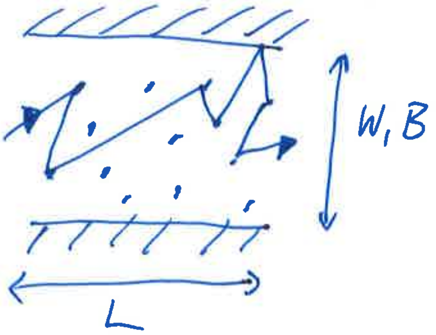
Quantum transport
Part 3: Scattering approach to quantum transport

Motivation: Boltzmann equation for diffusive transport requires the distribution function f and the conductivity σ to be well-defined at any given point in real- and k-space; i.e. $f = f(\vec{r}, \vec{p}, E)$ and $\sigma = \sigma(\vec{r})$

Picture:



$L, W, B \gg \ell_{el}, \ell_{inel}, \dots$

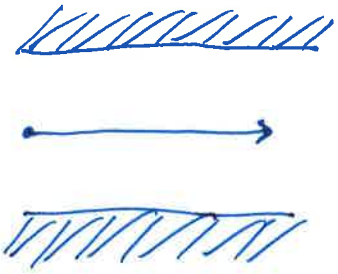
$\Rightarrow$ phase, momentum, energy, ... randomized and in (local) equilibrium

$\Rightarrow$ „large samples"

But: what happens when we have a very clean and/or very small system? (L or W or $B \approx \ell_{el}, \dots$) More than 2 contacts?

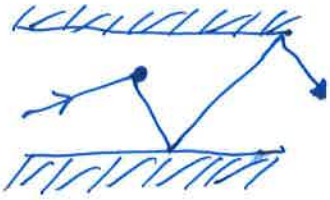
Pictures:

i)



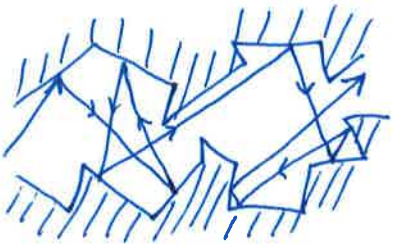
ballistic transport, „no scattering":
↳ $\sigma(\vec{r}) \to \infty$? Resistance of device $R \to 0$?

ii)



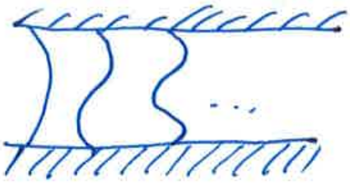
one or few scatterers:
↳ $\sigma(\vec{r}) = 0$ for most $\vec{r}$? And then?

iii)



cavities / billiards:
↳ $\sigma(\vec{r}) = 0$ for all accessible $\vec{r}$, „resistance" given by geometry...

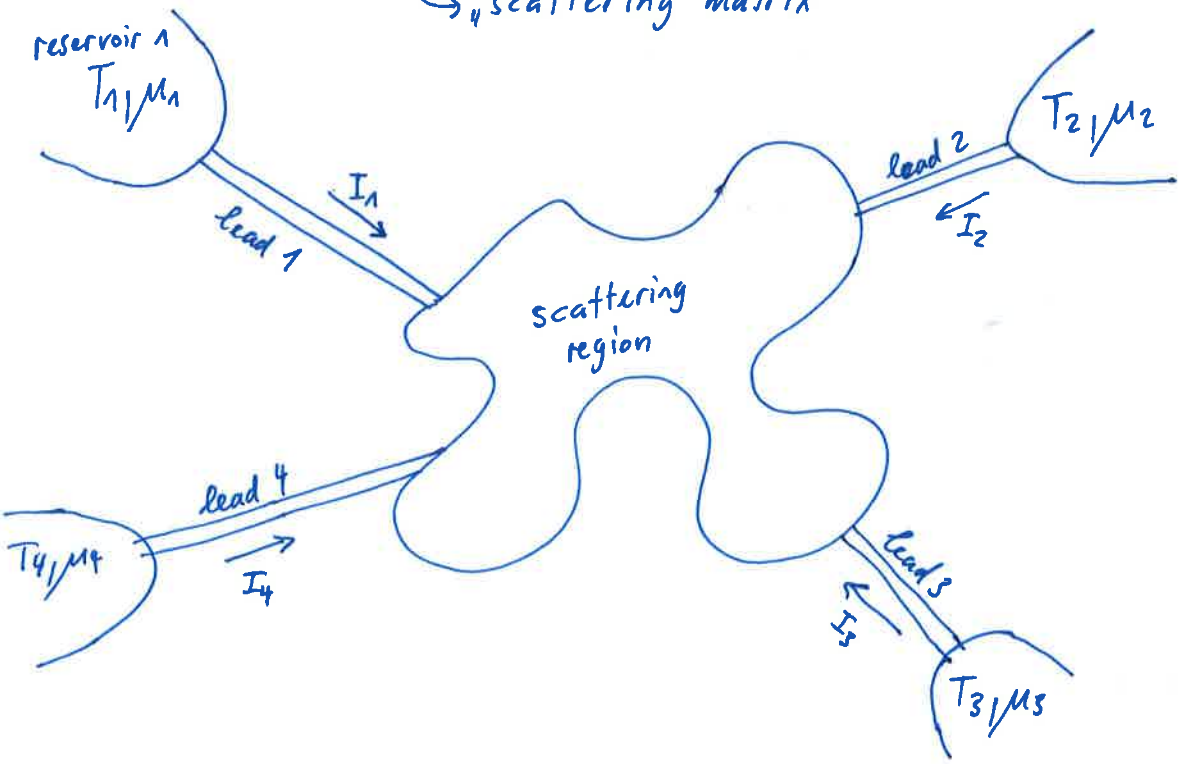
iv)



quantum mechanics?
↳ wave functions?
interference?
→ what is conductance/resistance?!

