``Enseigner la recherche en train de se faire''

COLLÈGE DE FRANCE
1530

Chaire de
Physique de la Matière Condensée

PETITS SYSTEMES THERMOELECTRIQUES: *CONDUCTEURS MESOSCOPIQUES ET GAZ D'ATOMES FROIDS*

Cycle « Thermoélectricité »
2012 - 2014

Antoine Georges

Séance du 5 novembre 2013

- Rappels: Effets thermoélectriques, etc…
- Généralités sur les systèmes mésoscopiques: conductance et transmission
- Coefficients thermoélectriques dans l'approche de Landauer -Büttiker

Séminaires :

10h45 **Jean-Louis Pichard** (SPEC – CEA Saclay) – *Conversion thermoélectrique à basse température dans des nano-fils désordonnés et des cavités quantiques chaotiques : l'intérêt des bords de spectres.*

11h45 - **Björn Sothmann** (DPT – Université de Genève) – *Three-terminal quantum-dot thermoelectrics.*

Outline of future lectures:

- Nov 12: *Thermoelectric effects in mesoscopic quantum devices* (+ 2 seminars by L.Molenkamp)
- Nov, 19: Energy Filtering, etc. (2 lectures)

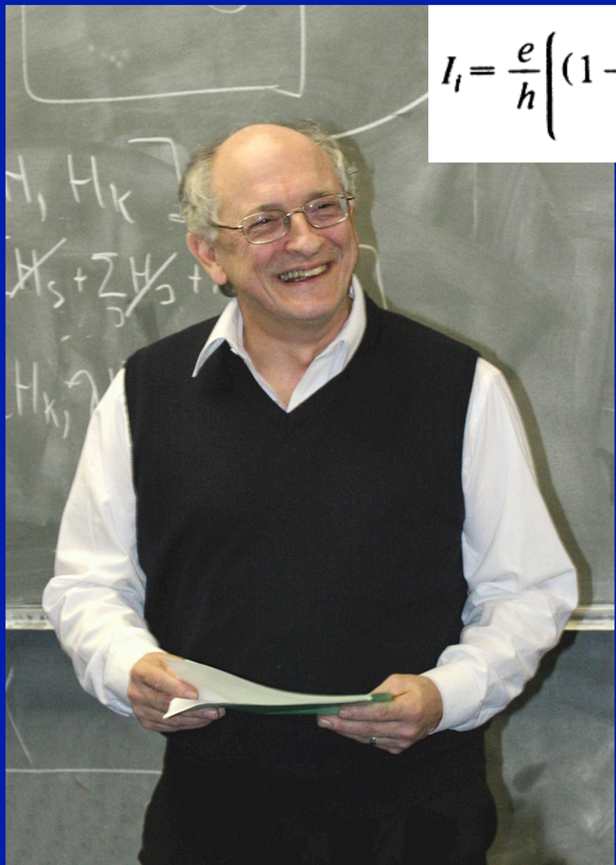
  (Seminar by O.Bourgeois on nano-phononics and thermal transport in small systems)
- NO LECTURES on Nov,26 and Dec,3
- Dec 10: *Cold atomic gases: transport and thermoelectric effects (I) (Two seminars by J-P Brantut and C.Grenier on recent experimental observations of these effects)*
- Dec 17: TE transport in cold gases (cont'd)

  Seminar by R.Grimm on observation of second-sound.

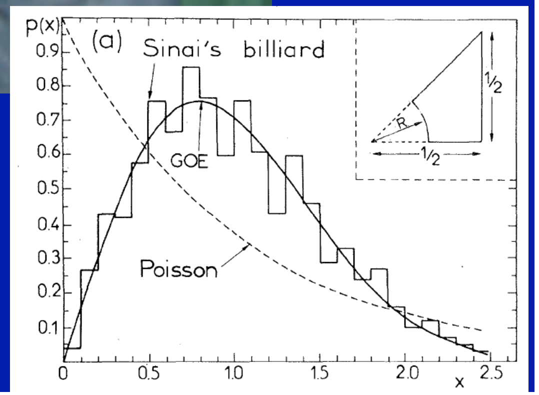
In memory of:

Oriol Bohigas (1937-2013)

Markus Büttiker (1950-2013)



$$I_i = \frac{e}{h}\left((1-R_{ii})\mu_i - \sum_{j\neq i} T_{ij}\mu_j\right).$$



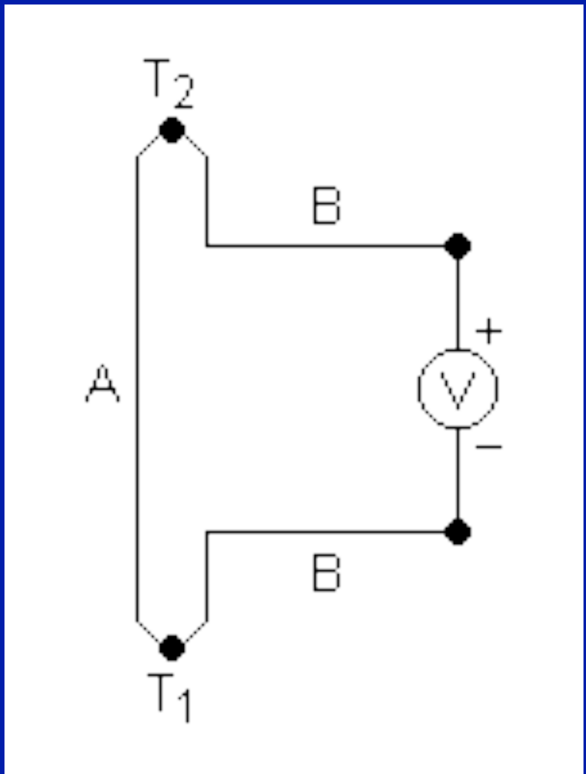
Reminders

(see lectures from last year on website)

Basic Thermolectric Effects

TWO KEY THERMOELECTRIC EFFECTS :
1. The Seebeck effect (1821)

A thermal gradient applied at the ends of an open circuit induces a finite voltage difference

