Lecture 2

General Model for Transport

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2.1 Introduction

In this chapter, we introduce a simple, but surprisingly useful model for electron transport. As sketched in Fig. 2.1, we first seek to understand the I–V characteristics of a nanoscale electronic device. The approach is due to R. Landauer in a form developed by Datta [1–3]. As indicated in Fig. 2.1, the contacts play an important role, but we will see that the final result can be generalized to describe transport in the bulk, for which the current is controlled by the properties of the material between the contacts. We shall not attempt to spatially resolve quantities within the device. In practice this can be important, especially for devices under moderate or high bias. Semiconductor devices are often described by the so-called semiconductor equations [4], that make use of the type of bulk transport equation that we shall discuss.

The heart of the device, the channel, is a material that is described by its density-of-states, the DOS, $D(E-U)$, where E is energy, and U a self-consistent electrostatic potential, U. An external gate may be used to

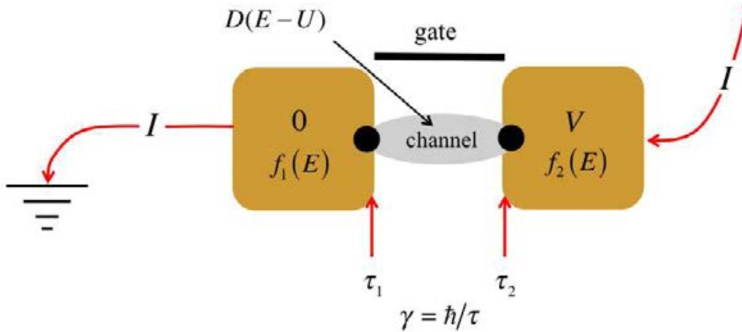

Fig. 2.1. Illustration of a model nanoscale electronic device. The voltage, V, lowers the Fermi level of contact 2 by an amount, qV.

move the states up and down in energy (as in a transistor), but in these lectures we will assume a two-terminal device and set $U = 0$.

The channel of our device is connected to two ideal contacts, which are assumed to be large regions in which strong scattering maintains near-equilibrium conditions. Accordingly, each contact is described by an equilibrium Fermi function (or occupation number),

$$f_0 = \frac{1}{1 + e^{(E-E_F)/k_B T_L}}, \tag{2.1}$$

where E_F is the Fermi level (chemical potential) of the contact, and T_L is the temperature of the lattice, which is also the temperature of the electrons because of the assumed near-equilibrium conditions. Each of the two contacts is in equilibrium, but if a voltage, V, is applied across the device, then $E_{F2} = E_{F1} - qV$.

The connection of the contacts to the channel is described by a characteristic time, τ, which describes how long it takes electrons to get in and out of the device. For a very small device (e.g. a single molecule), τ is controlled by the contact. For longer devices with good contacts, we will see that τ becomes the transit time for electrons to cross the channel. In general, the two connections might be different, so τ_1 and τ_2 may be different. Sometimes it is convenient to express τ in units of energy according to $\gamma = \hbar/\tau$. If the channel is a single molecule, γ has a simple physical interpretation; it represents the "broadening" of the molecular energy levels due to the finite lifetimes of the electrons in a molecular level.

Although this model is very simple, we shall see that it is also very powerful. We shall be concerned with two questions:

(1) How is the electron density in the device related to the Fermi levels in the contacts, to the density of states, and to the characteristic times?
(2) How is the electron current through the device related to the same parameters?

Before we develop the mathematical model, we briefly summarize the key assumptions. For a fuller discussion of these assumptions, see Refs. [1–3].

(1) The channel of the device is described by a band structure, $E(k)$. This assumption is not necessary; for the more general case, see Ref. [1].
(2) The contacts are large with strong inelastic scattering that maintain near-equilibrium conditions.
(3) We assume that electrons feel a self-consistent (mean-field) potential, U, due to the other electrons and the applied biases. (This assumption breaks down for "strongly correlated transport", such as single electron charging.) In practice, we would find the self-consistent potential by solving the Poisson equation. It is important for devices like transistors, but in these notes, we restrict our attention to two-terminal devices and set $U = 0$.
(4) All inelastic scattering takes place in the contacts. Electrons flow from left to right (or right to left) in independent energy channels.
(5) The contacts are reflectionless (absorbing). Electrons that enter the contact from the channel are equilibriated according to the Fermi level of the contact.

Although these assumptions may appear restrictive, we will find that they describe a large class of problems. Having specified the model device, we turn next to the mathematical analysis.

