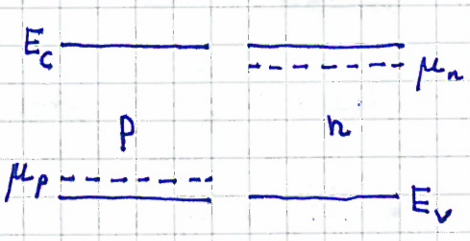
08.03.10

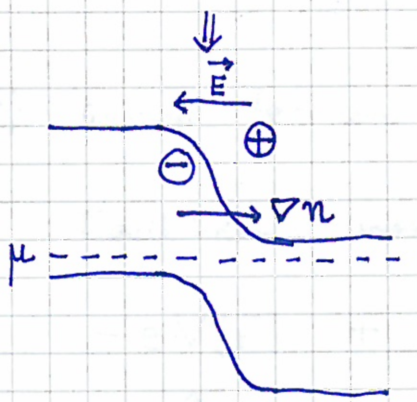
Drift vs diffusion: Einstein relations

We know that drift and diffusion are intimately related.

Ex: pn-junction



diffusion (+ recombination) near interface $\Rightarrow$ built-in field $\vec{E}$ $\Rightarrow$ drift



Equilibrium: $\vec{j} = 0$

Diffusion: $\vec{j}_D = -D \nabla n$ (defines D)

Drift: $\vec{j}_F = n \mu \vec{F}$ (defines μ)

Particle current densities $\vec{j}_D, \vec{j}_F$

D = diffusion constant $[m^2/s]$

μ = particle mobility $[s/kg]$

We have:

1) Classically: $D = k_B T \cdot \mu$

2) QM $(T=0)$: $D = \dfrac{1}{e^2 \cdot g(E_F)} \cdot \sigma$

} Einstein relations [A. Einstein, 1905-1911, Brownian motion]

Proofs:

1) $\vec{j} = 0 \Rightarrow -D \nabla n + n \mu \vec{F} = 0$

Equilibrium statistical mechanics: $n(T) = n_0 \, e^{-U/k_B T}$

$\vec{F} = -\nabla U$

$$\Rightarrow \nabla n = n_0\, e^{-U/k_BT} \cdot \left(\frac{-\nabla U}{k_BT}\right) = \frac{n}{k_BT} \cdot \vec{F}$$

$$\Rightarrow -D \cdot \frac{n}{k_BT} \vec{F} + n\mu \vec{F} = 0$$

$$\Rightarrow D = k_BT \cdot \mu$$

Note: $\vec{v}_d = \mu \vec{F}$ and $\vec{v}_d = -\mu_e \vec{E}$

$\vec{F} = q\vec{E} = -e\vec{E}$ $\Bigg\} \Rightarrow \mu_e = \mu \cdot e$

$$\Rightarrow D = (k_BT/e) \cdot \mu_e$$

2) assume fermions at $T = 0$

Equilibrium, with field $\vec{E}$ and density gradients present:

$$\underbrace{-eV(\vec{r})}_{\text{electrostatic potential } (\vec{E} = -\nabla V)} + \underbrace{E_F(\vec{r})}_{\text{Local chemical potential}} = \underbrace{\text{constant}}_{\text{global "electrochemical potential"}}$$

electrostatic potential ($\vec{E} = -\nabla V$)

Local chemical potential (measured relative to conduction band edge, accounts for $n(\vec{r})$)

global "electrochemical potential"

DOS pr unit area (or volume if 3D): $\rho(E) = D(E)/A$

$$n = \int_{-\infty}^{\infty} dE\, \rho(E)\, f(E) \overset{T=0}{=} \int_{-\infty}^{E_F} dE\, \rho(E)$$

