Yu. A. Kruglyak

Department of Information Technologies, Odessa State Environmental University, 15, Lvivska Str., Odessa, 65016, Ukraine

Yu. A. Kruglyak

ELECTRIC CURRENT, THERMOCURRENT, AND HEAT FLUX IN NANO- AND MICROELECTRONICS: TRANSPORT MODEL

The Landauer – Datta – Lundstrom modern electron and heat transport model is briefly summarized. If a band structure is chosen analytically or numerically, 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 for 1D, 2D, and 3D resistors of any size in ballistic, quasi-ballistic, and diffusive linear response regimes when there are differences in both voltage and/or temperature across the device.

Modes of conduction and transmission concepts are introduced. A new expression for resistivity is suggested providing a different view of resistivity in terms of the specific number of modes (per unit cross-sectional area) and the mean-free-path for backscattering. Fermi conduction window functions for electrons and phonons are formulated and compared. Whether a conductor is good or bad is determined only by the availability of the conductor energy states in an energy window ~ ± 2kT around the equilibrium electrochemical potential, which can vary widely from one material to another. Special attention is given to the near-equilibrium transport.

A general expression for thermocurrent is introduced which is suitable for analysis of conductivity of any materials from metals and semiconductors up to modern nanoresistors and nanocomposites. This general expression is simplified for the case of a linear response regime. Thermocurrent is expressed in terms of three transport coefficients -the conductivity, the Soret electro-thermal diffusion coefficient, and the electronic heat conductance under the short circuit conditions.

Heat transfer by phonons is treated in detail. The basic equation for the heat current is formulated. Electrical and thermal conductances are similar in structure, namely both are proportional to corresponding quantum of conductance, times an integral over the transmission, times the number of modes, times a window function. Moreover, the thermal broadening functions for electrons and phonons have similar shapes and each has a width of a few kT. Along with the number of modes determined by the dispersion relation, these two window functions play a key role in quantitative determination of the electrical and thermal conductivities.

Keywords: nanoelectronics, microelectronics, microelectronics, conductivity modes, transmission coefficient, Fermi windows, near-equilibrium transport, ballistic transport, quasi-ballistic transport, diffusive transport.

Introduction

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

We begin with two well known basic equations – for current and for the total number of electrons in the channel of a conductor under steady-state conditions and introduce a concept of conduction modes for resistors of different dimensions. Then introduce a concept of transmission coefficient as the relation of two transit times – ballistic to diffusive. It is shown that transmission coefficient is the relation of the mean-free-path for backscattering to the resistor length or in the most general case is the relation of the mean-free-path for backscattering to the sum of resistor length and the mean-free-path for backscattering. Now one can specify three transport regimes: diffusive, ballistic, and quasi-ballistic. Then new expression for a specific resistivity is suggested providing a different view of resistivity in terms of the specific number of modes (per unit cross-sectional area) and the mean-free-path for backscattering.

Further we treat only the near-equilibrium transport known also as the low field linear response regime which is most important practically and strongly influences and controls the performance of most electronic devices. Fermi conduction window function is introduced as a negative derivative of the equilibrium Fermi function over energy. Whether a conductor is good or bad is determined only by the availability of the conductor energy states in an energy window ~ $\pm 2kT$ around the equilibrium electrochemical potential, which can vary widely from one material to another. Current is driven by the difference of the Fermi functions in the "agenda" of the two contacts which for low bias is proportional to the Fermi conduction window function but not by so called "external electric field" as assumed in the Drude model still being useful and used in research and teaching. Thus famous Landauer expression for conductivity is introduced. Transport in a massive 3D conductor is treated.

It is shown that the conductance is always the product of the quantum of conductance, times the average transmission, times the number of modes in the Fermi windows which is one of the basic results of the LDL transport model.

Finally, the LDL model is generalized for thermocurrent. A general expression for thermocurrent is introduced which is suitable for analysis of conductivity of any materials from metals to semiconductors up to modern nanoresistors and nanocomposites. This general expression is simplified for the case of the linear response regime when there are differences in both voltage and temperature across the device. Thermocurrent is expressed through three transport coefficients – conductivity, the Soret electro-thermal diffusion coefficient, and the electronic heat conductance under the short circuit conditions as well as via these three specific transport coefficients. These equations are also valid for 1D and 2D resistors, but the units of the various terms differ. In summary, when a band structure is given, the number of modes can be

evaluated and, if a model for the mean-free-path for backscattering can be chosen, then the near-equilibrium transport coefficients can be evaluated using the expressions derived.

