Introduction to electrical transport theory in nanoscale systems

Krzysztof Byczuk

Institute of Theoretical Physics,
Physics Faculty,
University of Warsaw

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www.fuw.edu.pl/~byczuk

Friction, dissipation ... every day experience

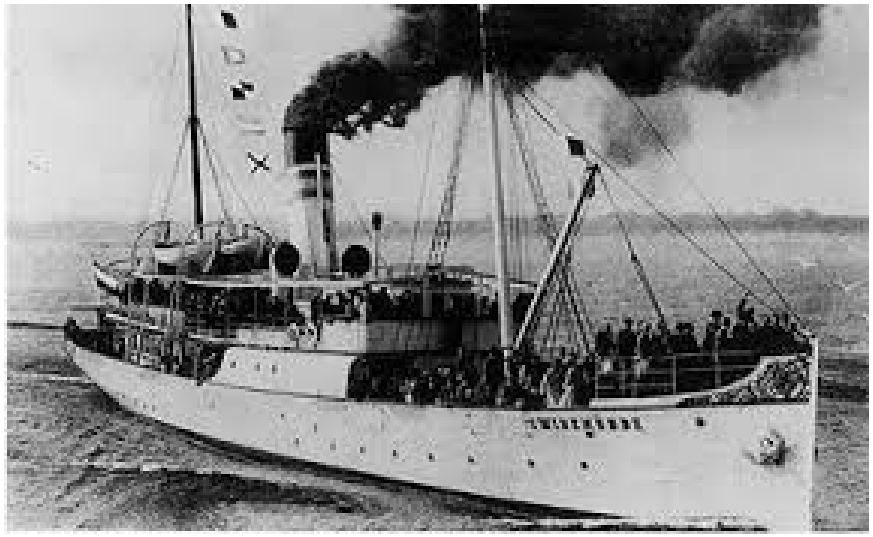
helps...

disturbs...

Friction dissipates energy

electric resistance

$$R \quad [\Omega = V/A]$$



viscosity

$$\eta \quad [Pa \cdot s]$$

Transport - generically non-equilibrium phenomenon!

Drude semi-classical approach to transport

$$\mathbf{E} = \rho \mathbf{j} \leftrightarrow \mathbf{j} = \sigma \mathbf{E}$$

linear response approach: ρ-**resistivity** and σ-**conductivity**

Ohm's law

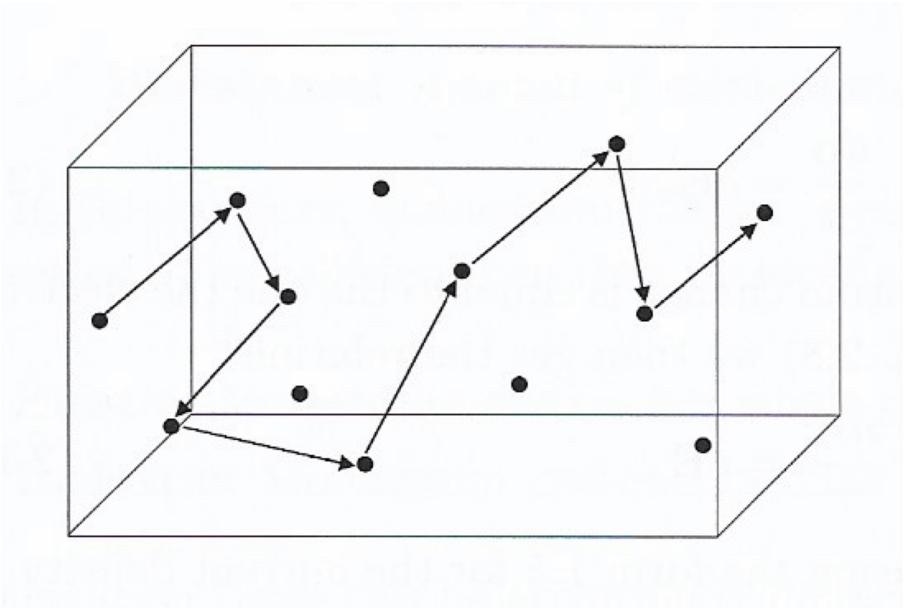
$$V = RI \leftrightarrow I = GV$$

R-**resistance** and G-**conductance**

Ohmic conductors

$$V = EL \text{ and } I = Sj \quad \text{then} \quad R = \rho \frac{L}{S} \quad \text{and} \quad G = \sigma \frac{S}{L}$$

Drude semi-classical approach to transport



relaxation time - average time τ between to successive collisions that change momentum $\mathbf{p}$

$$\frac{d\mathbf{p}}{dt} = \frac{1}{\tau}\mathbf{p} \quad \text{due to collisions,} \qquad \frac{d\mathbf{p}}{dt} = e\mathbf{E} \quad \text{between collisions}$$

Since $\mathbf{j} = en\mathbf{v}$ at steady state we get $\rho = \frac{m}{ne^2\tau}$ and $\sigma = \frac{ne^2\tau}{m}$.

