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LANDAUER – DATTA – LUNDSTROM GENERALIZED ELECTRON TRANSPORT MODEL

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This article briefly summarizes the Landauer – Datta – Lundstrom electron transport model. Provided a band structure is given, number of conduction modes can be evaluated and, if a model for a mean free pass 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, quasi-ballistic 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.

Keywords: nanoelectronics, conduction modes, transmission coefficient, ballistic transport, diffusive transport, thermoelectric coefficients.

1. INTRODUCTION

The objectives for these short notes is to give a condensed summary of Landauer – Datta – Lundstrom electron transport model [1 – 5] which works at the nanoscale as well as at 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.

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:

$$\begin{aligned} I &= \frac{2q}{h}\int \gamma(E)\pi\frac{D(E)}{2}\left(f_1-f_2\right)dE, \\ I &= \frac{2q}{h}\int T(E)M(E)\left(f_1-f_2\right)dE, \end{aligned} \tag{1}$$

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

$$\gamma(E) \equiv \frac{\hbar}{\tau(E)}, \tag{2}$$

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

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

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

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

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:

Diffusive: $L >> \lambda;\ T = \lambda/L << 1$,
Ballistic: $L << \lambda;\ T \to 1$,
Quasi-ballistic: $L \approx \lambda;\ T < 1$.

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

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

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

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

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

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

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

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

with a new expression for specific resistivity

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

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

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

$$M(E)=WM_{2D}(E)=W\frac{h}{4}\left\langle v_x^+(E)\right\rangle D_{2D}(E),\quad(5)$$

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

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

For parabolic energy bands

$$E(k)=E_C+\frac{\hbar^2k^2}{2m^*}\quad(6)$$

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

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

$$D(E)=D_{2D}(E)A=A\frac{m^*}{\pi\hbar^2}H(E-E_C),\quad(7)$$

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

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

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

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

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

where gv is the valley degeneracy.

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

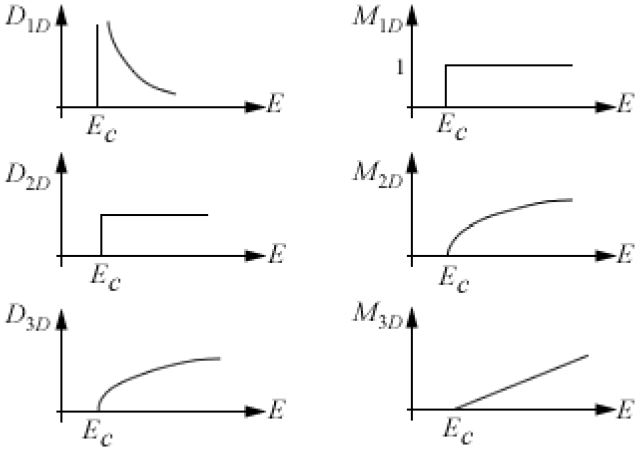

Fig. 1 – Comparison of the density of states $D(E)$ and number of modes $M(E)$ for 1D, 2D, and 3D resistors with parabolic dispersion.

For linear dispersion in grapheme

$$E(k)=\pm\hbar v_F k,\quad(9)$$

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),

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

Density of states in grapheme

$$D(E)=\frac{2|E|}{\pi\hbar^2 v_F^2} \qquad (11)$$

and number of modes

$$M(E)=W\frac{2|E|}{\pi\hbar v_F}\,. \qquad (12)$$

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

$$\sigma(E)=q^2\bar{D}(E)\frac{D(E)}{L}\left\{1,\frac{1}{W},\frac{1}{A}\right\}, \qquad (13a)$$

where

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

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

$$\sigma(E)=\frac{q^2}{h}M(E)\lambda(E)\left\{1,\frac{1}{W},\frac{1}{A}\right\}, \qquad (13b)$$

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

Although Eq. (13b) is not well known, the equivalent version in (13a) is a standard result that is derived in textbooks. Both Eqs (13) are far more generally applicable compared with traditional Drude model. For example, these equations give sensible answers even for materials like graphene whose non-parabolic bands make the meaning of electron mass somewhat unclear, causing considerable confusion when using Drude model. In general we must really use Eqs (13) 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

$$D\left(E\right)v\left(E\right)p\left(E\right)=N\left(E\right)\cdot d\,, \qquad (14)$$

where d is the number of dimensions. Being combined with (13a) it gives one more fundamental equation for conductivity