2.2 Mathematical model

To develop the mathematical model, consider first the case where only the first (left) contact is connected to the channel. Contact 1 will seek to fill up the states in the channel according to E_{F1}. Eventually, contact 1 and the channel will be in equilibrium with number of electrons between E and

$E + dE$ given by

$$N'_{01}(E)dE = D(E)dEf_1(E)\,, \tag{2.2}$$

where $D(E)$ is the density-of-states at energy, E, in the channel and $f_1(E)$ is the equilibrium Fermi function of contact 1. Note that $N'_{01}(E)dE$ is the total number of electrons, not the number density. The density-of-states includes the factor of two for spin degeneracy. We can also write a simple rate equation to describe the process by which equilibrium between the contact and channel is achieved. The rate equation is

$$F_1 = \left.\frac{dN'(E)}{dt}\right|_1 = \frac{N'_{01}(E) - N'(E)}{\tau_1(E)}\,. \tag{2.3}$$

According to eqn. (2.3), dN'/dt is positive if the number of the electrons in the channel is less than the equilibrium number and negative if it is more. If the channel is initially empty, the channel fills up until equilibrium is achieved, and if is initially too full of electrons, it empties out until equilibrium with the contact is reached.

On the other hand, if only contact 2 is connected to the channel, a similar set of equations can be developed,

$$N'_{02}(E)dE = D(E)dEf_2(E)\,, \tag{2.4}$$

$$F_2 = \left.\frac{dN'(E)}{dt}\right|_2 = \frac{N'_{02}(E) - N'(E)}{\tau_2(E)}\,. \tag{2.5}$$

In practice, both contacts are connected at the same time and both inject or withdraw electrons from the channel. The total rate of change of the electron number in the device is

$$\left.\frac{dN'(E)}{dt}\right|_{tot} = F_1 + F_2 = \left.\frac{dN'(E)}{dt}\right|_1 + \left.\frac{dN'(E)}{dt}\right|_2\,. \tag{2.6}$$

In steady-state, $dN'/dt = 0$, and we can solve for the steady-state number of electrons in the channel as

$$N'(E)dE = \frac{D(E)dE}{2}f_1(E) + \frac{D(E)dE}{2}f_2(E)\,, \tag{2.7}$$

where we have assumed that $\tau_1 = \tau_2$ and used eqns. (2.2) and (2.4). Finally, we obtain the total, steady-state number of electrons in the channel by integrating over all of the energy channels,

$$N = \int N'(E)dE = \int \left[\frac{D(E)}{2} f_1(E) + \frac{D(E)}{2} f_2(E)\right] dE\,. \tag{2.8}$$

Equation (2.8) is the answer to our first question. It gives the number of electrons in the channel of the device in terms of the density-of-states of the channel and the Fermi functions of the two contacts. Finally, a word about notation. The quantity, N' has units of number / energy; it is the differential carrier density, $N'(E) = dN/dE|_E$.

We should note the similarity of eqn. (2.8) to the standard expression for the equilibrium electron number in a semiconductor [4],

$$N_0 = \int D(E) f_0(E) dE\,. \tag{2.9}$$

The difference is that eqn. (2.9) refers to the number of electrons in equilibrium whereas eqn. (2.8) describes a device that may be in equilibrium (if $E_{F1} = E_{F2}$) or very far from equilibrium if the Fermi levels are very different.

We should remember that N is the total *number* of electrons in the channel, and $D(E)$ is the total density-of-states, the number of states per unit energy. In 1D, $D \propto L$, the length of the channel. In 2D, $D \propto A$, the area of the channel, and in 3D, $D \propto \Omega$, the volume of the channel. For device work we usually prefer to express the final answers in terms of the electron density (per unit length in 1D, per unit area in 2D, and per unit volume in 3D).

Having answered our first question, how the electron number is related to the properties of the channel and contacts, we now turn to the second question, the steady-state current. When a steady-state current flows, one contact tries to fill up states in the channel and the other tries to empty them. If $E_{F1} > E_{F2}$, contact 1 injects electrons and contact 2 removes them, and vice versa if $E_{F1} < E_{F2}$.

The rates at which electrons enter or leave contacts 1 and 2 are given by eqns. (2.3) and (2.5). In steady state,

$$F_1 + F_2 = 0\,. \tag{2.10}$$

The current is *defined* to be positive when it flows into contact 2, so

$$I' = qF_1 = -qF_2\,. \tag{2.11}$$

Using our earlier results, eqns. (2.2) and (2.4), we find

$$I'(E) = \frac{q}{2\tau(E)}\left(N'_{01} - N'_{02}\right) = \frac{2q}{h}\frac{\gamma(E)}{2}\,\pi\, D(E)\left(f_1 - f_2\right)\,, \tag{2.12}$$

where

$$\gamma \equiv \frac{\hbar}{\tau(E)}\,, \tag{2.13}$$

Finally, the total current is found by integrating over all of the energy channels,

$$I = \int I'(E)dE = \frac{2q}{h}\int \gamma(E)\pi\frac{D(E)}{2}\left(f_1 - f_2\right)dE\,. \tag{2.14}$$

According to eqn. (2.14), current only flows when the Fermi levels of the two contacts differ. In that case, there is a competition — one contact keeps trying to fill up the channel while the other one keeps trying to empty it.

