} \right) \mathfrak{F}_{r-1/2}(\eta_F) \left. \right], \\
 K &= WT \left(\frac{k}{q} \right)^2 \frac{2q^2}{h} \left(\frac{\lambda_0}{L} \right) \frac{\sqrt{2m^*kT}}{\pi h} \Gamma \left(r + \frac{5}{2} \right) \\
 &\quad \times \left[\left(r + \frac{5}{2} \right) \mathfrak{F}_{r+3/2}(\eta_F) - \frac{(r+3/2) \mathfrak{F}_{r+1/2}^2(\eta_F)}{\mathfrak{F}_{r-1/2}(\eta_F)} \right]. \tag{A.7}
 \end{aligned}$$

Conductivity $G = \sigma_{2D}W/L$ is given in *Siemens*: $[\sigma_{2D}] = 1 \text{ S}$. Similarly for other specific coefficients: $s_T = S_T L/W$; $\kappa_0 = K_0 L/W$; $\kappa = KL/W$.

Thermoelectric coefficients for 3D ballistic resistors are:

$$\begin{aligned}
 G &= A \frac{2q^2}{h} \frac{m^*kT}{2\pi\hbar^2} \mathfrak{F}_0(\eta_F), \\
 S_T &= -A \frac{k}{q} \frac{2q^2}{h} \frac{m^*kT}{2\pi\hbar^2} [2\mathfrak{F}_1(\eta_F) - \eta_F \mathfrak{F}_0(\eta_F)], \\
 S &= -\frac{k}{q} \left[\frac{2\mathfrak{F}_1(\eta_F)}{\mathfrak{F}_0(\eta_F)} - \eta_F \right], \\
 K_0 &= AT \left(\frac{k}{q} \right)^2 \frac{2q^2}{h} \frac{m^*kT}{2\pi\hbar^2} \\
 &\quad \times [6\mathfrak{F}_2(\eta_F) - 4\eta_F \mathfrak{F}_1(\eta_F) + \eta_F^2 \mathfrak{F}_0(\eta_F)], \\
 K &= AT \left(\frac{k}{q} \right)^2 \frac{2q^2}{h} \frac{m^*kT}{2\pi\hbar^2} \left[6\mathfrak{F}_2(\eta_F) - \frac{4\mathfrak{F}_1^2(\eta_F)}{\mathfrak{F}_0(\eta_F)} \right]. \tag{A.8}
 \end{aligned}$$

Thermoelectric coefficients for 3D diffusive resistors are:

$$\begin{aligned}
 G &= A \frac{2q^2}{h} \left(\frac{\lambda_0}{L} \right) \frac{m^*kT}{2\pi\hbar^2} \Gamma(r+2) \mathfrak{F}_r(\eta_F), \\
 S &= -\frac{k}{q} \left[\frac{(r+2) \mathfrak{F}_{r+1}(\eta_F)}{\mathfrak{F}_r(\eta_F)} - \eta_F \right], \\
 S_T &= -A \frac{k}{q} \frac{2q^2}{h} \left(\frac{\lambda_0}{L} \right) \frac{m^*kT}{2\pi\hbar^2} \\
 &\quad \times [\Gamma(r+3) \mathfrak{F}_{r+1}(\eta_F) - \eta_F \Gamma(r+2) \mathfrak{F}_r(\eta_F)], \\
 K_0 &= AT \left(\frac{k}{q} \right)^2 \frac{2q^2}{h} \left(\frac{\lambda_0}{L} \right) \frac{m^*kT}{2\pi\hbar^2} \\
 &\quad \times [\Gamma(r+4) \mathfrak{F}_{r+2}(\eta_F) - 2\eta_F \Gamma(r+3) \mathfrak{F}_{r+1}(\eta_F) \\
 &\quad + \eta_F^2 \Gamma(r+2) \mathfrak{F}_r(\eta_F)], \\
 K &= AT \left(\frac{k}{q} \right)^2 \frac{2q^2}{h} \left(\frac{\lambda_0}{L} \right) \frac{m^*kT}{2\pi\hbar^2} \Gamma(r+3) \\
 &\quad \times \left[(r+3) \mathfrak{F}_{r+2}(\eta_F) - \frac{(r+2) \mathfrak{F}_{r+1}^2(\eta_F)}{\mathfrak{F}_r(\eta_F)} \right]. \tag{A.9}
 \end{aligned}$$

Conductivity $G = \sigma_{3D}A/L$ is given in *Siemens*: $[\sigma_{3D}] = 1 \text{ S/m}$. Similarly for other specific coefficients: $s_T = S_T L/A$; $\kappa_0 = K_0 L/A$; $\kappa = KL/A$.

B. Thermoelectric Coefficients for Graphene with Linear Dispersion for Ballistic and Diffusive Regimes

Graphene is a 2D conductor with a unique linear band structure (15). Its transport coefficients are calculated from (40a), (40b), (40c), (40d), (42a), (42b), (42c), (42d), and (42e) with the number of modes given by (18). The power law scattering for diffusive regime (A.3) is used.

Conductivity $G = \sigma W/L$ is given in *Siemens*: $[\sigma] = 1 \text{ S}$. Similarly for other specific coefficients: $s_T = S_T L/W$; $\kappa_0 = K_0 L/W$; $\kappa = KL/W$.

