

GENERALIZED ELECTRON TRANSPORT MODEL FOR MICRO- AND NANOELECTRONICS

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The objectives for this report is to give a condensed summary of Generalized electron transport model [1, 2] which works well 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.

The generalized expression for current can be easily 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

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

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

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

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:

Diffusive: $L \gg \lambda$; $T = \lambda/L \ll 1$,

Ballistic: $L \ll \lambda$; $T \rightarrow 1$,

Quasi-ballistic: $L \approx \lambda$; $T < 1$.

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

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 is increased. Ballistic limit is obvious for $L \ll \lambda$, while for $L \gg \lambda$ it reduces into standard Ohm's law

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

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

$$M(E) = M_{1D}(E) = \frac{h}{4} \langle v_x^+(E) \rangle D_{1D}(E), \quad (5a)$$

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

$$M(E) = AM_{3D}(E) = A \frac{h}{4} \langle v_x^+(E) \rangle D_{3D}(E) \quad (5c)$$

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 bands

$$E(k) = E_c + \hbar^2 k^2 / 2m^* \quad (6)$$

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

$$D(E) = D_{1D}(E)L = \frac{L}{\pi\hbar} \sqrt{\frac{2m^*}{E - E_c}} H(E - E_c), \quad (7a)$$

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

$$D(E) = D_{3D}(E)\Omega = \Omega \frac{m^* \sqrt{2m^*(E - E_c)}}{\pi^2 \hbar^3} H(E - E_c), \quad (7c)$$

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

$$\begin{aligned}
M(E) &= M_{1D}(E) = H(E - E_C), \\
M(E) &= WM_{2D}(E) = Wg_v \frac{\sqrt{2m^*(E - E_C)}}{\pi\hbar} H(E - E_C), \\
M(E) &= AM_{3D}(E) = Ag_v \frac{m^*(E - E_C)}{2\pi\hbar^2} H(E - E_C),
\end{aligned} \tag{8}$$

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.

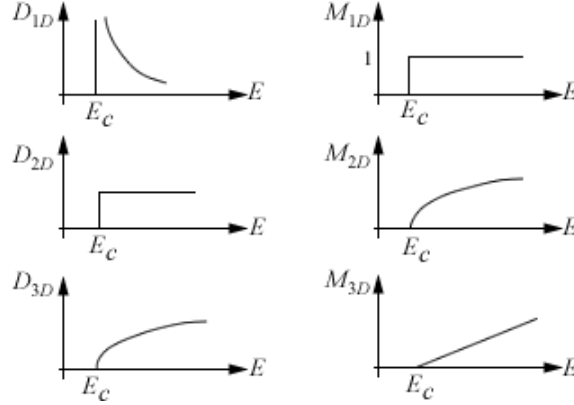


Fig. 1. Comparison of the density of states $D(E)$ and number of modes $M(E)$ for 1D, 2D, and 3D resistors with parabolic dispersion.

For linear dispersion in graphene

$$E(k) = \pm\hbar v_F k, \tag{9}$$

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),

$$v(k) = \frac{1}{\hbar} \frac{\partial E}{\partial k} \equiv v_F \approx 1 \times 10^6 \text{ m/s}. \tag{10}$$

Density of states in graphene

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

and number of modes

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

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

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

where

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

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

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

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

$$D(E)v(E)p(E) = N(E) \cdot d, \quad (14)$$

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

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

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

$$m^* = E_F / v_F^2. \quad (16)$$

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

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

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

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

is small enough. Using Taylor expansion under constant temperature condition

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

and property of the Fermi function

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

one finds

$$f_1 - f_2 = \left(-\frac{\partial f_0}{\partial E}\right)qV. \quad (21)$$

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

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

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

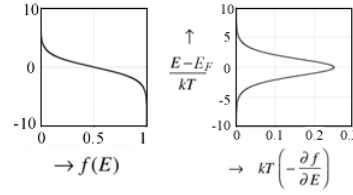


Fig. 2. Fermi function and the dimensionless normalized thermal broadening function.

If one integrates F_T over all energy range the total area

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

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 (21). With this near-equilibrium assumption for current (1) we have

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

with conductivity

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

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

References

1. S. Datta, Lessons from Nanoelectronics: A New Perspective on Transport, Hackensack, New Jersey: World Scientific Publishing Company, 2012.
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