This concludes the mathematical derivation that answers our two questions about how the steady-state number of electrons and current are related to the properties of the channel and contacts. The key results, eqns. (2.8) and (2.14) are repeated below.

$$\boxed{\begin{aligned} N &= \int \frac{D(E)}{2}\left(f_1 + f_2\right)dE \\ I &= \frac{2q}{h}\int \gamma(E)\pi\frac{D(E)}{2}\left(f_1 - f_2\right)dE\,. \end{aligned}} \tag{2.15}$$

The remainder of these lecture notes largely consists of understanding and applying these results.

2.3 Modes

The fact that the current is proportional to $(f_1 - f_2)$ makes sense, and $2q/h$ is a set of fundamental constants that we shall see is important, but what is the product, $\gamma\pi D/2$? It is an important quantity. According to eqn. (2.13),

γ has units of energy. The density-of-states, $D(E)$, has units of 1/energy. (Recall that we deal with total electron numbers, not electron densities, so the 3D density-of-states here does not have units of 1/energy-volume, as is customary in semiconductor physics.) Accordingly, we conclude that the product, $\gamma\pi D/2$ is dimensionless. We shall see that it is the number of conducting channels at energy, E.

Figure 2.2 is a sketch of a two-dimensional, ballistic channel.

The total density-of-states is

$$D(E)/A = D_{2D}(E) = g_v \frac{m^*}{\pi\hbar^2}\,, \tag{2.16}$$

where D_{2D} is the 2D density-of-states per unit area, the number of states per J-m^2. The final result assumes parabolic energy bands with an effective mass of m^* and occupation of a single subband (due to confinement in the vertical direction) with a valley degeneracy of g_v.

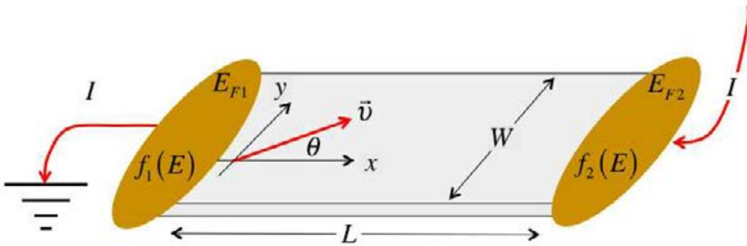

Fig. 2.2. A simple, 2D electronic device with channel width, W and length, L. For the calculation of the average x-directed velocity, ballistic transport is assumed, i.e. the channel is much shorter than a mean-free-path for scattering.

Let's do an "experiment" to determine the characteristic time, τ. From eqns. (2.7) and (2.12), we find

$$\frac{qN'(E)dE}{I'(E)dE} = \frac{\hbar}{\gamma}\frac{(f_1+f_2)}{(f_1-f_2)}\,. \tag{2.17}$$

Now in our experiment we apply a large voltage to contact 2, which makes $E_{F2} \ll E_{F1}$ so $f_2 \ll f_1$, and eqn. (2.17) becomes

$$\frac{qN'(E)dE}{I'(E)dE} = \frac{\text{stored charge}}{\text{current}} = \frac{\hbar}{\gamma} = \tau(E)\,. \tag{2.18}$$

The number of electrons in the channel is $N'(E) = n'_s(E)WL$, where n_s is the electron density per unit area. The differential current can be written as $I'(E) = qWn'_s(E)\left\langle \upsilon_x^+(E)\right\rangle$, so from eqn. (2.18), we find

$$\tau(E) = \frac{L}{\left\langle \upsilon_x^+(E)\right\rangle}\,, \tag{2.19}$$

which is just the average transit time of carriers across the channel.

To evaluate $\tau(E)$, we need $\left\langle \upsilon_x^+(E)\right\rangle$, the average velocity in the $+x$ direction. From Fig. 2.2, we see that for ballistic transport, in which electrons travel across the device without changing direction,

$$\left\langle \upsilon_x^+(E)\right\rangle = \upsilon(E)\left\langle \cos\theta\right\rangle\,. \tag{2.20}$$

A simple calculation gives

$$\left\langle \cos\theta\right\rangle = \frac{\int_{-\pi/2}^{\pi/2}\cos\theta d\theta}{\pi} = \frac{2}{\pi}\,, \tag{2.21}$$

so we find the average ballistic velocity in the $+x$ direction as

$$\left\langle \upsilon_x^+(E)\right\rangle = \frac{2}{\pi}\upsilon = \frac{2}{\pi}\sqrt{\frac{2(E-E_C)}{m^*}}\,, \tag{2.22}$$

where the final result assumes parabolic energy bands. (We also assumed isotropic conditions, so that $\upsilon(E)$ is not a function of θ.) Defining

$$M(E) \equiv \gamma(E)\pi\frac{D(E)}{2} \tag{2.23}$$

and using $\gamma = \hbar/\tau$ and $D = D_{2D}WL$, we find

$$M(E) = WM_{2D}(E) = W\frac{h}{4}\left\langle \upsilon_x^+(E)\right\rangle D_{2D}(E)\,. \tag{2.24}$$

Similar arguments in 1D and 3D yield

$$\boxed{\begin{aligned} M(E) &= M_{1D}(E) = \frac{h}{4}\left\langle \upsilon_x^+(E)\right\rangle D_{1D}(E) \\ M(E) &= WM_{2D}(E) = W\frac{h}{4}\left\langle \upsilon_x^+(E)\right\rangle D_{2D}(E) \\ M(E) &= AM_{3D}(E) = A\frac{h}{4}\left\langle \upsilon_x^+(E)\right\rangle D_{3D}(E)\,. \end{aligned}} \tag{2.25}$$

Note that the number of conducting channels at energy, E, is proportional to the width of the conductor in 2D and to the cross-sectional area in 3D.

