Chaire de Physique de la Matière Condensée

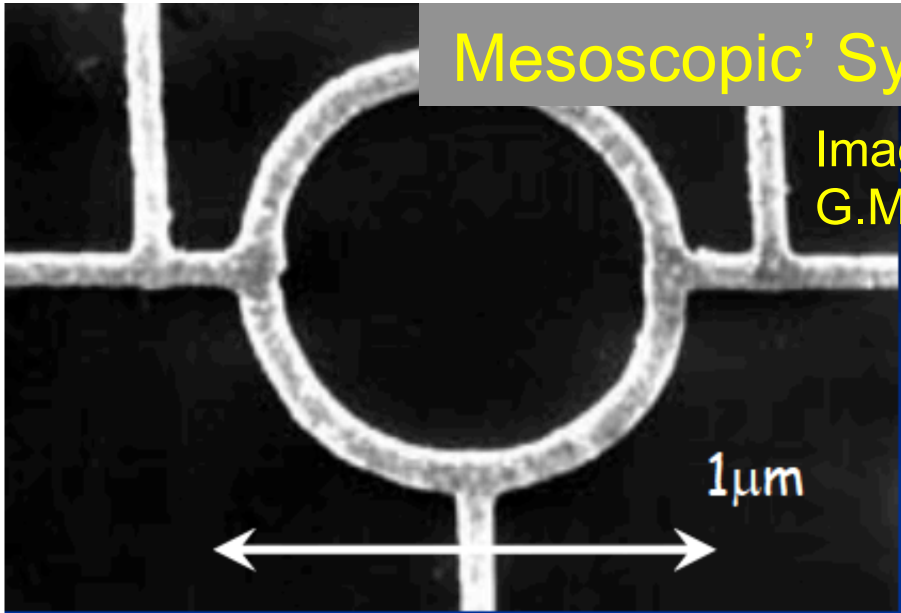
III.2 Systèmes mésoscopiques: coefficients thermoélectriques dans le formalisme de Landauer-Büttiker et quelques exemples

Antoine Georges

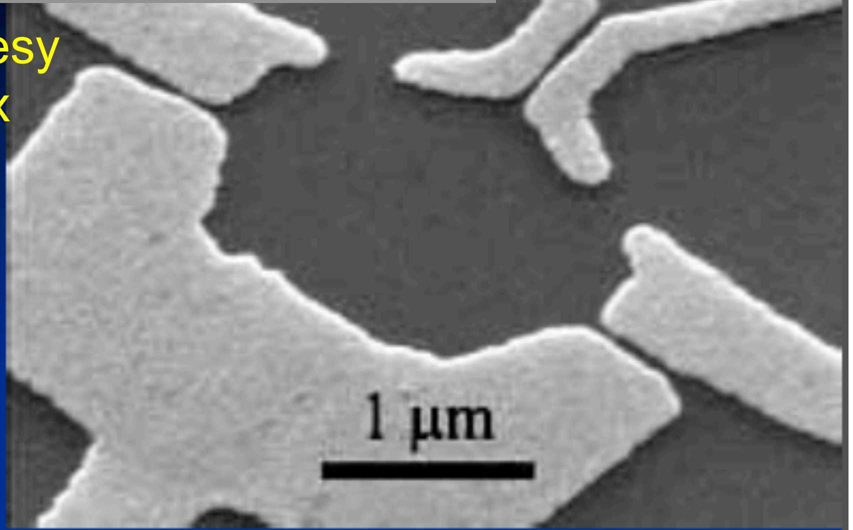
Cycle 2014-2015
1er juin 2015 – III.2

Mesoscopic' Systems: Some Examples

Images: Courtesy G.Montambaux

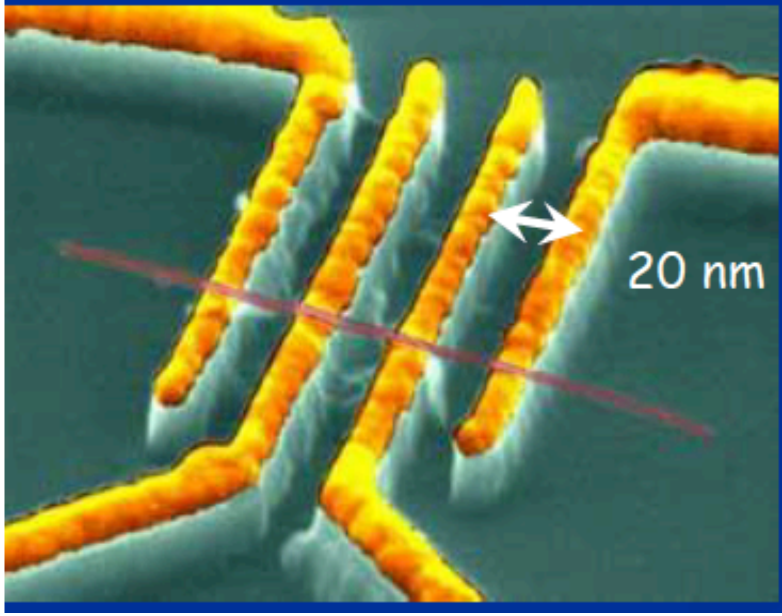


anneau métallique Cu

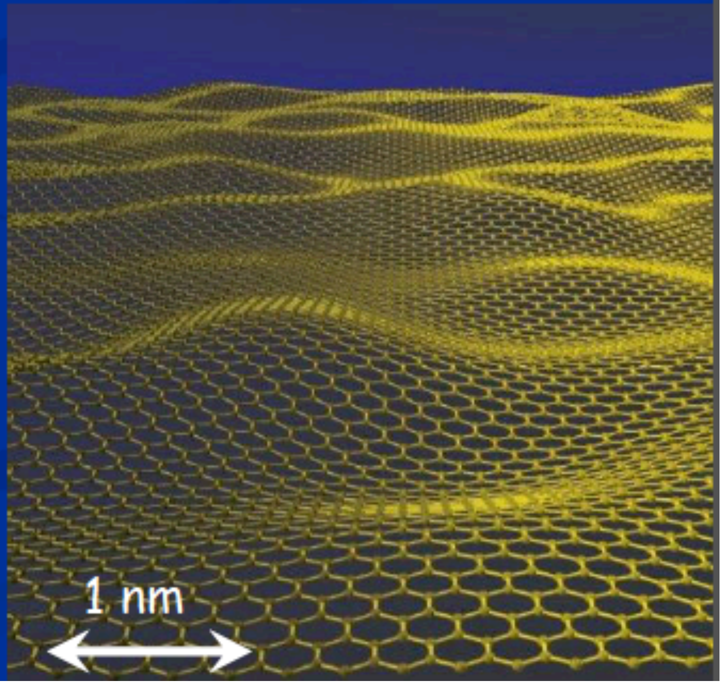


Gaz 2D, semiconducteur (AlGaAs)

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 $\sim k_B T$)

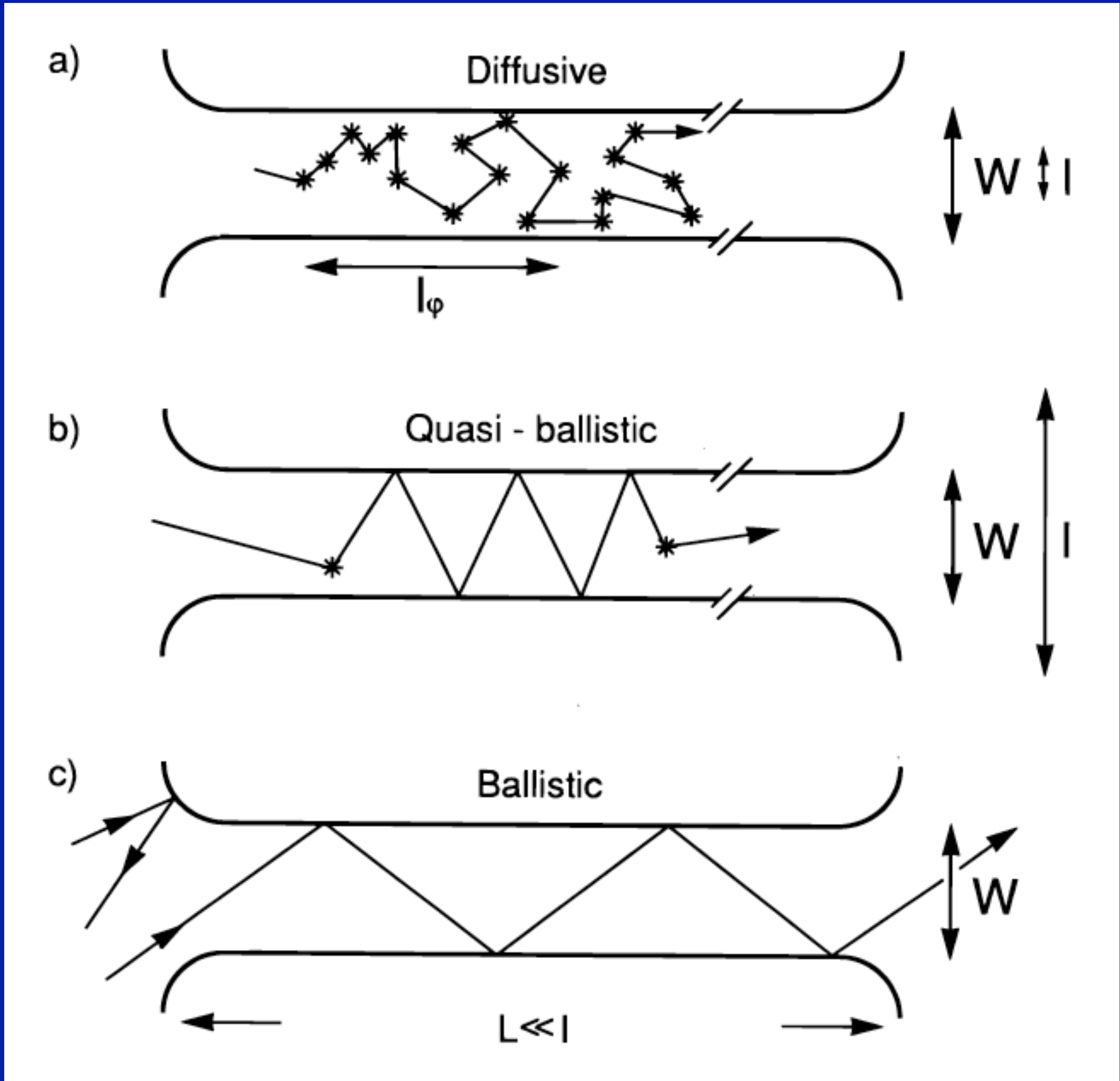
Elastic scattering length: ℓ_e (10-10^3 nm)

(Distance an electron travels between elastic scattering events)

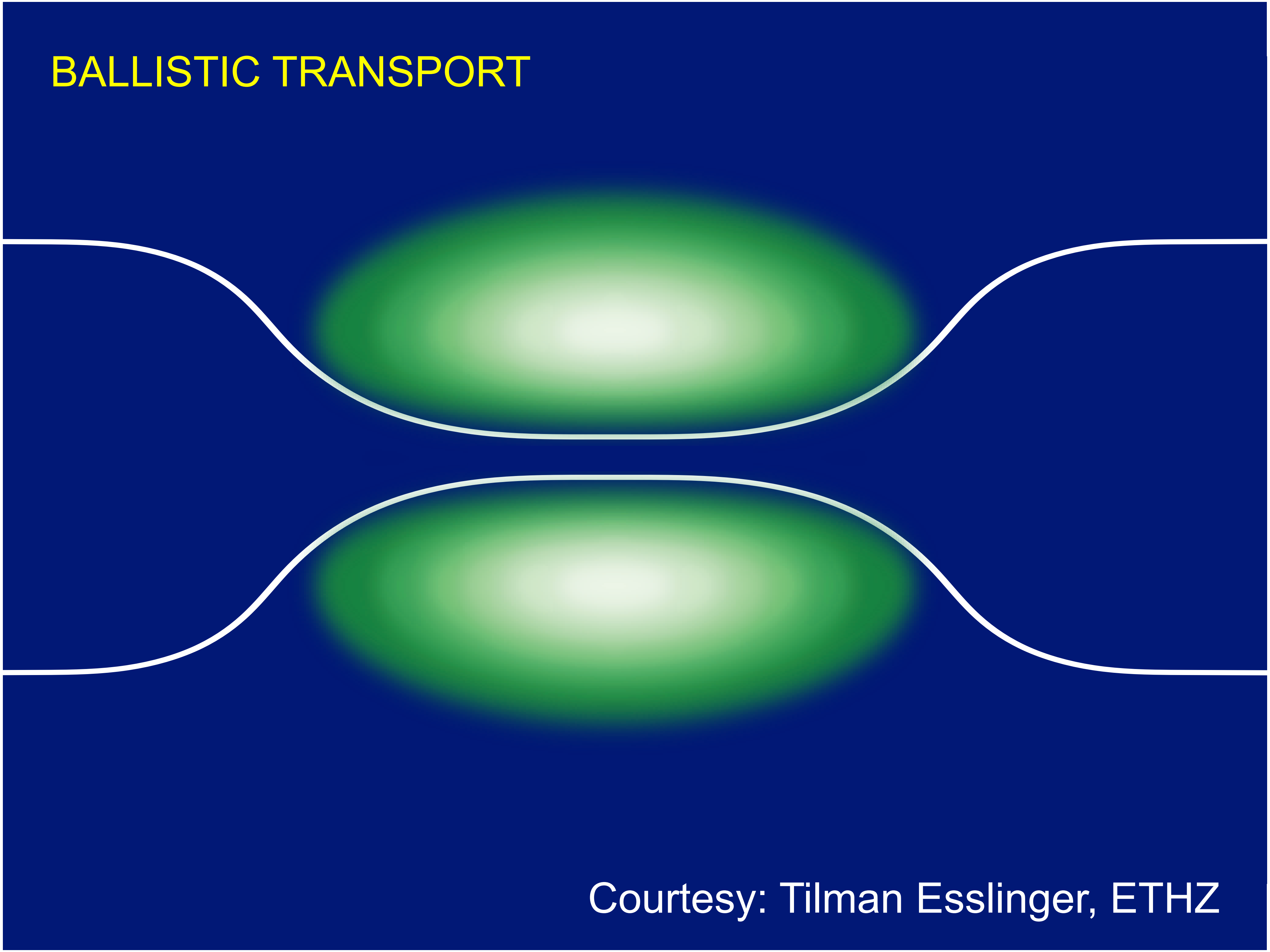
Macroscopic Conductor: $\ell_e \ll \ell_{in}, \ell_\phi \ll L$