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

where electron mass is defined as

$$m(E)=\frac{p(E)}{v(E)}\,. \qquad (15)$$

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

$$m^*=\frac{E_F}{v_F^2}\,. \qquad (16)$$

3. 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 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

$$f_0(E)\approx f_1(E)>f_2(E)\approx f_0(E)\,, \qquad (17)$$

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

$$V=\Delta E_F/q=(E_{F1}-E_{F2})/q \qquad (18)$$

is small enough. Using Taylor expansion under constant temperature condition

$$f_2=f_1+\frac{\partial f_1}{\partial E_F}\Delta E_F=f_1+\frac{\partial f_1}{\partial E_F}qV \qquad (19)$$

and property of the Fermi function

$$+\frac{\partial f}{\partial E_F} = -\frac{\partial f}{\partial E} \qquad (20)$$

one finds

$$f_1 - f_2 = (-\frac{\partial f_0}{\partial E})qV \,. \qquad (21)$$

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

$$F_T\left(E, E_F\right) = kT\left(-\frac{\partial f}{\partial E}\right) \qquad (22)$$

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

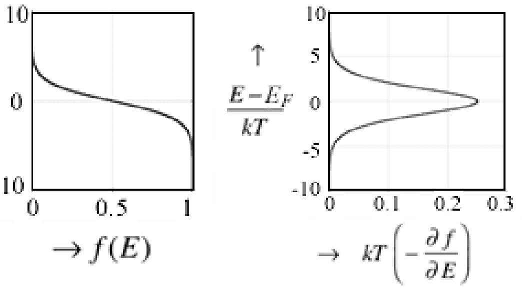

Fig. 2 – Fermi function and the dimensionless normalized thermal broadening function.

If one integrates F_T over all energy range the total area

$$\int_{-\infty}^{+\infty} dE F_T\left(E, E_F\right) = kT \,, \qquad (23)$$

so that we can approximately visualize F_T as a rectangular pulse centered around $E=F_T$ 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 ~ ± $2kT$ 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 (21). With this near-equilibrium assumption for current (1) we have

$$I = \left[\frac{2q^2}{h}\int T(E)M(E)\left(-\frac{\partial f_0}{\partial E}\right)dE\right]V = GV \,, \qquad (24)$$

with conductivity

$$G = \frac{2q^2}{h}\int T(E)M(E)\left(-\frac{\partial f_0}{\partial E}\right)dE \,, \qquad (25)$$

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 equation (3). For a conductor much longer than a mean free pass the current density equation for diffusive transport is

$$J_x = \frac{\sigma}{q}\frac{d\left(E_F\right)}{dx} \,, \qquad (26)$$

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

For a 2D conductor the surface specific conductivity is

$$\sigma_S = \frac{2q^2}{h}\int M_{2D}(E)\lambda(E)\left(-\frac{\partial f_0}{\partial E}\right)dE \qquad (27)$$

or in a different form

$$\sigma_S = \int \sigma_S'(E)dE \,, \qquad (28)$$

where differential specific conductivity

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

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:

$$G = \frac{2q^2}{h}\langle\langle T\rangle\rangle\langle M\rangle \,, \qquad (29)$$

$$\langle M\rangle = \int M(E)(-\frac{\partial f_0}{\partial E})dE \,,$$

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

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

$$G = \int G'(E)dE \,, \ [S] \qquad (30)$$

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

4. THERMOCURRENT AND THERMOELECTRIC COEFFICIENTS

Electrons carry both charge and heat. The charge current is given by Eqn. (1). 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)* 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

$$I_Q = \frac{2}{h}\int (E-E_F)\,T(E)\,M(E)\left(f_1 - f_2\right)dE . \quad (31)$$

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

$$f_1 - f_2 \approx \left(-\frac{\partial f_0}{\partial E}\right) q\Delta V - \left(-\frac{\partial f_0}{\partial E}\right)\frac{E-E_F}{T}\Delta T , \quad (32)$$

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

$$I = \int I'(E)\,dE , \quad (33)$$

where the differential current is

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

Using Eqn. (32) we obtain

$$I'(E) = G'(E)\Delta V + S'_T(E)\Delta T , \quad (34)$$

where

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

is the differential conductance and

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

is the Soret coefficient for electro-thermal 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 Eqn. (34) over all energy modes and find

$$I = G\Delta V + S_T \Delta T , \; [A] \quad (35)$$

$$I_Q = -T\,S_T\,\Delta V - K_0\,\Delta T , \; [W]$$

with three transport coefficients – conductivity given by Eqs. (30) , the Soret electro-thermal diffusion coefficient