We now have expressions for the number of channels at energy, E in 1D, 2D, and 3D, but we should try to understand the result. For parabolic energy bands, we can evaluate (2.24) to find

$$WM_{2D}(E) = g_v W \frac{\sqrt{2m^*(E - E_c)}}{\pi\hbar}\,, \tag{2.26}$$

where g_v is the valley degeneracy. Parabolic energy bands are described by

$$E(k) = E_C + \frac{\hbar^2 k^2}{2m^*}\,, \tag{2.27}$$

which can solved for k to write

$$WM_{2D}(E) = g_v \frac{Wk}{\pi} = g_v \frac{W}{\lambda_B(E)/2}\,, \tag{2.28}$$

where $\lambda_B = 2\pi/k$ is the de Broglie wavelength of electrons at energy, E. We now see how to interpret eqn. (2.24); $M(E)$ is simply the number of electron half wavelengths that fit into the width of the conductor. This occurs because the boundary conditions insist that the wavefunction goes to zero at the two edges of the conductor.

We can now re-write eqns. (2.15) as

$$\boxed{\begin{aligned} N &= \int \frac{D(E)}{2}\,(f_1 + f_2)\,dE \\ I &= \frac{2q}{h}\int M(E)\,(f_1 - f_2)\,dE \end{aligned}}\,, \tag{2.29}$$

which shows that to compute the number of electrons and the current, we need two different quantities, $D(E)$ and $M(E)$. The density-of-states is a familiar quantity. For parabolic energy bands, we know that the 1D, 2D, and 3D densities-of-states are given by

$$\begin{aligned} &\text{1D}: \quad D(E) = D_{1D}(E)L = \frac{L}{\pi\hbar}\sqrt{\frac{2m^*}{(E-E_c)}}H(E-E_c) \\ &\text{2D}: \quad D(E) = D_{2D}(E)A = A\frac{m^*}{\pi\hbar^2}H(E-E_c) \\ &\text{3D}: \quad D(E) = D_{3D}(E)\Omega = \Omega\frac{m^*\sqrt{2m^*(E-E_c)}}{\pi^2\hbar^3}H(E-E_c)\,, \end{aligned} \tag{2.30}$$

where L is the length of the 1D channel, A is the area of the 2D channel, Ω is the volume of the 3D channel, and H is the Heaviside step function. We now also know how to work out the corresponding results for $M(E)$; for parabolic energy bands they are

$$\begin{aligned} M(E) &= M_{1D}(E) = H(E - E_c) \\ M(E) &= W M_{2D}(E) = W g_v \frac{\sqrt{2m^*(E - E_c)}}{\pi\hbar} H(E - E_c) \\ M(E) &= A M_{3D}(E) = A g_v \frac{m^*}{2\pi\hbar^2}(E - E_c) H(E - E_c)\,, \end{aligned} \tag{2.31}$$

where W is the width of the 2D channnel and A is the cross sectional area of the 3D channel. Figure 2.3 compares the density-of-states and number of modes (conducting channels) in 1D, 2D, and 3D for the case of parabolic energy bands ($E(k) = E_c + \hbar^2 k^2/2m^*$).

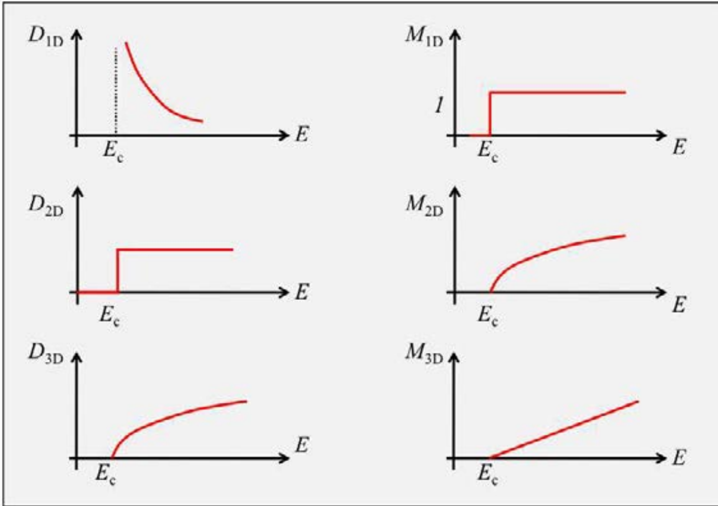

Fig. 2.3. Comparison of the density-of-states, $D(E)$, and number of channels, $M(E)$, in 1D, 2D, and 3D. Parabolic energy bands are assumed in each case.