Scattering approach: divide system into 3 sub-systems

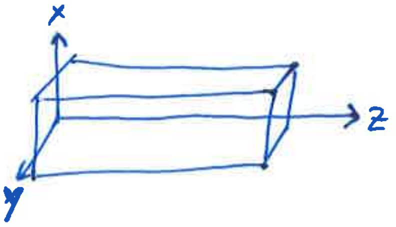
- reservoirs ≡ contacts → equilibrium; $\mu, T, f, \ldots$
- leads (≡ terminals) → well-defined (quantum) states
- scattering region
  - ↳ connects different states in different leads
  - ↳ „scattering matrix"



Reservoirs:
- thermodynamic equilibrium (here: Fermi distribution)
- electrochemical potential μ_i and temperature T_i
- „large": μ_i and T_i do not change with number of (quasi-) particles.
- „fast" (energy) relaxation by inelastic scattering
  - ↳ equilibrium
- completely uncorrelated particles (loss of any information, e.g. phase)

Leads:
- some well-defined, well-understood (quantum-) system
  - ↳ eigenmodes
- semi-infinite
- simplest version: wave-guide, hard-wall confinement potential

quantum states in leads and subbands:



particle-in-a-box (see „background_knowledge")

$$-\frac{\hbar^2}{2m^*}\vec{\nabla}^2\Psi + U(x,y,z)\Psi = E\Psi \Rightarrow \text{eigenstates}$$

assumption U independent of z (no confinement, no back-scattering)

⇒ separation into transverse (x,y) and longitudinal parts:

$$\Psi(x,y,z) = X(x,y)\cdot \underset{\substack{\uparrow\\ \text{plane wave along } z}}{e^{ik_z\cdot z}}$$

$$\Rightarrow -\frac{\hbar^2}{2m^*}(\partial_x^2+\partial_y^2)\cancel{X}_n + U(x,y)X_n = \underset{\substack{\uparrow\\ \text{„subband" energy}}}{\mathcal{E}_n}\cdot X_n \quad \Rightarrow \quad k_z^{(n)} = \overset{\substack{\text{incoming and outgoing}\\ \text{plane wave in } z\\ \downarrow}}{\pm}\sqrt{\frac{2m^*}{\hbar^2}(E-\mathcal{E}_n)}$$

cases $E<\mathcal{E}_n$: $k_z^{(n)}$ imaginary → evanescent wave → no transport!

$E>\mathcal{E}_n$: $k_z^{(n)}\in\mathbb{R}$ → group velocity $V_n^{(n)} = \frac{1}{\hbar}\frac{\partial E}{\partial k_z} = \frac{1}{\hbar}\frac{\partial}{\partial k_z}\left(\frac{\hbar^2 k_z^2}{2m^*}\right) = \frac{\hbar k_z^{(n)}}{m^*}$

(intuitive: $v = p/m = \hbar k/m$)

Transverse modes: depend on geometry, confinement potential, ...

↳ have usually no strong affects on physics.

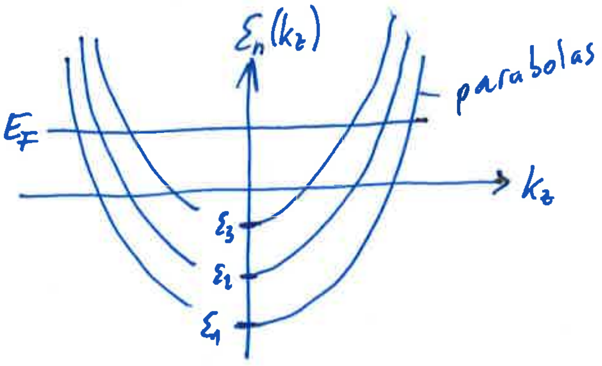
hard-wall potential: $X(x=0,y)=0$; $X(x=L_x,y)=0$; $X(x,y=0)=0$; $X(x,y=L_y)=0$

$$\Rightarrow X_n = A_n\cdot\sin(k_{nx}\cdot x)\cdot\sin(k_{ny}\cdot y) \quad ; \quad k_{nx} = n_x\cdot\frac{\pi}{L_x} \; ; \; k_{ny} = n_y\cdot\frac{\pi}{L_y}$$

$$\mathcal{E}_n = \frac{\hbar^2}{2m^*}\left(k_{nx}^2 + k_{ny}^2\right)$$

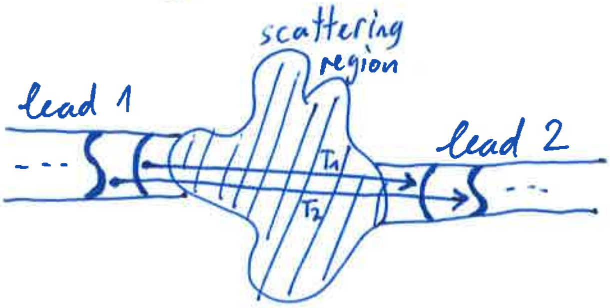
normalization: one particle per length ⇒ $A_n = \sqrt{v_n}$