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

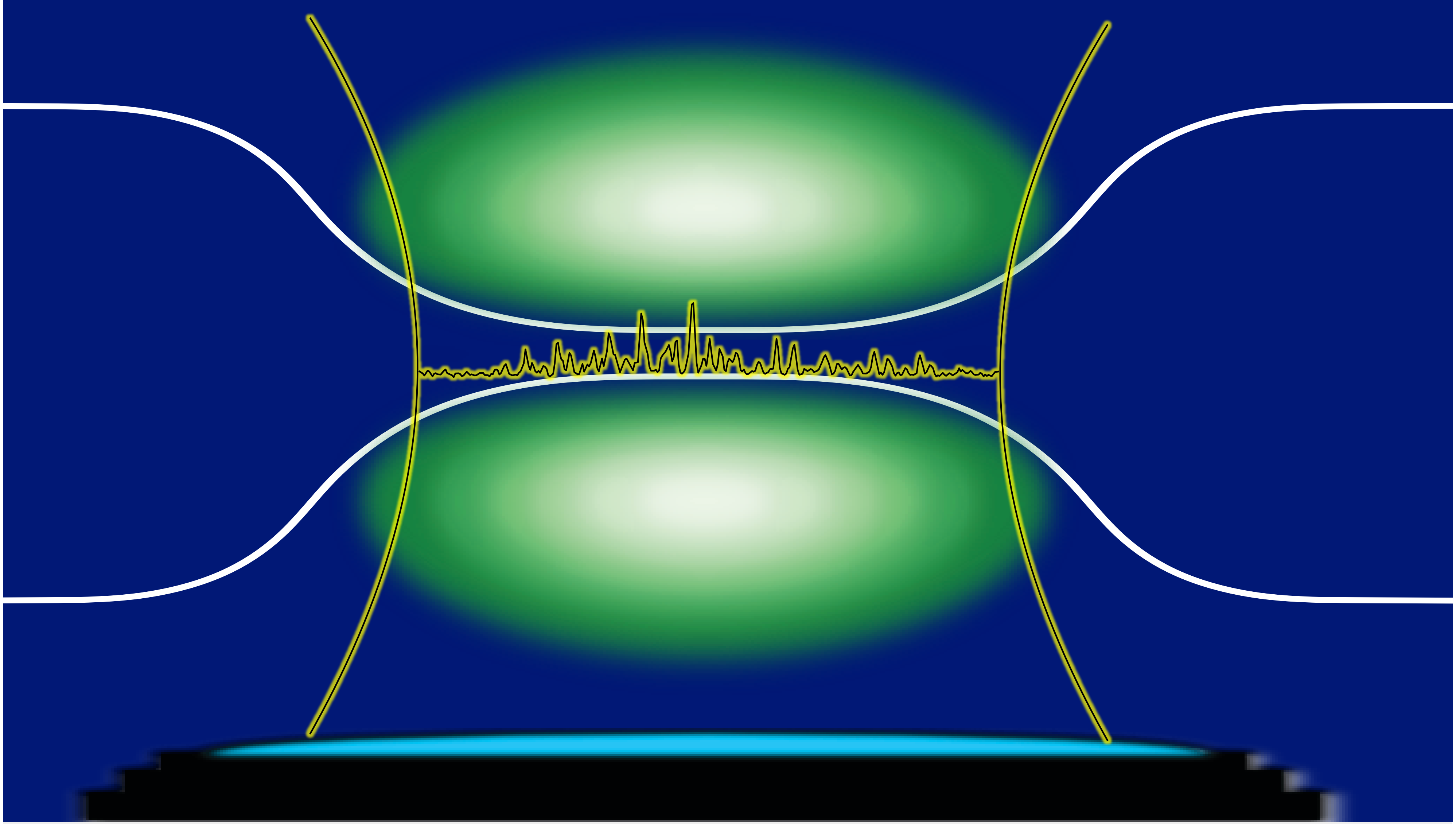
Ballistic regime: $L \ll \ell_e$ Diffusive regime: $\ell_e \ll L$



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


BALLISTIC TRANSPORT
Courtesy: Tilman Esslinger, ETHZ

scattering (impurities→ random potential): diffusive



See use of specle in experiments by: Aspect, Inguscio, Hulet, DeMarco

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

Classically (Ohm’s law + Drude) :

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

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

$$\Rightarrow G = G_0 \frac{\ell_e}{L} \to \infty \quad (L \ll \ell_e)$$

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' -

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

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

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

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

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

A simple derivation (1-channel)

→ Notes on College de France website (2013-2014 lectures)

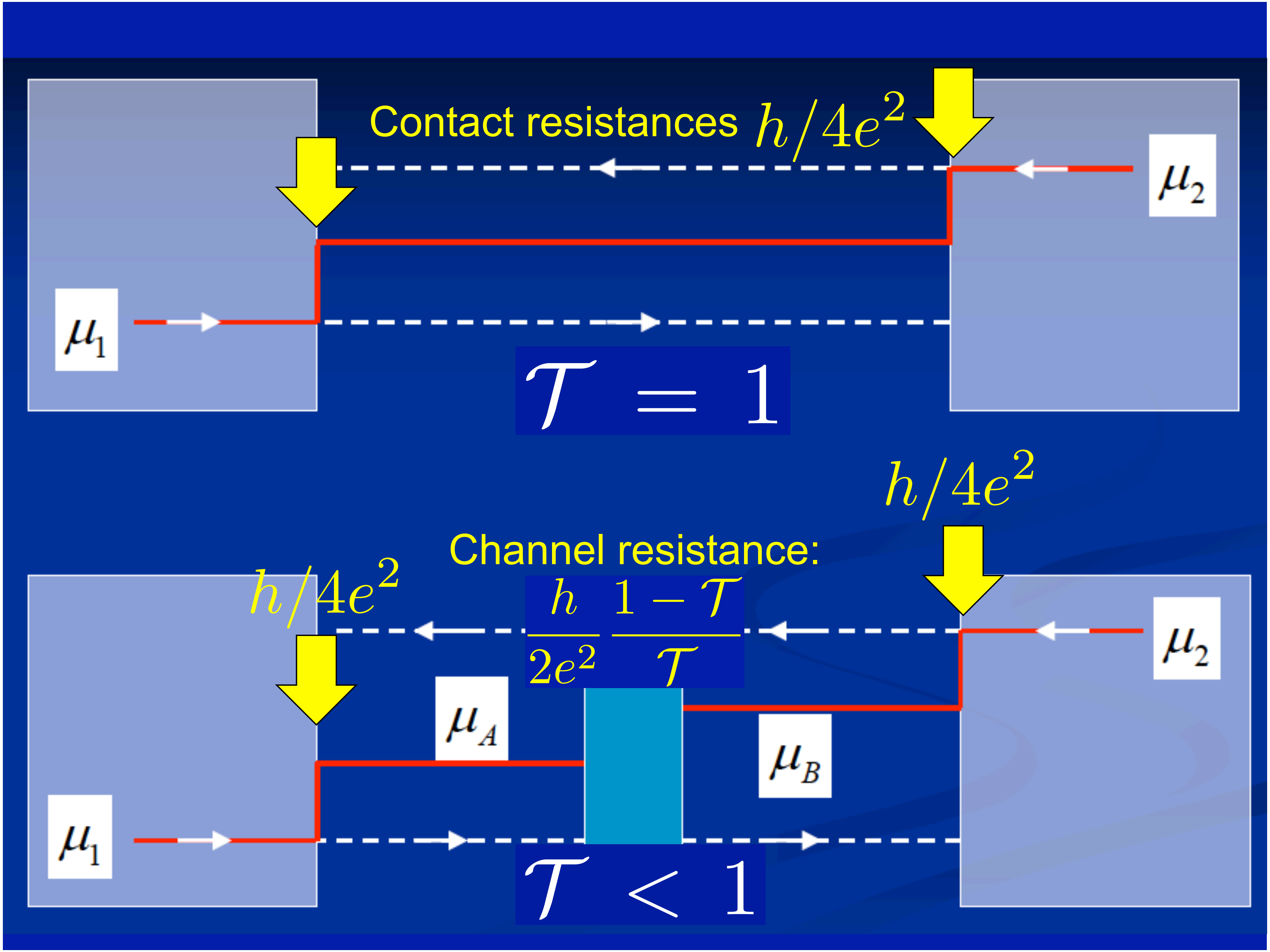
Where does the potential drop ?

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

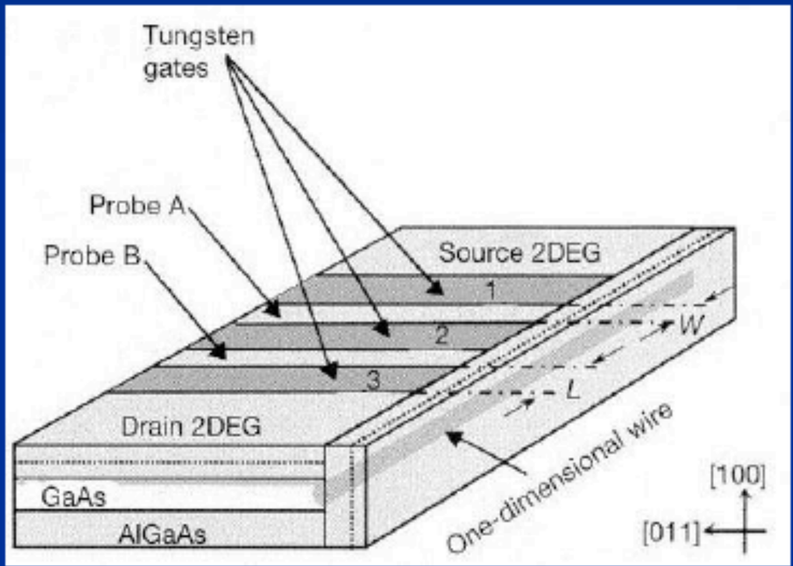
Note: Channel conductance → Infinity for perfect transmission

Four-terminal resistance of a ballistic quantum wire

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

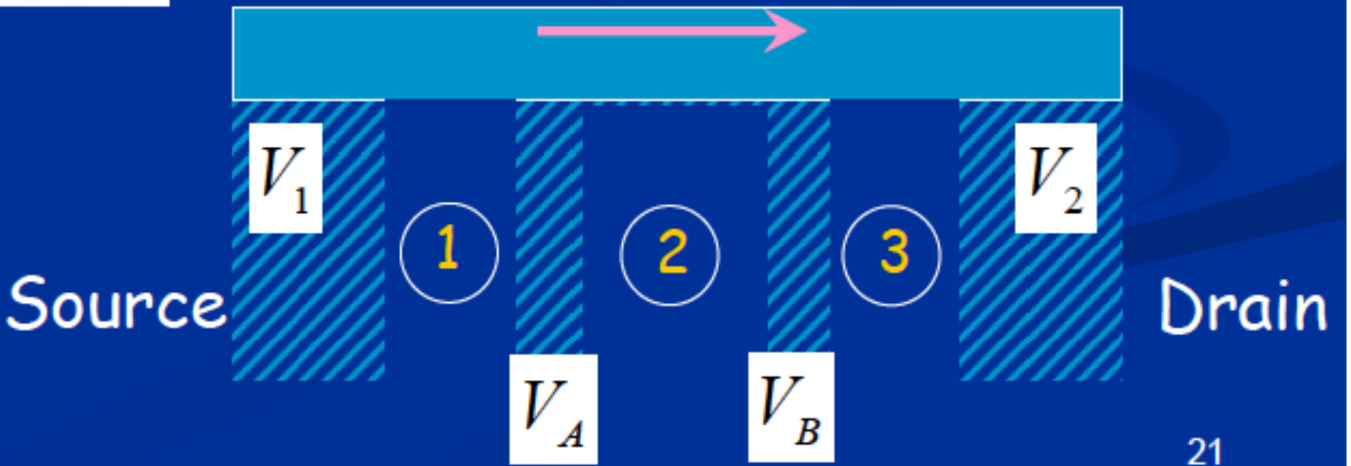
Bell-Labs, Lucent Technologies, Murray Hill, New Jersey 07974, USA
† Departments of Physics and Applied Physics, Columbia University, New York 10003, USA

Nature 411, 51 (2001)