We can summarize the main points of this section as follows.

(1) The density-of-states vs. E is used to compute carrier densities.
(2) The number of modes (channels) vs. E is used to compute the current.

(3) The number of modes at energy, E, is proportional to the average velocity (in the direction of transport) at energy, E, times the density-of-states, $D(E)$.
(4) $M(E)$ depends on the band structure and on dimensionality.

Although we assumed parabolic energy bands to work out examples, the main results, eqn. (2.25), are general. See Lecture 10 — the graphene case study to see how to work out $M(E)$ for graphene. For general band structures, a numerical procedure can be used [5].

2.4 Transmission

Figure 2.2 showed how electrons flow from contact 1 to contact 2 under ballistic conditions. Figure 2.4 shows the diffusive case.

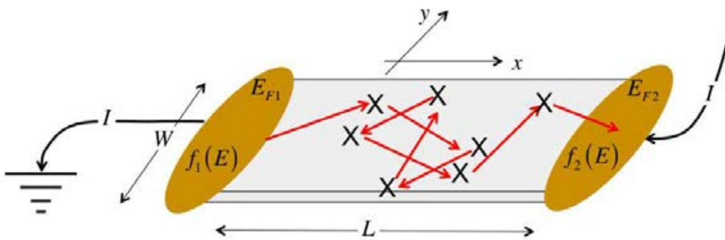

Fig. 2.4. A simple, 2D electronic device with channel width, W and length, L. In this case, diffusive transport is assumed — the channel is many mean-free-paths long.

Electrons injected from contact 1 (or 2) undergo a random walk. Some of these random walks terminate at the injecting contact and some at the other contact. If there is a positive voltage on contact 2, then a few more of the random walks terminate on contact 2. The average distance between scattering events is known as the mean-free-path. Transport is "diffusive" when the sample length is much longer than the mean-free-path. A key parameter in our model is the quantity $\gamma\pi D/2$, which we have seen is $M(E)$ for ballistic transport. The broadening, γ, is related to the transit time according to $\gamma = \hbar/\tau$. We expect the transit time to increase when transport is diffusive, so $\gamma\pi D/2$ will decrease. In this section, we will show that for diffusive transport $\gamma\pi D/2 = M(E)T(E)$, where $T(E) \leq 1$ is known as the "transmission".

For ballistic transport, there is a distribution of transit times because carriers are injected into the channel at different angles. Accordingly, we evaluated γ from the average transit time and found

$$\gamma(E) = \frac{\hbar}{\langle \tau(E) \rangle}\,, \tag{2.32}$$

where

$$\langle \tau(E) \rangle = \frac{L}{\left\langle \upsilon_x^+(E) \right\rangle} = \frac{L}{\upsilon(E)\,\langle \cos\theta \rangle} = \frac{L}{\upsilon(E)\,(2/\pi)}\,. \tag{2.33}$$

Our challenge now is to determine $\langle \tau(E) \rangle$ for the case of diffusive transport.

Consider a device with a very long channel ($L \gg \lambda$), then Fick's Law of diffusion should apply. If we inject electrons from contact 1 and collect them from contact 2, then the current in our 2D device should be given by

$$J = qD_n \frac{dn_s}{dx} \quad \text{A/cm}\,. \tag{2.34}$$

As shown in Fig. 2.5, there is a finite concentration of injected electrons at $x = 0$, $\Delta n_s(0)$, and for a long channel, $\Delta n_s(L) \to 0$. The electron profile is linear because no recombination-generation is assumed. The total number of electrons in the device is $N = n_s(0)WL/2$, where W is the width of the conductor in the direction normal to current flow, and L is the length. From our definition of transit time, we find

$$\tau = \frac{qN}{I} = \frac{Wq\Delta n_s(0)L/2}{WqD_n\Delta n_s(0)/L} = \frac{L^2}{2D_n}\,, \tag{2.35}$$

where we have used $I = JW$ and $dn_s/dx = \Delta n_s(0)/L$. We conclude that the diffusive transit time is

$$\tau_D = \frac{L^2}{2D_n}\,, \tag{2.36}$$

while the ballistic transit time was

$$\tau_B = \frac{L}{\left\langle \upsilon_x^+ \right\rangle}\,. \tag{2.37}$$

Putting this all together, we find

$$\gamma(E)\pi\frac{D(E)}{2} = \frac{\hbar}{\tau_D}\pi\frac{D}{2} = \frac{\hbar}{\tau_B}\pi\frac{D}{2} \times \frac{\tau_B}{\tau_D} \equiv M(E)T(E)\,, \tag{2.38}$$

where

$$T(E) = \frac{\tau_B}{\tau_D}\,. \tag{2.39}$$

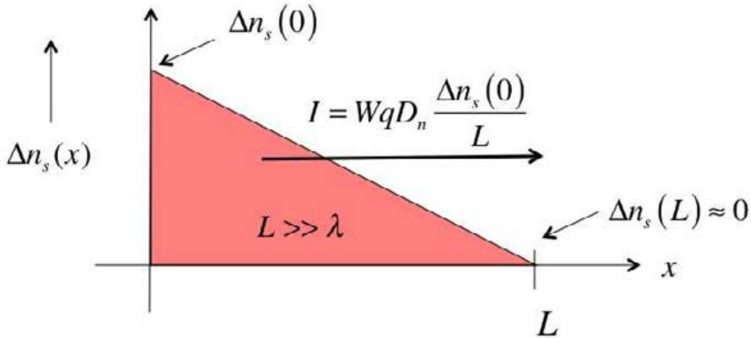

Fig. 2.5. Illustration of diffusion in a channel many mean-free-paths long.