Resistance - amount of momentum change during collisions (**momentum relaxation**).

Relaxation processes

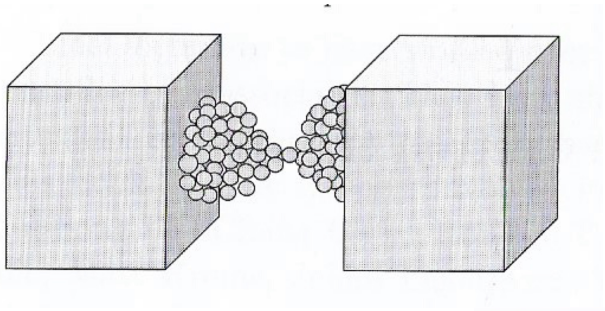
- **elastic scattering** - momentum relaxes, single-particle energy conserved (τ)
- **inelastic scattering** - momentum and single particle energy relaxes (τ_E), **incoherent transport**, phase of the wave function changed
- **dephasing process** - a change of the phase without change of energy considerably (τ_ϕ)

All these relaxation processes lead to approaching a local equilibrium of the system.

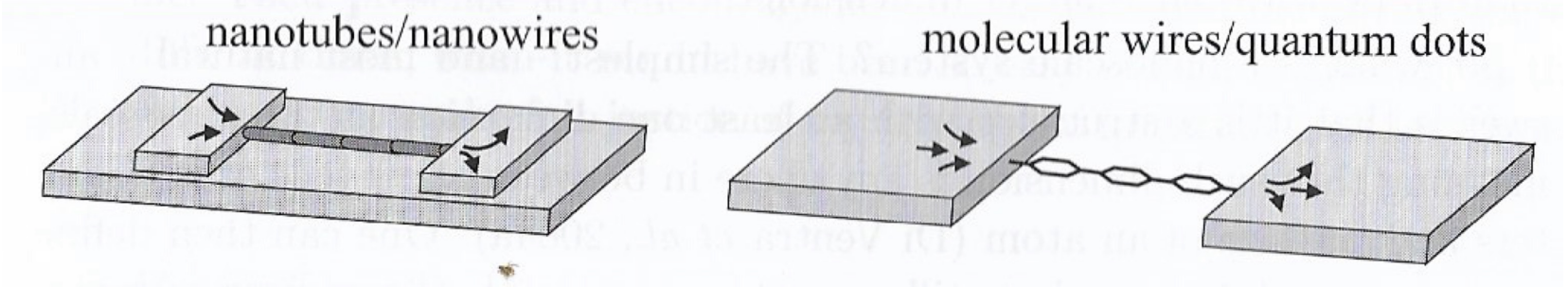
Typical theoretical approaches describing transport: semi-classical Drude model, Kubo formalism, Boltzmann kinetic equation, **Landauer approach**,...

Nanosystems

Nanoscale dimension $1nm = 10^{-9}m$ at least in one direction



If $I = 1\mu A$ and $S = 10\mathring{A}^2$ then $j = I/A = 10^9 A/cm^2$!



Landauer quantum scattering theory takes into account quantum effects in this transport.

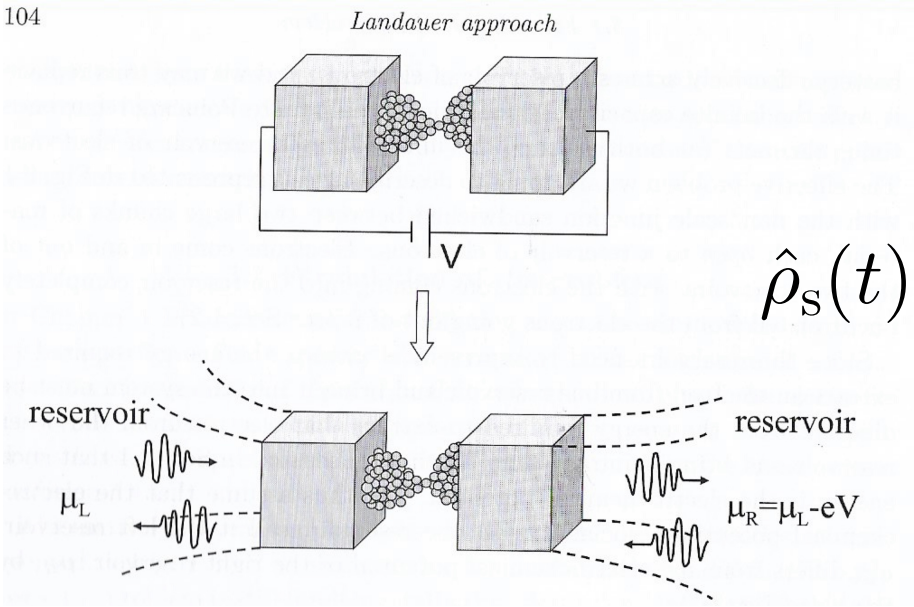
Quantum of conductance:

$$I = \frac{e}{\Delta t}, \quad V = \frac{\Delta E}{e}, \quad \Delta E \Delta t = h, \quad \text{hence} \quad G = \frac{I}{V} = \frac{e^2}{\Delta E \Delta t} = \frac{e^2}{h} = \frac{1}{25,8k\Omega}$$