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

$$G_4 = \infty$$



Slide: courtesy G.Montambaux

2-terminal conductance is quantized

4-terminal Conductance is infinite

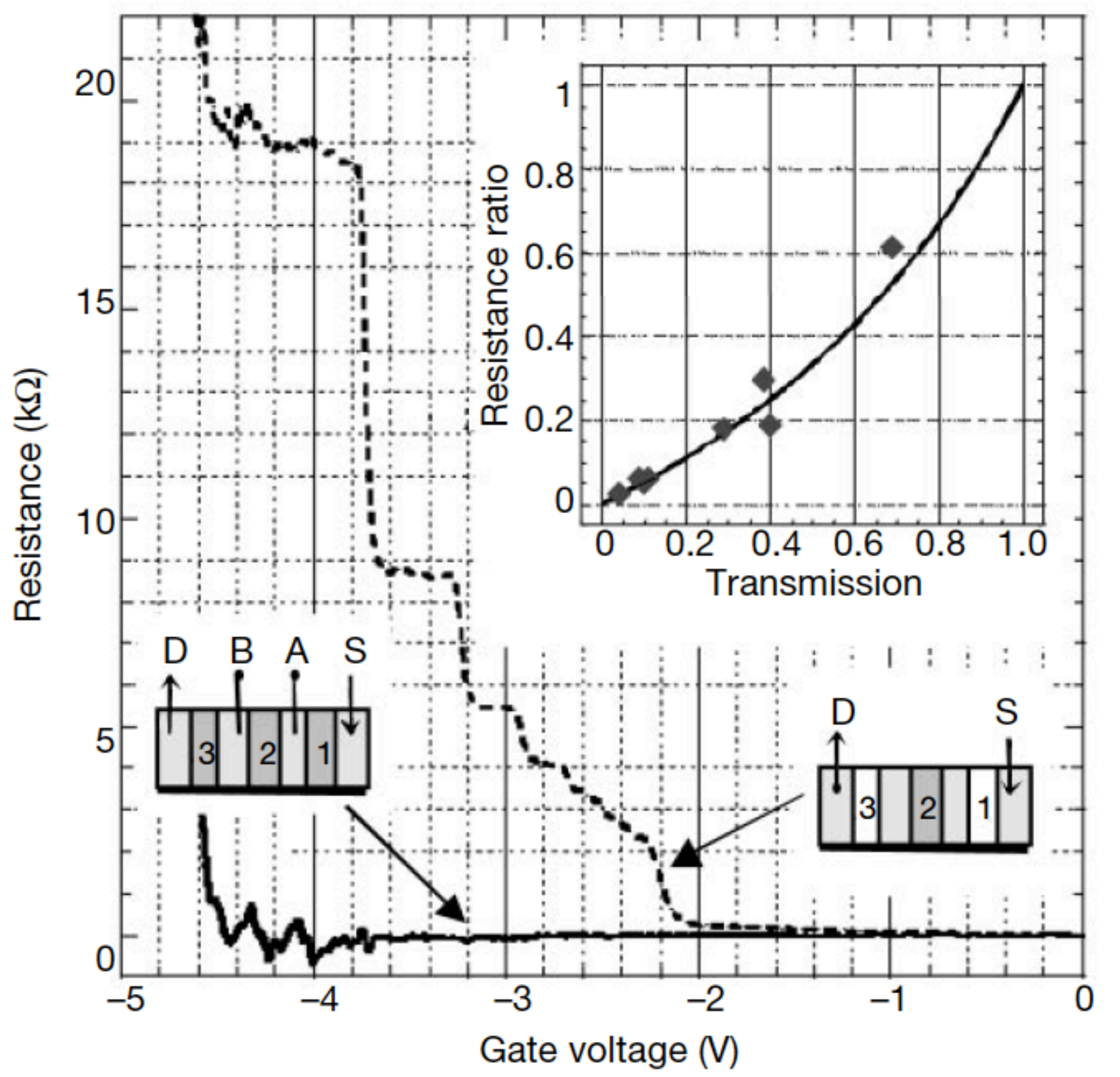
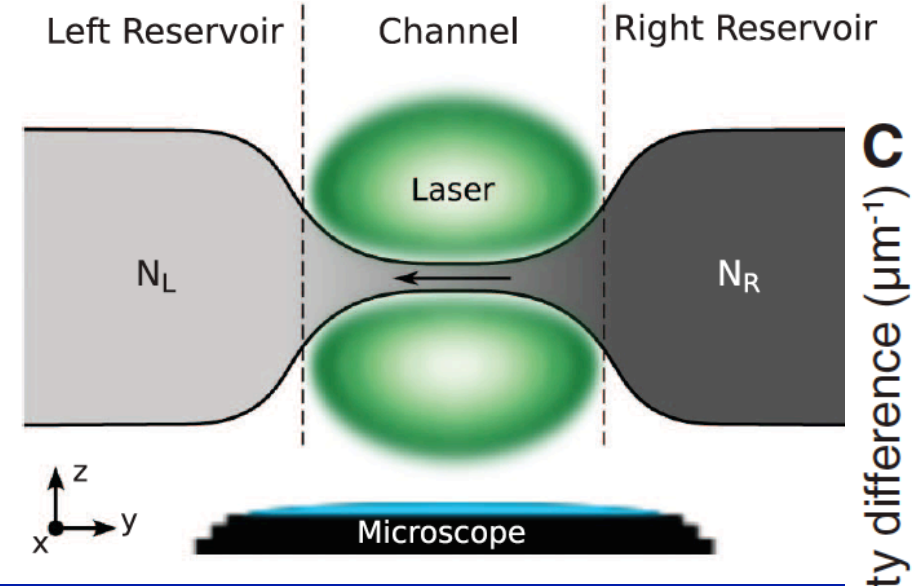
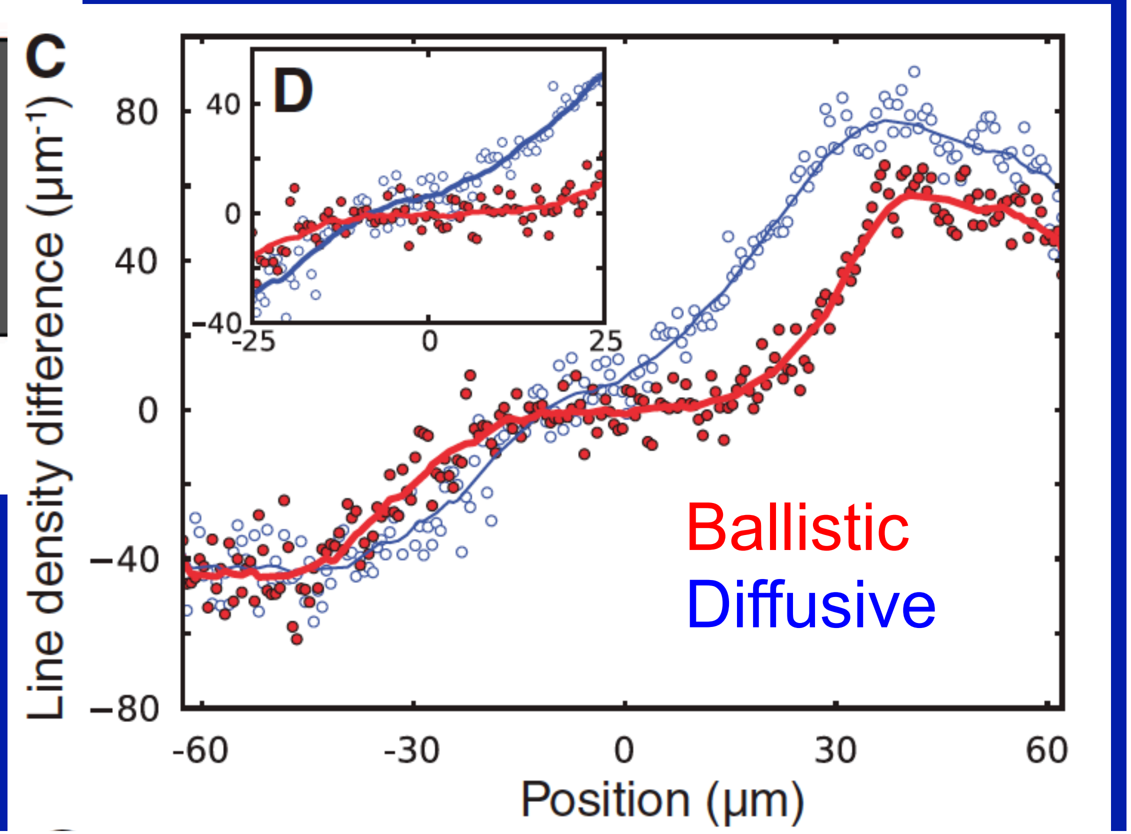


Figure 2 Two- and four-terminal resistances of a ballistic quantum wire. The dashed line shows the two-terminal resistance of the 2-μm-long central section of the wire versus the voltage applied to the associated gate 2. Gates 1 and 3 are not activated. The solid line shows the four-terminal resistance,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

Anticipating on the following lecture: 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

Generalization of the Landauer formula to thermoelectric transport

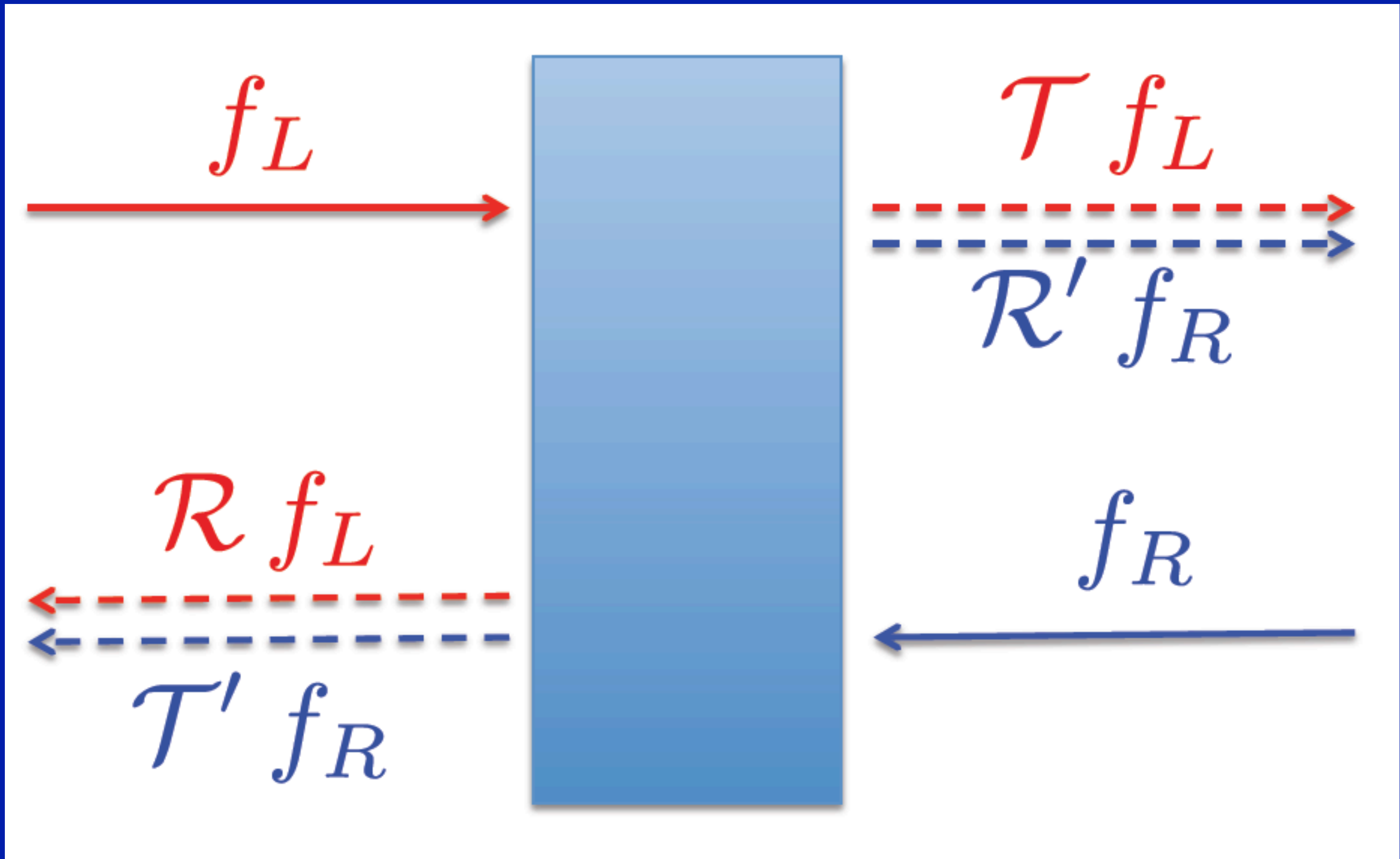
Thermal: HL Engquist and PW Anderson Phys Rev B 24, 1151 (1981)

Thermoelectric effects:
U.Sivan and Y.Imry Phys Rev B 33, 551 (1986)
P.N. Butcher J. Phys Cond Matt 2, 4869 (1990)

Particle, Energy and Entropy Currents

For a detailed discussion, see notes

Reconsidering the entropy current…



Linear Response Regime:

$$\frac{\partial}{\partial \mu} f\left(\frac{\varepsilon-\mu}{k_B T}\right) = \left(-\frac{\partial f}{\partial \varepsilon}\right) \;,\; \frac{\partial}{\partial T} f\left(\frac{\varepsilon-\mu}{k_B T}\right) = \frac{\varepsilon-\mu}{T}\left(-\frac{\partial f}{\partial \varepsilon}\right)$$

$$\frac{\partial}{\partial \alpha} s = \frac{\partial s}{\partial f}\frac{\partial}{\partial \alpha} f = [-k_B \ln \frac{f}{1-f}]\frac{\partial}{\partial \alpha} f = \frac{\varepsilon-\mu}{T}\frac{\partial}{\partial \alpha} f$$

$$\begin{aligned} I_N &= \frac{2}{h}\int d\varepsilon\, \mathcal{T}(\varepsilon)\left[\Delta\mu + \frac{\varepsilon-\mu}{T}\Delta T\right]\left(-\frac{\partial f}{\partial \varepsilon}\right) \\ I_S &= \frac{2}{h}\int d\varepsilon\, \mathcal{T}(\varepsilon)\left[\frac{\varepsilon-\mu}{T}\Delta\mu + \left(\frac{\varepsilon-\mu}{T}\right)^2 \Delta T\right]\left(-\frac{\partial f}{\partial \varepsilon}\right) \end{aligned}$$