We see that in the presence of scattering, we just need to replace $M(E)$ by $M(E)T(E)$.

To evaluate $T(E)$, we use eqn. (2.39) with eqns. (2.36) and (2.37) and find

$$T(E) = \frac{2D_n}{L\left\langle \upsilon_x^+ \right\rangle}\,. \tag{2.40}$$

The diffusion coefficient describes the random walk of electrons; it is related to the carrier velocity and the mean-free-path for backscattering, λ, according to

$$D_n = \frac{\left\langle \upsilon_x^+ \right\rangle \lambda}{2} \quad \mathrm{cm}^2/\mathrm{s}\,. \tag{2.41}$$

(This expression is not obvious. You can check that it is dimensionally correct but will have to wait until Lecture 6 for the derivation and for a precise definition of the mean-free-path for backscattering.) Finally, using eqns. (2.40) and (2.41), we find a simple expression for the transmission:

$$T(E) = \frac{\lambda}{L} \ll 1\,. \tag{2.42}$$

As expected, the product $\gamma\pi D/2 = M(E)T(E)$ is greatly reduced from its ballistic value.

Our "derivation" of $T(E)$ here is no more than a plausibility argument. As we will discuss in Lecture 6, the transmission is the probability that an electron at energy, E injected from contact 1 exits in contact 2 (or vice versa). It must be a number between 0 and 1. Equation (2.42) is accurate

in the diffusive limit that we have considered ($L \gg \lambda$), but it fails when L is short. The correct, general expression is

$$\boxed{T(E) = \frac{\lambda(E)}{\lambda(E) + L}}, \tag{2.43}$$

which reduces to eqn. (2.42) for the diffusive limit of $L \gg \lambda$, but for the ballistic limit of $L \ll \lambda$ it approaches 1. This expression is reasonable, but we will see in Lecture 6 that it can be derived with relatively few assumptions and that it is valid not only in the ballistic and diffusive limits, but in between as well.

To summarize, we can write in general

$$\gamma(E)\pi\frac{D(E)}{2} = M(E)T(E)\,, \tag{2.44}$$

with $M(E)$ being given by eqns. (2.25) and $T(E)$ by eqn. (2.43). People speak of three different transport regimes:

$$\begin{array}{lll} \text{Diffusive}: & L \gg \lambda & T = \lambda/L \ll 1 \\ \text{Ballistic}: & L \ll \lambda & T \to 1 \\ \text{Quasi}-\text{ballistic}: & L \approx \lambda & T < 1\,. \end{array} \tag{2.45}$$

Our simple transport model can be used to describe all three regions.

2.5 Near-equilibrium (linear) transport

To summarize, we have developed an expression for the current in a nanoscale device that can be expressed in two different ways:

$$\begin{aligned} I &= \frac{2q}{h}\int \gamma(E)\pi\frac{D(E)}{2}\,(f_1 - f_2)\,dE \\ I &= \frac{2q}{h}\int T(E)M(E)\,(f_1 - f_2)\,dE\,. \end{aligned} \tag{2.46}$$

There is no limitation to small applied biases yet, but if we apply a large bias, then there could be a lot of inelastic scattering that would invalidate our assumption that the current flows in independent energy channels. Since our interest is in near-equilibrium transport, we now simplify these equations for low applied bias.

The two Fermi functions in eqn. (2.46) are different when there is an applied bias. Recall that an applied bias lowers the Fermi level by $-qV$. If the applied bias is small, we can write

$$(f_1 - f_2) \approx -\frac{\partial f_0}{\partial E_F} \Delta E_F \,. \tag{2.47}$$

From the form of the equilibrium Fermi function,

$$f_0 = \frac{1}{1 + e^{(E-E_F)/k_B T_L}} \,, \tag{2.48}$$

we see that

$$\frac{\partial f_0}{\partial E_F} = -\frac{\partial f_0}{\partial E} \,. \tag{2.49}$$

Equations (2.49) and (2.47) can be used in eqn. (2.46) along with $\Delta E_F = -qV$ to obtain

$$I = \left[\frac{2q^2}{h} \int T(E) M(E) \left(-\frac{\partial f_0}{\partial E} \right) dE \right] V = GV \,. \tag{2.50}$$

The final result,

$$\boxed{G = \frac{2q^2}{h} \int T(E) M(E) \left(-\frac{\partial f_0}{\partial E} \right) dE \,,} \tag{2.51}$$

is just the conductance in Ohm's Law, but now we have an expression that relates the conductance to the properties of the material. It is important to remember that this expression is valid in 1D, 2D, or 3D, if we use the appropropiate expression for $M(E)$.