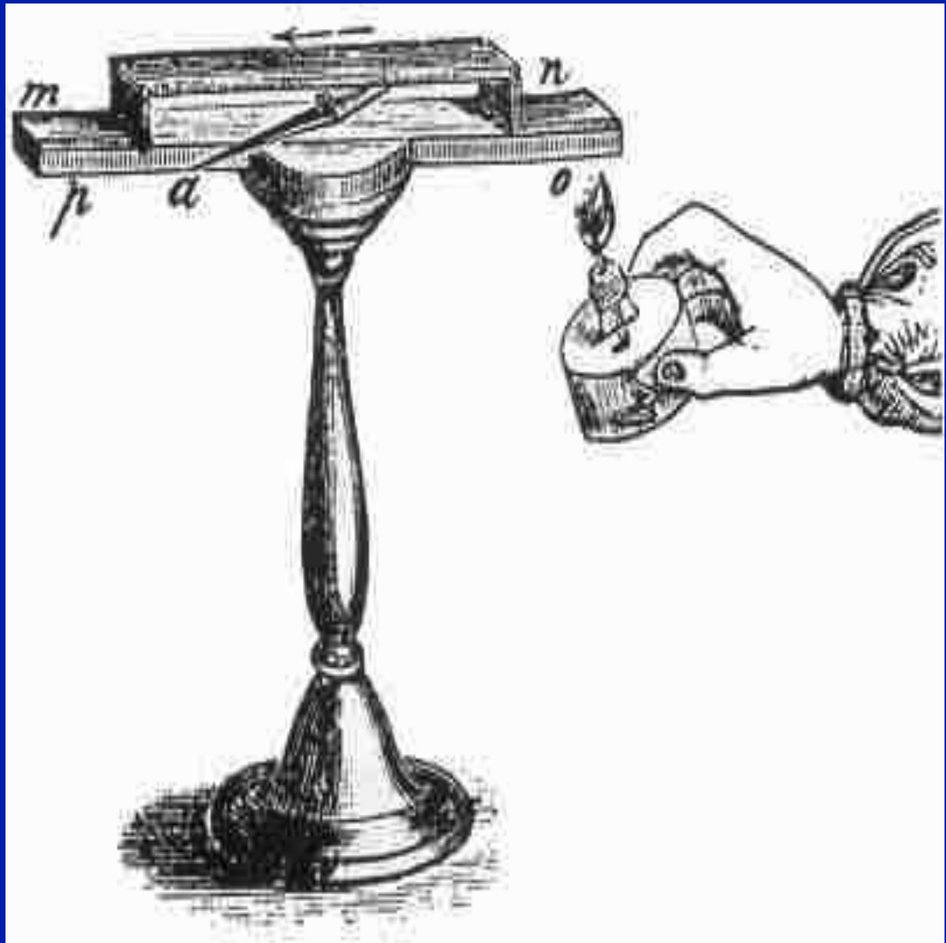


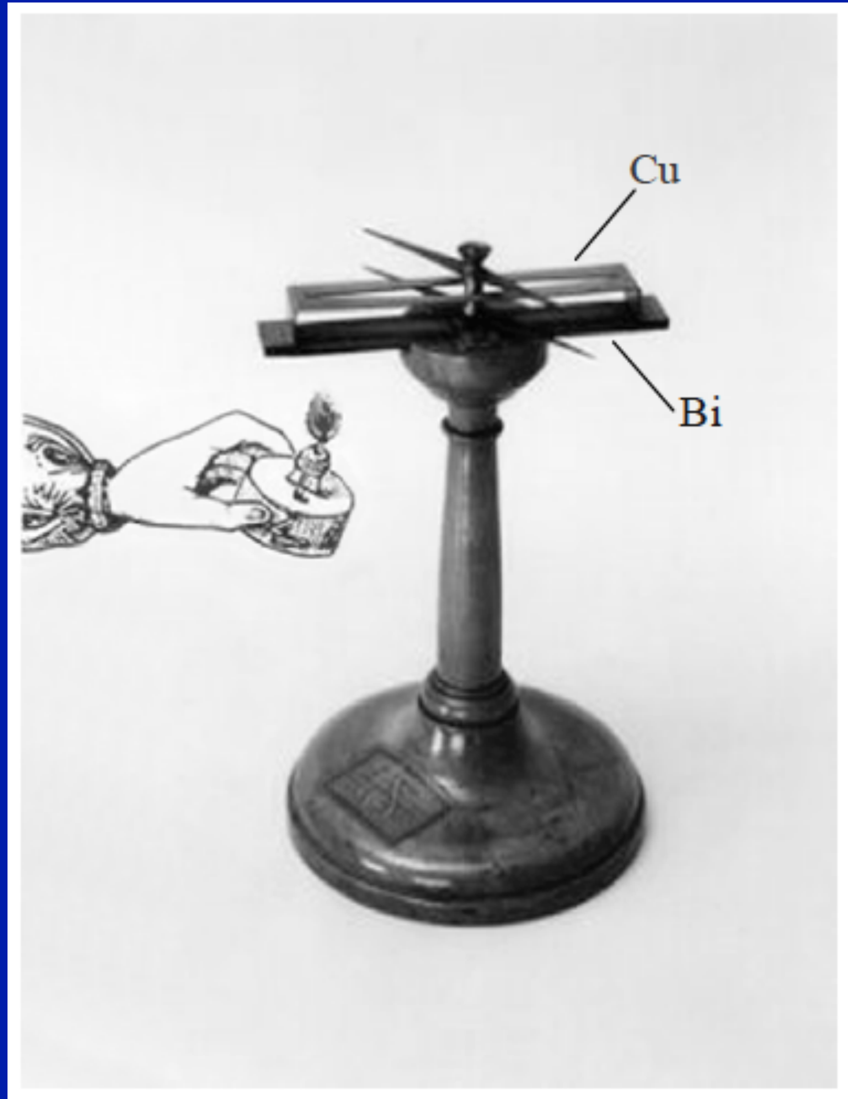
$$\Delta V = -\alpha\,\Delta T$$

α: Seebeck coefficient (thermopower)

Actual observation: junction between two metals, voltage drop:

$$V = (\alpha_B - \alpha_A)\,(T_2 - T_1)$$





Seebeck's original instrument: deflection of a compass needle
Heated junction of two metals (o,n)

Or, actually, Alessandro Volta in 1794…

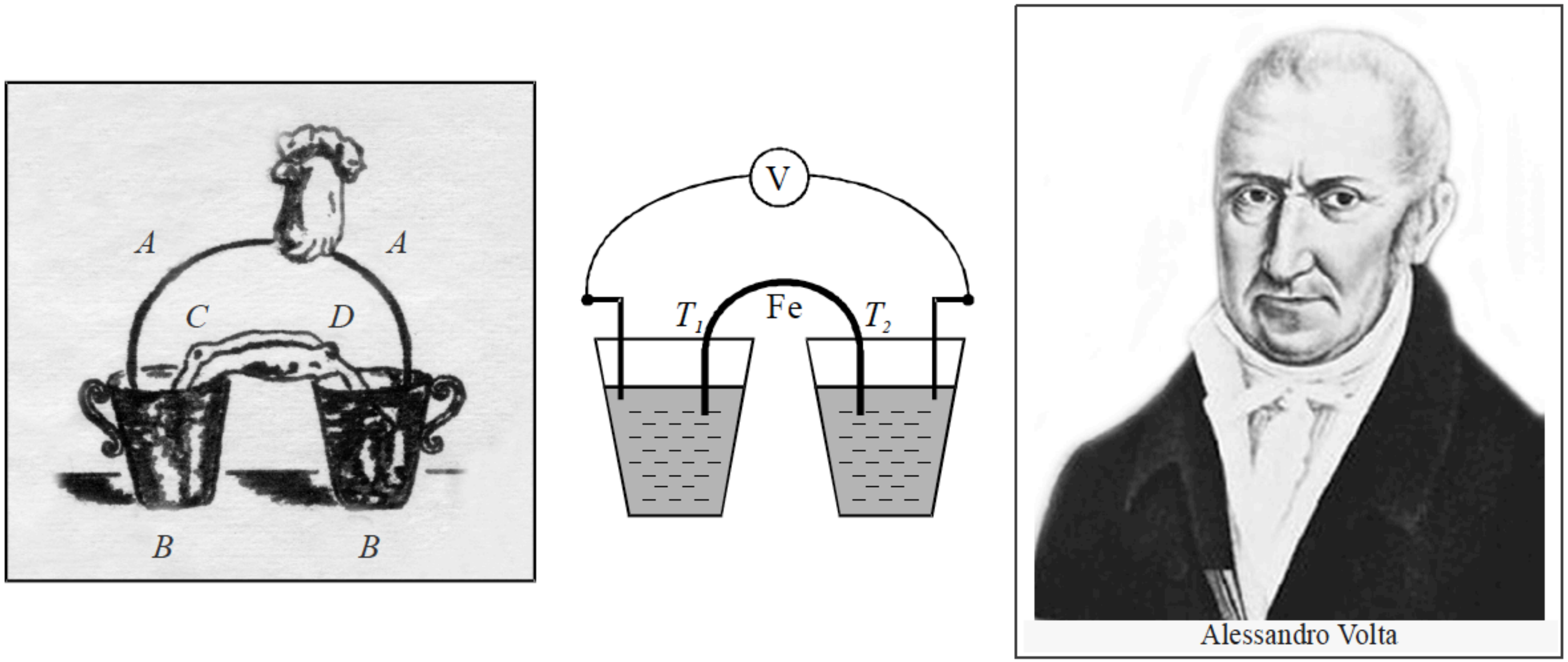
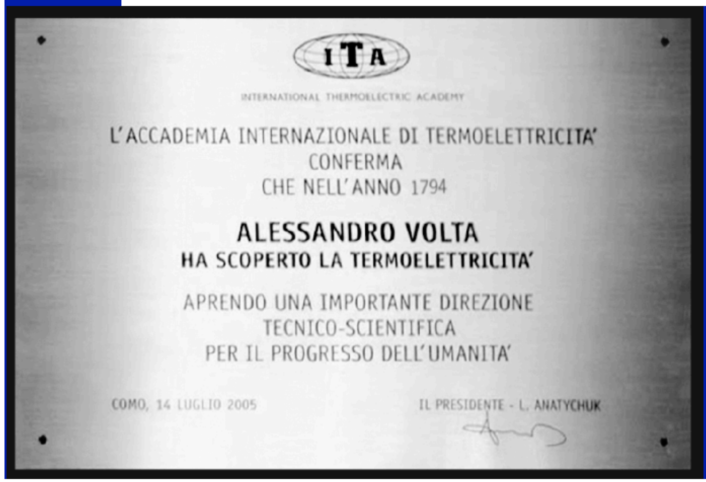


Fig. 3. Discovery of thermoelectricity by Volta on February 10, 1794.

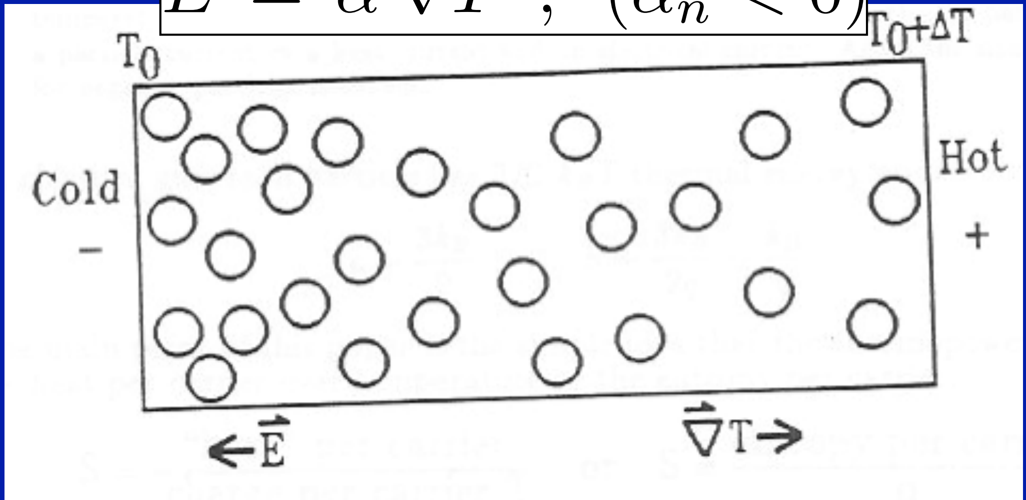


cf. e.g. LI Anatychuk,
Journal of Thermoelectricity, 1994
G.Pastorino, ibid., 2009

Qualitative picture:

cf: PM Chaikin, An introduction to thermopower for those who might want to use it…in `Organic superconductors', 1990

$$\vec{E} = \alpha \vec{\nabla} T \ , \ (\alpha_n < 0)$$

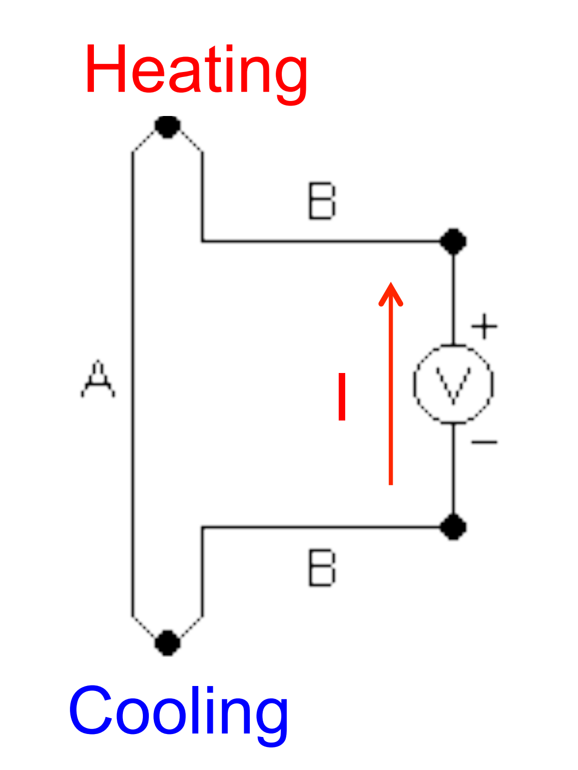


- Higher density of carriers on the cold side, lower on hot side
- → an electric field is established
- `Stopping condition': balance electric field and thermal gradient to get zero particle flow.
- In this cartoon: carriers are negatively charged, hence field is <u>opposite</u> to thermal gradient
- Electron-like (hole-like) carriers correspond to negative (positive) Seebeck coefficient → Seebeck useful probe of nature of carriers

TWO KEY THERMOELECTRIC EFFECTS : 2. The Peltier effect (1834)

Heat production at the junction of two conductors in which a current is circulated.

