Lecture 3:
General model for transport

Professor Mark Lundstrom
Electrical and Computer Engineering
Purdue University, West Lafayette, IN USA
\[ \ln \left[ \mathcal{F}_{1/2}(\eta_F) \right] \]

\[ \mathcal{F}_{1/2}(\eta_F) = \frac{1}{\sqrt{\pi}} \int_0^\infty \frac{\eta^{1/2}}{1 + e^{\eta - \eta_F}} \ d\eta \]

\[ \eta_F = (E_F - E_C)/k_B T \]

\[ \mathcal{F}_{1/2}(0) = 0.7652 \]
lecture 2: periodic boundary conditions

\[ k_x = \frac{2\pi}{L_x} j \quad L_x = N_A a \quad k_x(\text{max}) = \frac{2\pi}{a} \]

\[ 0 < k_x < \frac{2\pi}{a} \]

\[ -\frac{\pi}{a} < k_x < +\frac{\pi}{a} \]
1) **General model for low-field transport**
2) Modes
3) Transmission
4) Linear (near equilibrium) transport
5) Summary
S. Datta, *Quantum Transport: Atom to Transistor*, Cambridge, 2005
(“Electronics from the Bottom Up” [nanohub.org](http://nanohub.org))
final result (near-equilibrium transport)

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

\[ f_1(E) \approx f_2(E) \approx f_0(E) \]

\[ 0 \leq T(E) \leq 1 \]

transmission

\[ M(E) \]

number of conducting channels
assumptions

1) Contacts are large with strong scattering, always very near equilibrium.

2) $U$, the self-consistent (mean-field) potential. (For ‘strongly correlated’ transport, see Datta.)

3) In this class, we will assume that the device can be described by an $E(k)$. For the more general case, see Datta.
4) Contacts are **reflectionless** (‘absorbing’). Any electron that enters from the device, stays in the contact and equilibrates with it.
5) Electrons flow from left to right (or right to left) in different energy channels (modes). **Energy channels are independent.** Elastic scattering may occur in the device, but electrons do not change energy channels. All inelastic scattering takes place in the contacts.
1) Contacts stay in equilibrium.
2) Electrons respond to the average potential, \( U \).
3) Device is described by an \( E(k) \) from which we can determine \( D(E) \) (not a necessary assumption).
4) Contacts are reflectionless.
5) Independent energy channels in the device (if scattering occurs, it is elastic).
fills states from the left contact

(ignores electrostatics for now; \( U = 0 \))

\[
\frac{dN(E)}{dt} \bigg|_1 = \frac{N_1^0(E) - N(E)}{\tau_1}
\]

\[
N_1^0(E) = D(E) f_1(E)
\]
filling states from the right contact

\[ \frac{dN(E)}{dt} \bigg|_2 = \frac{N_2^0(E) - N(E)}{\tau_2} \]

\[ N_2^0(E) = D(E) f_2(E) \]
steady-state

\[ \frac{dN(E)}{dt}_\text{tot} = \frac{dN(E)}{dt}_1 + \frac{dN(E)}{dt}_2 = \frac{N_1^0 - N}{\tau_1} + \frac{N_2^0 - N}{\tau_2} = 0 \]

\[ N(E) = \frac{(1/\tau_1)}{(1/\tau_1) + (1/\tau_2)} N_1^0(E) + \frac{(1/\tau_2)}{(1/\tau_1) + (1/\tau_2)} N_2^0(E) \]

\[ \begin{cases} \quad N_1^0(E) \equiv D(E) f_1(E) \quad \gamma_1 = h/\tau_1 \\ \quad N_2^0(E) \equiv D(E) f_2(E) \quad \gamma_2 = h/\tau_2 \end{cases} \]
steady-state electron number, $N(E)$

$$N(E) = \frac{\gamma_1}{\gamma_1 + \gamma_2} D(E) f_1(E) + \frac{\gamma_2}{\gamma_1 + \gamma_2} D(E) f_2(E)$$

$$N(E) = D_1(E) f_1(E) + D_2(E) f_2(E)$$

\[
\begin{align*}
D_1(E) &= \frac{\gamma_1}{\gamma_1 + \gamma_2} D(E) & \text{DOS that can be filled by contact 1} \\
D_2(E) &= \frac{\gamma_2}{\gamma_1 + \gamma_2} D(E) & \text{DOS that can be filled by contact 2}
\end{align*}
\]
The steady-state electron number, $N$,

$$N = \int \left[ D_1(E)f_1(E) + D_2(E)f_2(E) \right] dE$$

Recall that in equilibrium, we use:

$$N_0 = \int D(E)f_0(E) dE$$

$D(E) \propto L$ (1D)  $D(E) \propto A$ (2D)  $D(E) \propto \Omega$ (3D)

$n_L$  $n_S$  $n$
steady-state current, $I$

$D(E-U)$

$E_{F1}$
$f_1(E)$

$E_{F2}$
$f_2(E)$

$F_1$  $F_2$

$I$

Contact 1 tries to fill up the device according to its Fermi level.