Landauer approach - Approximation 1

$$\hat{H}_{\rm tot} = \hat{H}_{\rm s} \otimes \hat{1}_{\rm battery} + \hat{1}_{\rm s} \otimes \hat{H}_{\rm battery} + \hat{H}_{\rm int}$$

$$V = \frac{\mu_L - \mu_R}{e}$$



$$\hat{\rho}_{\rm s}(t) = {\rm Tr}_{\rm battery}\hat{\rho}_{\rm tot}(t)$$

The **closed system**, battery and electrode-junction-electrode structure, is replaced by **open system**, electrode-junction-electrode structure dynamically coupled to two reservoirs at different chemical potentials.

Landauer approach - Approximation 2

Lindblad type evolution

$$\frac{d}{dt}\hat{\rho}_{\mathrm{s}}(t) = \mathcal{L}\hat{\rho}_{\mathrm{s}}(t)$$

with initial condition $\hat{\rho}_{\mathrm{s}}(t = t_0)$.

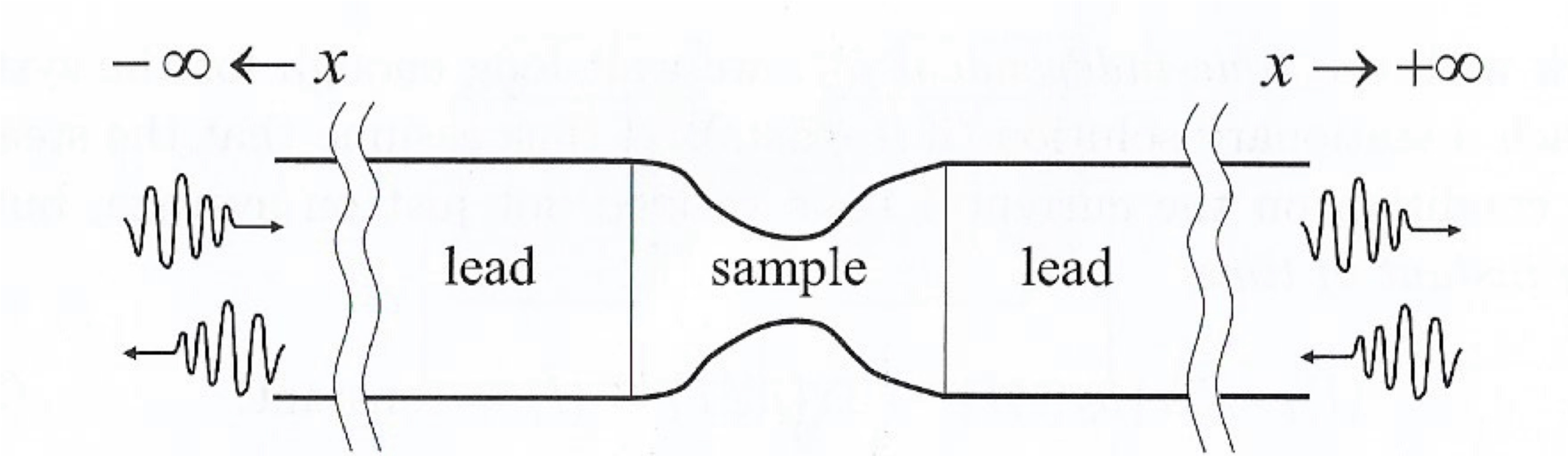
Assume that the ideal steady-state (time independent) solution exists $\hat{\rho}_{\mathrm{s}}^{ss}$ that at every instant of time

$$\langle \hat{I} \rangle_t = \mathrm{Tr}\left(\hat{\rho}_{\mathrm{s}}(t)\hat{I}\right) \to \mathrm{Tr}\left(\hat{\rho}_{\mathrm{s}}^{ss}\hat{I}\right) = \langle \hat{I} \rangle = \mathrm{constant}.$$

The problem is **ideally stationary** but $\hat{\rho}_{\mathrm{s}}^{ss}$ is practically not obtainable.

Landauer approach - Approximation 3

We are going to work with $\hat{H}_{\mathrm{s}}$ only.



We replace dynamical coupling with reservoirs with **scattering boundary conditions** at infinity. The system is closed but infinite.