2.6 Transport in the bulk

In this lecture, we have developed a model for the current or conductance of a device whose channel length may be short or long. When the channel is long, the contacts play no role, and the current is limited by the material properties of the channel. We can develop an expression for the current in a bulk conductor from either of the two forms of the current equations, eqn. (2.46). Let's use the first form.

Assuming near-equilibrium conditions, we can use eqn. (2.47) to write eqn. (2.46) as

$$I = \frac{2q}{h} \int \left[\gamma(E) \pi \frac{D(E)}{2} \left(-\frac{\partial f_0}{\partial E_F} \right) \Delta E_F \right] dE \,. \tag{2.52}$$

A bulk conductor is, by definition, in the diffusive limit, so

$$\gamma(E) = \frac{\hbar}{\tau(E)} = \frac{\hbar}{L^2/2D_n(E)} \,. \tag{2.53}$$

To be specific, let's assume a 2D conductor for which we can write

$$D(E) = WLD_{2D}(E) \,. \tag{2.54}$$

Now using eqns. (2.53) and (2.54) in (2.52), we find

$$J_{nx} = I/W = \left[\int qD_n(E)D_{2D}(E)\left(-\frac{\partial f_0}{\partial E_F}\right)dE\right]\frac{\Delta E_F}{L} \,. \quad \text{A/cm} \tag{2.55}$$

Figure 2.6 illustrates how we think about a bulk resistor. In a conventional resistor, the potential and electrochemical potential (or quasi-Fermi level) drop linearly along the length. In our model device, the Fermi levels are only defined in the two contacts. Since the bulk resistor is assumed to be under low bias and near-equilibrium everywhere, we can conceptually place two contact separated by a length, $L \gg \lambda$, anywhere along the length of the resistor. The average electrochemical potential in the first contact, becomes E_{F1} for our "device", and the average electrochemical potential in the second contact, our E_{F2}. Because the electrochemical potential drops linearly with position, $\Delta E_F/L$ becomes dF_n/dx, and we can write (2.55) as

$$\boxed{J_{nx} = \sigma_n \frac{d(F_n/q)}{dx} \,,} \tag{2.56}$$

where the conductivity is

$$\boxed{\sigma_n = \int q^2 D_n(E)D_{2D}(E)\left(-\frac{\partial f_0}{\partial E}\right)dE \,.} \tag{2.57}$$

Equations (2.56) and (2.57) are standard results that are conventionally obtained from irreversible thermodynamics or by solving the Boltzmann Transport Equation [7]. We have obtained the standard expressions for bulk materials by assuming that the channel of our model device is much longer that a mean-free-path.

Real resistors can be linear even when quite large voltages are applied. How does this occur? It occurs because when the resistor is long, electrons do not drop down the total potential drop in one step. Instead, they continually gain a little energy and then dissipate it by emitting phonons. If the resistor is long and the voltage drop not too large, then the electrons

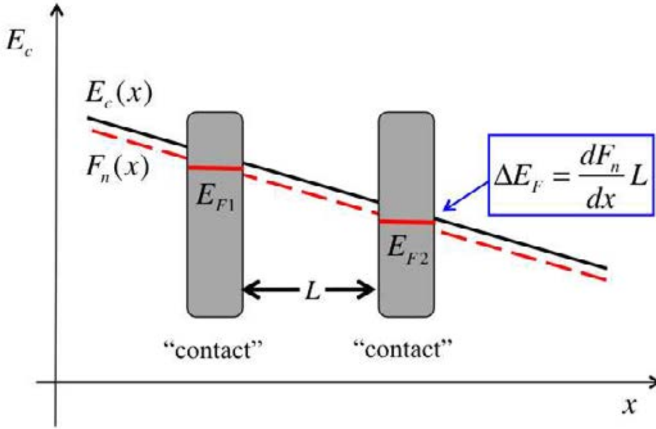

Fig. 2.6. Illustration of how a near-equilibrium bulk conductor is conceptually treated as a device with two contacts.

are always near-equilibrium, and we can conceptually divide up the resistor into sub-devices, as sketched in Fig. 2.6, where only a fraction of the potential drop occurs.

Equation (2.56) can also be written differently. Conventional semiconductor theory tells us that for a non-degenerate, n-type semiconductor

$$\begin{aligned} n_s &= N_{2D} e^{(F_n - Ec)/k_B T_L} \\ N_{2D} &= g_v \frac{m^* k_B T_L}{\pi \hbar^2} \\ F_n &= E_c + k_B T_L \ln \frac{N_{2D}}{n_s} \\ \sigma_n &= n_s q \mu_n \,. \end{aligned} \tag{2.58}$$

(Note that the units of the 2D conductivity, σ_n, are Siemens or $1/\Omega$.) Using eqns. (2.58), the current equation, (2.56) becomes

$$\boxed{J_{nx} = n_s q \mu_n \mathcal{E}_x + q D_n \frac{dn_s}{dx}}\,, \tag{2.59}$$

where

$$\boxed{\frac{D_n}{\mu_n} = \frac{k_B T_L}{q}} \tag{2.60}$$

is the Einstein relation. Equation (2.59) is the well-known "drift-diffusion" equation, which is often the starting point for analyzing semiconductor devices [4]. We see that it assumes steady-state, near-equilibrium, non-degenerate conditions (and we have also assumed a uniform temperature along the resistor).