From which we immediately identify the Onsager coefficients defined as (cf 2012-2013 lectures):

$$\begin{pmatrix} I_N \\ I_S \end{pmatrix} = \begin{pmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{pmatrix}\begin{pmatrix} \Delta\mu \\ \Delta T \end{pmatrix}$$

$$L_{11} = \frac{2}{h} I_0 \;,\; L_{12} = L_{21} = \frac{2}{h} k_B I_1 \;,\; L_{22} = \frac{2}{h} k_B^2 I_2$$

in which the *dimensionless* integrals read:

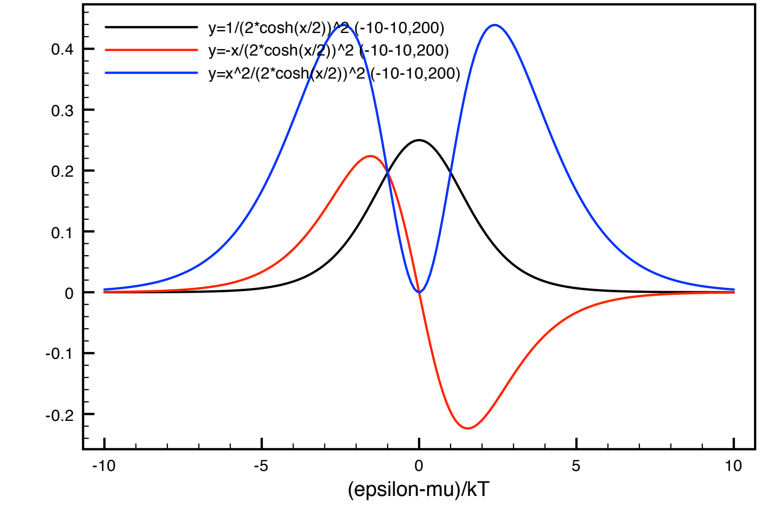
$$I_n \equiv \int d\varepsilon\, \mathcal{T}(\varepsilon)\left(\frac{\varepsilon-\mu}{kT}\right)^n\left(-\frac{\partial f}{\partial \varepsilon}\right)$$

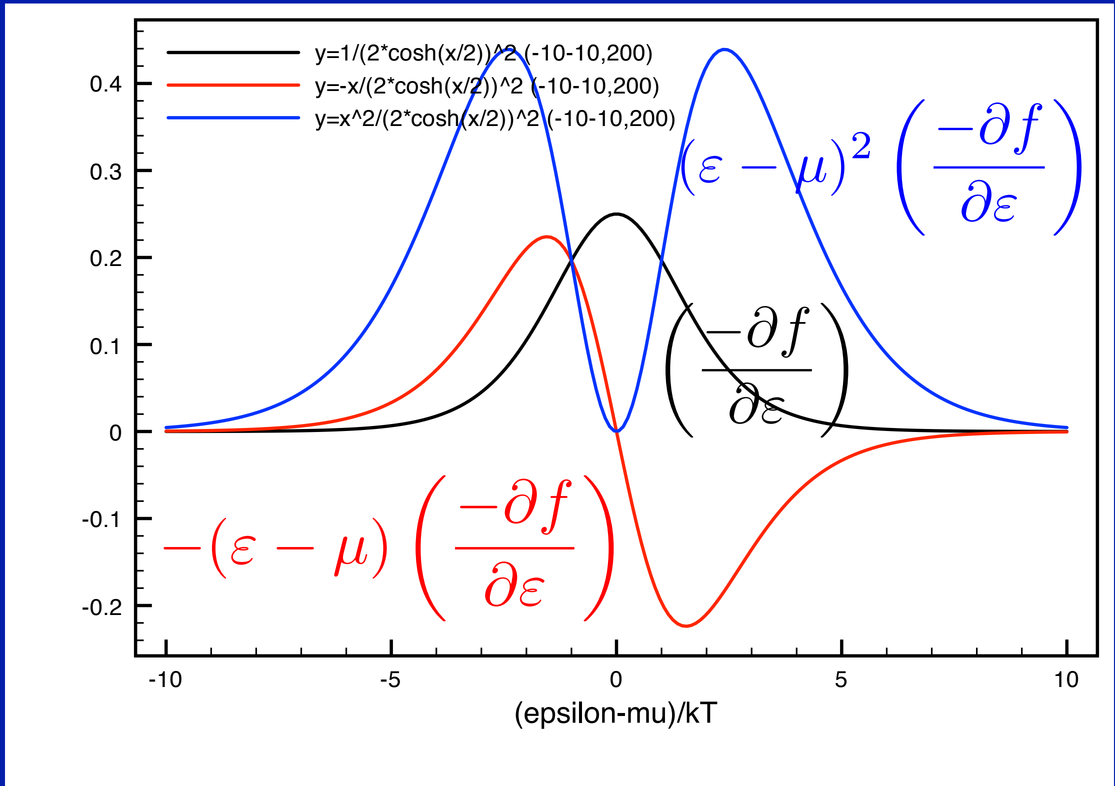
Conductance, Thermopower and Thermal Conductance:

$$\boxed{\begin{aligned}
G &= \frac{2e^2}{h} I_0 \;, \quad \left(\frac{h}{e^2} = 25.81 k\Omega \right) \\
\alpha &= -\frac{k_B}{e} \frac{I_1}{I_0} \;, \quad \left(\frac{k_B}{e} = 86.3\, \mu V K^{-1} \right) \\
\frac{G_{th}}{T} &= \frac{2}{h} k_B^2 \left[I_2 - \frac{I_1^2}{I_0} \right] \\
\mathcal{L} \equiv \frac{G_{th}}{TG} &= \left(\frac{k_B}{e} \right)^2 \left[\frac{I_2}{I_0} - \left(\frac{I_1}{I_0} \right)^2 \right]
\end{aligned}}$$

Dimensionless integrals:

$$\boxed{I_n \equiv \int d\varepsilon\, \mathcal{T}(\varepsilon) \left(\frac{\varepsilon - \mu}{k_B T} \right)^n \left(-\frac{\partial f}{\partial \varepsilon} \right)}$$





Different coefficients probe different range of energy:

- Conductance probes the immediate vicinity of E_F, in a symmetric way for particles and holes
- Thermopower probes a difference between contributions from holes (>0) and particles (<0). *It vanishes if particles and hole have the same transmission.*
- Thermal conductance probes a few kT from E_F

Low Temperature expressions

(from Sommerfeld's expansion – see notes

Warning: assumes no or weak intrinsic T-dependence of transmission
– OK for elastic scattering

$$G = \frac{2e^2}{h}\mathcal{T}(\mu = \varepsilon_F)$$ Landauer

$$\alpha = -\frac{k_B}{e}\frac{\pi^2}{3}k_B T\,\frac{\mathcal{T}'(\varepsilon_F)}{\mathcal{T}(\varepsilon_F)}$$

$$= -\frac{k_B}{e}\frac{\pi^2}{3}k_B T\,\frac{\partial}{\partial\mu}\ln\mathcal{T}(\mu)\Big|_{\mu=\varepsilon_F}$$ Mott-Cutler

$$\frac{G_{th}/T}{G} \equiv \mathcal{L} \to \left(\frac{k_B}{e}\right)^2\frac{\pi^2}{3}\quad (T\to 0)$$

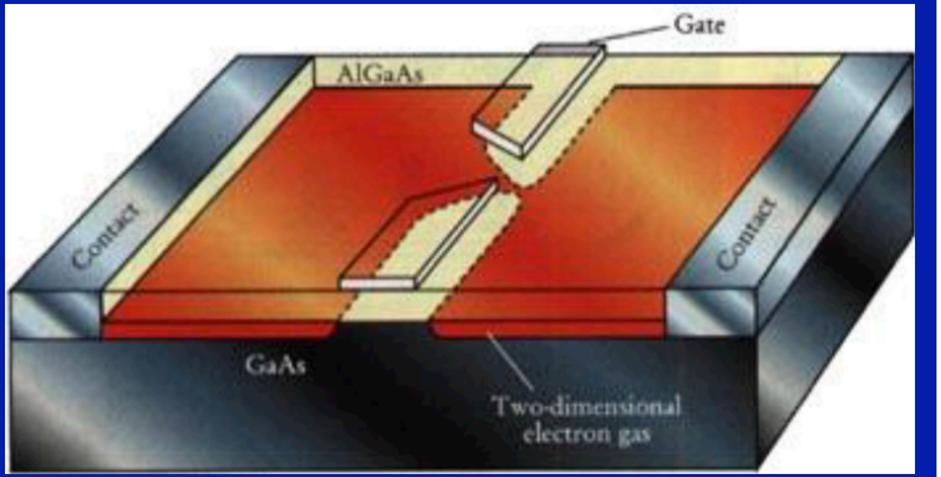
Wiedemann-Franz law

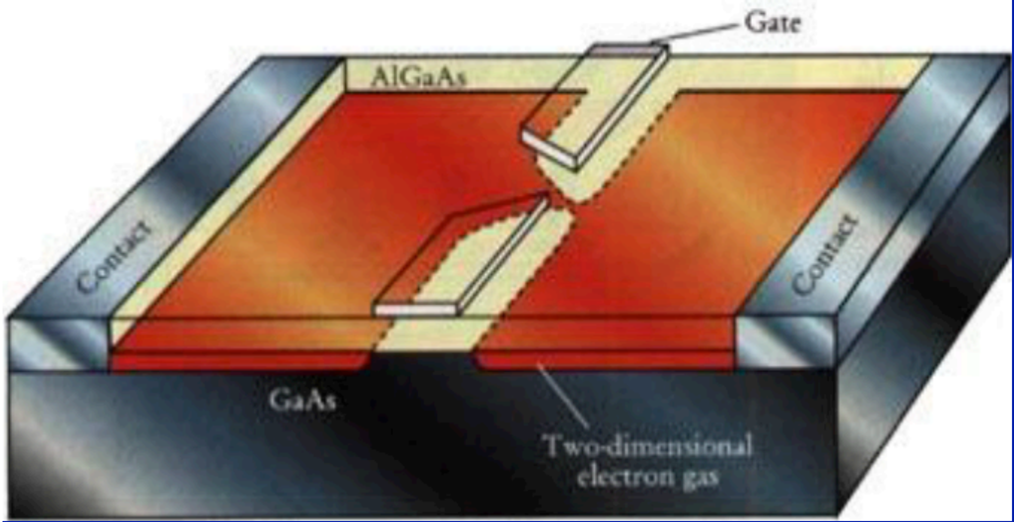
Two examples

- Quantum Point Contact
- Quantum Dot

Quantum Point Contacts (QPC) The first evidence of conductance quantization

Van Wees et al. PRL 60, 848 (1988)
Quantized Conductance of Point Contacts in a Two-Dimensional Electron Gas
cf. also:
Wharam et al.
One-dimensional transport and the quantization of the ballistic resistance
J.Phys C 21 L209 (1988)





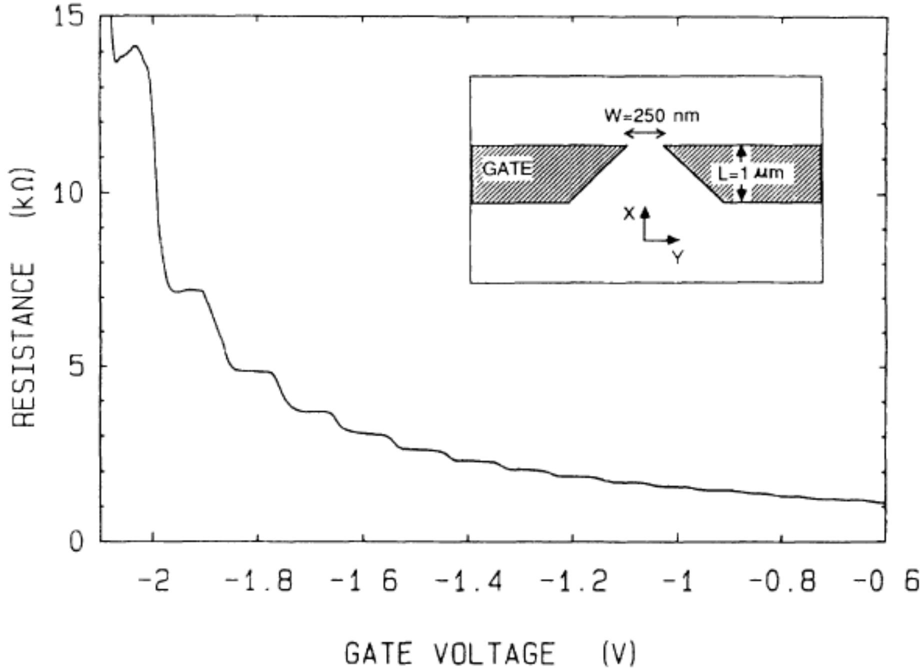


FIG. 1. Point-contact resistance as a function of gate voltage at 0.6 K. Inset: Point-contact layout.

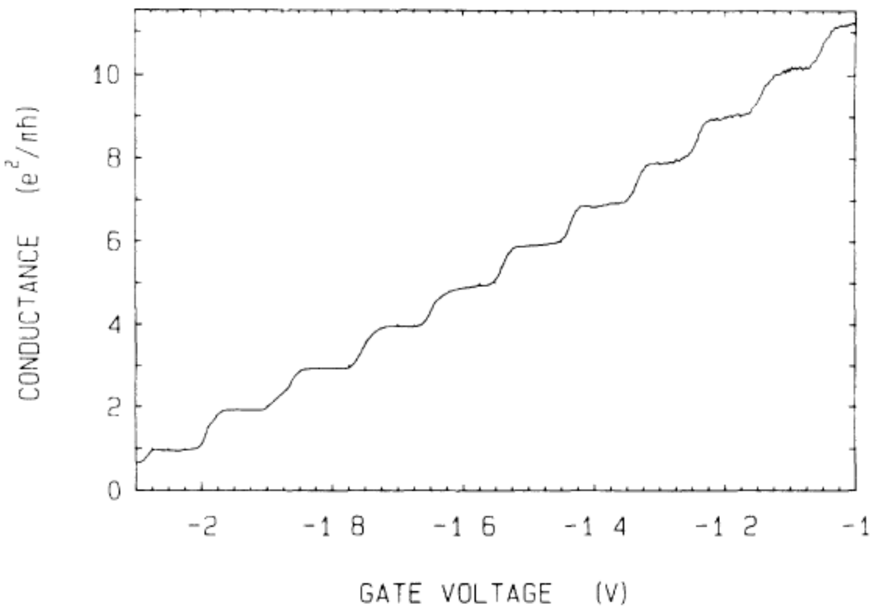


FIG. 2. Point-contact conductance as a function of gate voltage, obtained from the data of Fig. 1 after subtraction of the lead resistance. The conductance shows plateaus at multiples of $e^2/\pi\hbar$.