(since $f(E) = \Theta(E_F - E)$ (step function!) at $T=0$)

$$\Rightarrow \frac{\partial n}{\partial E_F} = \frac{\partial}{\partial E_F}\left\{\int_{-\infty}^{E_F} dE\, \rho(E)\right\} = \rho(E_F)$$

$$\Rightarrow \nabla E_F = \frac{\partial E_F}{\partial n} \nabla n = \frac{1}{\rho(E_F)} \cdot \nabla n$$

$$\Rightarrow e \cdot \vec{E} + \frac{\nabla n}{\rho(E_F)} = 0$$

Equil: $\vec{j} = 0 \Rightarrow \underbrace{-D\,\nabla n}_{\text{diffusion}} \underbrace{- n\mu_e \vec{E}}_{\text{drift}} = 0$

(particle currents)

$$\nabla n = -e\,\rho(E_F)\,\vec{E}$$

$$\Rightarrow \quad + e\rho(E_F) D \cdot \vec{E} - n\mu_e \vec{E} = 0$$

$$\Rightarrow \quad D = \frac{n\mu_e}{e\,\rho(E_F)}$$

Electric current density: $\vec{j}_e = -e \cdot \vec{j}_F = -e \cdot n\,\vec{v}_d$

$$\left.\begin{aligned} &= -e \cdot n \cdot (-\mu_e \vec{E}) \\ \text{and } \vec{j}_e &= \sigma \vec{E} \quad (\text{Ohm's law}) \end{aligned}\right\} \Rightarrow \sigma = e n \mu_e$$

$$\Rightarrow \quad D = \frac{1}{e^2 \rho(E_F)} \cdot \sigma$$

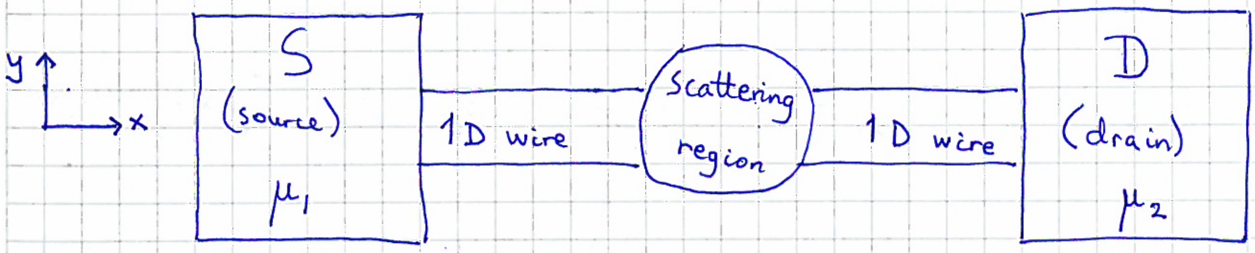
Remarks:

- D can be measured by measuring μ_e or σ (and vice versa)
- μ_e, σ, D are equilibrium properties of the system
  In general: Linear transport coefficients are equilibrium properties
- electron transport can be viewed as drift or diffusion:
  Drift: $\vec{j} = -n\mu_e \vec{E}$ ("all electrons contribute")
  Diffusion: $\vec{j} = -D\,\rho(E_F)\,\nabla E_F$ ("only electrons at Fermi Level contribute")

Conductance in terms of transmission

Landauer formula

Typical configuration ('patterned' in the 2DEG):



S, D: Large regions in the 2DEG ("contacts", "reservoirs") at separate equilibrium; chemical potentials μ_1 and μ_2. [We assume a common (low!) temp. T]

1D wires ("channels"):

- Assumed to be perfectly ballistic (i.e. no scattering)
- Electrostatically defined by split gate electrodes at potential V_G (see pp 47-48); more negative V_G $\Rightarrow$ more narrow channel.

Confining potential: $U(y)$ (assumed to be independent of x)

Possible models for $U(y)$: Box; Harmonic etc.