Heat transfer by phonons is treated in details. Basic equation for the heat current due to phonons is formulated. The rest is concerned with the linear response conditions. By analogy with the Fermi window function for electrons, the Fermi window function for phonons is introduced. As a result, an expression for the lattice thermal conductance is obtained which is proportional to the quantum of thermal conductance. It is valuable that the electrical and thermal conductivities are similar in structure, namely: both are proportional to corresponding quantum of conductance, times an integral over the transmission, times the number of modes, times a window function. Moreover, the thermal broadening functions for electrons and phonons have similar shapes and each has a width of a few kT. 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 conductivities.

1. LDL model for current

Two basic equations for electric current

$$N = \int \frac{D(E)}{2}\left(f_1 + f_2\right)dE\,, \tag{1}$$

$$I = \frac{2q}{h}\int \gamma(E)\pi\frac{D(E)}{2}\left(f_1 - f_2\right)dE \tag{2}$$

are easily derived [5 – 7], where N is the total, steady-state number of electrons in the channel, $D(E)$ is the density-of-states with the spin degeneracy factor $g_s = 2$ included, the Fermi function

$$f\left(E\right) = \frac{1}{e^{(E-E_F)/kT}+1} \tag{3}$$

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, "broadening" $\gamma(E)$ relates to transit time for electrons to cross the resistor channel

$$\gamma(E) \equiv \frac{\hbar}{\tau(E)}\,. \tag{4}$$

Proportionality of current to $\left(f_1 - f_2\right)$ makes sence, and fundamental constant $2q/h$ is important and known as the Klitzing constant. According to (4), γ is measured in energy units, the density-of-states has units of (energy)$^{-1}$, thus the product $\gamma(E)\pi D(E)/2$ is dimensionless. We shall see now that $\gamma(E)\pi D(E)/2 \equiv M(E)$ has a physical meaning of the number of the resistor conduction modes (channels) at energy E.

1.1. Conduction modes

Let us consider 2D ballistic resistor of length L which is much shorter than a mean-free-pass for back-scattering λ, oriented along the x axis and having width W along the y axis. The total density-of-states is

$$D(E) = D_{2D}\,(\mathrm{E})\,L\cdot W, \tag{5}$$

$$D_{2D}(E) = g_v \frac{m^*}{\pi\hbar^2},\ [1/J{\cdot}m^2] \tag{6}$$

where $D_{2D}(E)$ is the specific density-of-states (per unit area $A = L\cdot W$) written for parabolic energy bands with an effective mass m^* and occupation of a single subband due to confinement in the z direction with a valley degeneracy g_v [8].

Let us determine the characteristic time τ. Equations (38) and (46) of [6] give

$$\frac{qN'(E)dE}{I'(E)dE} = \frac{\hbar}{\gamma}\frac{(f_1 + f_2)}{(f_1 - f_2)}, \tag{7}$$

where $N'(E)dE$ is the steady-state number of electrons in the channel in differential form

$$N'(E)dE = \frac{D(E)dE}{2} f_1(E) + \frac{D(E)dE}{2} f_2(E) \tag{8}$$

and current in differential form

$$I'(E)\,dE = \frac{q}{2\tau(E)}\left(N'_{01}\,dE - N'_{02}\,dE\right) = \frac{2q}{h}\frac{\gamma(E)}{2}\pi D(E)\,dE(f_1 - f_2) \tag{9}$$

with

$$N'_{01}(E)\,dE = D(E)\,dE\,f_1(E) \tag{10}$$

and

$$N'_{02}(E)\,dE = D(E)\,dE\,f_2(E) \tag{11}$$

as the number of electrons being in equilibrium between channel and contact 1, as well as channel and contact 2, between energy E and $E + dE$. We have assumed that current is defined to be positive when it flows from the outside into contact 2 with electrons moving from contact 1 to contact 2 (standard agreement).

Let us now apply a large enough voltage $V = (E_{F1} - E_{F2})/q$ to contact 2 which makes $E_{F2} << E_{F1}$, thus $f_2 << f_1$. Then Eq. (7) becomes

$$\frac{qN'(E)\,dE}{I'(E)\,dE} = \frac{\text{stored charge}}{\text{current}} = \frac{\hbar}{\gamma} = \tau(E). \tag{12}$$

The number of electrons in the resistor is

$$N'(E) = n_S'(E)\,L \cdot W\,, \tag{13}$$

where n_S' is the specific electron density (per unit area) and differential current

$$I'(E) = qWn_S'(E)\left\langle v_x^+(E)\right\rangle. \tag{14}$$

Thus Eq. (12) gives

$$\tau(E) = \frac{L}{\left\langle v_x^+(E)\right\rangle}, \tag{15}$$

which is simply the average transit time of electrons across the channel.