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

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

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

where current *I* is defined to be positive when it flows 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 (35) for long diffusive resistors can be written in the common form used to describe bulk transport as

$$J_x = \sigma \frac{d\left(E_F / q\right)}{dx} - s_T \frac{dT}{dx} , \; [A/m^2] \quad (36)$$

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

with three specific transport coefficients

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

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

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

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

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

The inverted form of Eqs (35) is often preferred in practice, namely:

$$\Delta V = RI - S\Delta T , \quad (37)$$

$$I_Q = -\Pi I - K\Delta T ,$$

where

$$S = S_T / G\,,$$

$$\Pi = TS\,,$$

$$K = K_0 - \Pi S G\,.$$

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 (36) become

$$\frac{d(E_F / q)}{dx} = \rho J_x + S\frac{dT}{dx}\,, \qquad (38)$$

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

with transport coefficients:

$$\rho = 1/\sigma\,,$$

$$S = s_T / \sigma\,,$$

$$\kappa = \kappa_0 - S^2\sigma T\,.$$

In summary, when a band structure is given, number of modes can be evaluated from Eqs (5) and, if a model for the mean free pass for backscattering *λ(E)* can be chosen, then the near-equilibrium transport coefficients can be evaluated using the expressions listed above.

5. BIPOLAR CONDUCTION

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

$$M_{3D}(E) = g_v\frac{m^*}{2\pi\hbar^2}(E - E_C) \quad (E \geq E_C) \quad (39)$$

and for the valence band

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

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

$$\sigma = \frac{q^2}{h}\int_{E_C}^{\infty} M_{3D}(E)\lambda(E)\left(-\frac{\partial f_0}{\partial E}\right)dE \qquad (40)$$

and for the valence band

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

The Seebeck coefficient for electrons in the conduction band follows from Eqs (36):

$$\sigma = \int_{E_C}^{\infty}\sigma'(E)dE\,, \qquad (41)$$

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

$$s_T = -\frac{k}{q}\int_{E_C}^{\infty}\left(\frac{E - E_F}{kT}\right)\sigma'(E)dE\,,\ S = S_T/\sigma.$$

Similarly, for electrons in the valence band we have:

$$\sigma_p = \int_{-\infty}^{E_V}\sigma_p'(E)dE\,, \qquad (42)$$

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

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

$$S_p = s_T^{(v)} / \sigma_p\,,$$

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 a narrow bandgap conductors or at high temperatures. In such a case, we have to simply integrate over all the modes and will find

$$\sigma^{tot} \equiv \sigma + \sigma_p = \frac{q^2}{h}\int_{E_1}^{E_2} M_{3D}^{tot}(E)\lambda(E)\left(-\frac{\partial f_0}{\partial E}\right)dE\,, \quad (43)$$

$$M_{3D}^{tot}(E) = M_{3D}(E) + M_{3D}^{v}(E)\,;$$

moreover, we have not 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 that in both cases we integrate the same expression with the appropriate *M*$_{3D}$*(E)* and *λ(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 remind that in the first direct form of the transport coefficients (36) the contributions from each mode are added in parallel so the total specific Soret coefficient

$$s_T^{tot} = -\frac{k}{q}\int_{-\infty}^{+\infty}\left(\frac{E-E_F}{kT}\right)\sigma'(E)dE = S\sigma + S_p\sigma_p; \quad (44)$$

then the Seebeck coefficient for bipolar conduction

$$S^{tot} = \frac{S\sigma + S_p\sigma_p}{\sigma + \sigma_p}.$$

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 pass for backscattering can be established, then the near-equilibrium transport coefficients can be calculated using final expressions listed above.

We also collect below the thermoelectric coefficients for parabolic band semiconductors and for grapheme [4, 5].

6. CONCLUGIONS

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 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 of 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 have also collected the thermoelectric coefficients for parabolic band semiconductors and for graphene.