Landauer approach - Approximation 3

Time dependent Schrodinger equation

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = \hat{H}_{\mathrm{s}}|\Psi(t)\rangle$$

with eigen-problems

$$\hat{H}_{\mathrm{s}}|\Psi_{E_i,\alpha}\rangle = E_i|\Psi_{E_i,\alpha}\rangle \quad \text{and} \quad \hat{H}_{\mathrm{s}}|\Psi_{E,\alpha}\rangle = E|\Psi_{E_i,\alpha}\rangle.$$

General stationary solution of time dependent Schrodinger equation:

$$|\Psi(t)\rangle = \sum_{E_i,\alpha} c_{E_i,\alpha}|\Psi_{E_i,\alpha}\rangle e^{-\frac{i}{\hbar}E_i t} + \sum_{\alpha}\int dE c_{E,\alpha}|\Psi_{E,\alpha}\rangle e^{-\frac{i}{\hbar}Et}.$$

Landauer approach - Approx. 2 & 3 - consequences

Approx. 2 - lost information on the **history** of the system.

No dynamical information on current density (clearly present in the real system) can be obtained after the static approximation is made. Capturing of the non-linear dynamical effects is impossible.

Approx. 3 - the amount of correlations lost in the process of going from a non-equlibrium mixed state to a pure stationary state

$$\hat{\rho}_{\mathrm{tot}}(t) \rightarrow \hat{\rho}_{\mathrm{s}}(t) \rightarrow \hat{\rho}_{\mathrm{s}}^{ss} \rightarrow \hat{H}_{\mathrm{s}}$$

cannot be determined even in principle.

Other methods, like Kubo formalism, let this perturbatively, at least in principle.

Landauer approach - Approximation 4

True many-body Hamiltonian of the system is replaced by some type of mean-field single-particle models

$$\hat{H}_{\rm s} = \hat{H}^{mf} + \hat{V}$$

E.g.,

Hartree model

$$\hat{H}_{\rm s} = -\frac{\hbar^2}{2m}\nabla^2 + e^2 \int \frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}' + \hat{V}_{\rm ext}(\mathbf{r})$$

or density-functional model

$$\hat{H}_{\rm s} = -\frac{\hbar^2}{2m}\nabla^2 + e^2 \int \frac{n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}' + \hat{V}_{\rm xc}(\mathbf{r}) + \hat{V}_{\rm ext}(\mathbf{r})$$

or single-particle model

$$\hat{H}_{\rm s} = -\frac{\hbar^2}{2m}\nabla^2 + \hat{V}_{\rm ext}(\mathbf{r})$$

as we will do.

Landauer approach - Approximation 5

Definition:

A **channel** - a set of quantum numbers $\{E, \alpha\}$ that describes a scattering solution.

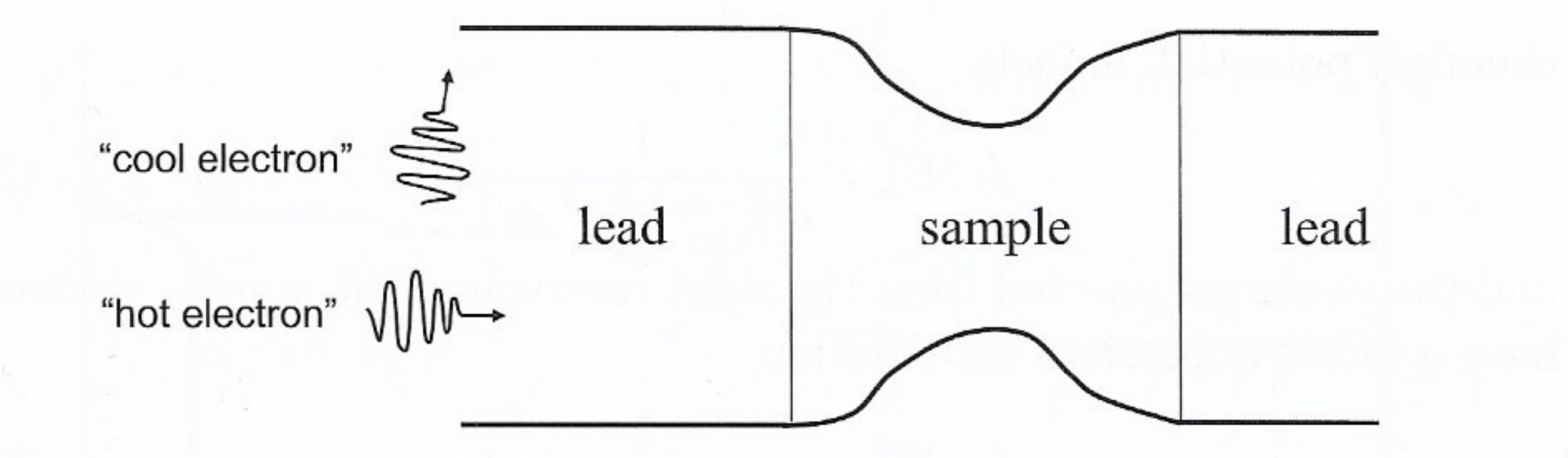
Approximation 5: We neglect correlations between different channels.

Off-diagonal elements of the density matrix connecting $\{E, \alpha\}$ and $\{E', \alpha'\}$ are exactly zero. The system evolved into a totally **incoherent** (**independent**) set of single-particle channels. This decoherence time must be extremely short.