To evaluate τ, one needs to calculate the average velocity of an electron in the +*x* direction, from contact 1 to contact 2. This velocity in our case of ballistic transport, in which electrons move across the resistor without changing direction

$$\left\langle v_x^+(E)\right\rangle = v(E)\left\langle\cos\theta\right\rangle, \tag{16}$$

where angle θ is counted out of positive direction of the *x* axis. The average

$$\left\langle\cos\theta\right\rangle = \frac{1}{\pi}\int_{-\pi/2}^{\pi/2}\cos\theta d\theta = \frac{2}{\pi}, \tag{17}$$

thus for parabolic dispersion and under isotropic conditions assumed one obtains

$$\left\langle v_x^+(E)\right\rangle = \frac{2}{\pi}v = \frac{2}{\pi}\sqrt{\frac{2(E-E_C)}{m^*}}. \tag{16}$$

Defining conduction modes as

$$M(E) \equiv \gamma(E)\pi\frac{D(E)}{2} \tag{17}$$

and using (4) and (5), one finally obtains

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

$$M(E) = WM_{2D}(E) = W\frac{h}{4}\left\langle v_x^+(E)\right\rangle D_{2D}(E)\,, \tag{18}$$

$$M(E) = AM_{3D}(E) = A\frac{h}{4}\left\langle v_x^+(E)\right\rangle D_{3D}(E)\,,$$

where similar arguments were used to get the final results also for 1D and 3D conductors. One may note that the number of conduction modes at energy *E* is proportional to the width of 2D resistor and to the cross-sectional area *A* of 3D resistor.

Let us now call attention to the physical meaning of the results summarized in (18). Thus, for 2D conductor accounting for (6) and (16) we have

$$WM_{2D}(E) = g_v W \frac{\sqrt{2m^*(E - E_C)}}{\pi\hbar}. \tag{19}$$

In the case of a parabolic dispersion

$$E(k) = E_C + \frac{\hbar^2 k^2}{2m^*} \tag{20}$$

with the wave vector expressed through the de Broglie wavelength of electrons at energy E

$$\lambda_B = 2\pi/k, \tag{21}$$

from general expression (19) for the number of modes for 2D conductor one obtains important relation

$$WM_{2D}(E) = g_v \frac{Wk}{\pi} = g_v \frac{W}{\lambda_B(E)/2} = M(E), \tag{22}$$

which opens up a possibility of physical interpretation of the number of modes for 2D conductor, namely: $M(E)$ is just the number (accounting also for the valley degeneracy g_v) of the de Broglie electron half wavelengths that fit into the width of the resistor. Integrality of the conduction mode numbers is assured by the boundary conditions with the imperative vanishing of the wave function at the two edges of the 2D conductor. A thorough discussion of conduction modes concept for 1D, 2D, and 3D nano- and mesoresistors can be found in [9 – 12].

To summarize, now we have two basic equations for current

$$N = \int \frac{D(E)}{2}(f_1 + f_2)\,dE,$$

$$I = \frac{2q}{h}\int M(E)(f_1 - f_2)\,dE, \tag{23}$$

according to which to compute the number of electrons and the current, one needs two quantities – $D(E)$ and $M(E)$.

For parabolic energy bands (20) the 1D, 2D, and 3D densities of states are well known and given by

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

$$D(E) = D_{2D}(E)A = A\frac{m^*}{\pi\hbar^2}H(E - E_C), \tag{24}$$

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

where Ω is the volume of the 3D resistor, and $H(E - E_c)$ is the Heaviside step function. The number of modes in this particular case of parabolic dispersion

$$M(E) = M_{1D}(E) = H\left(E - E_C\right),$$

$$M(E) = WM_{2D}(E) = Wg_v \frac{\sqrt{2m^*(E - E_C)}}{\pi\hbar} H\left(E - E_C\right), \tag{25}$$

$$M(E) = AM_{3D}(E) = Ag_v \frac{m^*(E - E_C)}{2\pi\hbar^2} H\left(E - E_C\right).$$

Although we have assumed a parabolic dispersion above, the expressions for $M(E)$ (18) have general meaning and valid for linear dispersion like in graphene. For an arbitrary band structure a numerical procedure might be used [13].

1.2. Transmission coefficient

We have treated ballistic transport above. Let us turn to diffusive case when $L >> \lambda$. Electrons injected from contacts 1 and 2 undergo a random walk. Some trajectories terminate at the injecting contact and some at the other contact. If a positive voltage is applied to contact 2, then a few more electrons terminate on contact 2.

A key parameter in the LDL transport model is a quantity $\gamma(E)\pi D(E)/2$ which is the number of conduction modes $M(E)$ in the case of ballistic transport. The broadening γ relates to the transit time as $\gamma = \hbar/\tau$. The transit time is being increased when transport becomes diffusive, thus $\gamma(E)\pi D(E)/2$ will decrease. It will be shown now that for diffusive transport $\gamma\pi D(E)/2 = M(E) \cdot T(E)$, where $T(E) \leq 1$ is known as the transmission coefficient.