$\Rightarrow$ We have a separable QM problem:

$$H = -\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial x^2} + \left(-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial y^2} + U(y)\right) = \mathcal{H}_x + \mathcal{H}_y$$

$$\Psi(x,y) = \phi(x)\cdot\chi(y)$$

$$E = E^t + E^l \qquad (t = \text{transv.};\ l = \text{longit.})$$

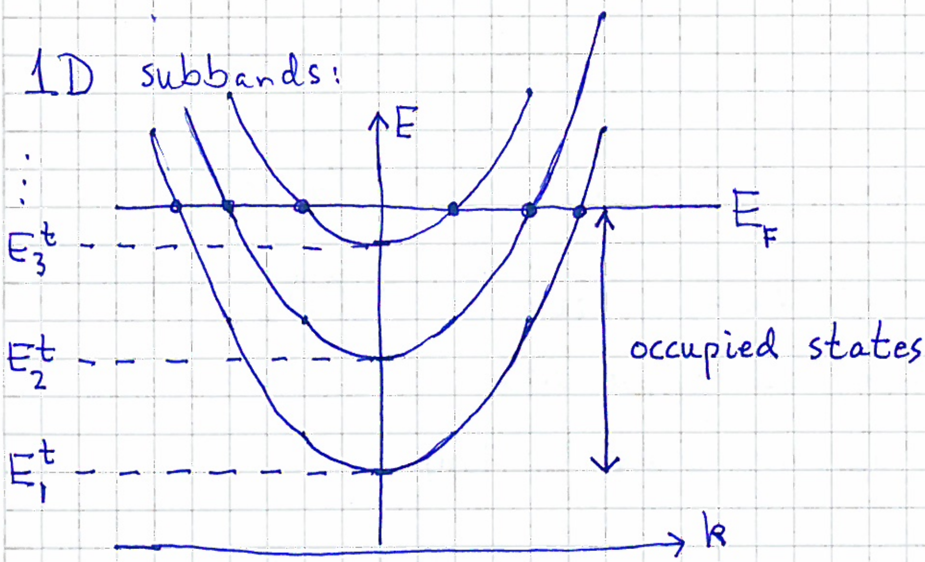
$$\mathcal{H}_x \, \phi_k(x) = E_k^l \, \phi_k(x)$$

$$\phi_k(x) = \frac{1}{\sqrt{L}} e^{ikx} \, , \qquad E_k^l = \frac{\hbar^2 k^2}{2m^*}$$

$$\mathcal{H}_y \, \chi_n(y) = E_n^t \, \chi_n(y) \qquad (n = 1, 2, \ldots)$$

$$\Rightarrow \psi_{nk}(x,y) = \frac{1}{\sqrt{L}} e^{ikx} \chi_n(y) \; ; \; E_{nk} = E_n^t + \frac{\hbar^2 k^2}{2m^*}$$

1D subbands:



States with ($E_1^t <$) $E < E_F$ will be occupied by electrons ($g_s = 2$).
States at (or "near") E_F contribute to net current when applied voltage between S and D is small.
In figure above: 3 states at $E = E_F$ with $v_x > 0$
——— " ——— $v_x < 0$

1D DOS pr unit length (see p10 and Exercise 1) in subband n:

PBC $\Rightarrow \Delta k = \frac{2\pi}{L} \rightarrow D(k) = \frac{2}{2\pi/L} \Rightarrow g(k) = \frac{D(k)}{L} = \frac{1}{\pi}$

$\Rightarrow$ # states with wavenr $< k$, pr unit length : $n(k) = g(k) \cdot 2k = 2k/\pi$

$\Rightarrow$ ——— " ——— energy $< E$, ——— " ——— : $n(E) = \frac{2}{\pi}\sqrt{2m^* E/\hbar^2}$

$\Rightarrow$ DOS pr unit length : $g(E) = dn/dE = (1/\pi\hbar) \cdot \sqrt{2m^*/E} = 4/h v(E)$