How are these independent channels populated?

Landauer approach - Approximation 5

The answer is not obvious:



"Hot electrons" with larger velocity component along the current flow will have less time to relax to local equilibrium energy-momentum distribution then "cold electrons" with smaller velocity component along the current flow.

In principle, they are described by different distribution functions! However, ...

Landauer approach - Approximation 5

...we assume that all electrons approaching from the left reservoir (**right-movers**) are populated with a **local equilibrium distribution** with a given chemical potential of the left reservoir

$$f_L(E) = \frac{1}{e^{\beta(E-\mu_L)}+1},$$

and similarly for **left-movers**

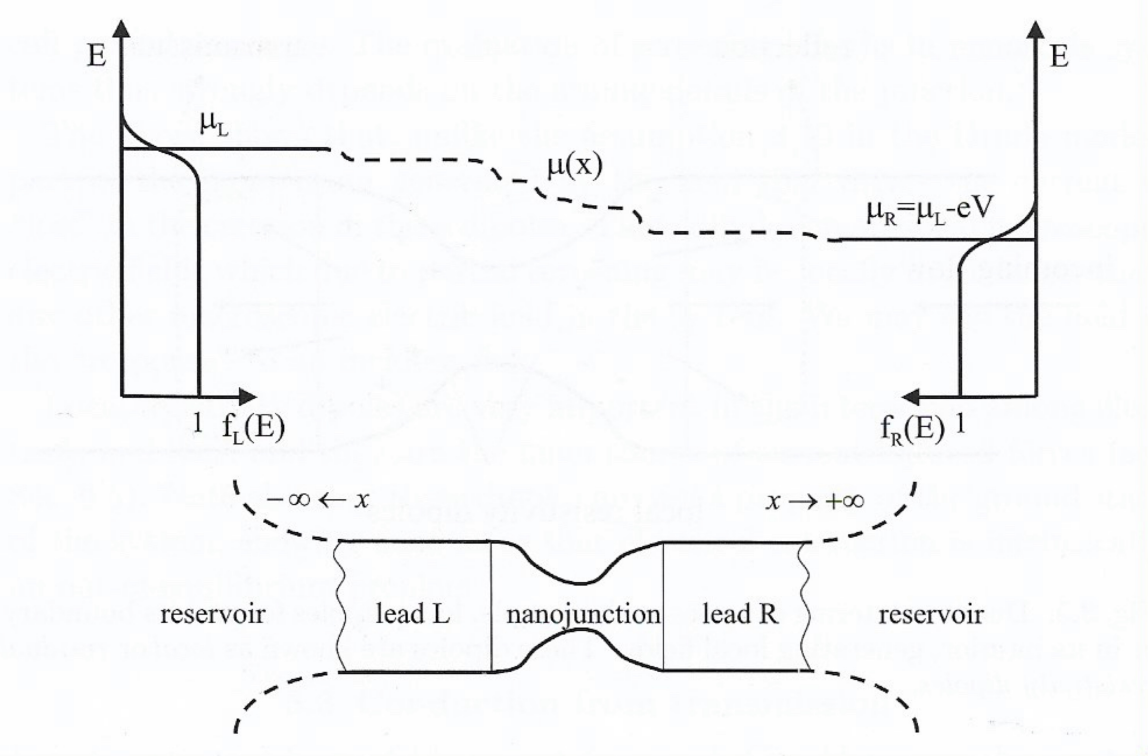
$$f_R(E) = \frac{1}{e^{\beta(E-\mu_R)}+1}.$$

Hence

$$\hat{\rho}_{\rm s}^{ss} = \sum_L |\Psi_L\rangle f_L \langle\Psi_L| + \sum_R |\Psi_R\rangle f_R \langle\Psi_R|.$$

Landauer approach - Summary

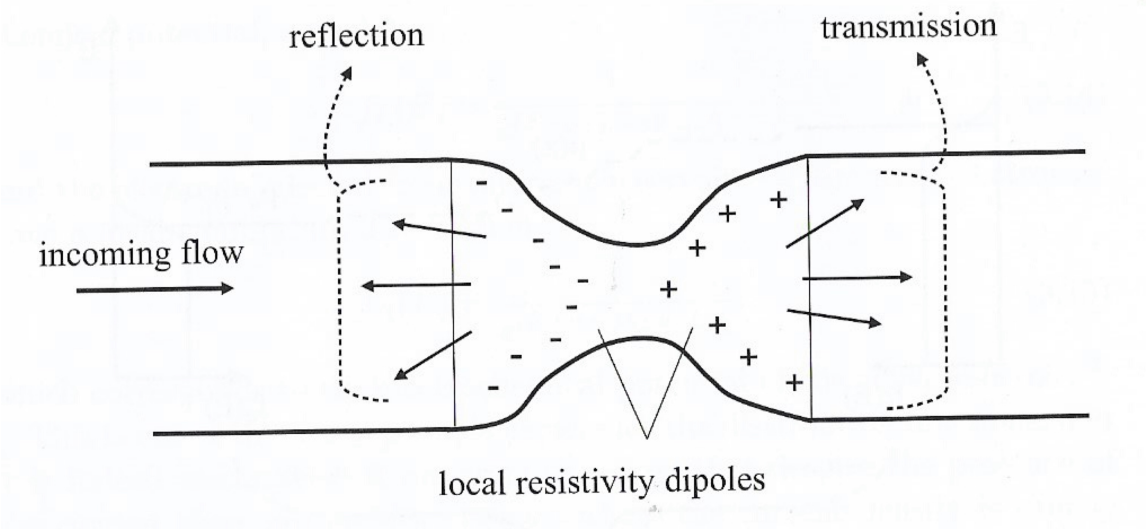
Cartoon of the system described within Landauer approach:



Particles are injected at infinities with two different local equilibrium distributions. The (macroscopic-averaged) local electrochemical potential $\mu(x)$ varies along the whole structure.

Landauer approach - Summary

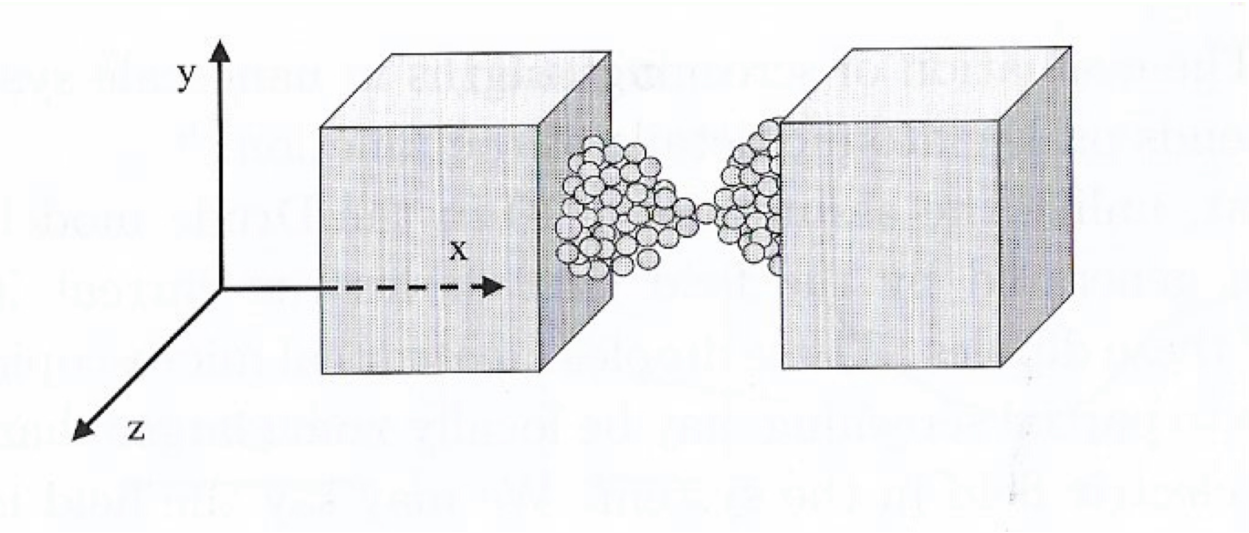
In Landauer approach the biased $V = (\mu_L - \mu_R)/e$ is not a perturbation to the system Hamiltonian. The biased here is a **boundary condition** on the system, where wave-packet with given momenta carry the current across the nano-junction. There is a finite probability that due to scattering the electron is transmitted in a given direction or reflected.

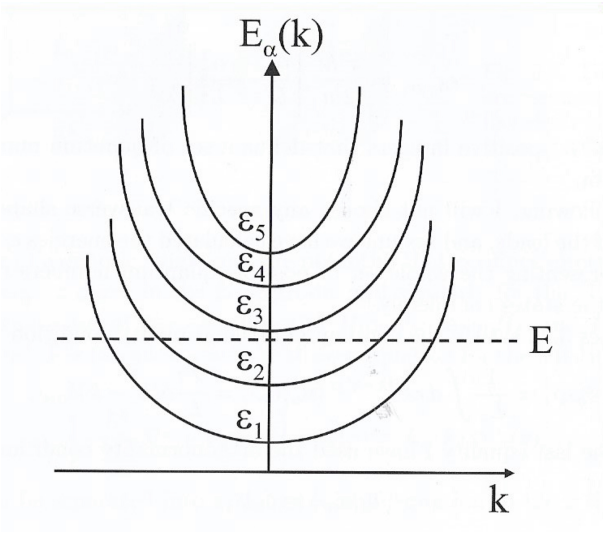


Due to back reflection the local accumulation of charges appear. It happens on the screening length distance $\sim 1\mathring{A}$ (metals) - $100\mathring{A}$ (semiconductors) or more in systems with reduced dimensions. **Local resistivity dipoles** are formed and some momentum is lost $\rightarrow$ **resistance**.