***Reversible**: heating or cooling as orientation of current is reversed.*



Heating rate: Π: Peltier coefficient

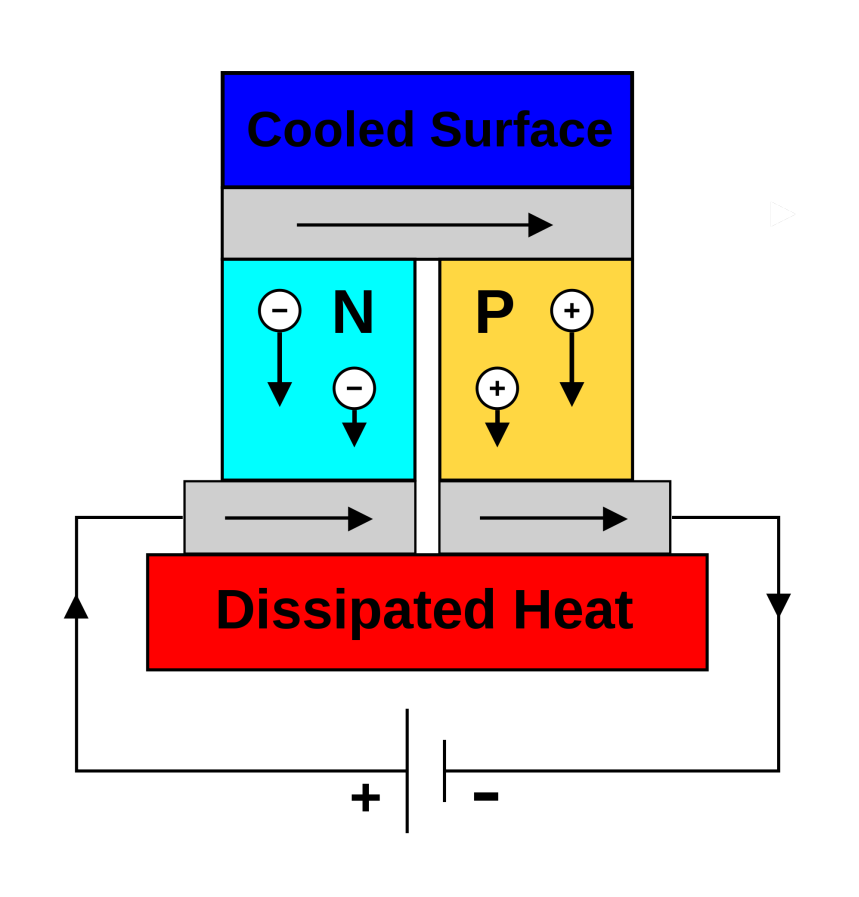
$$\dot{Q} = \Pi_{AB}\, I$$

2nd Kelvin relation (Onsager):

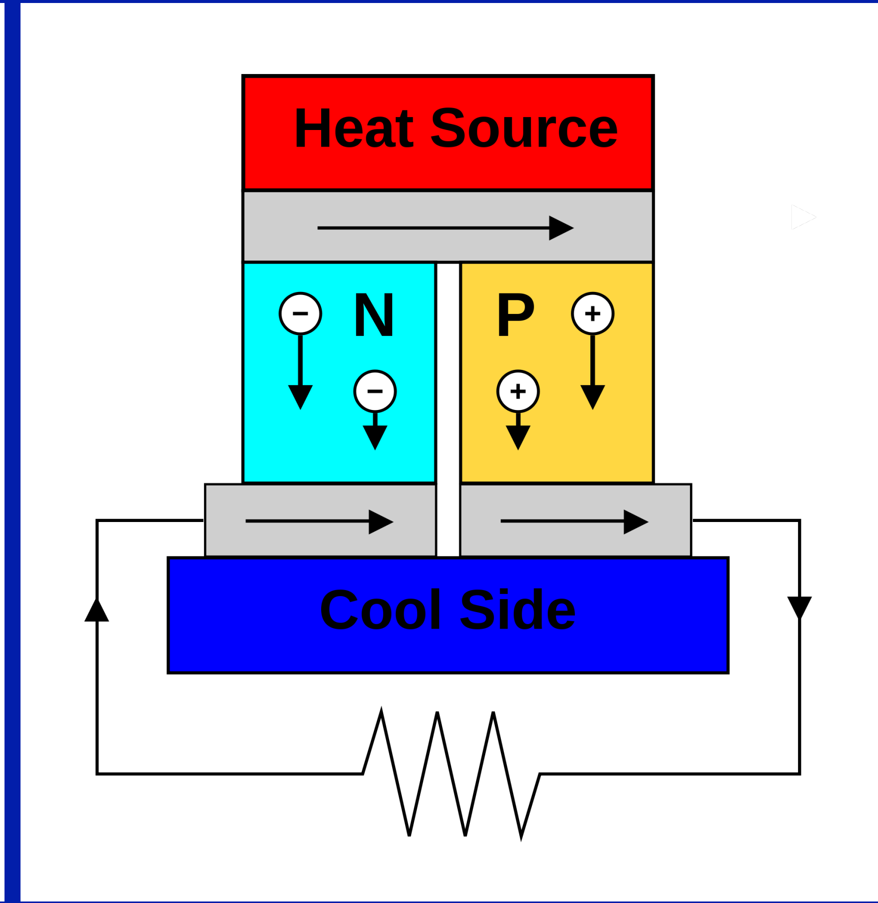
$$\Pi = T\,\alpha$$

<u>Note: thermoelectric coefficients are actually intrinsic to a single conductor (ex: B is a superconductor)</u>

Two basic applications of the Peltier and Seebeck effects: Coolers and Generators

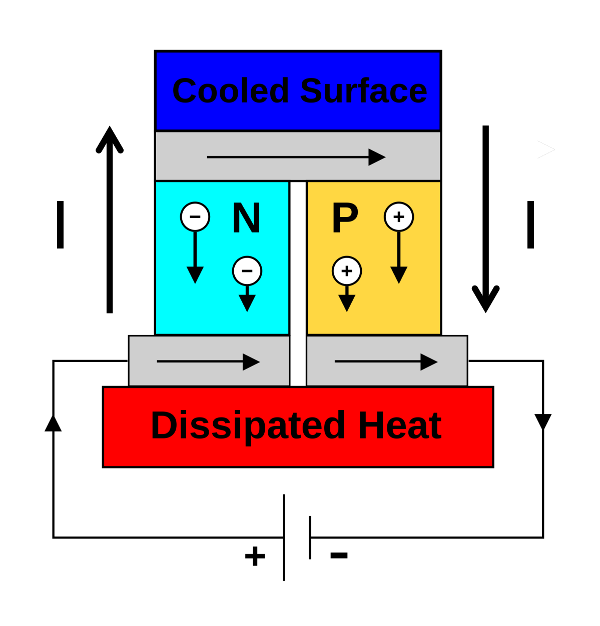


Cooling module [Peltier]

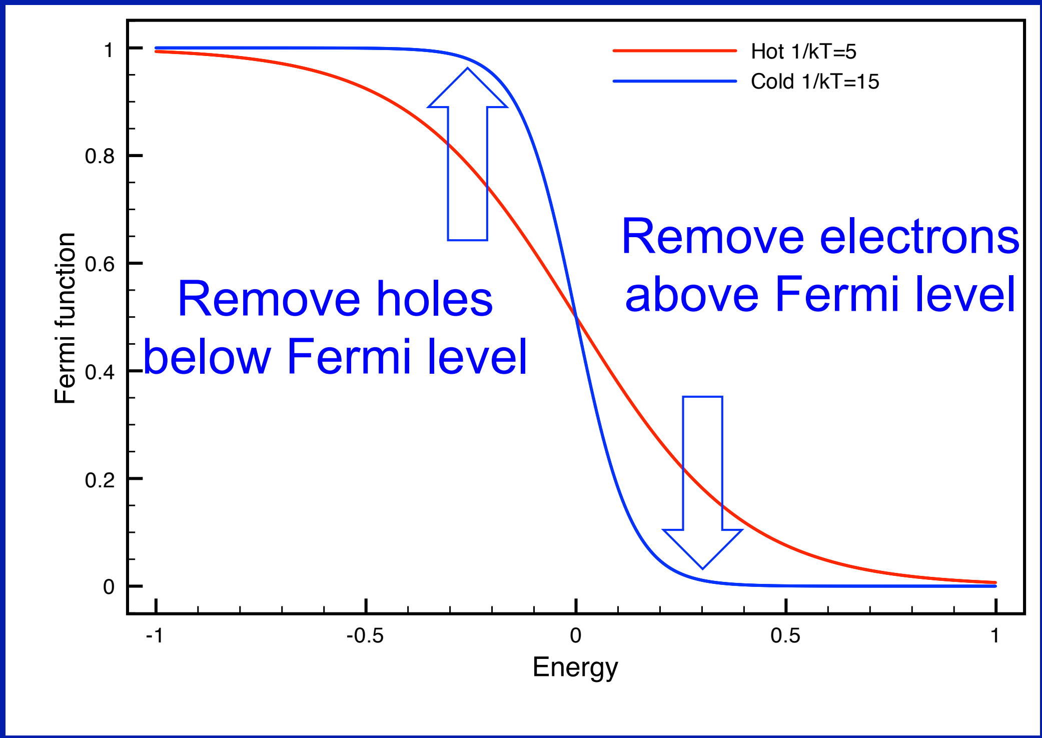


Power generation module [Seebeck]