Finally, you may be wondering: "What about holes?" In standard semiconductor physics, the conduction and valence bands are described by two different electrochemical potentials (or quasi-Fermi levels), F_n and F_p. This occurs because we have two separate populations of carriers that are in equilibrium with carriers in the same band but not with carriers in the other band. The recombination-generation processes that couple the two populations are typically slow in comparison to the scattering processes that establish equilibrium within each band. For electrons in the conduction band, we have

$$\begin{aligned} J_{nx} &= \sigma_n \frac{d(F_n/q)}{dx} \\ \sigma_n &= \int q^2 D_n(E) D_{2D}(E) \left(-\frac{\partial f_0}{\partial E_F}\right) dE \\ f_0 &= \frac{1}{1+e^{(E-F_n(x))/k_B T_L}}\,, \end{aligned} \tag{2.61}$$

and for electrons in the valence band, we have

$$\begin{aligned} J_{px} &= \sigma_p \frac{d(F_p/q)}{dx} \\ \sigma_p &= \int q^2 D_p(E) D_{2D}(E) \left(-\frac{\partial f_0}{\partial E_F}\right) dE \\ f_0 &= \frac{1}{1+e^{(E-F_p(x))/k_B T_L}}\,. \end{aligned} \tag{2.62}$$

The total current is the sum of the contributions from each band. It is important to note that these equations refer to *electrons* in both the conduction and valence bands. The occupation factor, f_0, describes the probability that an *electron* state is occupied. It is often useful to visualize the resulting current flow in the valence band in terms of holes, but the expressions that we used were derived for electrons, and we did not inquire as to whether they were in the conduction or valence bands because it does not matter.

2.7 Summary

This has been a long lecture, but the final result is a simple one that we shall see is very powerful. Equation (2.51) describes the conductance of a linear resistor very generally. The conductance is proportional to some fundamental constants, $(2q^2/h)$, which we will see in the next lecture is the "quantum of conductance", that is associated with the contacts. The conductance is related to the number of conducting channels at energy, E, $M(E)$, and to the transmission, $T(E)$, which is the probability that an electron with energy, E, injected from one contact exits to the other contact. We find the total conductance by integrating the contributions of all of the energy channels. Equation (2.51) is valid in 1D, 2D, or 3D — we simply need to use the correct expressions for $M(E)$. It is valid for very short (ballistic) resistors or very long (diffusive) resistors and for the region in between. The next lecture will begin with eqn. (2.51). Finally, it should be mentioned, that we have assumed isothermal conditions — the two contacts are at the same temperature. The implications of temperature gradients will be discussed in Lectures 4 and 5.

2.8 References

The approach summarized in this chapter is described much more fully by Datta.

[1] Supriyo Datta, *Electronic Transport in Mesoscopic Systems*, Cambridge Univ. Press, Cambridge, UK, 1995.

[2] Supriyo Datta, *Quantum Transport: Atom to transistor*, Cambridge Univ. Press, Cambridge, UK, 2005.

[3] Supriyo Datta, *Lessons from Nanoelectronics: A new approach to transport theory*, World Scientific Publishing Company, Singapore, 2011.

The standard approach to semiconductor devices is clearly presented by Pierret.

[4] Robert F. Pierret *Semiconductor Device Fundamentals*, Addison-Wesley, Reading, MA, USA, 1996.

Jeong describes how to evaluate $M(E)$ for an arbitrary $E(k)$.

[5] Changwook Jeong, Raseong Kim, Mathieu Luisier, Supriyo Datta, and Mark Lundstrom, "On Landauer vs. Boltzmann and Full Band vs. Effective Mass Evaluation of Thermoelectric Transport Coefficients", *J. Appl. Phys.*, **107**, 023707, 2010.

Two classic references on low-field transport are:

[6] J.M. Ziman, *Principles of the Theory of Solids*, Cambridge Univ. Press, Cambridge, U.K., 1964.

[7] N.W. Ashcroft and N.D. Mermin, *Solid–State Physics*, Saunders College, Philadelphia, PA, 1976.

A collection of additional resources on carrier transport can be found at:

[8] M. Lundstrom, S. Datta, and M.A. Alam, "Electronics from the Bottom Up", http://nanohub.org/topics/ElectronicsFromTheBottomUp, 2011.

Hear a lecture on this chapter at:

[9] M. Lundstrom, "General Model for Transport", http://nanohub.org/topics/LessonsfromNanoscience, 2011.