APPENDIX 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

$$\Im_j(\eta_F) = \frac{1}{\Gamma(j+1)}\int_0^{\infty}\frac{\eta^j}{\exp(\eta-\eta_F)+1}d\eta, \quad (45)$$

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

$$\eta_F = \frac{E_F - E_C}{kT}. \quad (46)$$

In expressions below thermoelectric coefficients (35) and (37) for diffusive regime were calculated with the power law scattering

$$\lambda(E) = \lambda_0\left(\frac{E}{kT}\right)^r. \quad (47)$$

1. Thermoelectric coefficients for 1D ballistic resistors:

$$G = \frac{2q^2}{h}\Im_{-1}(\eta_F);$$

$$S_T = -\frac{k}{q}\frac{2q^2}{h}[\Im_0(\eta_F) - \eta_F\Im_{-1}(\eta_F)];$$

$$S = -\frac{k}{q}\left[\frac{\Im_0(\eta_F)}{\Im_{-1}(\eta_F)} - \eta_F\right];$$

$$K_0 = T\left(\frac{k}{q}\right)^2 \frac{2q^2}{h}\begin{bmatrix} 2\Im_1(\eta_F) - 2\eta_F\Im_0(\eta_F) + \\ +\eta_F^2\,\Im_{-1}(\eta_F) \end{bmatrix};$$

$$K = T\left(\frac{k}{q}\right)^2 \frac{2q^2}{h}\left[2\Im_1(\eta_F) - \frac{\Im_0^2(\eta_F)}{\Im_{-1}(\eta_F)}\right]$$

2. Thermoelectric coefficients for 1D diffusive resistors:

$$G = \frac{2q^2}{h}\left(\frac{\lambda_0}{L}\right)\Gamma(r+1)\Im_{r-1}(\eta_F);$$

$$S_T = -\frac{k}{q}\frac{2q^2}{h}\left(\frac{\lambda_0}{L}\right)\Gamma(r+1)\times$$
$$\times\left[(r+1)\Im_r(\eta_F) - \eta_F\Im_{r-1}(\eta_F)\right];$$

$$S = -\frac{k}{q}\left[\frac{(r+1)\Im_r(\eta_F)}{\Im_{r-1}(\eta_F)} - \eta_F\right];$$

$$K_0 = T\left(\frac{k}{q}\right)^2 \frac{2q^2}{h}\left(\frac{\lambda_0}{L}\right)\begin{bmatrix} \Gamma(r+3)\Im_{r+1}(\eta_F) - \\ -2\eta_F\Gamma(r+2)\Im_r(\eta_F) + \\ +\eta_F^2\,\Gamma(r+1)\Im_{r-1}(\eta_F) \end{bmatrix};$$

$$K = T\left(\frac{k}{q}\right)^2 \frac{2q^2}{h}\left(\frac{\lambda_0}{L}\right)\Gamma(r+2)\times$$
$$\times\left[(r+2)\Im_{r+1}(\eta_F) - \frac{(r+1)\Im_r^2(\eta_F)}{\Im_{r-1}(\eta_F)}\right].$$

Conductivity $G = \sigma_{1D}/L$ is given in *Siemens*: $[\sigma_{1D}] = 1S\cdot m$. Similarly for other specific coefficients: $S_T = S_TL$; $k_0 = K_0L$; $k = KL$.

3. Thermoelectric coefficients for 2D ballistic resistors:

$$G = W\frac{2q^2}{h}\frac{\sqrt{2\pi m^* kT}}{h}\Im_{-1/2}(\eta_F);$$

$$S_T = -W\frac{k}{q}\frac{2q^2}{h}\frac{\sqrt{2\pi m^* kT}}{h}\times$$
$$\times\left[\frac{3}{2}\Im_{1/2}(\eta_F) - \eta_F\Im_{-1/2}(\eta_F)\right];$$

$$S = -\frac{k}{q}\left[\frac{3\Im_{1/2}(\eta_F)}{2\Im_{-1/2}(\eta_F)} - \eta_F\right];$$

$$K_0 = W\,T\left(\frac{k}{q}\right)^2 \frac{2q^2}{h}\frac{\sqrt{2\pi m^* kT}}{h}\times$$
$$\times\left[\frac{15}{4}\Im_{3/2}(\eta_F) - 3\eta_F\Im_{1/2}(\eta_F) + \eta_F^2\,\Im_{-1/2}(\eta_F)\right];$$

$$K = W\,T\left(\frac{k}{q}\right)^2 \frac{2q^2}{h}\frac{\sqrt{2\pi m^* kT}}{h}\times$$
$$\times\left[\frac{15}{4}\Im_{3/2}(\eta_F) - \frac{9\Im_{1/2}^2(\eta_F)}{4\Im_{-1/2}(\eta_F)}\right].$$