Simple intuition about thermoelectric cooling



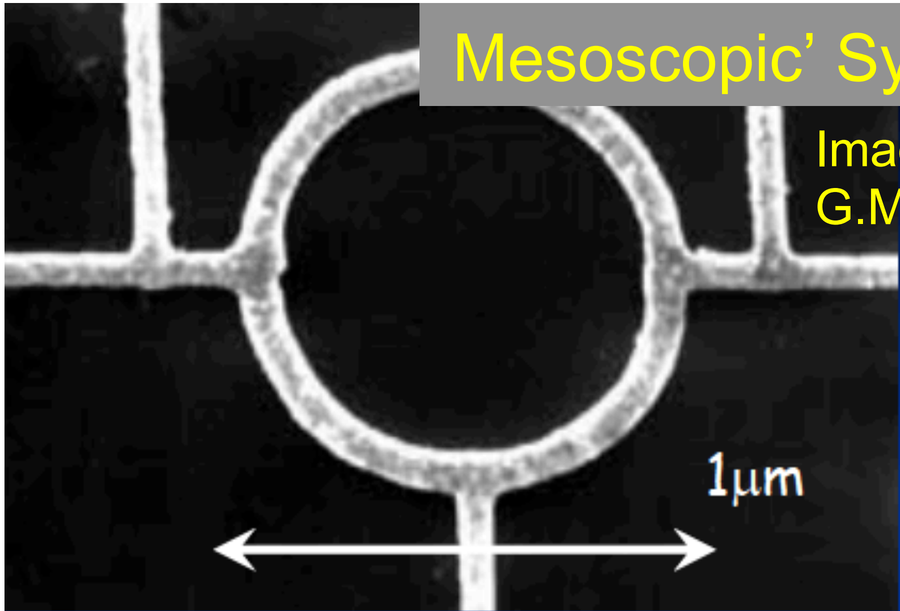
- Electrons move against current
- Holes move along current
- BOTH electrons and holes leave cold end to reach hot end
- BOTH processes correspond to lowering of entropy of cold end



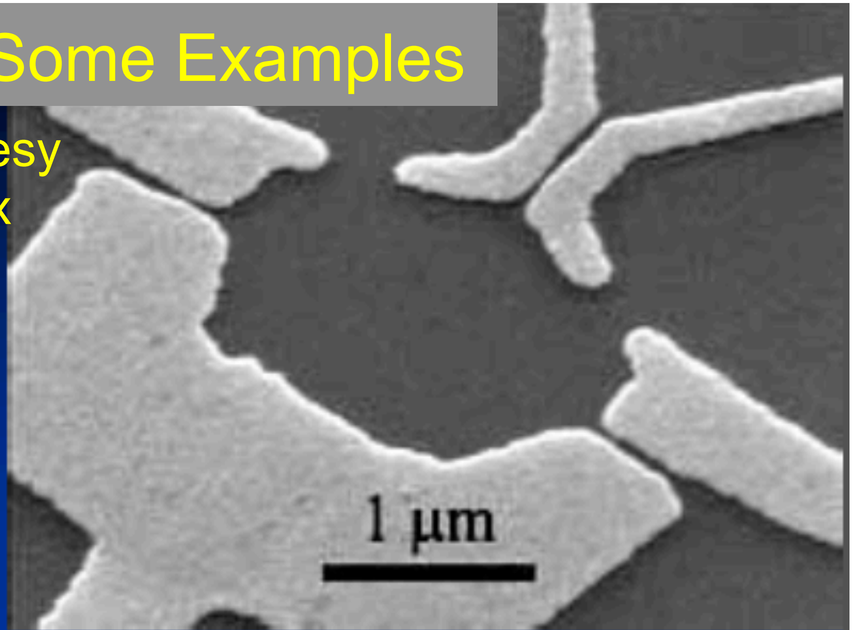
First part of these lectures:
Thermoelectric effects
in the context of
"Mesoscopic"
Electronic Systems

Mesoscopic' Systems: Some Examples

Images: Courtesy
G.Montambaux

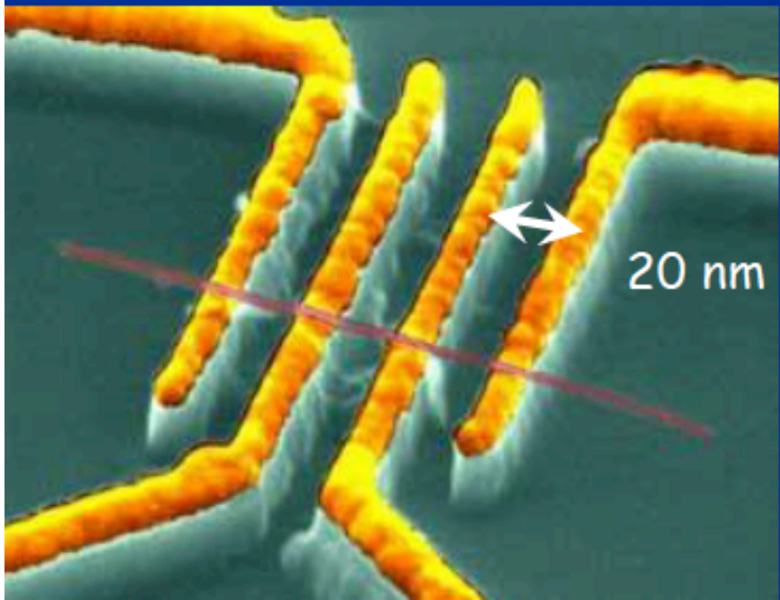


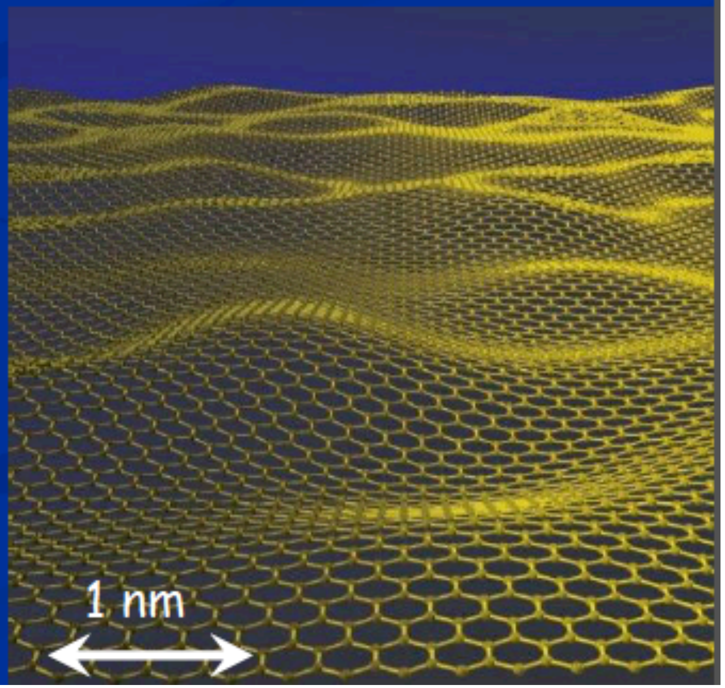
anneau métallique Cu



Gaz 2D, semiconducteur (AlGaAs)

Nanotube de carbone





Graphène

Mesoscopic Systems : Lengthscales

Geometrical dimension: L

(Size of conductor)

Phase coherence length: ℓ_ϕ

(Distance an electron travels before its phase changes by 2π)

Inelastic scattering length: ℓ_{in} (~10^3 nm ~ 1μm)

(Distance an electron travels before its energy changes by $\sim k_B T$)

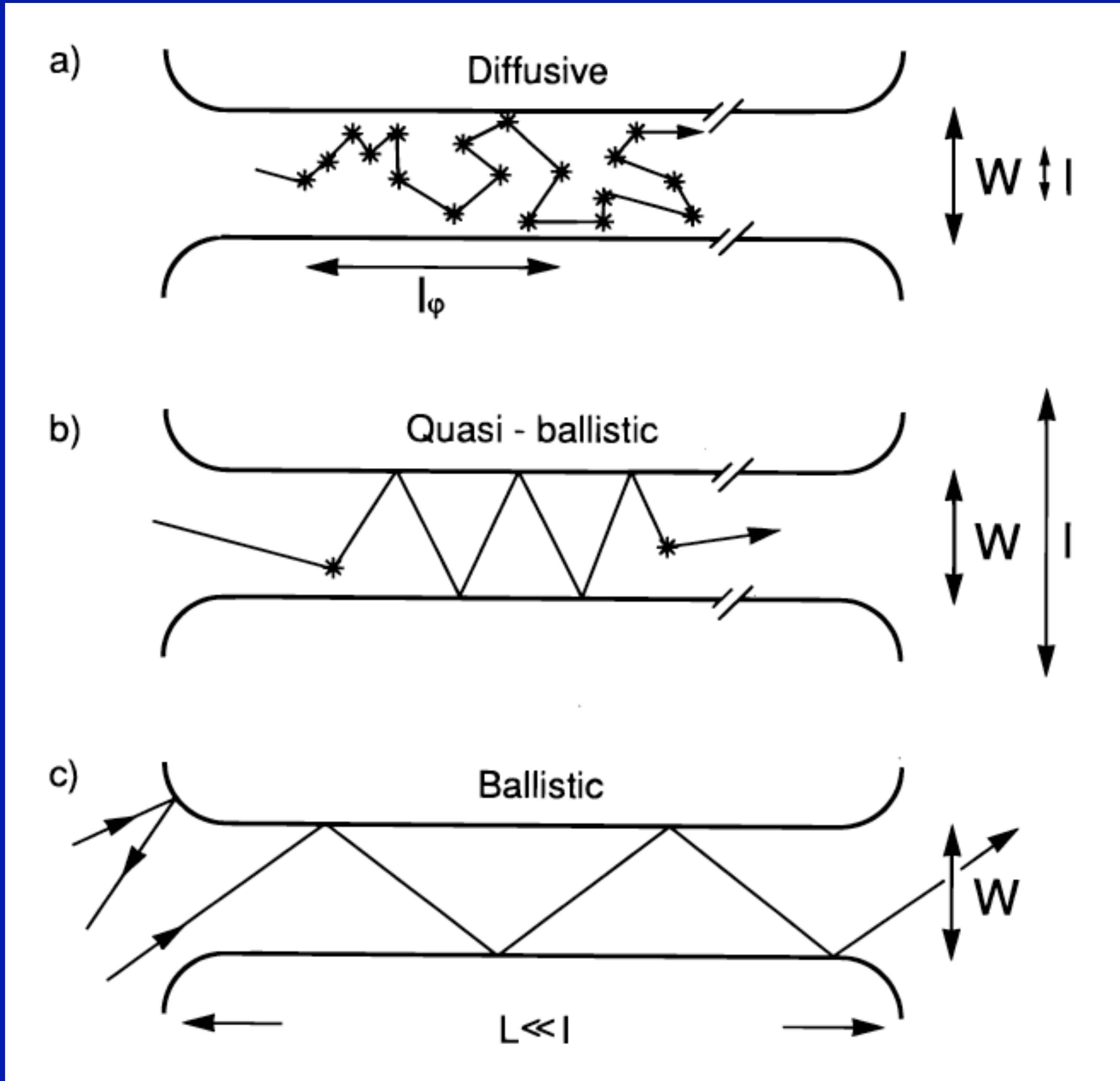
Elastic scattering length: ℓ_e (10-10^3 nm)