In ballistic regime electrons are injected into channel at different angles. Accordingly, there is a certain distribution of transit times. Thus, the value of γ is found through the average transit time

$$\gamma(E) = \frac{\hbar}{\langle \tau(E) \rangle}, \tag{26}$$

where for 2D conductor

$$\langle \tau(E) \rangle = \frac{L}{\langle v_x^+(E) \rangle} = \frac{L}{v(E)\langle \cos\vartheta \rangle} = \frac{L}{v(E)(2/\pi)}. \tag{27}$$

What would be $\langle \tau(E) \rangle$ for diffusive transport?

When $L >> \lambda$, then the first Fick's law of diffusion would be applied. In case of 2D conductor the current flux

$$J = q\bar{D}\frac{dn_S}{dx}, \tag{28}$$

where current density is proportional to the surface electron density gradient and $\bar{D}$ is a diffusion coefficient.

Let electrons be injected into a channel mostly by contact 1. Then $f_1 \approx 1$ and $f_2 \approx 0$. There is a finite concentration of injected electrons $\Delta n_S(0)$ at the left side ($x = 0$) of the conductor. For a long channel $\Delta_S(L) \to 0$ due to $f_2 \approx 0$. The electron profile is linear, because no recombination-generation processes are assumed.

Transit time according to (12) is determined by the stored charge relative to current

$$\tau_D = \frac{qN}{I} = \frac{Wq\Delta n_S(0)L/2}{Wq\bar{D}\Delta n_S(0)/L} = \frac{L^2}{2\bar{D}}, \tag{29}$$

where the total number of electrons in the conductor is $N = n_S(0)WL/2$ and current $I = J \cdot W$ with $dn_s/dx = \Delta n_S(0)/L$. From (29) and (28) we conclude that the diffusive transit time is

$$\tau_D = \frac{L^2}{2\bar{D}}, \tag{30}$$

while the ballistic transit time

$$\tau_B = \frac{L}{\langle v_x^+ \rangle}. \tag{31}$$

Gathering all together and remembering definition of γ (26) for both regimes, one obtains

$$\gamma(E)\pi\frac{D(E)}{2} = \frac{\hbar}{\tau_D}\pi\frac{D(E)}{2} = \frac{\hbar}{\tau_B}\pi\frac{D(E)}{2}\frac{\tau_B}{\tau_D} \equiv M(E)T(E), \tag{32}$$

where we see that transmission coefficient is the relation of two transit times – ballistic to diffusive

$$T(E) = \frac{\tau_B}{\tau_D}. \tag{34}$$

In other words, in the presence of electron scattering the number of modes $M(E)$ just needs to be replaced by $M(E) \cdot T(E)$. A thorough discussion of transition from ballistic transport to diffusion regime for 1D and 3D conductors may be found in [7, 9, 10, 14, 15].

From (34) together with (30) and (31) we obtain

$$T(E) = \frac{2\bar{D}}{L\langle v_x^+ \rangle}. \tag{35}$$

Random walks theory [16] gives

$$\bar{D} = \frac{\langle v_x^+ \rangle \lambda}{2}, \tag{36}$$

and finally one obtains a simple expression for the transmission coefficient

$$T(E) = \frac{\lambda}{L} \ll 1, \tag{37}$$

with λ as the mean-free-path for backscattering. As it was already noted,

$$\gamma \pi D(E)/2 = M(E) \cdot T(E) \tag{38}$$

is greatly reduced in diffusion regime relative to ballistic one.

Equation (37) is accurate in the diffusion limit ($L >> \lambda$), but it fails when length of a conductor is short enough. In the most general case [4, 5]

$$T(E) = \frac{\lambda(E)}{\lambda(E) + L}, \tag{39}$$

which is valid for both diffusive and ballistic regimes, as well as between

$$\begin{gathered} \text{Diffusive: } L >> \lambda;\ \ T = \lambda/L << 1, \\ \text{Ballistic: } L << \lambda;\ \ T \to 1, \\ \text{Quasi-ballistic: } L \approx \lambda;\ \ T < 1. \end{gathered} \tag{40}$$

It is remarkable that such a simple transport model works well in all three regimes.