Ballistic regime are:

$$\begin{aligned}
 G^{\text{ball}} &= W \frac{2q^2}{h} \left(\frac{2kT}{\pi\hbar v_F} \right) [\mathfrak{F}_0(\eta_F) + \mathfrak{F}_0(-\eta_F)], \\
 S^{\text{ball}} &= -\frac{k}{q} \left\{ \frac{2[\mathfrak{F}_1(\eta_F) - \mathfrak{F}_1(-\eta_F)]}{\mathfrak{F}_0(\eta_F) + \mathfrak{F}_0(-\eta_F)} - \eta_F \right\}, \\
 S_T^{\text{ball}} &= -W \frac{2q^2}{h} \left(\frac{2kT}{\pi\hbar v_F} \right) \left(\frac{k}{q} \right) \\
 &\quad \times \{2[\mathfrak{F}_1(\eta_F) - \mathfrak{F}_1(-\eta_F)] \\
 &\quad - \eta_F [\mathfrak{F}_0(\eta_F) + \mathfrak{F}_0(-\eta_F)]\},
 \end{aligned}$$

$$\begin{aligned}
K^{\text{ball}} &= WT \frac{2q^2}{h} \left(\frac{2kT}{\pi \hbar v_F} \right) \left(\frac{k}{q} \right)^2 \\
&\times \left\{ 6 [\mathfrak{F}_2(\eta_F) + \mathfrak{F}_2(-\eta_F)] \right. \\
&\quad \left. - \frac{4[\mathfrak{F}_1(\eta_F) - \mathfrak{F}_1(-\eta_F)]^2}{\mathfrak{F}_0(\eta_F) + \mathfrak{F}_0(-\eta_F)} \right\}, \\
K_0^{\text{ball}} &= WT \frac{2q^2}{h} \left(\frac{2kT}{\pi \hbar v_F} \right) \left(\frac{k}{q} \right)^2 \\
&\times \left\{ 6 [\mathfrak{F}_2(\eta_F) + \mathfrak{F}_2(-\eta_F)] \right. \\
&\quad - 4\eta_F [\mathfrak{F}_1(\eta_F) - \mathfrak{F}_1(-\eta_F)] \\
&\quad \left. + \eta_F^2 [\mathfrak{F}_0(\eta_F) + \mathfrak{F}_0(-\eta_F)] \right\}. \tag{B.1}
\end{aligned}$$

Diffusive regime are:

$$\begin{aligned}
G^{\text{diff}} &= W \frac{2q^2}{h} \left(\frac{2kT}{\pi \hbar v_F} \right) \left(\frac{\lambda_0}{L} \right) \Gamma(r+2) \\
&\times [\mathfrak{F}_r(\eta_F) + \mathfrak{F}_r(-\eta_F)], \\
S^{\text{diff}} &= -\frac{k}{q} \left\{ \frac{(r+2) [\mathfrak{F}_{r+1}(\eta_F) - \mathfrak{F}_{r+1}(-\eta_F)]}{\mathfrak{F}_r(\eta_F) + \mathfrak{F}_r(-\eta_F)} - \eta_F \right\}, \\
S_T^{\text{diff}} &= -W \frac{2q^2}{h} \frac{k}{q} \left(\frac{2kT}{\pi \hbar v_F} \right) \left(\frac{\lambda_0}{L} \right) \\
&\times \left\{ \Gamma(r+3) [\mathfrak{F}_{r+1}(\eta_F) - \mathfrak{F}_{r+1}(-\eta_F)] \right. \\
&\quad \left. - \eta_F \Gamma(r+2) [\mathfrak{F}_r(\eta_F) + \mathfrak{F}_r(-\eta_F)] \right\}, \\
K &= WT \frac{2q^2}{h} \left(\frac{k}{q} \right)^2 \left(\frac{2kT}{\pi \hbar v_F} \right) \left(\frac{\lambda_0}{L} \right) \\
&\times \Gamma(r+3) \\
&\times \left\{ (r+3) [\mathfrak{F}_{r+2}(\eta_F) + \mathfrak{F}_{r+2}(-\eta_F)] \right. \\
&\quad \left. - \frac{(r+2) [\mathfrak{F}_{r+1}(\eta_F) - \mathfrak{F}_{r+1}(-\eta_F)]^2}{\mathfrak{F}_r(\eta_F) + \mathfrak{F}_r(-\eta_F)} \right\}, \\
K_0 &= WT \frac{2q^2}{h} \left(\frac{k}{q} \right)^2 \left(\frac{2kT}{\pi \hbar v_F} \right) \left(\frac{\lambda_0}{L} \right) \\
&\times \left\{ \Gamma(r+4) [\mathfrak{F}_{r+2}(\eta_F) + \mathfrak{F}_{r+2}(-\eta_F)] \right. \\
&\quad - 2\eta_F \Gamma(r+3) [\mathfrak{F}_{r+1}(\eta_F) + \mathfrak{F}_{r+1}(-\eta_F)] \\
&\quad \left. + \eta_F^2 \Gamma(r+2) [\mathfrak{F}_r(\eta_F) + \mathfrak{F}_r(-\eta_F)] \right\}. \tag{B.2}
\end{aligned}$$

Conflict of Interests

The author declares that there is no conflict of interests regarding the publication of this paper.

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