Subbands: $$\mathcal{E}_n(k_z^{(n)}) = \underset{\substack{\uparrow\\ \text{subband}\\ \text{energy}}}{\mathcal{E}_n} + \frac{\hbar^2 k_z^{(n)2}}{2m^*}$$



occupied modes (T=0): $\mathcal{E}_n < E_F \Rightarrow M(E_F) = \sum_n \overset{\substack{\text{step function}\\ \downarrow}}{\Theta}(E_F-\mathcal{E}_n)$

Transmission: the scattering region „connects" modes in different terminals (leads)



transmission of mode n

$$\overline{T}(E) = \sum_n \overset{\downarrow}{T_n} \cdot \theta(E - \varepsilon_n)$$ (only elastic processes)

$$\overline{R}(E) = M(E) - \overline{T}(E)$$

total reflection — number of channels — total transmission of lead

Some math: in principle we should sum over all k_z, n, spin

↳ infinitely long leads: length L + periodic boundary conditions:

$$\psi_z(z) = \psi_z(z+L)$$

$$\psi_z = e^{ik_z z}, \quad k_z = n_z \cdot \frac{2\pi}{L}, \quad \text{spacing } \Delta k = \frac{2\pi}{L}$$

$$\Rightarrow \text{any sum } \underline{\sum_{k_z, \text{spin}} g(k_z)} \xrightarrow{} 2 \cdot \frac{1}{\Delta k} \int g(k_z)\, dk_z = \underline{\frac{L}{\pi} \int g(k_z)\, dk_z}$$

↑ if $g(k)$ is „smooth" on Δk

current carried by one transverse mode from reservoir

quasi-classical: carrier density $\rho = \frac{1}{L}$ (normalization; note that the wave functions are completely delocalized along z!)

$$\Rightarrow I_m^{(in)} = -e \sum_{k,s} \rho_m \cdot v_m(k) \cdot f(E(k))$$

lead — given by contact

integral

$$= -\frac{eL}{L\pi} \int v_k \cdot f(E_k)\, dk$$

from ρ

$$= -\frac{e}{\pi} \int \underbrace{\frac{1}{\hbar} \frac{\partial E_k}{\partial k}}_{v_k} \cdot f(E_k)\, dk = -\frac{e}{\pi\hbar} \int \frac{\partial E}{\partial k} \cdot f(E) \cdot \underbrace{N(E)\, dE}_{dk} = -\frac{2e}{h} \int_{\varepsilon_m}^{\infty} \frac{dE}{dk} \cdot \overbrace{\frac{1}{\partial E/dk}}^{N(E)} \cdot f(E)\, dE$$

density of states $N(E) = \frac{dk}{dE}$ — $h = 2\pi\hbar$ — $N(E) = 0$ for $E < \varepsilon_m$

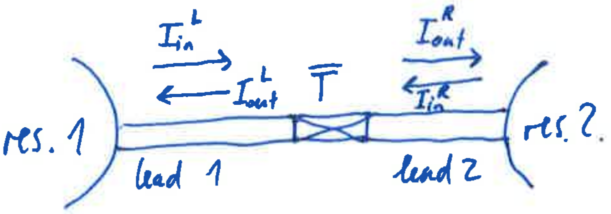
$$= -\frac{2e}{\hbar} \int_{\varepsilon_m}^{\infty} f(E)\, dE$$

counts modes accessible in lead

All modes in lead: $\underline{\underline{I^{(in)} = -\frac{2e}{h} \int_{-\infty}^{\infty} M(E) \cdot f(E)\, dE}}$

But: total current contains also current scattered <u>into</u> the lead

simplest example: <u>quantum wire between two reservoirs</u>:



assume: $\bar{T} = \bar{T}_R = \bar{T}_L$ (symmetric) $\rightarrow$ $\bar{R} = \bar{R}_L = \bar{R}_R = M - \bar{T}$

$$\Rightarrow I_{out}^L = -\frac{2e}{h}\int_{-\infty}^{\infty}\Big[\underset{\substack{\uparrow\\ \text{from R}}}{\bar{T}(E)}\cdot \underset{\substack{\uparrow\\ \text{filled}\\ \text{from }\mu_R}}{f_R(E)} + \underset{\substack{\uparrow\\ \text{from L}\\ \hookrightarrow\text{backscattered}}}{\bar{R}(E)}\cdot \underset{\substack{\uparrow\\ \text{filled from }\mu_L}}{f_L(E)}\Big]dE$$

$$\Rightarrow \text{Total current: } I = I_{in}^L - I_{out}^L = -\frac{2e}{h}\int_{-\infty}^{\infty}\Big[\underbrace{M(E) f_L(E)}_{I_{in}^L} - \bar{T}(E) f_R(E) - \overset{M-\bar{T}}{\widetilde{\bar{R}(E)}} f_L(E)\Big]dE$$

$$= -\frac{2e}{h}\int_{-\infty}^{\infty}\bar{T}(E)\big[f_L(E) - f_R(E)\big]dE$$

$$\underset{\substack{\uparrow\\ \text{for } T\equiv 0}}{=} -\frac{2e}{h}\int_{\mu_R}^{\mu_L}\bar{T}(E)\,dE$$