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

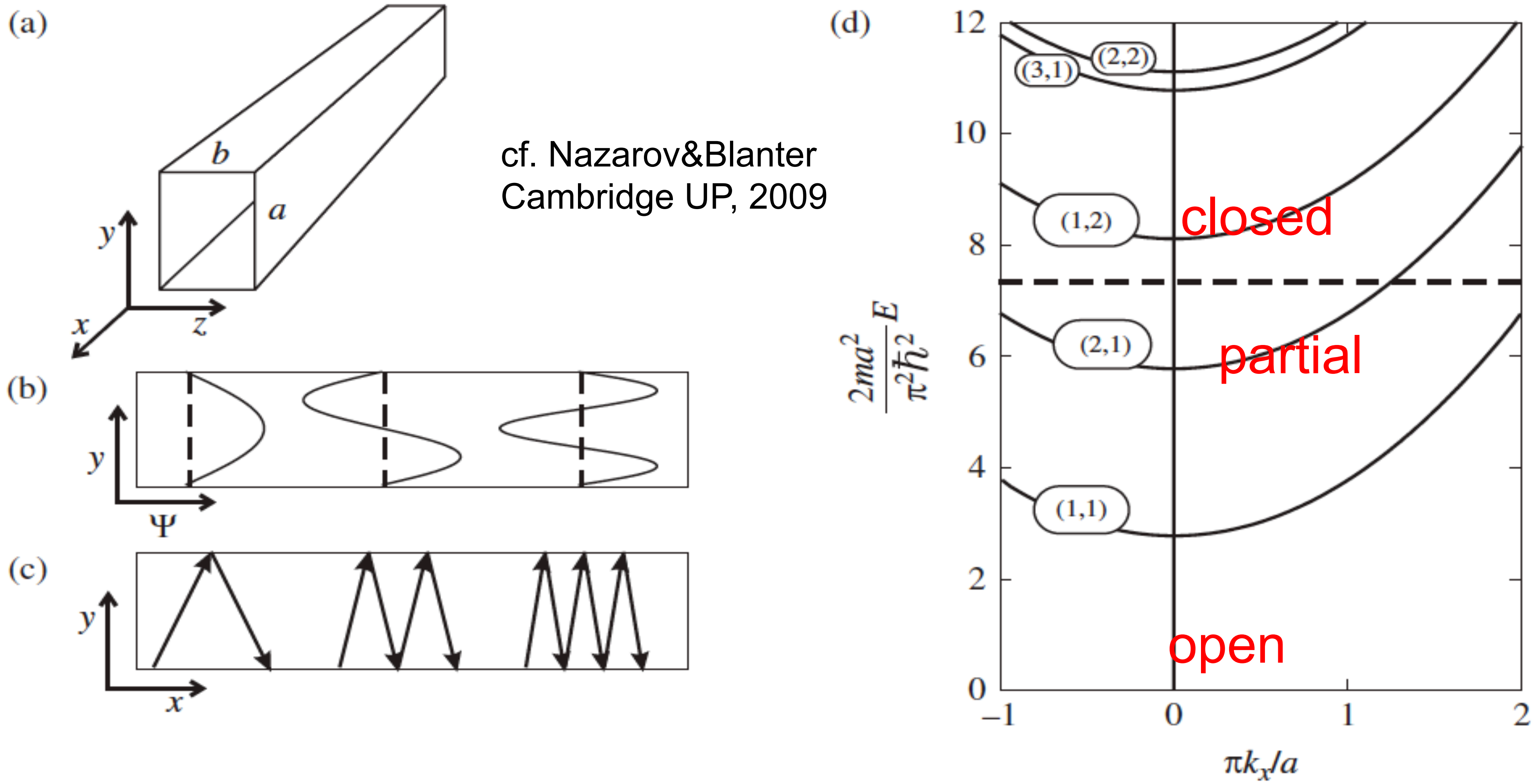
$$\mathcal{T}_{nm} = |t_{nm}|^2$$

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

Total current finally involves transmission coefficient:

$$\mathcal{T}(\varepsilon) = \sum_{nm} \mathcal{T}_{nm} = \sum_{nm} t_{nm} t^*_{nm} = \mathrm{Tr}\, tt^\dagger$$

$$= \sum_\lambda \mathcal{T}_\lambda$$ sum of eigenvalues of tt^+ matrix



cf. Nazarov&Blanter
Cambridge UP, 2009

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

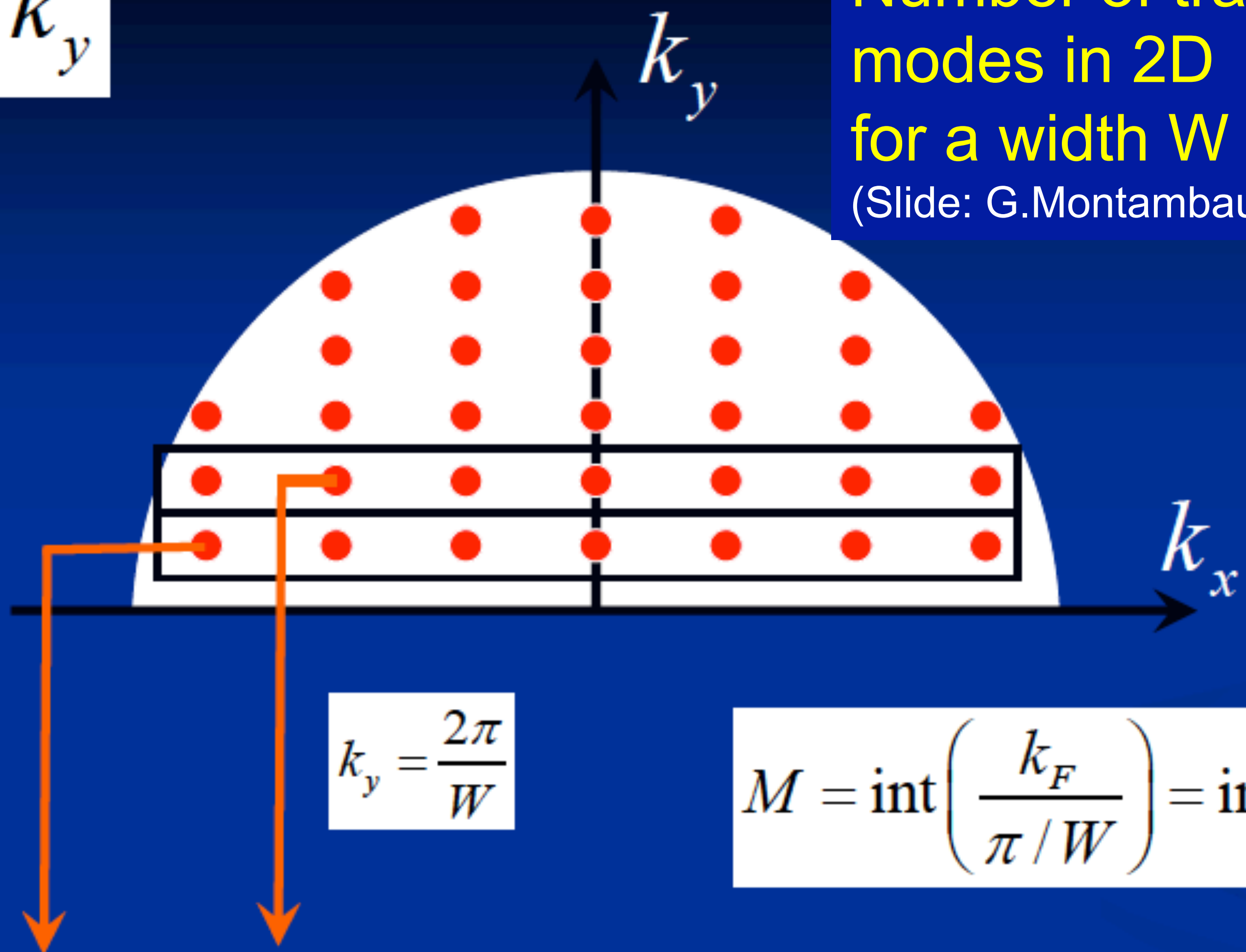
$$3D: \quad \varepsilon_{n_y,n_z}(k_x) = \frac{\hbar^2}{2m}\left[k_x^2 + n_y^2\left(\frac{\pi}{a}\right)^2 + n_z^2\left(\frac{\pi}{b}\right)^2\right] \quad (n_y, n_z > 0)$$

Number of transverse modes in 2D for a width W

(Slide: G.Montambaux)

$$k_F^2 = k_x^2 + k_y^2$$

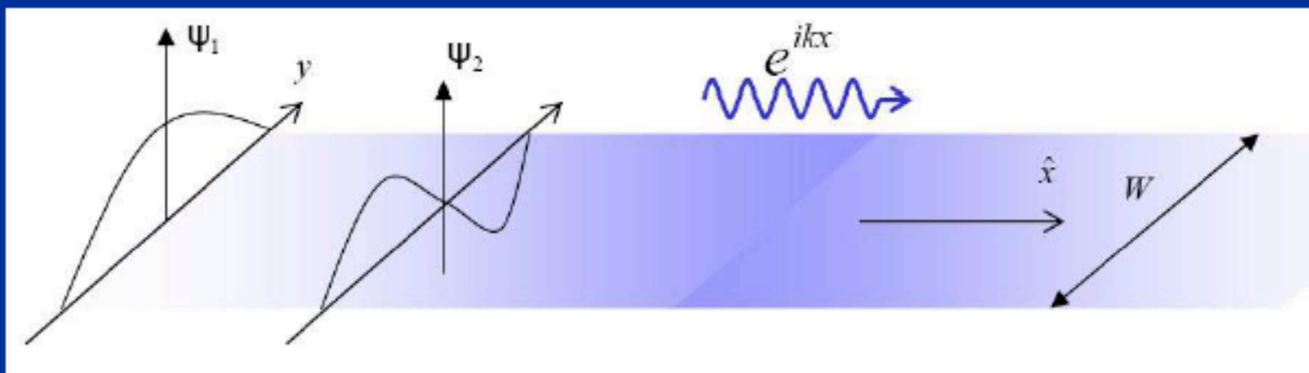
$$k_y = \frac{n_y \pi}{W}$$



$$k_y = \frac{\pi}{W}$$

$$k_y = \frac{2\pi}{W}$$

$$M = \mathrm{int}\left(\frac{k_F}{\pi / W}\right) = \mathrm{int}\left(\frac{k_F W}{\pi}\right)$$

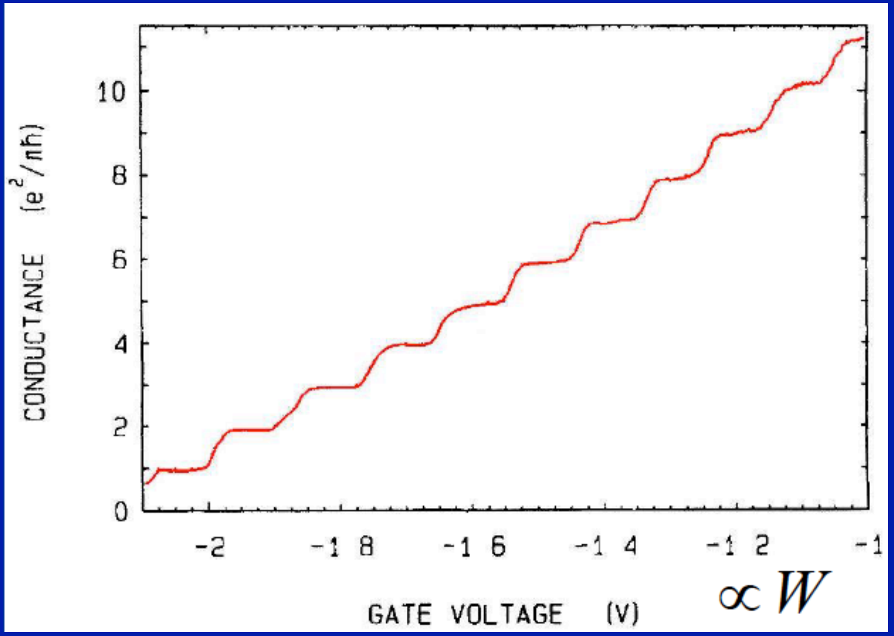


Simplest model: only fully open or fully closed channels

(`Il faut qu'une porte soit ouverte ou fermée', Alfred de Musset)

$$\mathcal{T}(\varepsilon) = \sum_n \theta(\varepsilon - \varepsilon_n)$$

$$G = \frac{2e^2}{h} \sum_n f(\varepsilon_n - \mu)$$



$\propto W$

Thermopower of a QPC

Theory: P.Streda J.Phys Cond Matt. 1, 1025 (1989), Proetto PRB 44, 9096 (1991)

First experiment: L.Molenkamp et al. PRL 65, 1052 (1990)