1.3. Ohm's law

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

$$R^{ball} = \frac{h}{q^2}\frac{1}{M(E)}. \tag{41}$$

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 as

$$R(E) = \frac{h}{q^2}\frac{1}{M(E)}\left(1 + \frac{L}{\lambda(E)}\right). \tag{42}$$

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

$$R \equiv \frac{V}{I} = \rho\frac{L}{A}. \tag{43}$$

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

$$R(E) = \frac{\rho(E)}{A}[L + \lambda(E)] \tag{44}$$

with a new expression for resistivity

$$\rho(E) = \frac{h}{q^2}\left(\frac{1}{M(E)/A}\right)\frac{1}{\lambda(E)}, \tag{45}$$

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

1.4. Linear response regime

Near-equilibrium transport or low field linear response regime corresponds to $\lim(dI/dV)_{V\to 0}$. There are several reasons to develop a 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 is used as 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.

Let us assume that under the low field condition

$$f_0(E) \approx f_1(E) > f_2(E), \tag{46}$$

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

$$V = \Delta E_F / q = (E_{F1} - E_{F2})/q \tag{47}$$

is small enough. Using the Taylor expansion under constant temperature condition

$$f_2 = f_1 + \frac{\partial f_1}{\partial E_1}\nabla E_F = f_1 + \frac{\partial f_1}{\partial E_1} qV \tag{48}$$

and the property of the Fermi function

$$+\frac{\partial f}{\partial E_F} = -\frac{\partial f}{\partial E} \tag{49}$$

one finds

$$f_1 - f_2 = (-\frac{\partial f_0}{\partial E})qV\,. \tag{50}$$

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

$$F_T\left(E, E_F\right) = kT\left(-\frac{\partial f}{\partial E}\right) \tag{51}$$

is known as thermal broadening function and shown in Fig. 1.

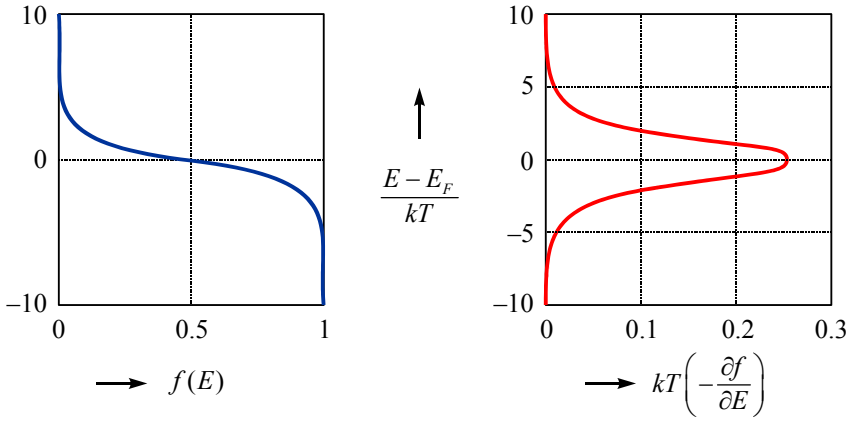

Fig. 1. Fermi function and the dimensionless normalized thermal broadening function.

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

$$\int_{-\infty}^{+\infty} dE F_T\left(E, E_F\right) = kT\,, \tag{52}$$

so that we can approximately visualize F_T as a rectangular pulse centered around $E = E_F$ with a peak value of ¼ and a width of ~ $4kT$.

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 ~ $\pm 2kT$ around the electrochemical potential E_{F0}, which can vary widely from one material to another. Current is driven by the difference $f_1 - f_2$ of the two contacts which for low bias is proportional to the derivative of the equilibrium Fermi function (50). Current generation concept based on experimental and theoretical results of modern nano- and mesophysics are discussed thoroughly in [4, 5, 9, 10, 17].

With the near-equilibrium assumption for current (23) instead of most general expression valid for both diffusive and ballistic regimes as well as in between

$$I = \frac{2q}{h}\int T(E)M(E)\left(f_1 - f_2\right)dE\,, \tag{53}$$

we have now

$$I = \left[\frac{2q^2}{h}\int T(E)M(E)\left(-\frac{\partial f_0}{\partial E}\right)dE\right]V = GV\,, \tag{54}$$

with conductivity

$$G = \frac{2q^2}{h}\int T(E)M(E)\left(-\frac{\partial f_0}{\partial E}\right)dE\,, \tag{55}$$

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

1.5. Transport in a massive conductor

For ballistic limit $T(E)=1$. For diffusive transport $T(E)$ is given by equation (39). For a conductor much longer than a mean-free-path the equation for current density is

$$J_x = \frac{\sigma}{q}\frac{d\left(E_F\right)}{dx} \tag{56}$$

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

For a 2D conductor the surface specific conductivity is

$$\sigma_S = \frac{2q^2}{h}\int M_{2D}(E)\lambda(E)\left(-\frac{\partial f_0}{\partial E}\right)dE\,. \tag{57}$$

or in a different form

$$\sigma_S = \int \sigma'_S(E)dE\,, \tag{58a}$$

where differential specific conductivity

$$\sigma'_S(E) = \frac{2q^2}{h}M_{2D}(E)\lambda(E)\left(-\frac{\partial f_0}{\partial E}\right). \tag{58b}$$