- net current determined by „transport window" between μ_R and μ_L
- For $\bar{T}(E) \equiv \bar{T}$ (independent of E) between μ_R and μ_L and with $\mu_L = \mu_R - eV_{sd}$ (applied bias):

$$I = -\frac{2e}{h}\int_{\mu_R}^{\mu_R - eV_{sd}}\bar{T}(E)\,dE = -\frac{2e}{h}\bar{T}\int_{\mu_R}^{\mu_R - eV_{sd}} dE = \frac{2e^2}{h}\cdot\bar{T}\cdot V_{sd}$$

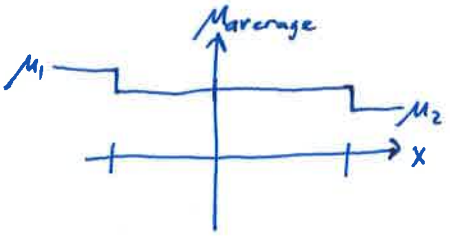
$\Rightarrow$ „Landauer Formula" for conductance: $\underline{\underline{G = \frac{I}{V_{sd}} = \frac{2e^2}{h}\cdot\bar{T}}}$

↳ „conductance from transmission"!

- Ballistic wire $(T_n \equiv 1) \Rightarrow T = M$
  ↳ each mode contributes $G_0 = \frac{2e^2}{h} \equiv \frac{1}{R_K}$ to the conductance
  $\underline{R_K \cong 12.9\,k\Omega}$ (von Klitzing constant)

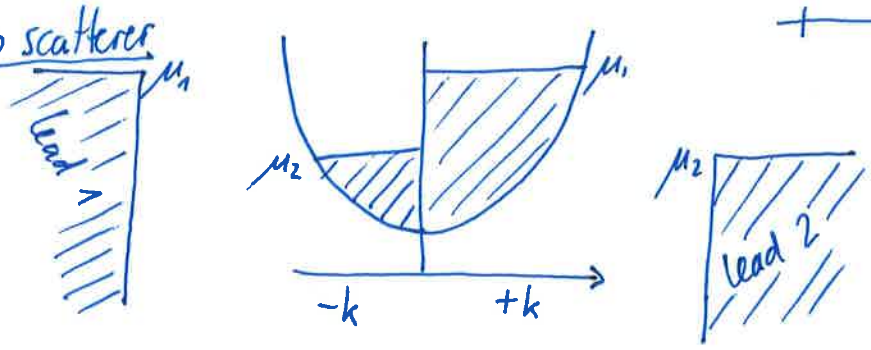
  ↳ independent of wire length!

So: „where *is* the resistance??"



- voltage drop; no scatterer

for a ballistic wire:



strength of scattering approach: e.g. Landauer Formula
↳ only distribution functions of leads (↔ contacts) enter, the distributions of particles moving *into* contacts are not relevant!

↳ the wave functions in the contacts are complicated, but *not* relevant!

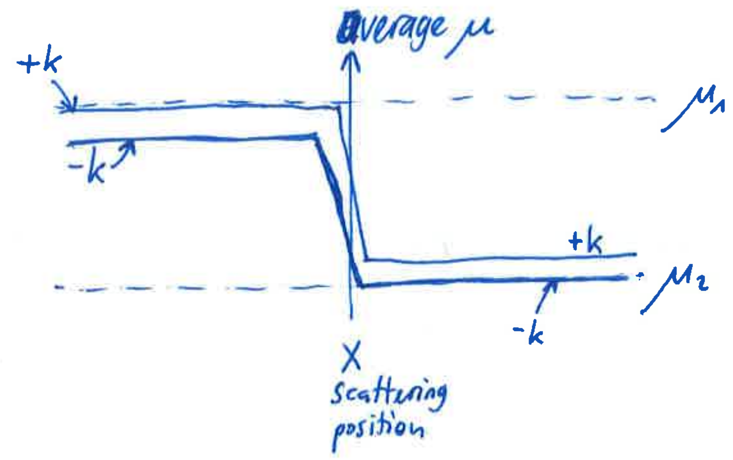
↳ require „reflection-less" contacts: no backscattering from contact into lead.

- Ohm's law → exercise class.

- "Resistance": no scatterer → $G_c = \frac{2e^2}{h}$ (single mode)
  1 scatterer → $G_s = \frac{2e^2}{h} T$

  if we choose $G_s = \frac{2e^2}{h} \cdot \frac{T}{1-T} \Rightarrow G^{-1} = G_c^{-1} + G_s^{-1}$ (see exercises)
  ↳ G_c is a „contact resistance" that applies to all modes.