Group velocity : $v(E) = \hbar^{-1} \, dE/dk = \sqrt{2E/m^*}$

Here, E is relative to bottom of 1D subband

Note: $g(E)$ and $v(E)$ indep. of subband n

Electric current from S to D ($1 \to 2$), subband n:

$$I_n^+ = -e \int_{E_n^t}^{\mu_1} dE \, \rho_n^+(E) \cdot v_n(E) \cdot T_n(E)$$

Remarks:

- $\rho_n^+(E) = \frac{1}{2}\rho_n(E) = \frac{1}{2}\rho(E)$ (indep. of n)

  since $\rho(E) = \rho^+(E) + \rho^-(E)$ and $\rho^+(E) = \rho^-(E)$

  (Here ρ^+ is for states with $k>0$, i.e., $v_x > 0$ and

  ρ^- —— " —— $k<0$, i.e., $v_x < 0$)

  $$\Rightarrow \rho_n^+(E) = \frac{2}{h \cdot v(E)}$$

- $v_n(E) = v(E)$ (also indep. of n)

- $T_n(E)$ = transmission probability for electron in subband n with energy E (relative to E_n^t), i.e., prob. of getting through scattering region

  [If <u>no</u> scatterers in 1D channel: $T_n(E) = 1$]

- We have here assumed $T \approx 0$, so $f(E) \approx \Theta(\mu_1 - E)$, i.e., step function

- The expression for I_n^+ is "natural, logical choice"

- I_n^+ is contribution to <u>total</u> I_n originating in right-going electrons in region S, with energy "appropriate" inside 1D channel, i.e., with $\rho_n^+(E) > 0$

- <u>Check</u> that the <u>unit</u> of the right hand side is <u>C/s</u>!

Similarly: El. current from D to S, subband n:

$$I_n^- = -(-e) \int_{E_n^t}^{\mu_2} dE \, \rho_n^-(E) \, v_n(E) \, T_n(E)$$

pos. I in pos. x direction!

Since $g_n^+(E)\cdot v_n(E) = \frac{2}{h\cdot v_n(E)}\cdot v_n(E) = \frac{2}{h}$,

we have

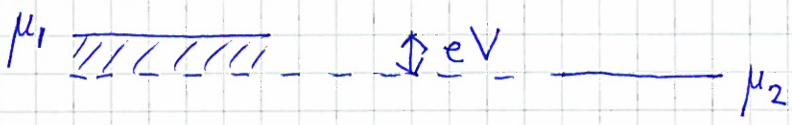
$$I_n^+ = -\frac{2e}{h}\int_{E_n^t}^{\mu_1} dE\, T_n(E) \;; \qquad I_n^- = +\frac{2e}{h}\int_{E_n^t}^{\mu_2} dE\, T_n(E)$$

Net current:

$$I_n = I_n^+ + I_n^- = -\frac{2e}{h}\int_{\mu_2}^{\mu_1} dE\, T_n(E)$$

Linear regime: $\mu_1 \approx \mu_2 \approx E_F$

$$\Rightarrow I_n \approx -\frac{2e}{h}\cdot T_n(E_F)\cdot(\mu_1-\mu_2)$$



Voltage between S and D:

$$V = V_1 - V_2 = \frac{\mu_1-\mu_2}{(-e)}$$

$$\Rightarrow I_n = \frac{2e^2}{h}\cdot T_n(E_F)\cdot V$$

$\Rightarrow$ Conductance G_n due to subband n: $\quad G_n = \frac{I_n}{V} = \frac{2e^2}{h} T_n(E_F)$

$\Rightarrow$ Total conductance:

$$\boxed{G = \sum_n G_n = \frac{2e^2}{h}\sum_n T_n(E_F)}$$

Landauer formula (here: $E_n^t < E_F$)

Quantum of resistance: $\boxed{\frac{h}{e^2} = 25.8\ \mathrm{k}\Omega}$

Ballistic wire $\Rightarrow T_1 = T_2 = \ldots = T_N = 1 \quad (E_N^t < E_F)$

$$\Rightarrow G = \frac{2e^2}{h}\cdot N$$