4. Thermoelectric coefficients for 2D diffusive resistors:

$$G = W\frac{2q^2}{h}\left(\frac{\lambda_0}{L}\right)\frac{\sqrt{2m^* kT}}{\pi h}\Gamma(r+\frac{3}{2})\Im_{r-1/2}(\eta_F);$$

$$S = -\frac{k}{q}\left[\frac{(r+3/2)\Im_{r+1/2}(\eta_F)}{\Im_{r-1/2}(\eta_F)} - \eta_F\right];$$

$$S_T = -W\frac{k}{q}\frac{2q^2}{h}\left(\frac{\lambda_0}{L}\right)\frac{\sqrt{2m^* kT}}{\pi h}\times$$
$$\times\left[\Gamma(r+\frac{5}{2})\Im_{r+1/2}(\eta_F) - \eta_F\Gamma(r+\frac{3}{2})\Im_{r-1/2}(\eta_F)\right];$$

$$K_0 = W\,T\left(\frac{k}{q}\right)^2 \frac{2q^2}{h}\left(\frac{\lambda_0}{L}\right)\frac{\sqrt{2m^* kT}}{\pi h}\times$$
$$\times\begin{bmatrix} \Gamma(r+\frac{7}{2})\Im_{r+3/2}(\eta_F) - 2\eta_F\Gamma(r+\frac{5}{2})\Im_{r+1/2}(\eta_F) + \\ +\eta_F^2\,\Gamma(r+\frac{3}{2})\Im_{r-1/2}(\eta_F) \end{bmatrix};$$

$$K = W\,T\left(\frac{k}{q}\right)^2 \frac{2q^2}{h}\left(\frac{\lambda_0}{L}\right)\frac{\sqrt{2m^* kT}}{\pi h}\times$$
$$\times\Gamma(r+\frac{5}{2})\left[(r+\frac{5}{2})\Im_{r+3/2}(\eta_F) - \frac{(r+\frac{3}{2})\Im_{r+1/2}^2(\eta_F)}{\Im_{r-1/2}(\eta_F)}\right].$$

Conductivity $G = \sigma_{2D}W/L$ is given in *Siemens*: $\left[\sigma_{2D}\right] = 1S$. Similarly for other specific coefficients: $S_T = S_TL/W$; $k_0 = K_0L/W$; $k = KL/W$.

5. Thermoelectric coefficients for 3D ballistic resistors:

$$G = A\frac{2q^2}{h}\frac{m^* kT}{2\pi\hbar^2}\Im_0(\eta_F);$$

$$S_T = -A\frac{k}{q}\frac{2q^2}{h}\frac{m^*kT}{2\pi\hbar^2}\left[2\Im_1(\eta_F) - \eta_F\Im_0(\eta_F)\right];$$

$$S = -\frac{k}{q}\left[\frac{2\Im_1(\eta_F)}{\Im_0(\eta_F)} - \eta_F\right];$$

$$K_0 = AT\left(\frac{k}{q}\right)^2\frac{2q^2}{h}\frac{m^*kT}{2\pi\hbar^2}\times$$
$$\times\left[6\Im_2(\eta_F) - 4\eta_F\Im_1(\eta_F) + \eta_F^2\Im_0(\eta_F)\right];$$

$$K = AT\left(\frac{k}{q}\right)^2\frac{2q^2}{h}\frac{m^*kT}{2\pi\hbar^2}\times$$
$$\times\left[6\Im_2(\eta_F) - \frac{4\Im_1^2(\eta_F)}{\Im_0(\eta_F)}\right].$$

6. Thermoelectric coefficients for 3D diffusive resistors:

$$G = A\frac{2q^2}{h}\left(\frac{\lambda_0}{L}\right)\frac{m^*kT}{2\pi\hbar^2}\Gamma(r+2)\Im_r(\eta_F);$$

$$S = -\frac{k}{q}\left[\frac{(r+2)\Im_{r+1}(\eta_F)}{\Im_r(\eta_F)} - \eta_F\right];$$

$$S_T = -A\frac{k}{q}\frac{2q^2}{h}\left(\frac{\lambda_0}{L}\right)\frac{m^*kT}{2\pi\hbar^2}\times$$
$$\times\left[\Gamma(r+3)\Im_{r+1}(\eta_F) - \eta_F\Gamma(r+2)\Im_r(\eta_F)\right];$$