Voltage drop; with a scatterer:



+k-states:

- left of scatterer: $\mu^L_{+k} = \mu_1$
  (filled only by contact 1)
- right of scatterer: $\mu^R_{+k} = \mu_2 + T(\mu_1 - \mu_2)$
  ↑ above μ_2: filled with probability T

-k-states:

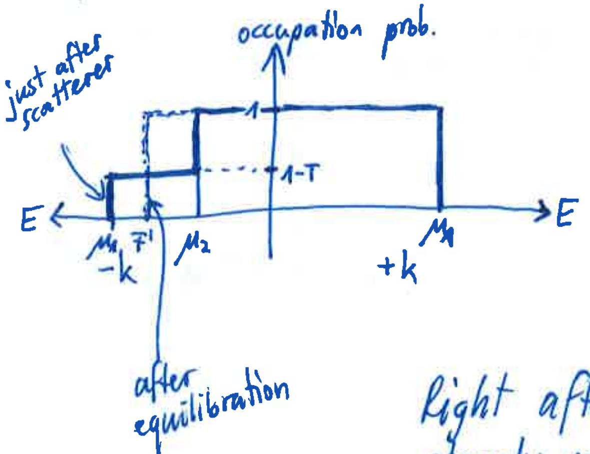
- right of scatterer: $\mu^R_{-k} = \mu_2$
  (filled by contact 2 only)
- left of scatterer: $\mu^L_{-k} = \mu_2 + \underbrace{(1-T)}(\mu_1 - \mu_2)$
  prob. for particles with μ_1 to be backscattered into a -k-state

⇒ electrochemical potential μ drops „sharply" over scatterer
↳ interaction volume

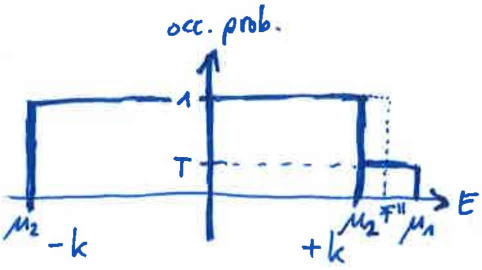
Joule heating / energy dissipation?

energy distribution on the

left of the scatterer:



right of the scatterer:



Right after the scatterer the electrons are in a strongly non-equilibrium situation⊛ (the transmitted electrons from the left can lower the energy on the right side and the back-scattered electrons can lower their energy because the are now in -k-states).

⊛ „hot electrons"

„Far" away from the scatterer a new equilibrium is established by inelastic scattering (elchem. potentials F' and F'': particle conservation → $F' = \mu_2 + (1-T)(\mu_1 - \mu_2)$)
↳ The heat is dissipated on the length l_{in}, the inelastic scattering length, on which the electron distribution relaxes to a Fermi-distribution.

Electrostatic potential at a scatterer?

from above: electrochemical potential μ drops sharply at scatterer (Δz)

But: electrical potential cannot follow as sharply:

electric field $|\vec{E}| \approx \Delta\mu_{el}/\Delta x$; if $\Delta\mu_{el} \approx \Delta\mu_{elch}$ $\Rightarrow$ very large ($\to\infty$) $|\vec{E}|$

↳ electrons are attracted to scatterer to screen the electric field

characteristic length: screening length; depends on dimensions, ...

eg. 2DEG: $\ell_{scr} \approx \sqrt{\frac{\varepsilon d}{e^2 N}}$ ← "thickness" of 2DEG

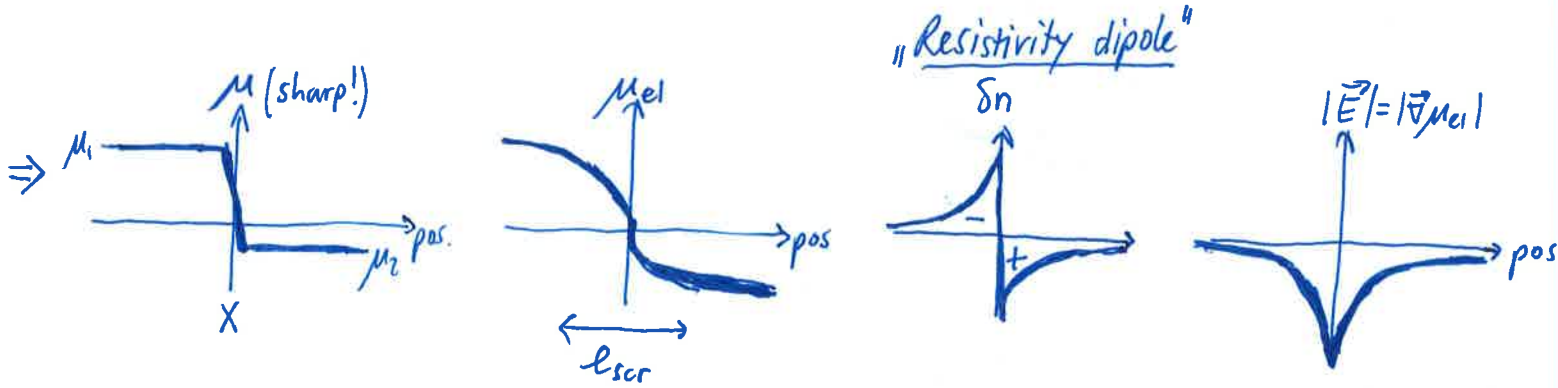
dielectric constant

density of states

eg. GaAs 2DEG: $\ell_{scr} \approx 5\,nm$

metals : $\ell_{scr} \sim$ Å

(due to large density of states)