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:

$$G = \frac{2q^2}{h}\left\langle\left\langle T\right\rangle\right\rangle\left\langle M\right\rangle, \tag{59a}$$

$$\left\langle M\right\rangle = \int M(E)(-\frac{\partial f_0}{\partial E})dE\,, \tag{59b}$$

$$\left\langle\left\langle T\right\rangle\right\rangle = \frac{\int T(E)M(E)\,(-\frac{\partial f_0}{\partial E})\,dE}{\int M(E)\,(-\frac{\partial f_0}{\partial E})\,dE} = \frac{\left\langle MT\right\rangle}{\left\langle M\right\rangle}\,. \tag{59c}$$

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

$$G = \int G'(E)dE\,,\ [S] \tag{60a}$$

$$G'(E) = \frac{2q^2}{h}M(E)T(E)\left(-\frac{\partial f_0}{\partial E}\right). \tag{60b}$$

2. LDL model for thermocurrent and thermoelectric coefficients

Electrons carry both charge and heat. The charge current is given by Eq. (53). 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

$$I_Q = \frac{2}{h}\int (E - E_F)T(E)M(E)\left(f_1 - f_2\right)dE\,. \tag{61}$$

It is important from practical point of view that both expressions – for the electric current (53) and thermocurrent (61) are suitable for analysis of conductivity of any materials from metals to semiconductors up to modern nanocomposites [18].

When there are differences in both voltage and temperature across the resistor, then we must expand the Fermi difference $\left(f_1 - f_2\right)$ in a Taylor series in both voltage and temperature and get

$$f_1 - f_2 \approx \left(-\frac{\partial f_0}{\partial E}\right)q\Delta V - \left(-\frac{\partial f_0}{\partial E}\right)\frac{E - E_F}{T}\Delta T\,, \tag{62}$$

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

$$I = \int I'(E)dE\,, \tag{63a}$$

where the differential current is

$$I'(E) = \frac{2q}{h}T(E)M(E)\left(f_1 - f_2\right). \tag{63b}$$

Using Eq. (62), we obtain

$$I'(E) = G'(E)\Delta V + S'_T(E)\Delta T\,, \tag{64a}$$

where

$$G'(E) = \frac{2q^2}{h}T(E)M(E)\left(-\frac{\partial f_0}{\partial E}\right) \tag{64b}$$

is the differential conductance and

$$S'_T(E) = -\frac{2q^2}{h}T(E)M(E)\left(\frac{E - E_F}{qT}\right)\left(-\frac{\partial f_0}{\partial E}\right) = -\frac{k}{q}\left(\frac{E - E_F}{kT}\right)G'(E) \tag{64c}$$

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

Now we integrate Eq. (64a) over all energy modes and find

$$I = G\Delta V + S_T \Delta T\,, \ [\mathrm{A}] \tag{65a}$$

$$I_Q = -T\,S_T\,\Delta V - K_0\,\Delta T\,, \ [\mathrm{W}] \tag{65b}$$

with three transport coefficients – conductivity given by Eqs. (60) , the Soret electro-thermal diffusion coefficient

$$S_T = \int S_T'(E)dE = -\frac{k}{q}\int\left(\frac{E-E_F}{kT}\right)G'(E)dE\,, \ [\mathrm{A/K}] \tag{65c}$$

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

$$K_0 = T\left(\frac{k}{q}\right)^2\int\left(\frac{E-E_F}{kT}\right)^2 G'(E)\,dE\,, \ [\mathrm{W/K}] \tag{65d}$$

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

Equations (65) for long diffusive resistors can be written in the common form used to describe bulk transport as

$$J_x = \sigma\frac{d\left(E_F/q\right)}{dx} - s_T\frac{dT}{dx}\,. \ [\mathrm{A/m^2}] \tag{66a}$$

$$J_{Qx} = T\,s_T\frac{d(E_F/q)}{dx} - \kappa_0\frac{dT}{dx} \ [\mathrm{W/m^2}] \tag{66b}$$

with three specific transport coefficients

$$\sigma = \int \sigma'(E)\,dE\,, \tag{66c}$$

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

$$s_T = -\frac{k}{q}\int\left(\frac{E-E_F}{kT}\right)\sigma'(E)dE\,, \ [\mathrm{A/m\cdot K}] \tag{66d}$$

$$\kappa_0 = T\left(\frac{k}{q}\right)^2\int\left(\frac{E-E_F}{kT}\right)^2\sigma'(E)dE\,. \ [\mathrm{W/m\cdot K}] \tag{66e}$$