Scattering boundary conditions

$$\lim_{x\to-\infty}\hat{H}_{\rm s}=-\frac{\hbar^2}{2m}\nabla^2+V_L(\mathbf{r}_\perp)\equiv\hat{H}_L \quad\text{and}\quad \lim_{x\to+\infty}\hat{H}_{\rm s}=-\frac{\hbar^2}{2m}\nabla^2+V_R(\mathbf{r}_\perp)\equiv\hat{H}_R$$





Separable problem in x and y-z directions with asymptotic solutions

$$\psi_{\alpha k}(\mathbf{r})=\sqrt{\frac{1}{L_x}}u_\alpha(\mathbf{r}_\perp)e^{ikx} \quad\text{with}\quad E_\alpha(k)=\epsilon_\alpha+\frac{\hbar^2k^2}{2m}$$

for either $\hat{H}_L$ or $\hat{H}_R$.

Transmission and reflection probabilities

We look for general solution of $\hat{H}_{\rm s}$, i.e.

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right)\Psi_{\alpha k}(\mathbf{r}) = E\Psi_{\alpha k}(\mathbf{r})$$

merging with asymptotic solutions with $\hat{H}_L$ and $\hat{H}_R$. From Approx. 5, there are right and left moving states. An initial right moving state $\psi_{ik_i}(\mathbf{r})$ with $E_i(k_i) = \epsilon_i + \frac{\hbar^2 k_i^2}{2m}$ is scattered by the full $\hat{H}_{\rm s}$, such that

$$\Psi^+_{ik_i}(\mathbf{r}) \to \sum_{f=1}^{N_c^R} \mathcal{T}_{if}\psi_{fk_f}(\mathbf{r}) \quad \text{at} \quad x \to +\infty$$

and

$$\Psi^+_{ik_i}(\mathbf{r}) \to \psi_{ik_i}(\mathbf{r}) + \sum_{f=1}^{N_c^L} \mathcal{R}_{if}\psi_{fk_f}(\mathbf{r}) \quad \text{at} \quad x \to -\infty.$$

Transmission and reflection probabilities

Current across the surface S perpendicular to x-direction

$$I(E_i) = \frac{e\hbar}{2im} \int\limits_S dydz \left(\Psi^+_{ik_i}(\mathbf{r})^* \partial_x \Psi^+_{ik_i}(\mathbf{r}) - \Psi^+_{ik_i}(\mathbf{r}) \partial_x \Psi^+_{ik_i}(\mathbf{r})^* \right)$$

Deep in the left lead it is

$$I_L(E_i) = I_i(E_i) + \sum_{f=1}^{N_c^L} |\mathcal{R}_{if}|^2 I_f(E_i) = I_i(E_i) - \sum_{f=1}^{N_c^L} |\mathcal{R}_{if}|^2 |I_f(E_i)| \equiv$$

$$\equiv I_i(E_i) \left(1 - \sum_{f=1}^{N_c^L} R_{if}(E_i) \right), \quad \text{where}$$

$R_{if}(E_i) \equiv |\mathcal{R}_{if}|^2 \frac{|I_f(E_i)|}{|I_i(E_i)|}$ is a **reflection probability**,
$I_i(E_i) = \frac{\hbar k_i}{m L_x}$ and $I_f(E_i) = \frac{\hbar k_f}{m L_x}$.

Transmission and reflection probabilities

Similarly

$$I_R(E_i) \equiv I_i(E_i) \sum_{f=1}^{N_c^R} T_{if}(E_i), \quad \text{where}$$

$T_{if}(E_i) \equiv |\mathcal{T}_{if}|^2 \frac{|I_f(E_i)|}{|I_i(E_i)|}$ is **transmission probability**.

In ideal steady state (Approx. 2) two currents $I_L(E_I) = I_R(E_i)$. Hence

$$\sum_{f=1}^{N_c^R} T_{if}(E_i) + \sum_{f=1}^{N_c^L} R_{if} = 1 \ \text{ for } \ \psi_{ik_i}(\mathbf{r}) \in \mathrm{L}.$$

By symmetry $L \leftrightarrow R$:

$$\sum_{f=1}^{N_c^L} T_{if}(E_i) + \sum_{f=1}^{N_c^R} R_{if} = 1 \ \text{ for } \ \psi_{ik_i}(\mathbf{r}) \in \mathrm{R}.$$

By symmetry $t \leftrightarrow -t$ (TRS) we get similar **conservation laws** with $i \leftrightarrow f$.

Total current

From Approx. 5, the total current is a sum of currents from all channels with given occupations

$$I = e\mathrm{Tr}\left(\hat{\rho}_{\mathrm{s}}^{ss}\hat{I}\right) = \frac{e}{\pi\hbar}\int_{-\infty}^{+\infty} dE[f_L(E) - f_R(E)]T(E),$$

where

$$T(E) = \tilde{T}_{RL}(E) = \tilde{T}_{LR}(E) \quad - \quad \text{flux conservation}$$

and

$$\tilde{T}_{RL}(E) = \sum_{i=1}^{N_c^R}\sum_{f=1}^{N_c^L} T_{if}(E)$$

$$\tilde{T}_{LR}(E) = \sum_{i=1}^{N_c^L}\sum_{f=1}^{N_c^R} T_{if}(E)$$

are **total transmission coefficients**.