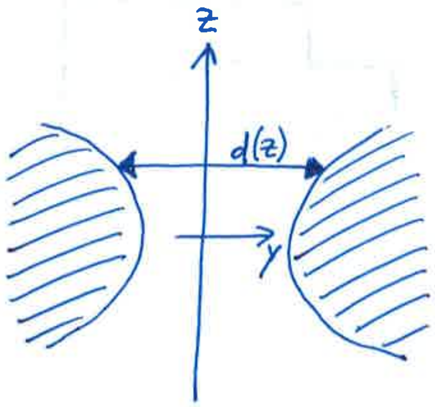


$\delta n = N \cdot \mu_{ch}$ (variation in electron density)

$\mu_{ch} = \mu - \mu_{el}$ (chemical potential)

Example of how to connect modes of two terminals: (later: scattering matrix)

Quantum point contact (QPC): (see also exercises)



- „split-gate" induced constriction in 2DEG
- solve Schrödinger equation

$$-\frac{\hbar^2}{2m^*}(\partial_y^2+\partial_z^2)\Psi(y,z) + U(y,z)\Psi(y,z) = E\Psi(y,z)$$

↑ induced confinement potential

- if $U(y,z)$ varies „slowly" with z (i.e. $U \approx U(y)$, not z)

↳ Ansatz: $\Psi(y,z) = \sum_n \chi_{n,z}(y) \cdot \phi_{n,E}(z)$

transverse modes; as a parameter

- assumption: hard-wall confinement at $y = \pm d(z)/2$

↳ $\chi_{n,z}(y) = \sin\left(n\pi \cdot \frac{y - \frac{d(z)}{2}}{d(z)}\right)$ and $\varepsilon_{n,z} = \frac{\hbar^2}{2m^*}\left(\frac{n\pi}{d(z)}\right)^2$ („subband" energies)

- Some uninteresting steps: insert $\chi_{n,z}$ into Schrödinger equation, multiply by $\chi_{m,z}$ and integrate over y

↳ $$\left(-\frac{\hbar^2}{2m^*}\partial_z^2 + \varepsilon_{n,z} - E\right)\phi_{n,E}(z) = \sum_m \underset{\substack{\uparrow \\ \frac{\hbar^2}{2m^*}\int dy\, \chi_{m,z}(y)\cdot\left[2\cdot\partial_z\chi_{n,z}\,\partial_z + \partial_z^2\chi_{n,z}\right]}}{\Lambda_{nm}}\phi_{n,E}(z)$$

- Λ_{nm} contains $\partial_z\chi_{n,z}$. If these changes are „small", we obtain plane waves as a solution for $\phi_{n,E}$. This is called the „adiabatic approximation".

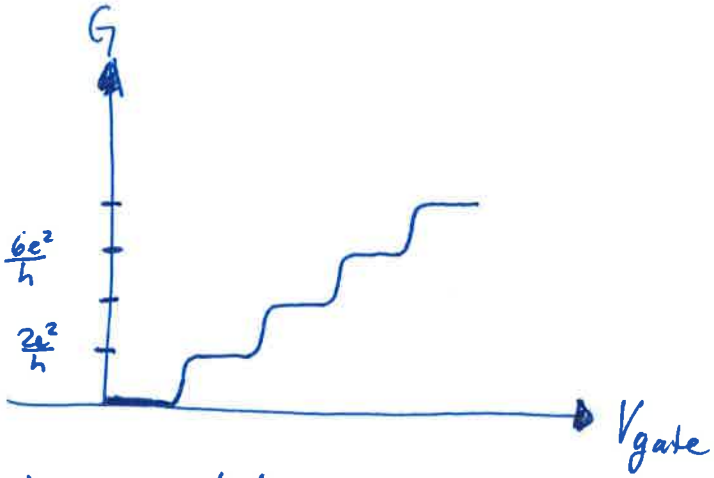
- „small": on scale of a Fermi-wave length; $\lambda_F \cdot \partial_z\chi_{n,z} \ll 1$

- propagating plane waves (i.e. not evanescent) for $\varepsilon_{n,z} - E < 0$ for all z

  ↳ transmission $T = 1$, otherwise $T = 0$ (back-scattering) ⇒ steps in G of $\frac{2e^2}{h}$

- adiabatic approximation breaks down for $\varepsilon_{n,z} \approx E$ ⇒ new mode starts to be transmitted

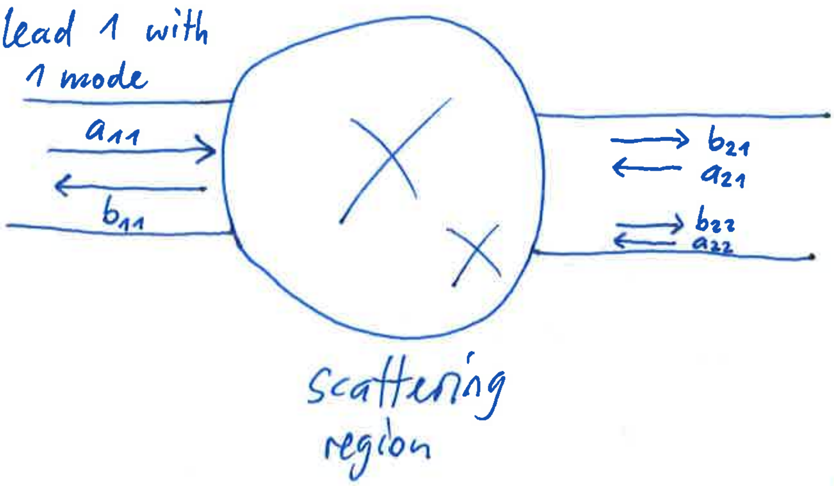
  ↳ needs to be modelled in detail, e.g.
    - hard-wall confinement with given curvature: Glazman et al., JETP Lett. 48, 238 (1988)
    - Taylor expansion along y and z ⇒ saddle point potential
      ↳ harmonic confinement: Büttiker, Phys. Rev. B 41, 7906 (1990)