$$K_0 = AT\left(\frac{k}{q}\right)^2\frac{2q^2}{h}\left(\frac{\lambda_0}{L}\right)\frac{m^*kT}{2\pi\hbar^2}\times$$
$$\times\begin{bmatrix}\Gamma(r+4)\Im_{r+2}(\eta_F) - 2\eta_F\Gamma(r+3)\Im_{r+1}(\eta_F) + \\ +\eta_F^2\Gamma(r+2)\Im_r(\eta_F)\end{bmatrix};$$

$$K = AT\left(\frac{k}{q}\right)^2\frac{2q^2}{h}\left(\frac{\lambda_0}{L}\right)\frac{m^*kT}{2\pi\hbar^2}\times$$
$$\times\Gamma(r+3)\left[(r+3)\Im_{r+2}(\eta_F) - \frac{(r+2)\Im_{r+1}^2(\eta_F)}{\Im_r(\eta_F)}\right].$$

Conductivity $G = \sigma_{3D}A/L$ is given in *Siemens*: $[\sigma_{3D}] = 1\ S/m$. Similarly for other specific coefficients: $S_T = S_TL/A$; $k_0 = K_0L/A$; $k = KL/A$.

APPENDIX B. THERMOELECTRIC COEFFICIENTS FOR GRAPHENE WITH LINEAR DISPERSION FOR BALLISTIC AND DIFFUSIVE REGIMES

Graphene is a 2D conductor with a unique linear band structure (9). Its transport coefficients are calculated from Eqs (35) and (37) with the number of modes given by Eqn (12). The power law scattering for diffusive regime (47) is used.

Conductivity $G = \sigma W/L$ is given in *Siemens*: $[\sigma] = 1S$. Similarly for other specific coefficients:

$$s_T = S_TL/W;\ k_0 = K_0L/W;\ k = KL/W.$$

1. Ballistic regime:

$$G^{ball} = W\frac{2q^2}{h}\left(\frac{2kT}{\pi\hbar v_F}\right)\left[\Im_0(\eta_F) + \Im_0(-\eta_F)\right];$$

$$S^{ball} = -\frac{k}{q}\left\{\frac{2\left[\Im_1(\eta_F) - \Im_1(-\eta_F)\right]}{\Im_0(\eta_F) + \Im_0(-\eta_F)} - \eta_F\right\};$$

$$S_T^{ball} = -W\frac{2q^2}{h}\left(\frac{2kT}{\pi\hbar v_F}\right)\left(\frac{k}{q}\right)\times$$
$$\times\begin{Bmatrix}2\left[\Im_1(\eta_F) - \Im_1(-\eta_F)\right] - \\ -\eta_F\left[\Im_0(\eta_F) + \Im_0(-\eta_F)\right]\end{Bmatrix};$$

$$K^{ball} = WT\frac{2q^2}{h}\left(\frac{2kT}{\pi\hbar v_F}\right)\left(\frac{k}{q}\right)^2\times$$
$$\times\begin{Bmatrix}6\left[\Im_2(\eta_F) + \Im_2(-\eta_F)\right] - \\ -\dfrac{4\left[\Im_1(\eta_F) - \Im_1(-\eta_F)\right]^2}{\Im_0(\eta_F) + \Im_0(-\eta_F)}\end{Bmatrix};$$

$$K_0^{ball} = WT\frac{2q^2}{h}\left(\frac{2kT}{\pi\hbar v_F}\right)\left(\frac{k}{q}\right)^2\times$$
$$\times\begin{Bmatrix}6\left[\Im_2(\eta_F) + \Im_2(-\eta_F)\right] - \\ -4\eta_F\left[\Im_1(\eta_F) - \Im_1(-\eta_F)\right] + \\ +\eta_F^2\left[\Im_0(\eta_F) + \Im_0(-\eta_F)\right]\end{Bmatrix}.$$