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

The inverted form of Eqs (65) is often preferred in practice, namely:

$$\Delta V = RI - S\Delta T\,, \tag{67a}$$

$$I_Q = -\Pi I - K\Delta T\,, \tag{67b}$$

where

$$S = S_T / G\,, \tag{67c}$$

$$\Pi = TS\,, \tag{67d}$$

$$K = K_0 - \Pi SG\,. \tag{67d}$$

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

Similarly, the inverted form of the bulk transport equations (66) become

$$\frac{d(E_F / q)}{dx} = \rho J_x + S\frac{dT}{dx}\,, \tag{68a}$$

$$J_{Qx} = TSJ_x - \kappa\frac{dT}{dx} \tag{68b}$$

with transport coefficients

$$\rho = 1/\sigma\,, \tag{68c}$$

$$S = s_T / \sigma\,, \tag{68d}$$

$$\kappa = \kappa_0 - S^2\sigma T\,, \tag{68e}$$

In summary, when a band structure is given, number of modes can be evaluated from Eqs (18) 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.

2.1. 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

$$J_{Qx}^{ph} = -\kappa_L\frac{dT}{dx}\ \ [\mathrm{W/m^2}] \tag{69}$$

with coefficient κ_L known as the specific lattice thermal conductivity. Such an exceptional thermal conductor like diamond has $\kappa_L \approx 2\cdot 10^3$ W/m·K while such a poor thermal conductor like glass has $\kappa_L \approx 1$ W/m·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.

To describe the phonon current, we need an expression like for the electron current (63) written now as

$$I = \frac{2q}{h}\int T_{el}(E)M_{el}(E)\left(f_1 - f_2\right)dE\,. \tag{70}$$

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

$$n_0(\hbar\omega) = \frac{1}{e^{\hbar\omega/kT} - 1}\,. \tag{71}$$

Let the temperatures for the left and 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 $T_{ph}(E)$ describes the phonon transmission across the entire channel.

It is easy now to rewrite Eq. (70) for 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 (70) by $\hbar\omega$ and move it inside the integral. The coefficient 2 in (70) reflects the spin degeneracy of electron. In the case of phonons we remove this coefficient, and instead of the number of phonon polarization types that contribute to the heat flow we include it to the number of phonon modes $M_{ph}(\hbar\omega)$. Finally, the heat current due to phonons is

$$Q = \frac{1}{h}\int(\hbar\omega)T_{ph}(\hbar\omega)M_{ph}(\hbar\omega)\left(n_1 - n_2\right)d(\hbar\omega)\,. \quad [W] \tag{72}$$

In the linear response regime by analogy with (50)

$$n_1 - n_2 \approx -\frac{\partial n_0}{\partial T}\Delta T\,, \tag{73}$$

where the derivative according to (71)

$$\frac{\partial n_0}{\partial T} = \frac{\hbar\omega}{T}\left(-\frac{\partial n_0}{\partial(\hbar\omega)}\right), \tag{74}$$

with

$$\frac{\partial n_0}{\partial(\hbar\omega)} = \left(-\frac{1}{kT}\right)\frac{e^{\hbar\omega/kT}}{(e^{\hbar\omega/kT} - 1)^2}\,. \tag{75}$$

Now Eq. (72) for small differences in temperature becomes

$$Q = -K_L\,\Delta T\,, \tag{76}$$

where the thermal conductance

$$K_L = \frac{k^2 T}{h} \int T_{ph}(\hbar\omega) M_{ph}(\hbar\omega) \left[\left(\frac{\hbar\omega}{kT} \right)^2 \left(-\frac{\partial n_0}{\partial(\hbar\omega)} \right) \right] d(\hbar\omega) . \quad [W/K] \tag{77}$$

Equation (52) is simply the Fourier's law stating that heat flows down to a temperature gradient. It is also useful to note that the thermal conductance (53) displays certain similarities with the electrical conductance

$$G = \frac{2q^2}{h} \int T_{el}(E) M_{el}(E) \left(-\frac{\partial f_0}{\partial E} \right) dE . \tag{78}$$

The derivative

$$W_{el}(E) \equiv \left(-\frac{\partial f_0}{\partial E} \right) \tag{79}$$

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

$$\int_{-\infty}^{+\infty} \left(-\frac{\partial f_0}{\partial E} \right) dE = 1 . \tag{80}$$

In case of phonons the term in square brackets of Eq.(53) acts as a window function specifying which modes carry the heat current. After normalization

$$W_{ph}(\hbar\omega) = \frac{3}{\pi^2} \left(\frac{\hbar\omega}{kT} \right) \left(\frac{\partial n_0}{\partial(\hbar\omega)} \right); \tag{81}$$

thus finally

$$K_L = \frac{\pi^2 k^2 T}{3h} \int T_{ph}(\hbar\omega) M_{ph}(\hbar\omega) W_{ph}(\hbar\omega) d(\hbar\omega) \tag{82}$$

with

$$g_0 \equiv \pi^2 k^2 T / 3h \approx (9.456 \times 10^{-13}\ W / K^2) T , \tag{83}$$

known as the quantum of thermal conductance experimentally observed first in 2000 [19].