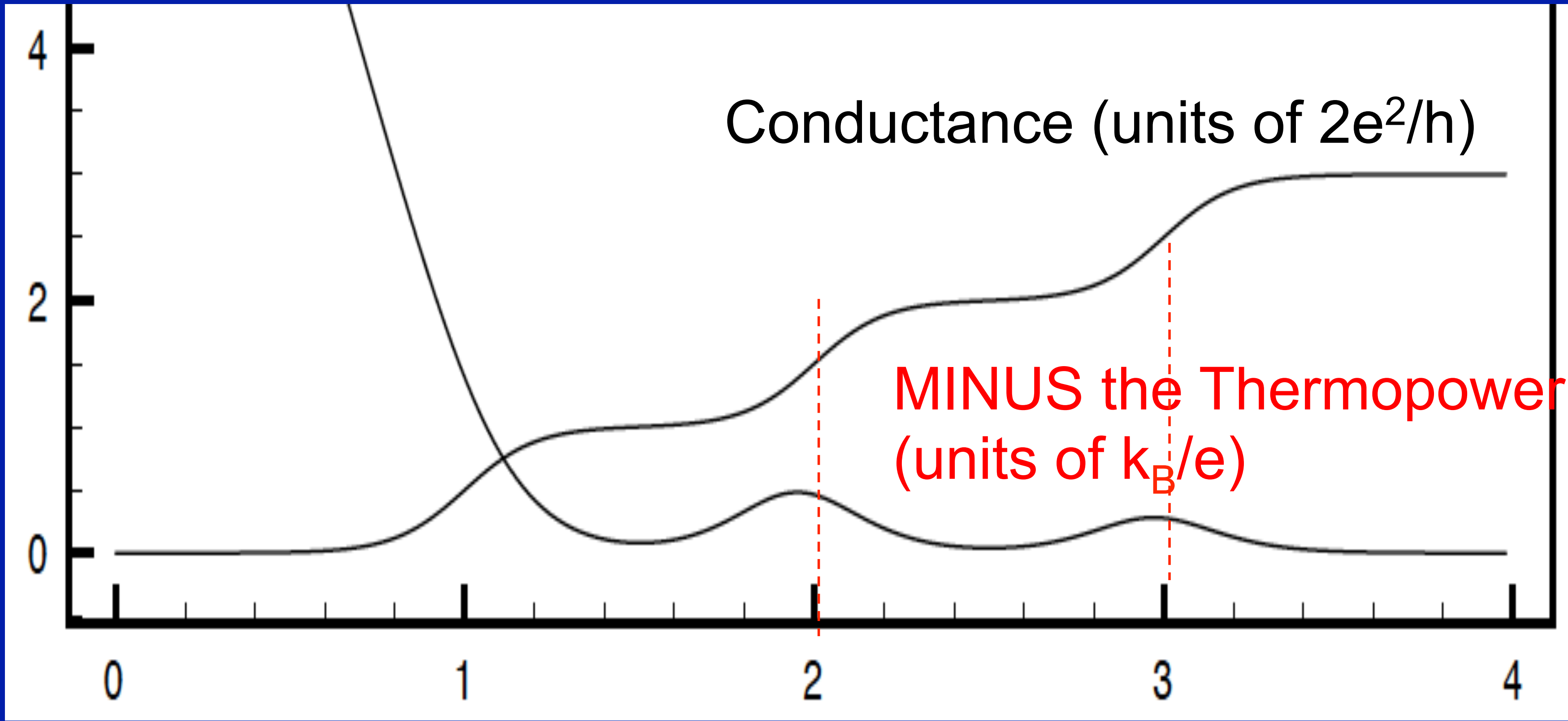
Use again simplest model (open or close channels only):

$$\mathcal{T}(\varepsilon) = \sum_{n=1}^{\infty} \theta(\varepsilon - \varepsilon_n)$$

$$x_n \equiv \frac{\varepsilon_n - \mu}{k_B T} \quad , \quad f(x) \equiv \frac{1}{1+e^x}$$

$$I_0 = \sum_n f(x_n)$$

$$I_1 = \sum_n \left[\frac{x_n}{1+e^{x_n}} + \ln(1+e^{-x_n}) \right]$$



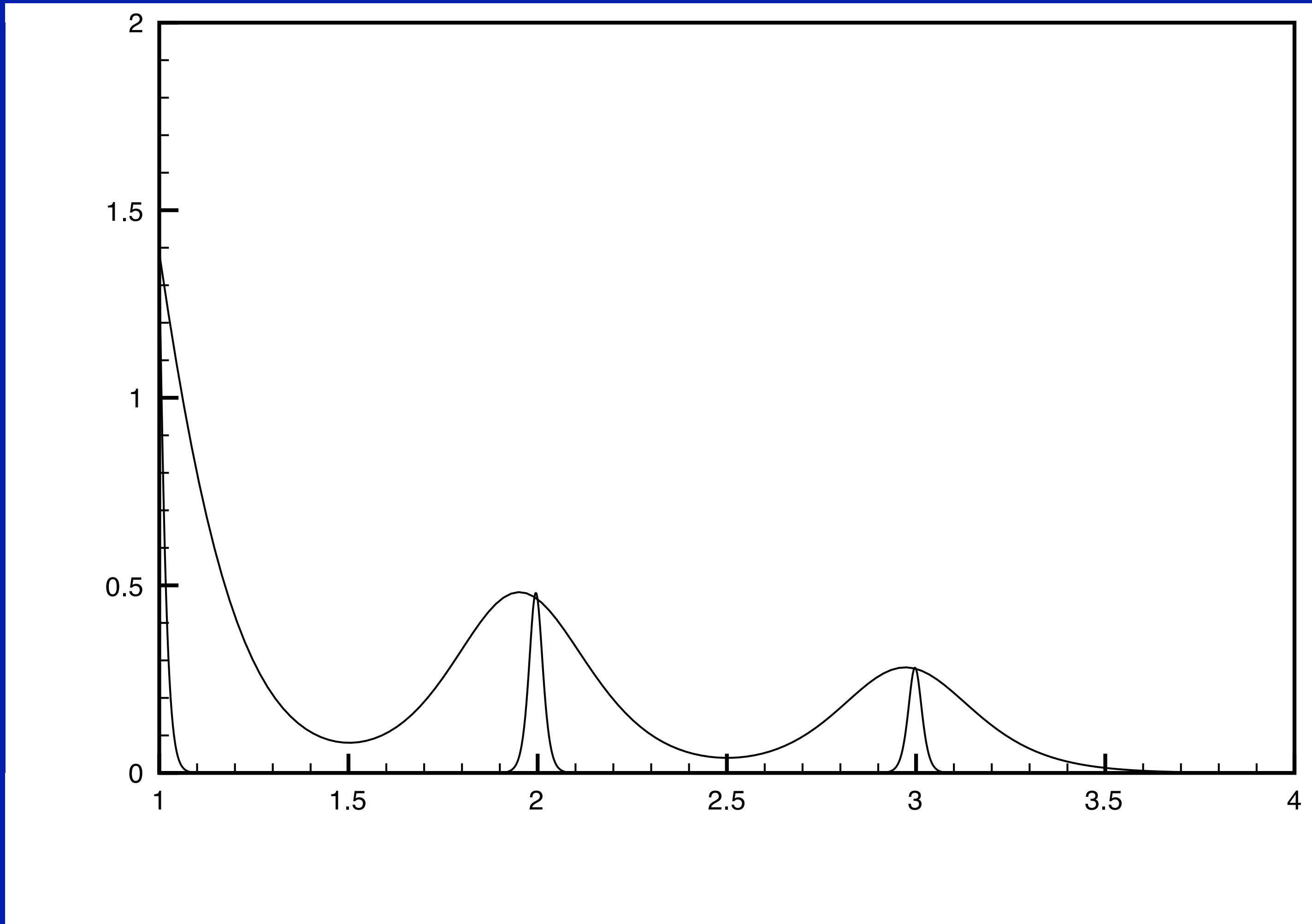
Recall at low-T: $\alpha \propto -\dfrac{1}{G}\dfrac{\partial G}{\partial \mu}$

Thermopower has a peak each time a new level becomes \`active' with ~ constant height

Parabolic well: $\mu \simeq \varepsilon_n \;:\; \alpha \simeq -\dfrac{k_B}{e}\,\dfrac{\ln 2}{n-1/2}\;,\; G \simeq \dfrac{2e^2}{h}(n-\dfrac{1}{2})$

<u>Experimental observation: see Laurens Molenkamp's seminar</u>

Temperature dependence



First Experiments: Thermopower of a QPC

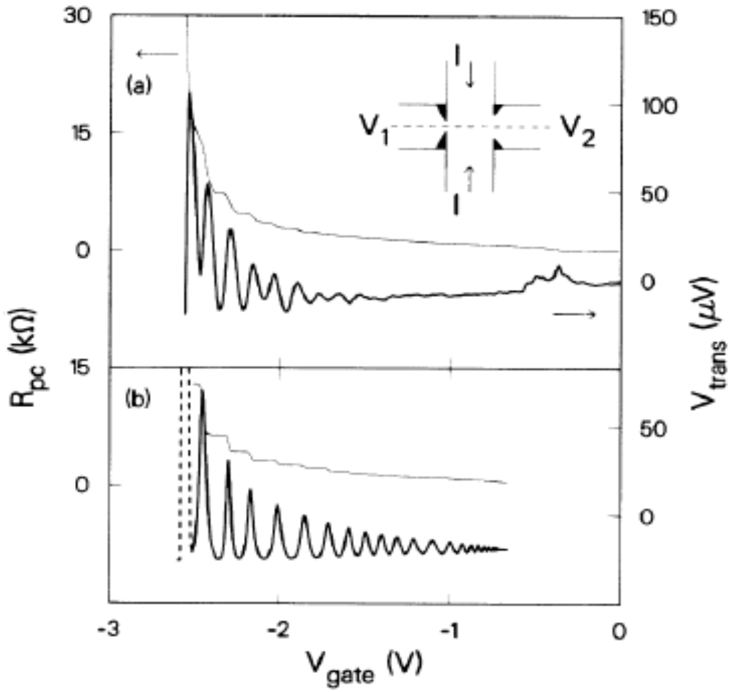
VOLUME 65, NUMBER 8 PHYSICAL REVIEW LETTERS 20 AUGUST 1990

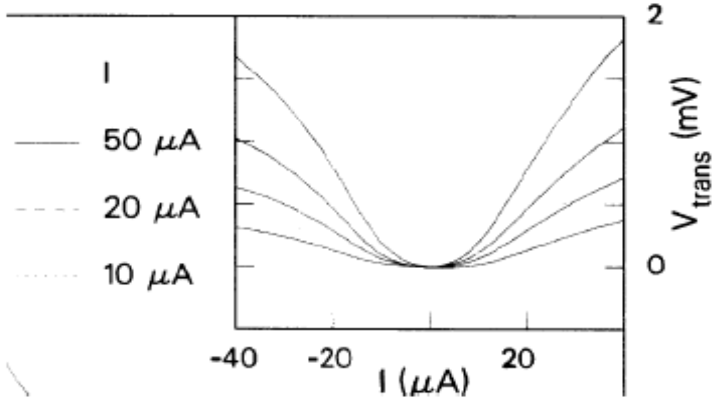
Quantum Oscillations in the Transverse Voltage of a Channel in the Nonlinear Transport Regime

L. W. Molenkamp, H. van Houten, C. W. J. Beenakker, and R. Eppenga
Philips Research Laboratories, 5600 JA Eindhoven, The Netherlands

C. T. Foxon
Philips Research Laboratories, Redhill, Surrey RH1 5HA, England

(Received 5 March 1990)





In semiconductors, at low T, $\tau_{e-p} \sim 100$ ps.

$\rightarrow$ nearly thermalized hot electron distribution in the heating channel

Slide: courtesy L.Molenkamp – see CdF website 2013-2014

Energy Filtering

cf. Mahan and Sofo, PNAS 93, 7436 (1996)

Think of:

$$p(\varepsilon) \equiv \frac{\mathcal{T}(\varepsilon)[-f'(\varepsilon)]}{\int d\varepsilon \mathcal{T}(\varepsilon)[-f'(\varepsilon)]} = \frac{g(\epsilon)}{G}$$

As a probability density, measuring the contribution to the total conductance of states around a given energy (for a given gate voltage)

Or even better:

$$x \equiv \frac{\varepsilon - \mu}{k_B T} \ , \ p(x) \equiv \frac{\mathcal{T}(\mu + k_B T\, x)}{4G \cosh^2 \frac{x}{2}} \ , \ \int dx\, p(x) = 1$$

Transmission coefficient (transport function) leading to $g^2 \rightarrow 1$ (Mahan-Sofo) :

$$g^2 = \frac{I_1^2}{I_0 I_2} = \frac{\langle(\varepsilon-\mu)\rangle_p^2}{\langle(\varepsilon-\mu)^2\rangle_p} = \frac{\langle x\rangle_p^2}{\langle x^2\rangle_p}$$

Clearly, a narrow transport function (transmission coefficient) - approaching asymptotically a δ-function - brings g close to unity

Note however:
This does not yield the best output power, since the power factor is ~ I_1^2/I_0