(Distance an electron travels between elastic scattering events)

Macroscopic Conductor: $\ell_e \ll \ell_{in}, \ell_\phi \ll L$

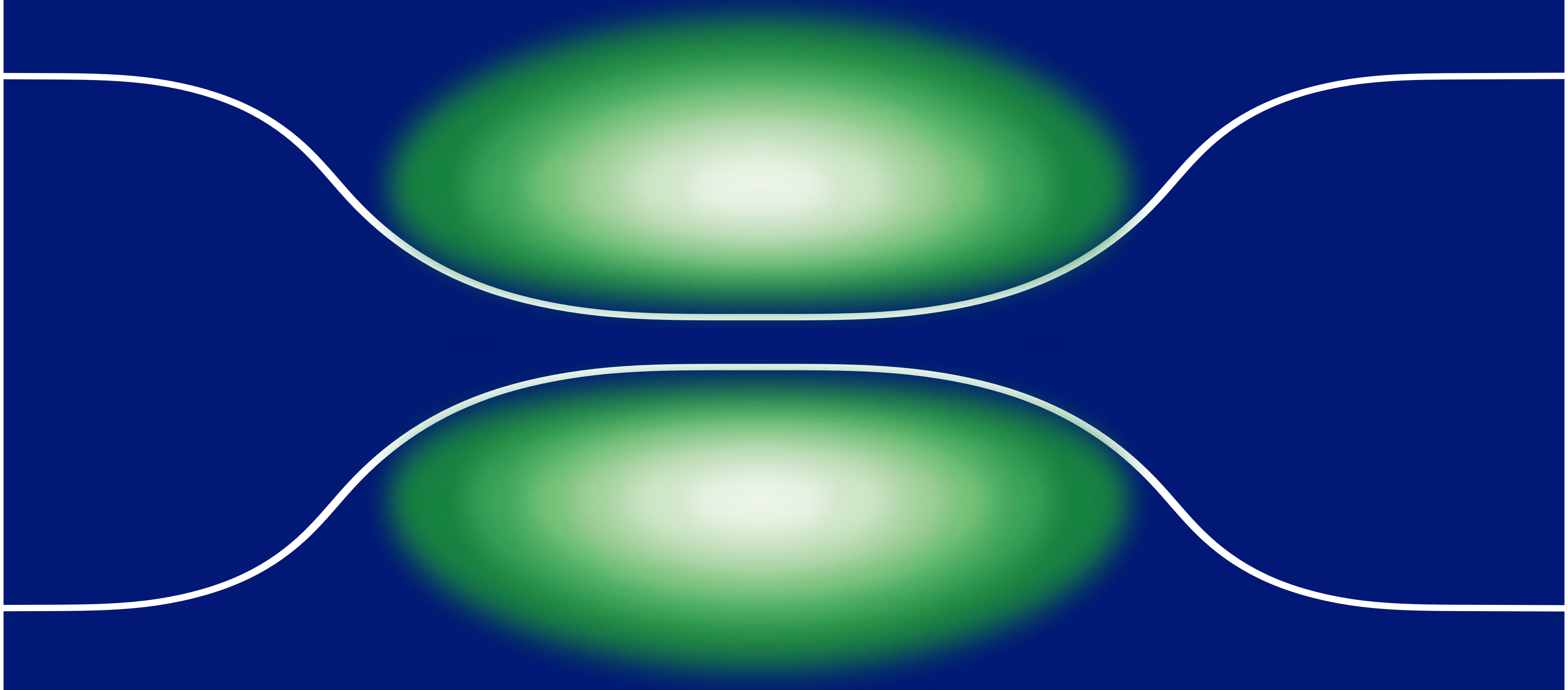
Mesoscopic Conductor: $\boxed{L \ll \ell_{in}, \ell_\phi}$

Ballistic regime: $L \ll \ell_e$ Diffusive regime: $\ell_e \ll L$



Cf. Beenakker and van Houten, arXiv:cond-mat 0412664

BALLISTIC TRANSPORT



Courtesy: Tilman Esslinger, ETHZ

What is the conductance of a perfectly ballistic conductor ? Is it infinite ?

Classically (Ohm's law + Drude) :

$$R = \rho \frac{L}{S} \quad , \quad G = \sigma \frac{S}{L}$$

$$\sigma = 1/\rho = \frac{ne^2 \tau_e}{m} = \frac{ne^2}{m v_F} \ell_e \;\; (\ell_e = v_F \tau_e)$$

$$\Rightarrow G = G_0 \frac{\ell_e}{L} \rightarrow \infty \;\; (L \ll \ell_e)$$

Conductance = Transmission

Rolf Landauer
(1927 Germany - 1999 USA)
IBM fellow

Author in particular of:

- The `Landauer principle' (1961)
(dissipation associated with the
Irreversible manipulation of information)
- The Landauer formula (1957)
Description of quantum transport
as transmission

A wave-like description of transport

The Landauer formula

Conductance as Transmission

- Case of a single conduction `channel' -

$$\mu_L - \mu_R = -e(V_L - V_R)$$

$$\boxed{T = 0: \quad G = \frac{2e^2}{h}\mathcal{T}(\varepsilon_F)}$$

$$T \neq 0: \quad G = \frac{2e^2}{h}\int d\varepsilon\, \mathcal{T}(\varepsilon)\left(-\frac{\partial f}{\partial \varepsilon}\right)$$

$$I = -\frac{2e}{h}\int d\varepsilon\, \mathcal{T}(\varepsilon)\left[f(\varepsilon - \mu_L) - f(\varepsilon - \mu_R)\right]$$

$\mathcal{T}(\varepsilon)$: Energy-dependent transmission coefficient

A simple derivation (1-channel)

→ On blackboard

[cf. Typed notes on website]

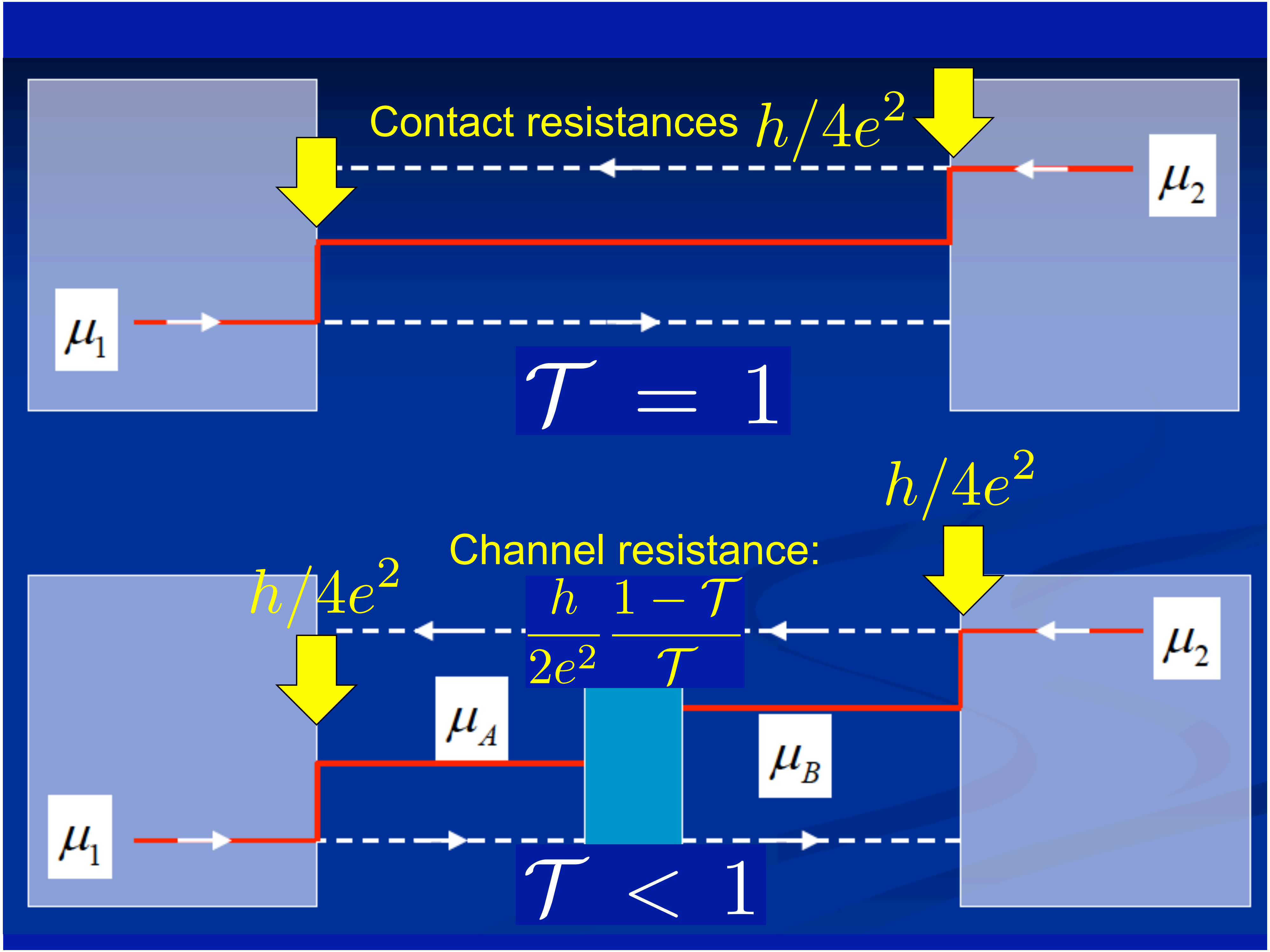
Where does the potential drop ?