2. Diffusive regime:

$$G^{diff} = W\frac{2q^2}{h}\left(\frac{2kT}{\pi\hbar v_F}\right)\left(\frac{\lambda_0}{L}\right)\times$$
$$\times\Gamma(r+2)\left[\Im_r(\eta_F) + \Im_r(-\eta_F)\right];$$

$$S^{diff} = -\frac{k}{q}\left\{\frac{(r+2)\left[\Im_{r+1}(\eta_F) - \Im_{r+1}(-\eta_F)\right]}{\Im_r(\eta_F) + \Im_r(-\eta_F)} - \eta_F\right\};$$

$$S_T^{diff} = -W\frac{2q^2}{h}\frac{k}{q}\left(\frac{2kT}{\pi\hbar v_F}\right)\left(\frac{\lambda_0}{L}\right)\times$$
$$\times\begin{Bmatrix}\Gamma(r+3)\left[\Im_{r+1}(\eta_F)-\Im_{r+1}(-\eta_F)\right]- \\ -\eta_F\Gamma(r+2)\left[\Im_r(\eta_F)+\Im_r(-\eta_F)\right]\end{Bmatrix};$$

$$K = WT\frac{2q^2}{h}\left(\frac{k}{q}\right)^2\left(\frac{2kT}{\pi\hbar v_F}\right)\left(\frac{\lambda_0}{L}\right)\times$$
$$\times\Gamma(r+3)\begin{Bmatrix}(r+3)\left[\Im_{r+2}(\eta_F)+\Im_{r+2}(-\eta_F)\right]- \\ -\dfrac{(r+2)\left[\Im_{r+1}(\eta_F)-\Im_{r+1}(-\eta_F)\right]^2}{\Im_r(\eta_F)+\Im_r(-\eta_F)}\end{Bmatrix};$$

$$K_0 = WT\frac{2q^2}{h}\left(\frac{k}{q}\right)^2\left(\frac{2kT}{\pi\hbar v_F}\right)\left(\frac{\lambda_0}{L}\right)\times$$
$$\times\begin{Bmatrix}\Gamma(r+4)\left[\Im_{r+2}(\eta_F)+\Im_{r+2}(-\eta_F)\right]- \\ -2\eta_F\Gamma(r+3)\left[\Im_{r+1}(\eta_F)+\Im_{r+1}(-\eta_F)\right]+ \\ +\eta_F^2\Gamma(r+2)\left[\Im_r(\eta_F)+\Im_r(-\eta_F)\right]\end{Bmatrix}.$$

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УЗАГАЛЬНЕНА ТРАНСПОРТНА МОДЕЛЬ ЕЛЕКТРОНІВ ЛАНДАУЕРА – ДАТТИ – ЛУНДСТРОМА

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Стисло викладена узагальнена модель транспорту електронів Ландауера – Датти – Лундстрома. Задавши зонну структуру, можна обчислити число мод провідності і при вибраної моделі розсіяння для середньої довжини вільного пробігу обчислюються термоелектричні транспортні коефіцієнти в режимі лінійного відгуку для 1D, 2D і 3D провідників в балістичному і дифузійному режимах як при різниці потенціалів, так і при різниці температур на контактах. Наведено кінцеві вирази для всіх термоелектричних транспортних коефіцієнтів через інтеграли Фермі – Дірака для 1D, 2D і 3D напівпровідників з параболічною дисперсією і для графену з лінійною дисперсією в балістичному і дифузійному режимах з урахуванням степеневого закону розсіювання.

Ключові слова: наноелектроніка, моди провідності, коефіцієнт проходження, балістичний транспорт, дифузійний транспорт, термоелектричні коефіцієнти.

ОБОБЩЕННАЯ МОДЕЛЬ ТРАНСПОРТА ЭЛЕКТРОНОВ ЛАНДАУЭРА – ДАТТЫ – ЛУНДСТРОМА

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Сжато изложена обобщенная модель транспорта электронов Ландауэра – Датты – Лундстрома. Задав зонную структуру, можно вычислить число мод проводимости и при выбранной модели рассеяния для средней длины свободного пробега вычисляются термоэлектрические транспортные коэффициенты в режиме линейного отклика для 1D, 2D и 3D проводников в баллистическом и диффузионном режимах как при различии потенциалов, так и при разности температур на контактах. Приведены конечные выражения для всех термоэлектрических транспортных коэффициентов через интегралы Ферми – Дирака для 1D, 2D и 3D полупроводников с параболической дисперсией и для графена с линейной дисперсией в баллистическом и диффузионном режимах с учетом степенного закона рассеяния.

Ключевые слова: наноэлектроника, моды проводимости, коэффициент прохождения, баллистический транспорт, диффузионный транспорт, термоэлектрические коэффициенты.

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