$F_1 + F_2 = 0$

$I = qF_1 = -qF_2$

Contact 2 tries to fill up the device according to its Fermi level.

Lundstrom ECE-656 F09
$F_1 = \left. \frac{dN(E)}{dt} \right|_1 = \frac{N_1^0(E) - N(E)}{\tau_1}$

$F_2 = \left. \frac{dN(E)}{dt} \right|_2 = \frac{N_2^0(E) - N}{\tau_2}$

$N(E) = \frac{\gamma_1}{\gamma_1 + \gamma_2} D(E) f_1(E) + \frac{\gamma_2}{\gamma_1 + \gamma_2} D(E) f_2(E)$

$N_1^0(E) \equiv D(E) f_1(E)$  \hspace{1cm} $N_2^0(E) \equiv D(E) f_2(E)$

$I(E) = +q \left. \frac{dN(E)}{dt} \right|_1 = -q \left. \frac{dN(E)}{dt} \right|_2$
results

\[ I(E) = \frac{q}{h} \left( \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} \right) D(E)(f_1 - f_2) \]

\[ \gamma_1 = \gamma_2 = \gamma \]

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

\[ N = \int N(E) dE = \int \left[ \frac{D(E)}{2}(f_1 + f_2) \right] dE \]
We will think of this “2” as representing the two degenerate spins.

When we compute the DOS, we usually include a factor of 2 for spin. \( D/2 \) is the DOS per spin.

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

\[
D(E)/2 = \text{density of states per spin}
\]
3) The device is described by some density-of-states.

5) For transistors, we use a gate to control the self-consistent potential, $U$.

1) Strong, inelastic scattering maintains equilibrium in the contacts.

2) Contacts are described by escape or transit times or by a ‘broadening’ energy.

4) Device may be ballistic, or there may be elastic scattering.
\( \gamma_1 = \gamma_2 = \gamma \)

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

\[
N = \int \frac{D(E)}{2} \left[ f_1(E) + f_2(E) \right] dE
\]

\[
\frac{D(E)}{2} : \text{ density-of-states per spin}
\]
1) A general model for low-field transport
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conducting channels

\[ I = \frac{2q}{\hbar} \int \gamma \pi \frac{D}{2} \left( f_1 - f_2 \right) dE \quad U = 0 \]

\[ \gamma(E) \pi D(E)/2 = ? \]

\[ \gamma(E) = \frac{\hbar}{\tau(E)} \]

is the ‘broadening’ and has units of energy.

\[ D(E) \]

has units of 1/energy.

\[ \gamma(E) \pi D(E)/2 = M(E) \]

is a number. We will show that \( M \) is the number of conducting channels at energy, \( E \).
Let's do an “experiment” to determine what $\gamma$ (or $\tau$) is.

$I(E) = \frac{2q}{h} \gamma(E) \pi \frac{D_{1D}(E)}{2} (f_1 - f_2)$

$N(E) = \frac{D_{1D}(E)}{2} \left[ f_1(E) + f_2(E) \right]$
the “experiment”

\[
I(E) = \frac{2q}{h} \gamma \pi \frac{D(E)}{2} (f_1 - f_2)
\]

\[
N(E) = \frac{D(E)}{2} [f_1(E) + f_2(E)]
\]

\[
\frac{qN}{I} = \frac{h (f_1 + f_2)}{\gamma (f_1 - f_2)}
\]

Apply \( V >> 0 \) to right contact, if \( f_2 << f_1 \) (injection from the source only), then:

\[
\frac{qN}{I} = \frac{\text{stored charge}}{\text{current}} = \frac{h}{\gamma} = \tau
\]
transit time

\[ \tau = \frac{\text{stored charge}}{\text{current}} \]