The `two' Landauer formulas...

Contact Resistance

(cf. Imry, 1986)

2-probe *vs*. 4-probe conductance



Contact resistances $h/4e^2$
μ_2
μ_1
$\mathcal{T} = 1$
$h/4e^2$
Channel resistance:
$h/4e^2$
$\frac{h}{2e^2}\frac{1-\mathcal{T}}{\mathcal{T}}$
μ_2
μ_A
μ_B
μ_1
$\mathcal{T} < 1$

Landauer formula

$$\frac{h}{4e^2} + \boxed{\frac{h}{2e^2}\frac{1-\mathcal{T}}{\mathcal{T}}} + \frac{h}{4e^2} = \frac{h}{2e^2}\frac{1}{\mathcal{T}}$$

Contact 1 + CHANNEL + Contact 2 = Total

Original 1957
Landauer formula

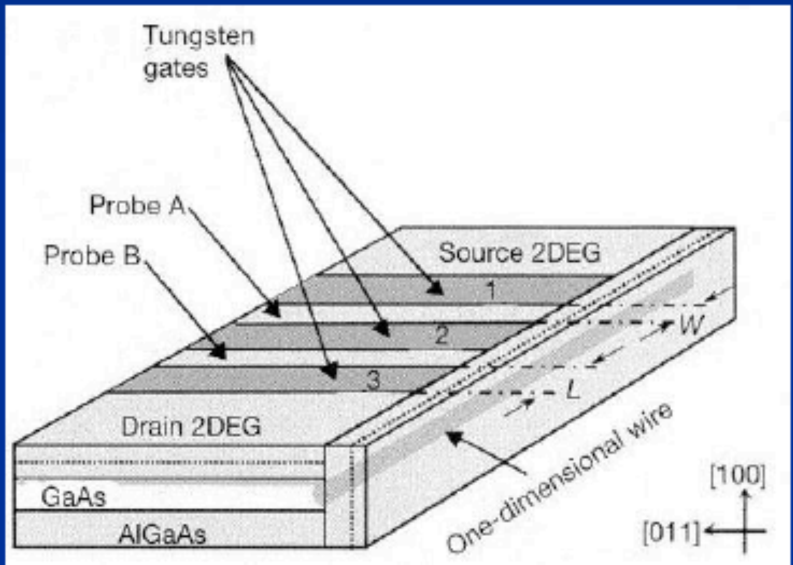
Note: Channel conductance → Infinity for perfect transmission

Four-terminal resistance of a ballistic quantum wire

R. de Picciotto*, H. L. Stormer*†, L. N. Pfeiffer*, K. W. Baldwin* & K. W. West*

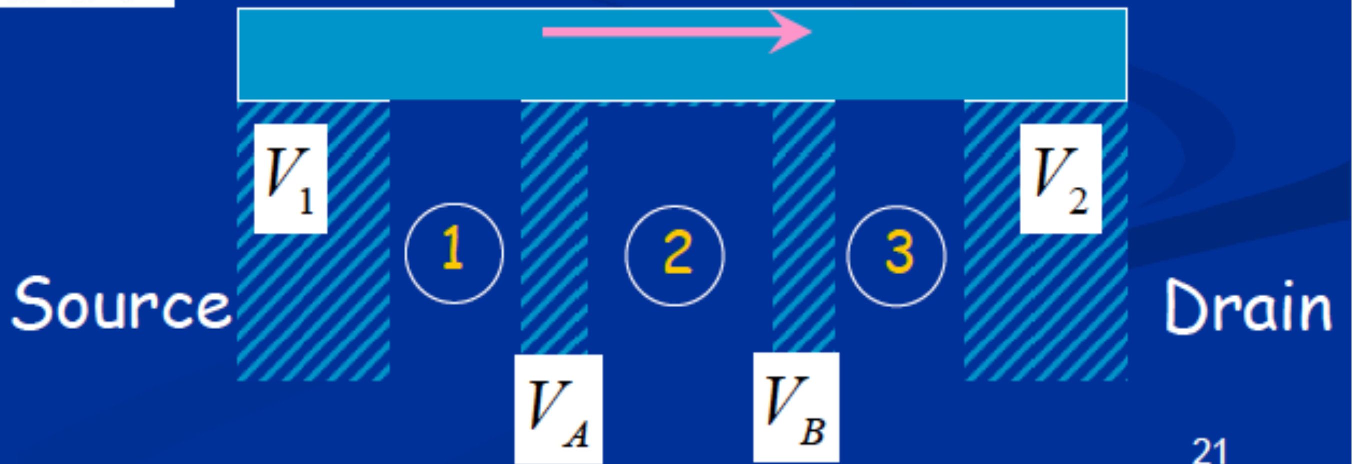
Nature 411, 51 (2001)

** Bell-Labs, Lucent Technologies, Murray Hill, New Jersey 07974, USA*
† Departments of Physics and Applied Physics, Columbia University, New York 10003, USA



$$G_2 = 2\frac{e^2}{h}$$

$$G_4 = \infty$$



Slide: courtesy G.Montambaux

2-terminal conductance is quantized

4-terminal Conductance is infinite

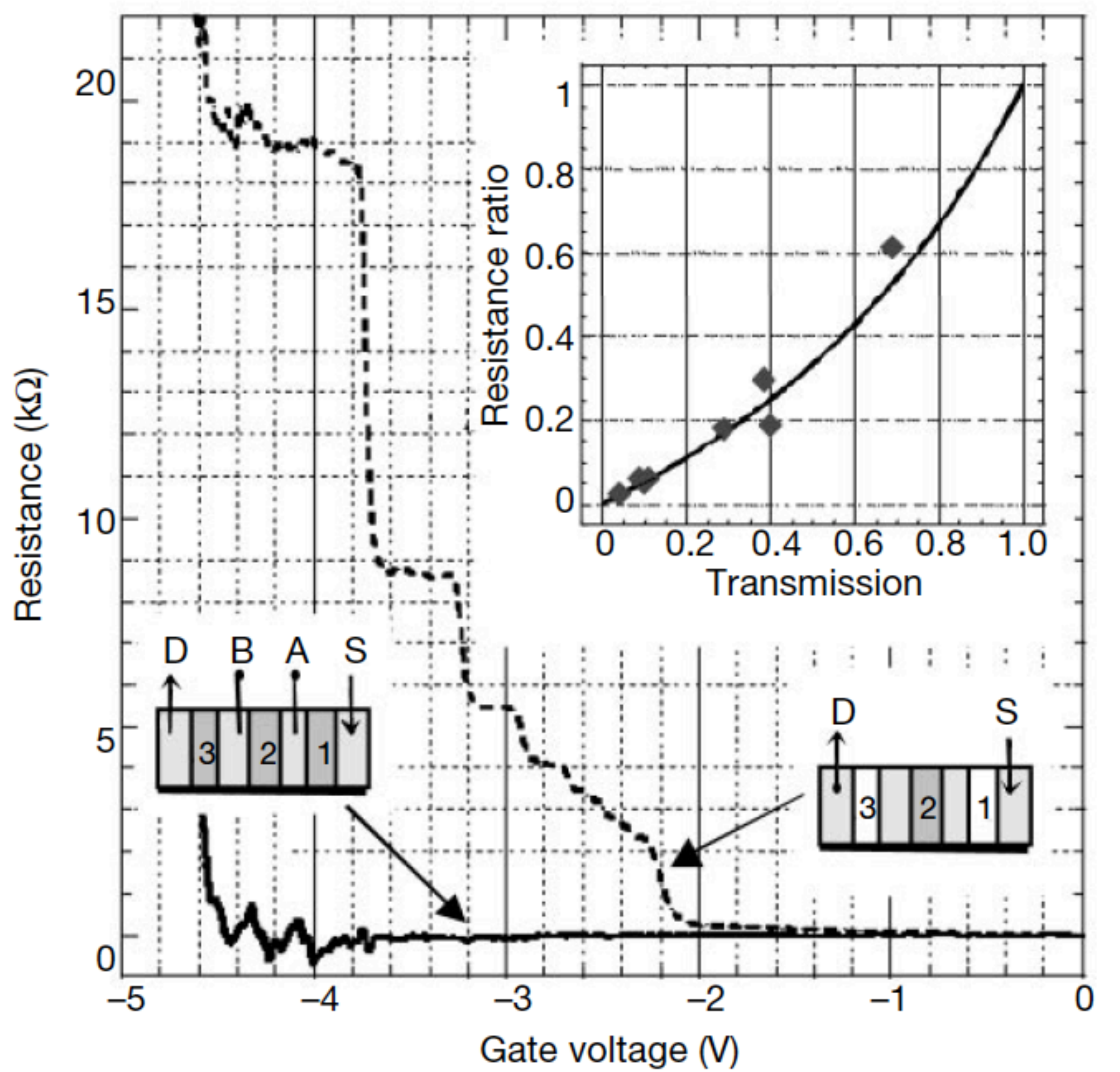
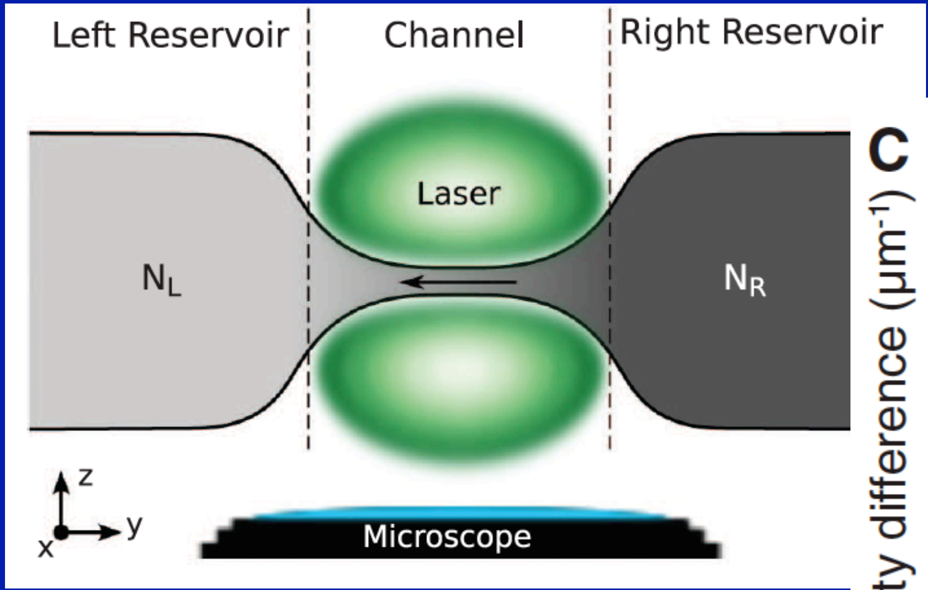
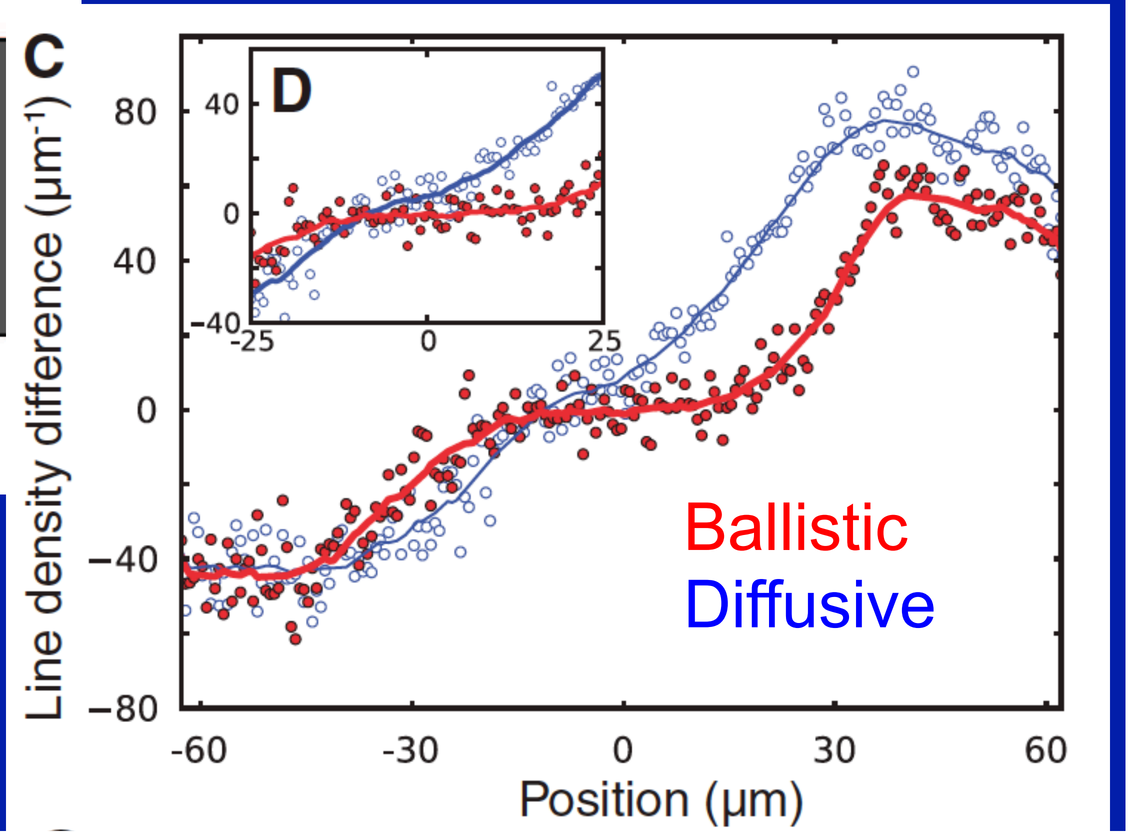