For optimization of transmission at finite power, see

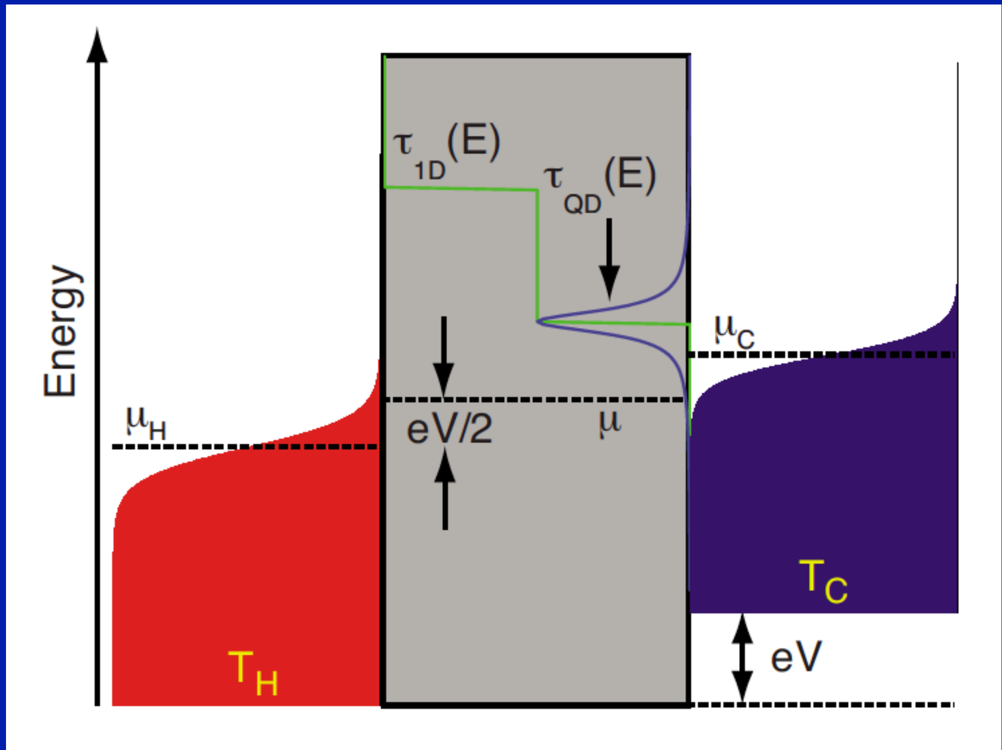
PRL **112**, 130601 (2014) PHYSICAL REVIEW LETTERS week ending 4 APRIL 2014

Most Efficient Quantum Thermoelectric at Finite Power Output

Robert S. Whitney
Laboratoire de Physique et Modélisation des Milieux Condensés (UMR 5493), Université Grenoble 1 and CNRS, Maison des Magistères, BP 166, 38042 Grenoble, France

Ilustrate this for a single resonant level In the context of mesoscopics: - Quantum Dots -

Early theory work: Beenakker and Staring PRB 46, 9667 (1992)
Experimental: Molenkamp et al., see seminar 12/11/2013
Efficiency: Nakpathomkun et al. PRB 82, 235428 (2010)
(see also: Mani et al. J. Elec. Mat 38, 1163 (2009)



Nakpathomkun et al.

Transmission coefficient is a Lorentzian:

$$\mathcal{T}(\varepsilon) = \frac{\Gamma_R \Gamma_L}{(\varepsilon-\varepsilon_r)^2 + (\Gamma_L+\Gamma_R)^2/4}$$

$$= \frac{(\Gamma/2)^2}{(\varepsilon-\varepsilon_r)^2 + (\Gamma/2)^2} \quad (\Gamma_R = \Gamma_L = \frac{\Gamma}{2})$$

Two control parameters: $\dfrac{\mu-\varepsilon_r}{k_B T}$, $\dfrac{\Gamma}{k_B T}$

$$I_n = \int dx \frac{x^n}{4\cosh^2 x/2} \frac{(\Gamma/2k_B T)^2}{\left(\frac{\mu-\varepsilon_r}{k_B T}+x\right)^2 + (\Gamma/2k_B T)^2}$$

Coupling constant $g^2 \left[\dfrac{\mu-\varepsilon_r}{k_B T}, \dfrac{\Gamma}{k_B T}\right]$

For fixed Γ/kT optimize over bias Δμ AND μ-ε_r

Nakpathomkun et al.
PRB 82, 235428 (2010)

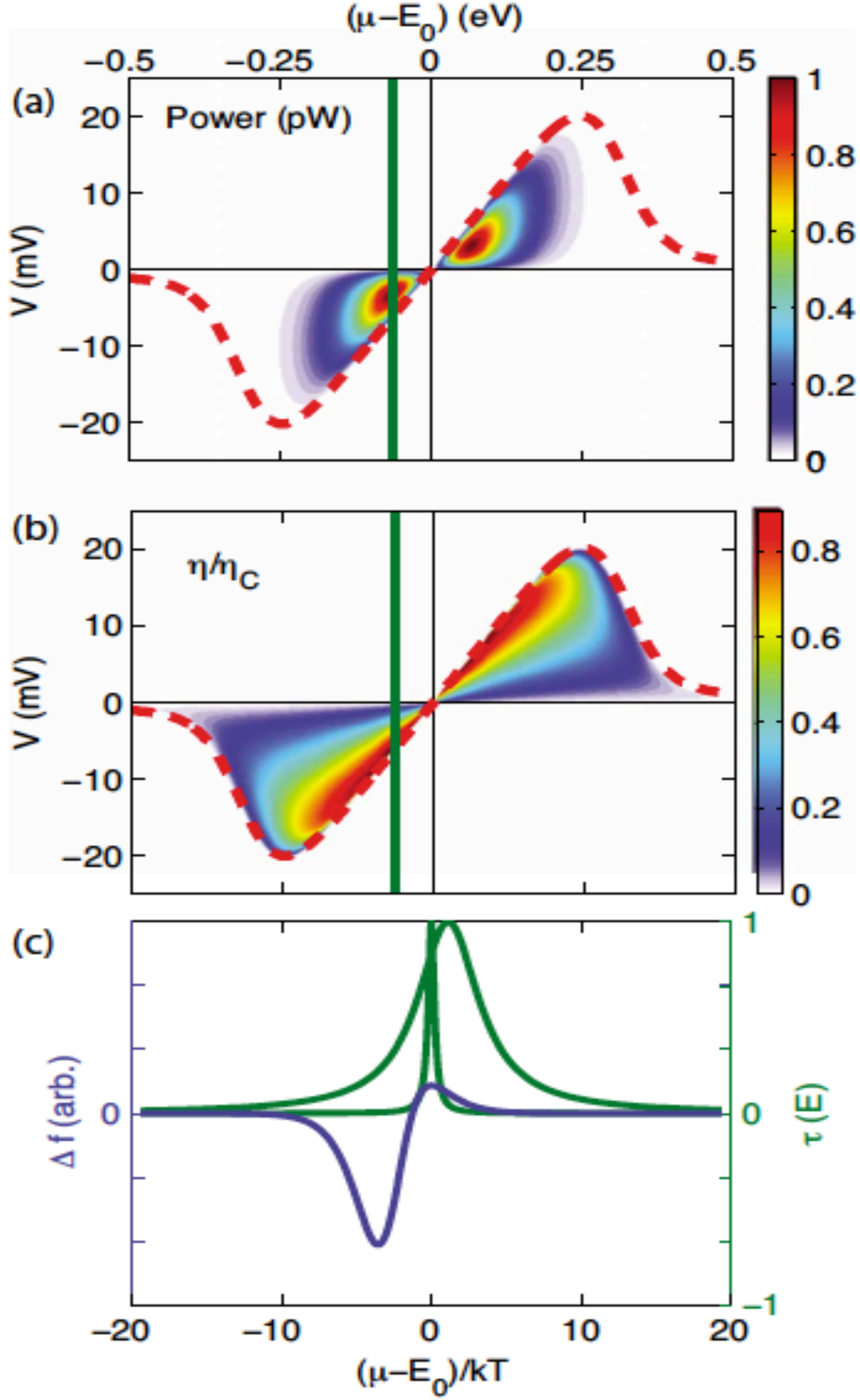
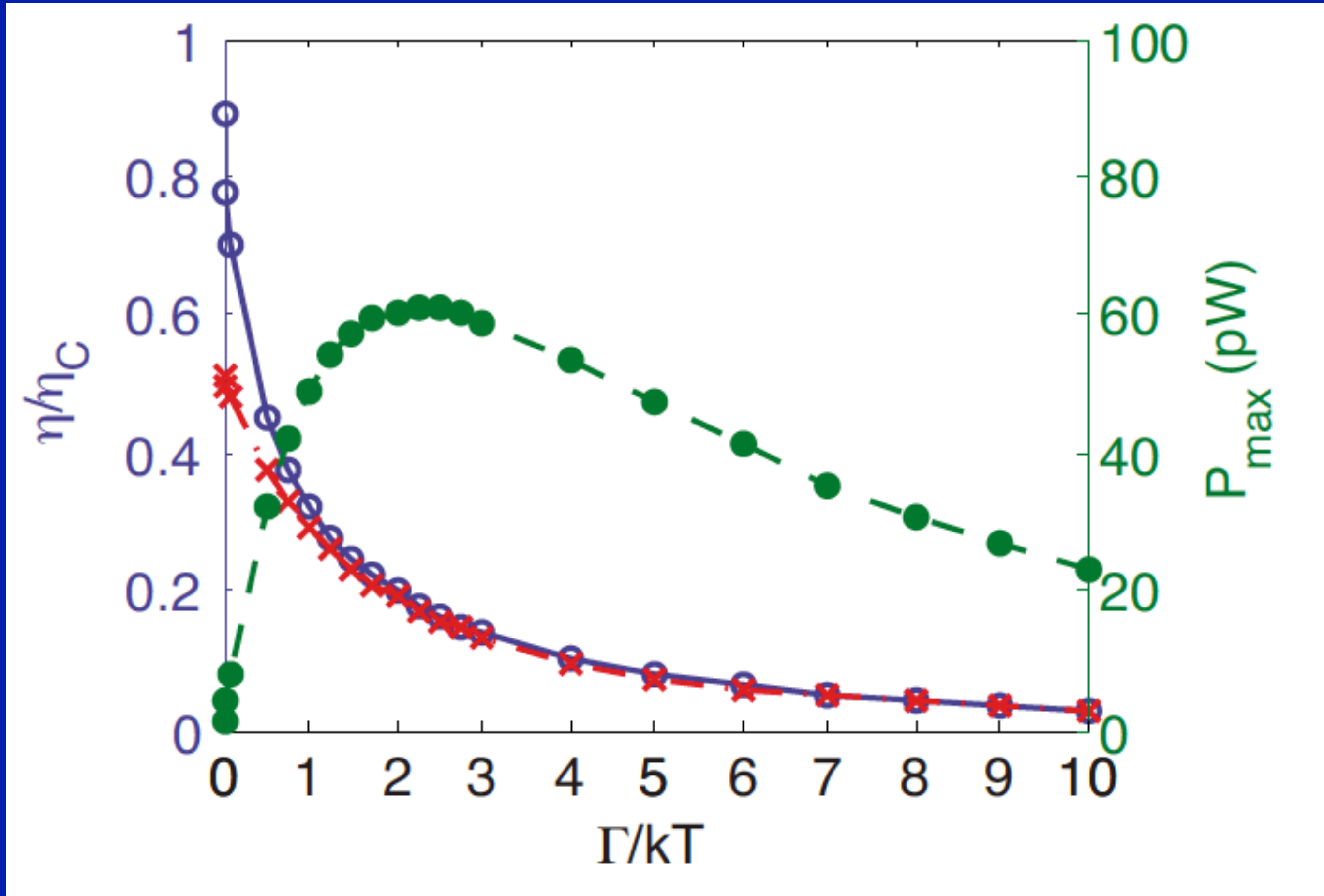


FIG. 2. (Color online) (a) Power and (b) efficiency normalized by Carnot efficiency, of a QD as a function of bias voltage V and average chemical potential μ, for T_C=300 K, T_H=330 K ($\Delta T/T_C$=0.1), and Γ=0.01kT. The open-circuit voltage, V_{oc} is highlighted in (red) dashed line (peak V_{oc} corresponds to $S \approx 2$ meV/K). The system works as a generator when the bias is between zero and V_{oc}. The vertical green line indicates the μ where maximum power occurs. (c) Current through a QD is the integral over the product of τ_{QD} (green) [Eq. (3)] and $\Delta f=(f_H-f_C)$, shown here in blue, using the μ and V that result in P_{max}. Two transmission widths, Γ=0.5kT and 5kT are plotted here in the approximate position where maximum power would be achieved.