(ballistic transport)

\[ N = n_L L \]

\[ I(E) = q n_L (E) \nu_x (E) \]

\[ \tau = \frac{q n_L L}{q n_L \nu_x} = \frac{L}{\nu_x} \]

‘transit time’

\[ (\gamma \tau = \hbar) \]
modes in 1D

\[ I = \frac{2q}{h} \int M(E)(f_1 - f_2) dE \]

\[ M(E) = \gamma(E) \pi \frac{D(E)}{2} \]

\[ \gamma \pi \frac{D(E)}{2} = \frac{h}{(L/\nu_x)\pi} \frac{L}{\pi h \nu_x} = 1 \]
\[ M(E) \text{ in 1D} \]

\[ E = \varepsilon_i + \frac{\hbar^2 k_x^2}{2m^*_i} \]

\[ M(E) \text{ is the number of subbands at energy, } E. \]
1) A general model for low-field transport
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1) **Ballistic:**
Electrons travel without scattering from the injecting contact to the absorbing contact.

\[
\langle \nu \rangle = \nu(E) = \sqrt{2(E - \varepsilon_1)/m^*}
\]
diffusive transport

\[ \gamma = \frac{h}{\langle \tau \rangle} \quad \langle \tau \rangle = ? \]

Assume a nanowire that is much longer than the mean-free-path for backscattering, \( L \gg \lambda \),

then, injected carriers diffuse to the other contact. Fick’s Law of diffusion should apply.
recall: base transit time of a BJT

\[ I = qD_n \frac{\Delta n(0)}{W_B} \]

\[ \Delta n(W_B) \approx 0 \]

\[ \tau = \frac{W_B^2}{2 D_n} \]


\[ \gamma = \frac{h}{\tau} \]

\[ \tau = \frac{L}{\nu} \]

\[ \gamma_{ball} = \frac{h}{L/\nu} \]

\[ \nu = \sqrt{\frac{2(E - \varepsilon_1)}{m^*}} \]
transmission (diffusive)

\[ \gamma = \frac{h}{\langle \tau \rangle} \]

\[ \langle \tau \rangle = \frac{L^2}{2 D_n} \]

\[ \gamma_{\text{Diff}} = \frac{h}{\frac{L^2}{2 D_n}} \rightarrow \gamma_{\text{Diff}} = \frac{h}{\frac{L^2}{(\nu \lambda)}} = \frac{\lambda}{L} \left( \frac{h}{L/\nu} \right) \]

\[ D_n = \frac{\nu \lambda}{2} \]

\[ \gamma_{\text{Diff}} = T \times \gamma_{\text{Ball}} \]

\[ T = \frac{\lambda}{L} << 1 \]
transmission

\[ I = \frac{2q}{h} \int M(E)(f_1 - f_2) \, dE \quad \Rightarrow \quad I = \frac{2q}{h} \int TM(E)(f_1 - f_2) \, dE \]

1) **Diffusive:** \( L >> \lambda \quad T = \frac{\lambda}{L} < 1 \)

2) **Ballistic:** \( L << \lambda \quad T = 1 \)

3) **Quasi-ballistic:** \( L \approx \lambda \quad T < 1 \)

\[ T(E) = \frac{\lambda(E)}{\lambda(E) + L} \]

\( \lambda \) is the ‘mean-free-path for backscattering’

This expression can be derived with relatively few assumptions.
outline

1) A general model for low-field transport
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Landauer expression for current

\[
I = \frac{2q}{h} \int TM(E) (f_1 - f_2) dE
\]

For small bias, we can linearize \((f_1 - f_2)\) and the current becomes proportional to \(V\) (linear, near-equilibrium, low-field response).
linear response

\[ I = \frac{2q}{h} \int T(E)M(E)(f_1 - f_2) dE \]

\[ f_2 = f_1 + \frac{\partial f_1}{\partial E} \Delta E_F = f_1 + \frac{\partial f_1}{\partial E} (-qV) \]

\[ f_1 - f_2 = \frac{\partial f_1}{\partial E} (qV) \]

\[ \frac{\partial f_1}{\partial E_F} = - \frac{\partial f_1}{\partial E} \]

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

\[ f_1(E) \approx f_2(E) \approx f_0(E) \]
1) A general model for low-field transport
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This lecture has presented a lot of equations. Don’t try to memorize them; try to understand the results.

“Mathematics is the language of clear thinking.”

Richard W. Hamming in 
questions

1) A general model for low-field transport
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