Figure 2 Two- and four-terminal resistances of a ballistic quantum wire. The dashed line shows the two-terminal resistance of the 2-μm-long central section of the wire versus the voltage applied to the associated gate 2. Gates 1 and 3 are not activated. The solid line shows the four-terminal resistance, $(V_A - V_B)/I$, versus the voltage applied to gate 2. Here

Anticipating on the Dec,10 lecture and seminars: ballistic transport in cold atomic gases





Conduction of Ultracold Fermions Through a Mesoscopic Channel
Jean-Philippe Brantut *et al.*
Science **337**, 1069 (2012);
DOI: 10.1126/science.1223175

Multi-Channel Generalization

Transport channel = mode of waveguide

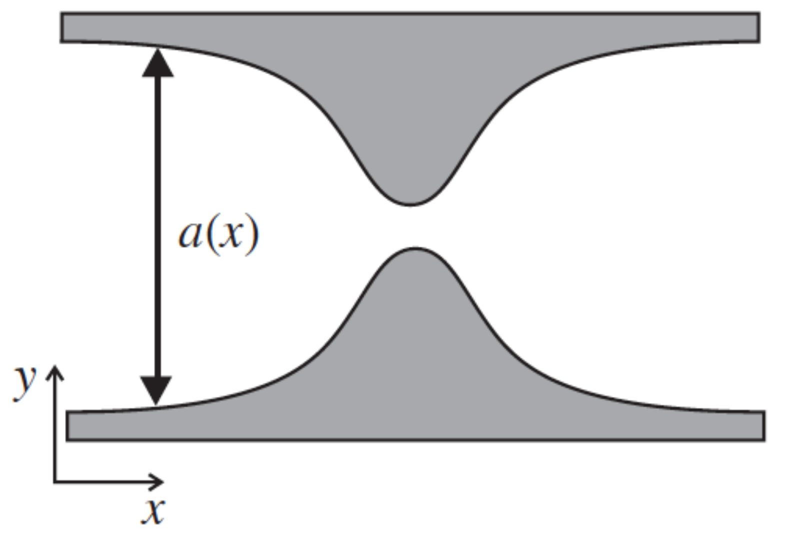
Adiabatic approximation: slow variation of potential along x:

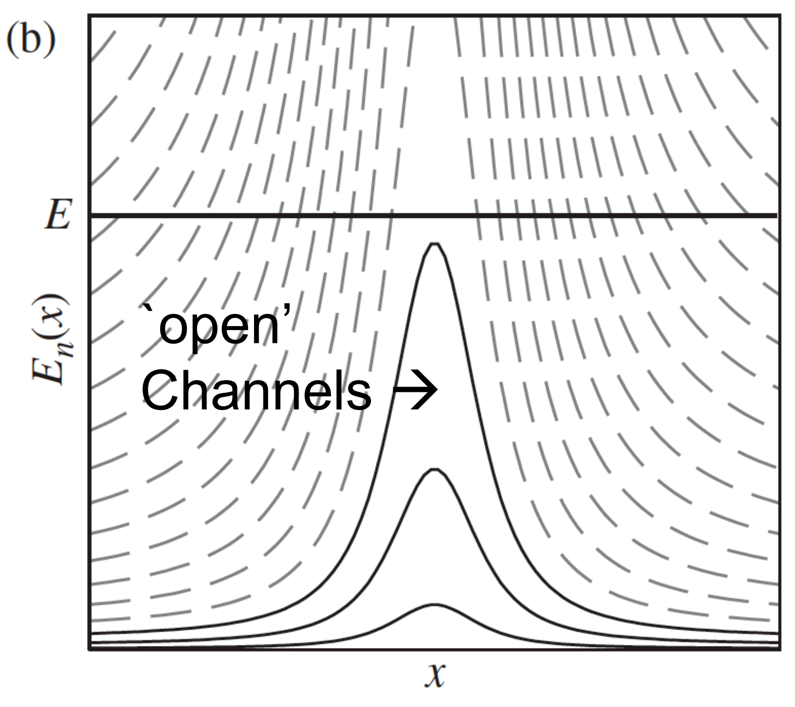
$$\Psi(x,y,z) \simeq \psi(x)\Phi_n(y,z)$$

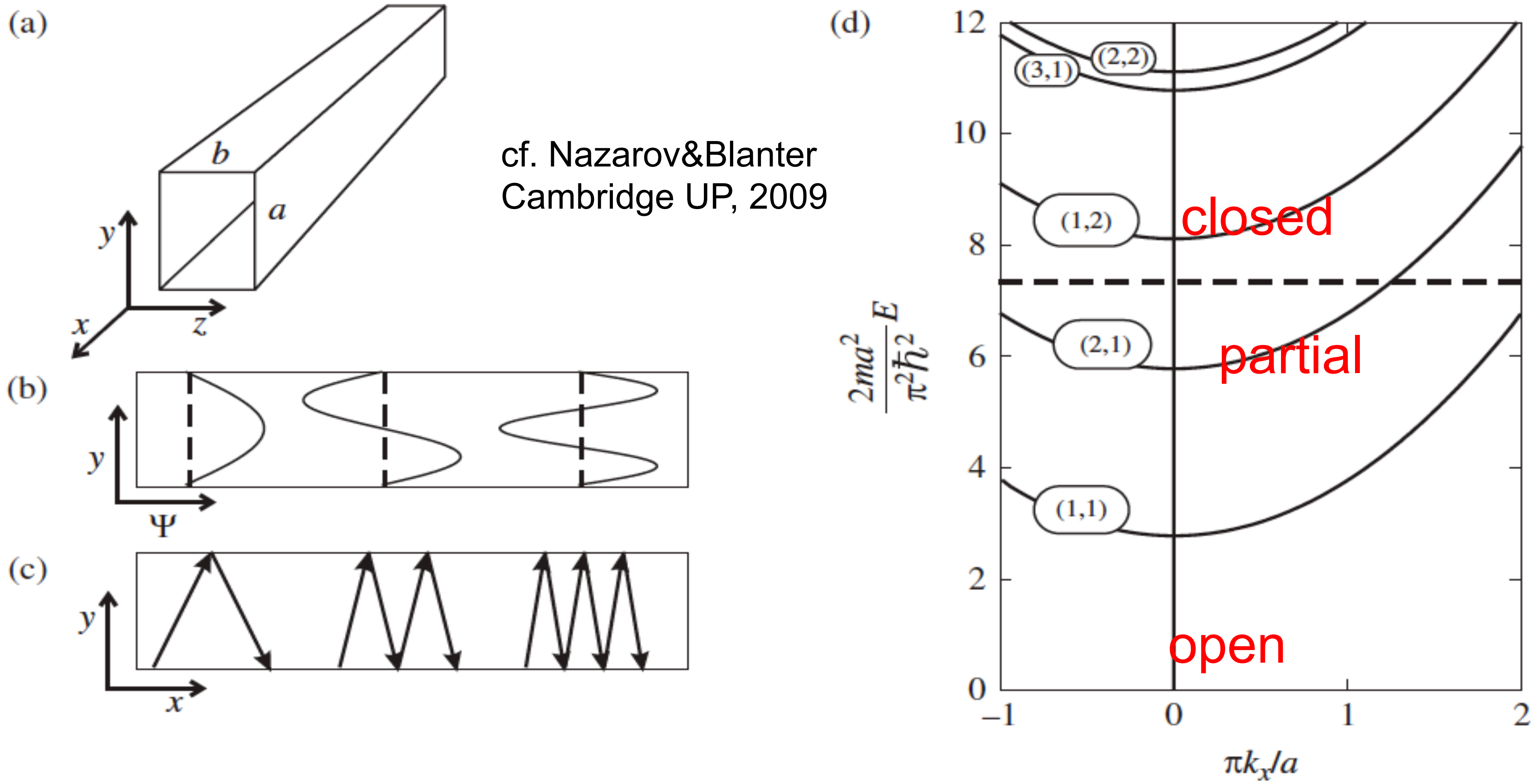
$$-\frac{\hbar^2}{2m}\nabla^2_{y,z}\Phi_n(y,z) + U_x(y,z)\Phi_n(y,z) = \varepsilon_n(x)\Phi_n(y,z)$$