Conductance from transmission

Zero-bias limit $\mu_L - \mu_R \to 0$, where $\mu_L = \epsilon_F + \epsilon$ and $\mu_R = \epsilon_F - \epsilon$, where $\epsilon \to 0$,

$$T(\epsilon_F \pm \epsilon) = T(\epsilon_F) \pm \frac{\partial T(E)}{\partial E}|_{\epsilon_F}\epsilon + ...$$

$$f_L(E) = f_R(E) - \frac{\partial f_R(E)}{\partial E}|_{\mu_R}(\mu_L - \mu_R) + ...$$

we obtain at $k_B T \to 0$

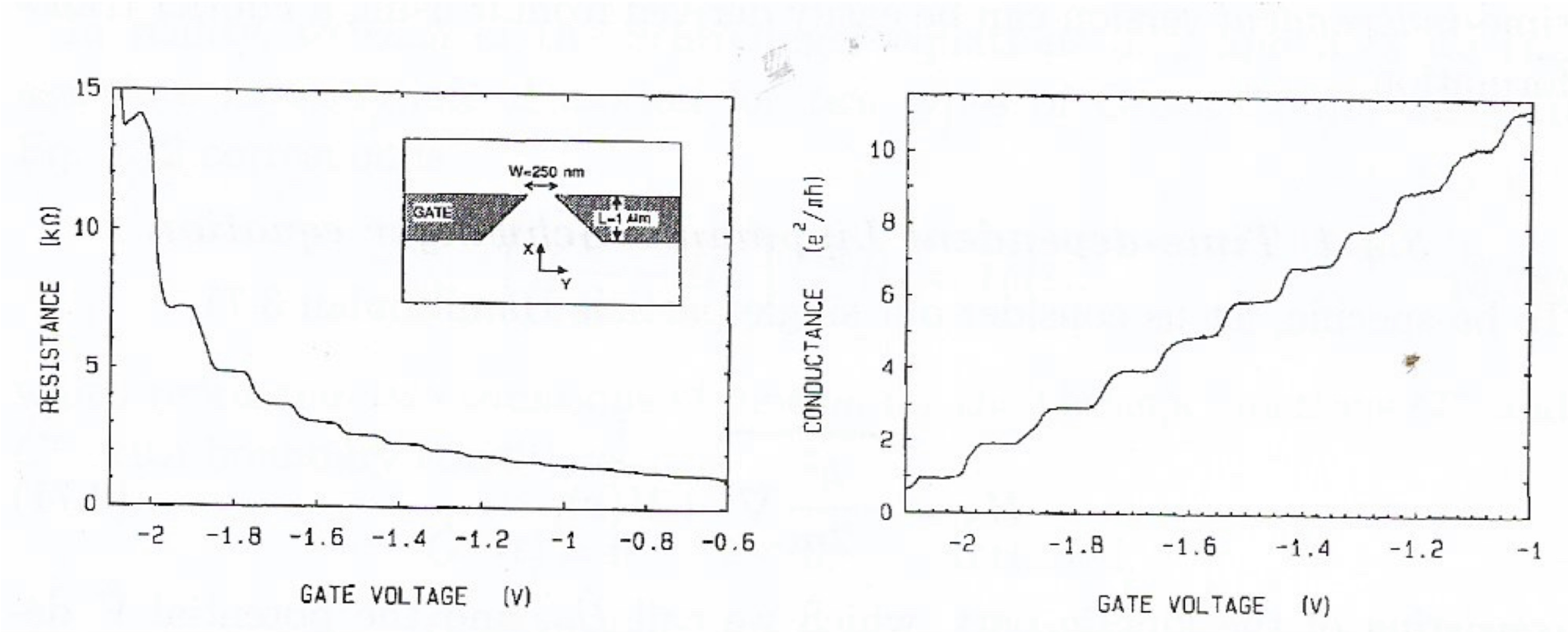
$$I = \frac{2e^2}{h}T(\epsilon_F)V.$$

Two probe conductance

$$G = \frac{dI}{dV} = \frac{2e^2}{h}T(\epsilon_F).$$

At resonance $T(E) \to 1$ very sharply $\to$ quantization of conductance.

Experimental verification of quantized conductance



Quantum point contact on a 2d electron gas. Wees et al. 1988.

Message to take home

In Landauer approach the external perturbation is replaced by boundary conditions and the scattering solution is obtained for quantum system. It is well suit approach to nano-scale systems and truly quantum effects are observable.

Multi-probe experiments, weak localization, universal quantum fluctuations, Aharonov-Bohm effect, and many other phenomena are described by Landauer theory.

Literature:
S. Datta, *Electronic transport in mesoscopic systems*
M. Di Ventra, *Electrical transport in nanoscale systems*