Experiment:
van Wees et al.,
Phys. Rev. Lett. 60,
848 (1988)
(see exercises)

- Each mode is connected to the same mode on the other side of the QPC and is mixed with other modes only if $\Lambda_{nm} \neq 0$ (e.g. sharp opening, new mode,...)

Idea of the <u>scattering matrix</u>; two contacts:



a: amplitude of in-going wave

b: amplitude of out-going wave

$$\boxed{a_{\underset{\text{lead}}{i}\underset{\text{mode}}{j}}}$$

scattering matrix: „connects" all out-going transverse modes with all in-coming modes in all leads

(contrast: „transfer matrix": connects all in- and out-going modes of one lead to the in- and out-going modes in another lead)

e.g.:
(above)

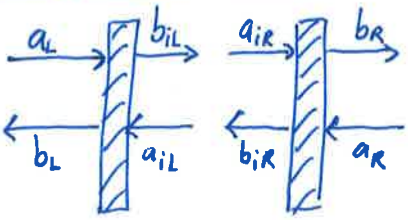
$$\begin{array}{l} \text{lead 1}\{ \\ \text{lead 2}\{ \end{array} \begin{pmatrix} b_{11} \\ b_{21} \\ b_{22} \end{pmatrix} = \overbrace{\begin{pmatrix} S^{11}_{11} & S^{12}_{11} & S^{12}_{12} \\ S^{21}_{11} & S^{22}_{11} & S^{22}_{12} \\ S^{21}_{21} & S^{22}_{21} & S^{22}_{22} \end{pmatrix}}^{S} \begin{pmatrix} a_{11} \\ a_{21} \\ a_{22} \end{pmatrix}$$

elements: $$S^{\alpha\overset{\text{in-coming}}{\beta}\leftarrow\text{leads}}_{\underset{\text{out-going}}{n}m\leftarrow\text{modes}}$$

dimension of scattering matrix S: $$\Big(\sum_{n=1}^{\overset{\text{number of leads}}{\downarrow}N}\overset{\text{modes of lead } n}{\downarrow}M_n\Big)\times\Big(\sum_{n=1}^{N}M_n\Big)$$

- Combine scattering matrices, 2-terminals, 1 mode in each lead

two barriers



individual scattering matrices: $\begin{pmatrix} b_L \\ b_{iL} \end{pmatrix} = \underbrace{\begin{pmatrix} r_L & \tilde{t}_L \\ t_L & \tilde{r}_L \end{pmatrix}}_{S_L} \begin{pmatrix} a_L \\ a_{iL} \end{pmatrix}$ („~": from the right „i": inner)

$$\begin{pmatrix} b_{iR} \\ b_R \end{pmatrix} = \underbrace{\begin{pmatrix} r_R & \tilde{t}_R \\ t_R & \tilde{r}_R \end{pmatrix}}_{S_R} \begin{pmatrix} a_{iR} \\ a_R \end{pmatrix}$$

We search for S such that $\begin{pmatrix} b_L \\ b_R \end{pmatrix} = S \cdot \begin{pmatrix} a_L \\ a_R \end{pmatrix}$, i.e. we want to eliminate all internal („i") amplitudes.

We have 6 unknowns (4 internal amplitudes + b_R and b_L) and first set $a_{iR} = b_{iL}$ and $a_{iL} = b_{iR}$ ⇒ 4 unknowns. We can use 2 of the 4 above equations to eliminate also b_{iL} and b_{iR} ⇒ two equations with b_L, b_R, a_L, a_R.

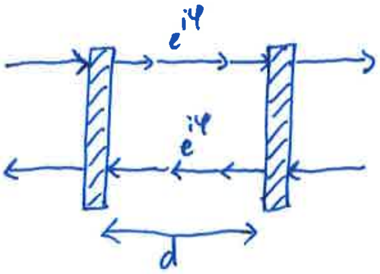
The result is $S = \begin{pmatrix} r & \tilde{t} \\ t & \tilde{r} \end{pmatrix}$ with $t = \dfrac{\tilde{t}_R t_L}{1 - \tilde{r}_L \tilde{r}_R}$; $r = r_L + \dfrac{\tilde{t}_L \tilde{r}_R \tilde{t}_L}{1 - \tilde{r}_R \tilde{r}_L}$

$$\tilde{t} = \frac{\tilde{t}_L t_R}{1 - \tilde{r}_R \tilde{r}_L} \; ; \; \tilde{r} = r_R + \frac{\tilde{t}_R \tilde{r}_L t_R}{1 - \tilde{r}_L \tilde{r}_R}$$

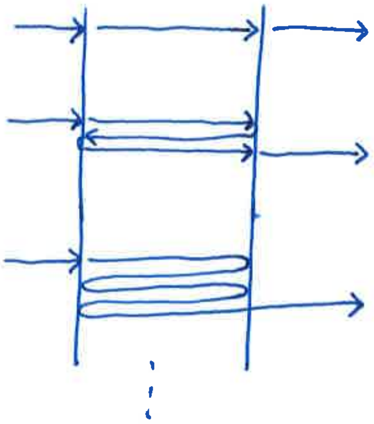
This result can be obtained in a more intuitive way using Feynman paths, where we add all possible ways that contribute to the out-going probability amplitude.