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \varepsilon_n(x)\psi(x) = \varepsilon\,\psi(x)}$$

cf. Nazarov&Blanter
Cambridge UP, 2009







cf. Nazarov&Blanter
Cambridge UP, 2009

$$2D: \quad \varepsilon_n(k_x) = \frac{\hbar^2}{2m}\left[k_x^2 + n^2\left(\frac{\pi}{a}\right)^2\right] \quad (n > 0)$$

$$3D: \quad \varepsilon_{n_y,n_z}(k_x) = \frac{\hbar^2}{2m}\left[k_x^2 + n_y^2\left(\frac{\pi}{a}\right)^2 + n_z^2\left(\frac{\pi}{b}\right)^2\right] \quad (n_y, n_z > 0)$$

Multi-channel Landauer formula

Transmission coefficient for an electron injected in channel m to go into channel n:

$$\mathcal{T}_{nm} = |t_{nm}|^2$$

Each mode n contributes a current proportional to $\sum_m \mathcal{T}_{nm}$

Total current finally involves transmission coefficient:

$$\boxed{\begin{aligned} \mathcal{T}(\varepsilon) &= \sum_{nm} \mathcal{T}_{nm} = \sum_{nm} t_{nm} t^*_{nm} = \mathrm{Tr}\, tt^\dagger \\ &= \sum_\lambda \mathcal{T}_\lambda \quad \text{sum of eigenvalues of } tt^+ \text{ matrix} \end{aligned}}$$

Notes on Thermoelectricity of Small Systems - Collège de France - Fall 2013

Antoine Georges

(Dated: Notes complementing lecture 1 - Nov 5, 2013)

Note: These are by no means intended as a self-contained set of notes. Instead, they are merely complements to the slides, covering the material presented in the blackboard during the lectures.

I. CONDUCTANCE AS TRANSMISSION: THE LANDAUER FORMULA

Useful books: Nazarov and Blanter[2], Montambaux[1].

A. Simple derivation for a single one-dimensional channel

Consider an incident wave coming from the left reservoir, which is partially reflected and partially transmitted, so that on the left side:

$$\psi_L(x) = \frac{1}{\sqrt{L}}\left[e^{+ikx} + r\,e^{-ikx}\right] \tag{1}$$

with r the reflection coefficient for the amplitude (a complex number in general). The corresponding particle current density reads:

$$\boldsymbol{j}_n \,=\, \frac{\hbar}{m}\,\mathrm{Re}\left[\frac{1}{i}\psi^*\partial_x\psi\right] \,=\, \frac{\hbar k}{mL}\,(1-|r|^2) \tag{2}$$

We could also have calculated the current from the transmitted wave:

$$\psi_R(x) \,=\, t\,\frac{1}{\sqrt{L}}\,e^{+ikx} \;\Rightarrow\; \boldsymbol{j}_n \,=\, \frac{\hbar k}{mL}\,|t|^2 \tag{3}$$

These two expressions are equivalent since the reflection and transmission coefficients for *probabilities* add up to unity:

$$\mathcal{R} \equiv |r|^2 \;\;,\;\; \mathcal{T} \equiv |t|^2 \;\;,\;\; \mathcal{R} + \mathcal{T} \,=\, 1 \tag{4}$$

The total current is the difference between the current originating from the left reservoir and that originating from the right reservoir (for a single-channel, the transmission coefficient in both cases is $\mathcal{T}$, see below):

$$I \,=\, 2_{spin}\,(-e)\,\frac{1}{L}\sum_{k>0}\frac{\hbar k}{m}\,\mathcal{T}(\varepsilon_k)\;[f(\varepsilon_k-\mu_L) - f(\varepsilon_k-\mu_R)] \tag{5}$$

We note that (beware of the subtleties with factors of 2: we consider only right-moving modes with $k > 0$!):

$$\frac{1}{L}\sum_{k>0}\frac{\hbar k}{m}\phi(\varepsilon_k) \to \int_0^{+\infty}\frac{dk}{2\pi}\,\frac{\hbar k}{m}\phi(\varepsilon_k) \,=\, \int d\varepsilon\,\frac{1}{2\pi\hbar}\,\phi(\varepsilon) \tag{6}$$

So that one finally gets:

$$\boxed{I \,=\, -\frac{2e}{h}\int d\varepsilon\,\mathcal{T}(\varepsilon)\;[f(\varepsilon-\mu_L) - f(\varepsilon-\mu_R)]} \tag{7}$$

This formula is actually valid for an arbitrary dispersion $\varepsilon(k_x)$, since the associated velocity reads $v_k = \frac{1}{\hbar}\frac{\partial\varepsilon_k}{\partial k}$ and $\int\frac{dk}{2\pi}\,v_k \to \int\frac{d\varepsilon}{h}$: the density of states does not appear in the final expression !

We recall - see the lectures of spring 2013 - that the (electro-) chemical potential difference is related to the tension between the left and right reservoirs by:

$$\mu_L - \mu_R = -eV \tag{8}$$

A common chemical potential can be defined such that:

$$\mu_L = \mu + \delta\mu_L \ , \ \mu_L = \mu + \delta\mu_R \ , \ \delta\mu_L - \delta\mu_R = -eV \tag{9}$$

The linear-response conductance is thus given by ($I = G\,V$):

$$\boxed{G = \frac{2e^2}{h}\int d\varepsilon\,\mathcal{T}(\varepsilon)\left(-\frac{\partial f}{\partial \varepsilon}\right) \quad , \quad G(T=0) = \frac{2e^2}{h}\,\mathcal{T}(\varepsilon_F)} \tag{10}$$

Quantum of resistance:

$$\boxed{R_Q \equiv \frac{h}{e^2} = 25.812807449(86)\,k\Omega} \tag{11}$$

The remarkable point is of course that a perfect 1-channel ballistic conductor does not have infinite conductance, but rather a conductance $2e^2/h$!

B. Where does the potential drop? Contact resistance.

Let us consider a 4-probe geometry as in the slides. We are going to evaluate the electron number at point A in two possible ways. By assuming local equilibrium at a local chemical potential μ_A. Or by stating that the electrons at A are either thos coming from the left reservoir and having undergone a reflexion of those coming from the right reservoir and having been transmitted. Thus:

$$\begin{aligned} N_A &= 2\sum_{k>0}\left[(1+\mathcal{R})f(\varepsilon_k-\mu_L) + \mathcal{T}f(\varepsilon_k-\mu_R)\right] \\ &= 2\sum_{k} f(\varepsilon_k - \mu_A) \end{aligned} \tag{12}$$

Beware that the first sum runs over $k > 0$ while the second one runs over all k's ! And $\sum_k = 2\sum_{k>0}$. Expanding for small departures from equilibrium, one obtains:

$$(1+\mathcal{R}+\mathcal{T})f(\varepsilon-\mu) + [(1+\mathcal{R})\delta\mu_L + \mathcal{T}\delta\mu_R]\left(-\frac{\partial f}{\partial \mu}\right) = 2f(\varepsilon-\mu) + \delta\mu_A\left(-\frac{\partial f}{\partial \mu}\right) \tag{13}$$

Hence (similar reasoning for B):

$$2\delta\mu_A = (1+\mathcal{R})\delta\mu_L + \mathcal{T}\delta\mu_R \ , \ 2\delta\mu_B = \mathcal{T}\delta\mu_L + (1+\mathcal{R})\delta\mu_R \tag{14}$$

So that the potential drop in the channel is given by:

$$\mu_A - \mu_B = \mathcal{R}\,(\mu_L - \mu_R) \tag{15}$$

Using the Landauer formula for the whole system: $V_L - V_R = \frac{h}{2e^2}\frac{1}{\mathcal{T}}I$, we obtain the conductance of the channel as (first Landauer formula, 1957):

$$\boxed{G_{ch} = \frac{2e^2}{h}\frac{\mathcal{T}}{\mathcal{R}} = \frac{2e^2}{h}\frac{\mathcal{T}}{1-\mathcal{T}}} \tag{16}$$

Calculating the potential drops at the contact $\mu_A - \mu_L$, we obtain that they are equal on each side, and that the resistance of each contact is given by:

$$\boxed{R_c = \frac{h}{4e^2}} \tag{17}$$

We check that $R_c + R_{ch} + R_c = 1/G = \frac{h}{2e^2}$.

[1] G. Montambaux, *Conduction quantique et physique mésoscopique*, Cours de l'Ecole Polytechnique, 2013.
[2] Yu. V. Nazarov and Blanter Y., *Quantum transport - introduction to nanoscience*, Cambridge University Press, 2009.