Comparison of Eq. (54) and Eq. (58) shows 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 Eq.(22) or

$$F_T(x) \equiv \frac{e^x}{\left(e^x + 1\right)^2} \tag{84}$$

with $x \equiv (E - E_F) / kT$ and shown in Fig. 2. This function for phonons is given by Eq.(57) or

$$F_T^{ph}(x) \equiv \frac{3}{\pi^2} \frac{x^2 e^x}{\left(e^x - 1\right)^2} \tag{85}$$

with $x \equiv \hbar\omega / kT$. Both functions are normalized to a unity and shown together in Fig. 2.

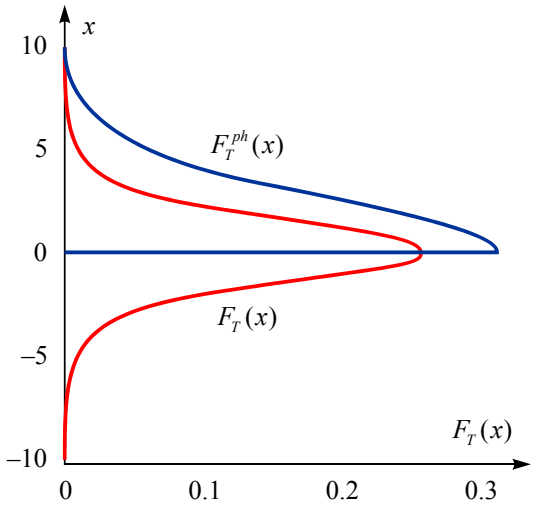

Fig. 2. Broadening function for phonons compared to that of electrons.

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 conductivities.

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 Lundstom gives correct quantitative description of transport processes for resistors of any nature, any dimension and size in ballistic, quasi-ballistic, 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 the 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, almost 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 on the temperature only. 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.

References

1. R. Landauer, *IBM J. Res. Dev*. **1**, 223 (1957).
2. R. Landauer, *J. Math. Phys*. **37**, 5259 (1996).
3. R. Landauer, *Philos. Mag*. **21**, 863 (1970).
4. S. Datta, *Lessons from Nanoelectronics: A New Perspective on Transport* (World Scientific, Singapore, 2012).
5. M. Lundstrom, J. Changwook, *Near-Equilibrium Transport: Fundamentals and Applications* (World Scientific, Singapore, 2013).
6. Yu. A. Kruglyak, *Nanosystems, Nanomaterials, Nanotechnologies*, **11**, 519 (2013); Erratum, **12**, 415 (2014).
7. Yu. A. Kruglyak, *ScienceRise*, **5:** N 3(5), 21 (2014).
8. C. Gang, *Nanoscale Energy Transport and Conversion: A Parallel Treatment of Electrons, Molecules, Phonons, and Photons* (Oxford University Press, New York, 2005).
9. Yu. A. Kruglyak, N.Yu. Kruglyak, M.V. Strikha, Sensor Electronics Microsys. Techn. **9**: N 4, 5 (2012).
10. Yu. A. Kruglyak, J. Nano- Electron. Phys. **5**: N 1, 01023 (2013).
11. Yu. A. Kruglyak, *Physics in Higher Education*, **19:** N 3, 99 (2013).
12. Yu. A. Kruglyak, Visnyk Odessa State Environ. Univ. N 15, 213 (2013).
13. C. Jeong, R. Kim, M. Luisier, S. Datta, and M. Lundstrom, *J. Appl. Phys.* **107**, 023707 (2010).
14. Yu. A. Kruglyak, *Physics in Higher Education*, **19:** N 2, 161 (2013).
15. Yu. A. Kruglyak, *Nanosystems, Nanomaterials, Nanotechnologies*, **11**, 655 (2013)
16. H. C. Berg, *Random Walks in Biology* (Princeton University Press, Princeton, 1993)
17. Yu. A. Kruglyak, *Physics in Higher Education*, **19:** N 1, 50 (2013).
18. L. I. Anatychuk, P. V. Gorsky, V. P. Mikhalchenko, *J. Thermoelectricity*, N 1, 5 (2014).
19. K. Schwab, E.A. Henriksen, J. M. Worlock, and M. L. Roukes, *Nature*, **404**, 974 (2000).

Submitted 21.11.2014