This method is demonstrated next for „resonant tunneling", which is almost identical to the described problem above.

Resonant tunneling: (no interactions, single-particle picture)



same probles as before, but with an additional phase between the barriers (e.g. $\varphi = k\cdot d$, d: distance between the barriers)



$t_{12} =$

$t_R e^{i\varphi} t_L$

$+$

$t_R (e^{i\varphi} \tilde{r}_L e^{i\varphi} \tilde{r}_R e^{i\varphi}) t_L$

$+$

$t_R (e^{i\varphi} \tilde{r}_L e^{i\varphi} \tilde{r}_R e^{i\varphi} \tilde{r}_L e^{i\varphi} \tilde{r}_R e^{i\varphi}) t_L$

$+$

$\vdots$

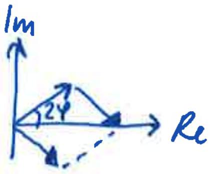
buzz-word: interference of different paths!

$$= t_R e^{i\varphi} t_L \cdot \sum_{n=0}^{\infty} \left(e^{2i\varphi} \cdot \tilde{r}_R \tilde{r}_L\right)^n$$

$$\underset{\text{geometric series}}{=} \frac{t_R t_L e^{i\varphi}}{1 - e^{2i\varphi} \tilde{r}_R \tilde{r}_L}$$

Transmission $T_{12} = |t_{12}|^2 = \frac{T_R T_L}{1 + R_L R_R - 2\sqrt{R_L R_R} \cdot \cos(2\varphi)}$

$T_i = |t_i|^2$, $R_i = |\tilde{r}_i|^2$



(for $\varphi = 0$ we obtain the previous result)

Discussion: For $T_i \ll 1$, $R_i \approx 1$ and for $\underline{\varphi \neq n\pi}$ $(n \in \mathbb{N})$

$\hookrightarrow T_{12} \approx 0$

For $\underline{\varphi \approx n\pi}$: $\varphi = n\pi + \delta\varphi \Rightarrow \cos(2\varphi) \approx 1 - \frac{1}{2} \cdot \delta\varphi^2 \Rightarrow 1 - \cos(2\varphi) \approx \frac{1}{2}\delta\varphi^2$

$\approx \frac{1}{2}\left(\frac{\partial\varphi}{\partial E}\right)^2 \cdot \Delta E^2$

$$\Rightarrow T_{12} = \frac{T_L T_R}{\underbrace{(1-\sqrt{R_L R_R})^2}_{1 + R_L R_R - 2\sqrt{R_L R_R}} + 2\sqrt{R_L R_R}(1 - \cos(2\varphi))} = \frac{T_L T_R}{\frac{1}{4}(T_L + T_R)^2 + \left(\frac{\partial\varphi}{\partial E}\right)^2 \cdot \Delta E^2}$$

$1 - \sqrt{R_L R_R} = \sqrt{(1-T_L)(1-T_R)} + 1$

$= \sqrt{1 - T_L - T_R - \cancel{T_L T_R}} + 1$ $(T_L T_R \ll T_i)$

$\approx 1 - (1 - \frac{1}{2}(T_L + T_R))$

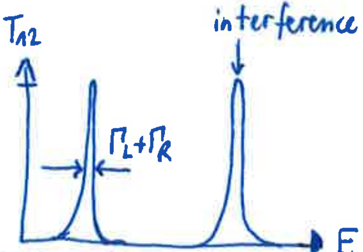
$= \frac{1}{2}(T_L + T_R)$

$$\frac{\partial E}{\partial \varphi} = \overbrace{\frac{\partial E}{\partial k}}^{\hbar v} \cdot \frac{\partial k}{\partial \varphi} = \hbar v \cdot \frac{1}{\partial\varphi/\partial k} \overset{\varphi = k\cdot d}{=} \hbar v \cdot \frac{1}{d} =: \hbar \cdot \underset{\text{attempt frequency}}{\nu}$$

$$\hookrightarrow \underline{\underline{T_{12}}} = \frac{T_L T_R \cdot (h\nu)^2}{\Delta E^2 + \frac{1}{4}(\hbar\nu T_L + \hbar\nu T_R)} = \underline{\underline{\frac{\Gamma_L \Gamma_R}{\Delta E^2 + \frac{1}{4}(\Gamma_L + \Gamma_R)}}}$$

def.: $\Gamma_i = \hbar\nu \cdot T_i$

(Lorentzian!)



$\boxed{T_{12} \text{ can be } 1! \ (\Gamma_L = \Gamma_R), \text{ though } T_i \ll 1}$