Max efficiency, Max Power, Efficiency at Max Power vs. Γ/kT



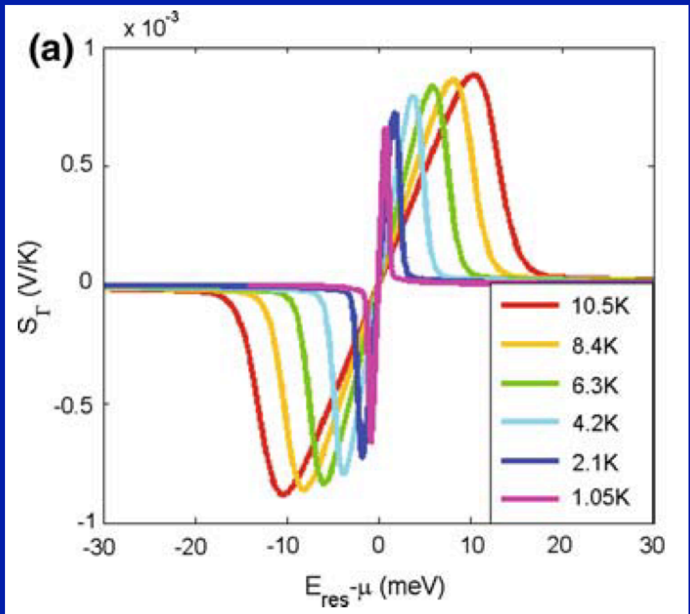
Efficiency is harmed by tails of the Lorentzian distribution causing too energetic electrons to waste heat in energy production and other electrons to travel in the wrong direction

Low-T limit kT<<Γ: Sommerfeld expansion as above

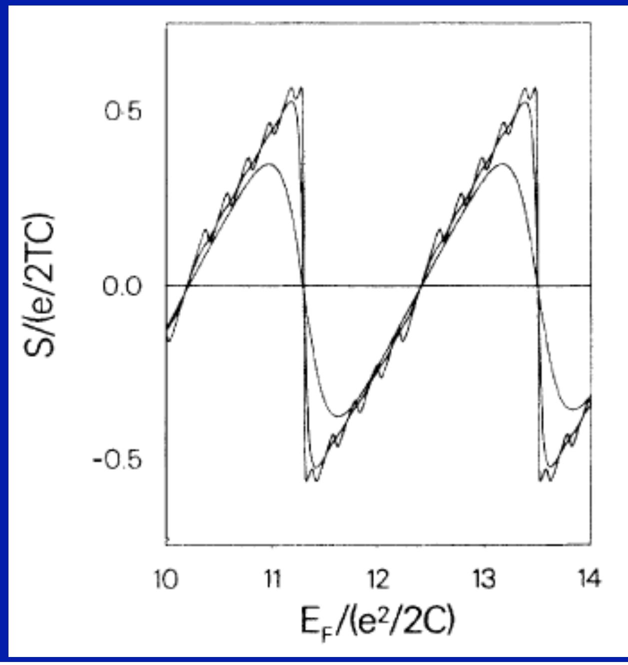
$$G = \frac{2e^2}{h}\mathcal{T}(\mu) = \frac{2e^2}{h}\,\frac{(\Gamma/2)^2}{(\mu-\varepsilon_r)^2+(\Gamma/2)^2}$$

$$\alpha \simeq -\frac{k_B}{e}\frac{\pi^2}{3}k_BT\,\frac{\partial}{\partial\mu}\ln\mathcal{T}(\mu)$$

$$= \frac{2\pi^2}{3}\frac{k_B}{e}\,\frac{(\mu-\varepsilon_r)/k_BT}{[(\mu-\varepsilon_r)/k_BT]^2+(\Gamma/2k_BT)^2}$$



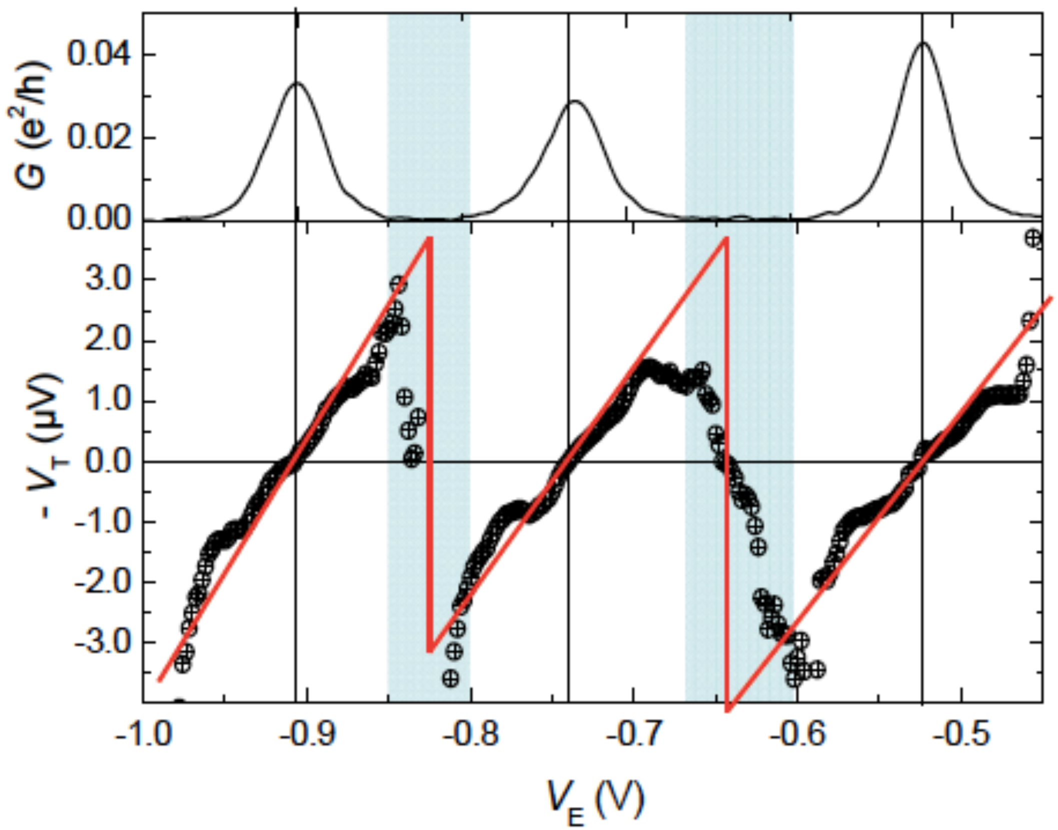
`sawtooth'



Thermopower of a QD

sequential tunneling

$\propto S$



small QD
$N \sim 15$
$T \sim 1.5$ K
$E_C \sim 2$ meV
$E_C / k_B T \sim 15$

Courtesy L.Molenkamp

Sample: Bo_I13C

Thermoelectricity of mesoscopic systems/nano-devices: New ideas and directions

Three-terminal devices

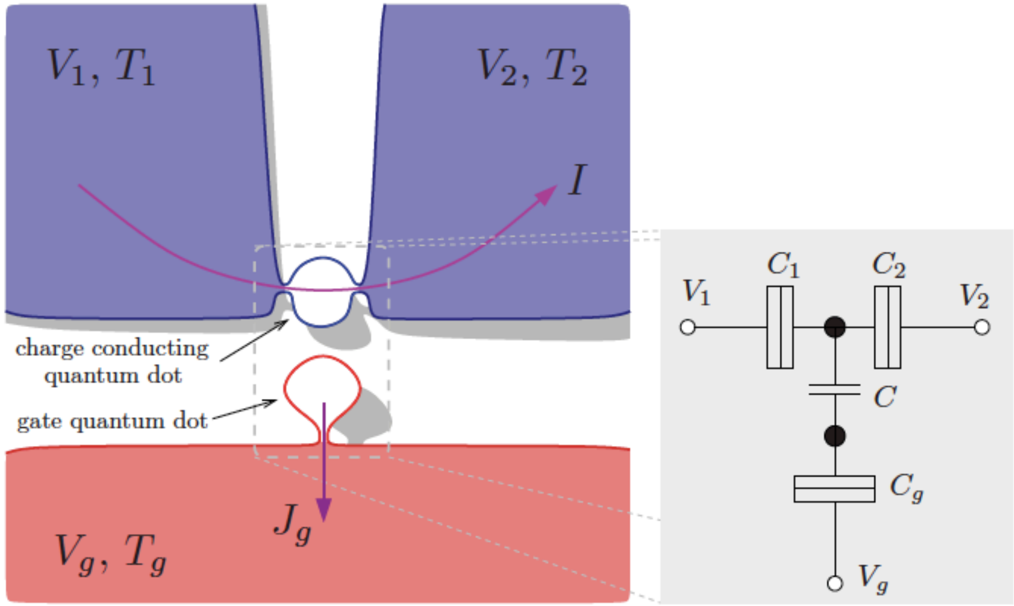
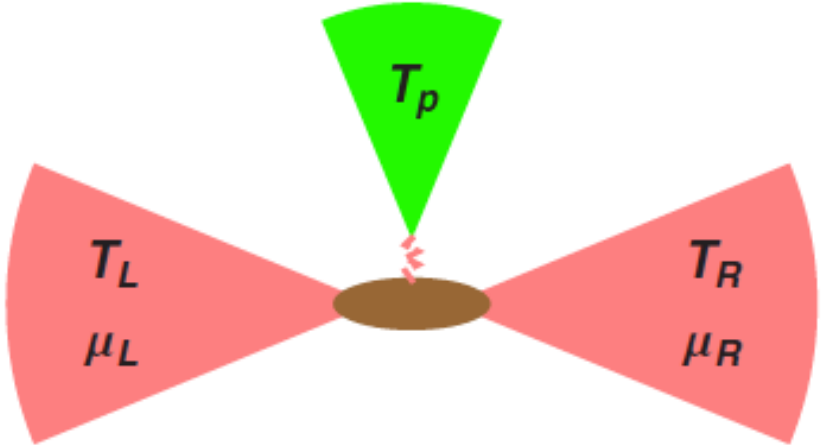


FIG. 1. (Color online) Energy to current converter. The conductor, a quantum dot open to transport between two fermionic reservoirs at voltages V_1 and V_2 and temperatures T_1 and T_2, is coupled capacitively to a second dot which acts as a fluctuating gate coupled to a reservoir at voltage V_g and temperature T_g. Here we discuss the case $T_1 = T_2 = T_s$.



For example:
3-terminal setup
Entin-Wohlman et al.
PRB 82 (2010) 115314

Sanchez & Buttiker PRB 83, 085428 (2011)

Recent experiment/device

PRL **114,** 146805 (2015) PHYSICAL REVIEW LETTERS week ending 10 APRIL 2015

Voltage Fluctuation to Current Converter with Coulomb-Coupled Quantum Dots

F. Hartmann,[1,*] P. Pfeffer,[1] S. Höfling,[1,2] M. Kamp,[1] and L. Worschech[1]
[1]*Technische Physik, Universität Würzburg, Physikalisches Institut and Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Am Hubland, D-97074 Würzburg, Germany*
[2]*SUPA, School of Physics and Astronomy, University of St. Andrews, St. Andrews, KY16 9SS, United Kingdom*
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We study the rectification of voltage fluctuations in a system consisting of two Coulomb-coupled quantum dots. The first quantum dot is connected to a reservoir where voltage fluctuations are supplied and the second one is attached to two separate leads via asymmetric and energy-dependent transport barriers. We observe a rectified output current through the second quantum dot depending quadratically on the noise amplitude supplied to the other Coulomb-coupled quantum dot. The current magnitude and direction can be switched by external gates, and maximum output currents are found in the nA region. The rectification delivers output powers in the pW region. Future devices derived from our sample may be applied for energy harvesting on the nanoscale beneficial for autonomous and energy-efficient electronic applications.

Recent review: Sothmann et al. arXiv:1406.5329

A note on the expression of transport coefficients in the bulk, in the Boltzmann equation approach

The Boltzmann equation approach

$F(\vec{k}, \vec{r}, t)$ Local distribution function

Relaxation-time approximation:

$$\frac{dF}{dt} = -\frac{F - F_0}{\tau}$$

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + \dot{\boldsymbol{k}} \cdot \nabla_{\boldsymbol{k}} F + \dot{\boldsymbol{r}} \cdot \nabla_{\boldsymbol{r}} F$$

For a bulk material, the Boltzmann equation leads to expressions that have complete formal similarity to the above ones. cf 2013-2014 lectures notes (website)

$$\mathcal{T}(\varepsilon) \equiv \frac{2}{\hbar}\int \frac{d^dk}{(2\pi)^d}\,\tau(\varepsilon_{\mathbf{k}}) \left[\frac{1}{d}\sum_a (\nabla^a_{\boldsymbol{k}}\varepsilon_{\mathbf{k}})^2\right] \delta(\varepsilon-\varepsilon_{\mathbf{k}})$$

(Dimensionality: L^{2-d})

Key difference: SQUARE of velocity enters here scattering – not ballistic Current-current correlator

$$\begin{aligned}
L_{11} &= \frac{1}{\hbar}\int d\varepsilon \left(-\frac{\partial f}{\partial \varepsilon}\right) \mathcal{T}(\varepsilon) \\
L_{12} &= \frac{1}{\hbar}\frac{1}{T}\int d\varepsilon \left(-\frac{\partial f}{\partial \varepsilon}\right) (\varepsilon-\mu)\,\mathcal{T}(\varepsilon) \\
L_{22} &= \frac{1}{\hbar}\frac{1}{T^2}\int d\varepsilon \left(-\frac{\partial f}{\partial \varepsilon}\right) (\varepsilon-\mu)^2\,\mathcal{T}(\varepsilon)
\end{aligned}$$

$$\sigma = e^2 L_{11} \quad , \quad \alpha = -\frac{L_{12}}{eL_{11}} \quad , \quad \kappa = T\left(L_{22} - \frac{L_{12}^2}{L_{22}}\right)$$

Consequences for a heavily doped small-gap semiconductor (see notes on the website)

These expressions are for a single type of carriers
(e.g. electrons in the conduction band)

Chemical potential
counted from the bottom of the conduction band :

$$\delta\mu \;\; , \;\; \left(\eta \equiv \frac{\delta\mu}{k_B T}\right)$$

Scattering time and Transport function:

$$\tau(\varepsilon) \sim (\varepsilon - \varepsilon_c)^r \;\; , \;\; \Phi(\varepsilon) \sim (\varepsilon - \varepsilon_c)^\phi$$

[Scattering by acoustic phonons: r = -1/2]
[Parabolic band: φ=3/2]

Thermopower:

(Note the first term δμ/kT)

$$\alpha = \frac{k_B}{e}\left[\eta - \frac{r+\phi+1}{r+\phi}\,\frac{F_{r+\phi}(\eta)}{F_{r+\phi-1}(\eta)}\right]$$

Lorenz number:

$$\left(\frac{e}{k_B}\right)^2 \mathcal{L}_e(\eta) = \frac{r+\phi+2}{r+\phi}\,\frac{F_{r+\phi+1}(\eta)}{F_{r+\phi-1}(\eta)} - \left(\frac{r+\phi+1}{r+\phi}\right)^2\left(\frac{F_{r+\phi}(\eta)}{F_{r+\phi-1}(\eta)}\right)^2$$

Fermi integrals:

$$F_n(\eta) \equiv \int_0^\infty dx\, \frac{x^n}{1+e^{x-\eta}}$$

- Density of carriers (parabolic band):

$$\boxed{n \;=\; 4\pi \left(\frac{2m_c k_B T}{h^2}\right)^{3/2} F_{1/2}(\eta)} \qquad (5$$

- Mobility (parabolic band) - not to be confused with chemical potential-:

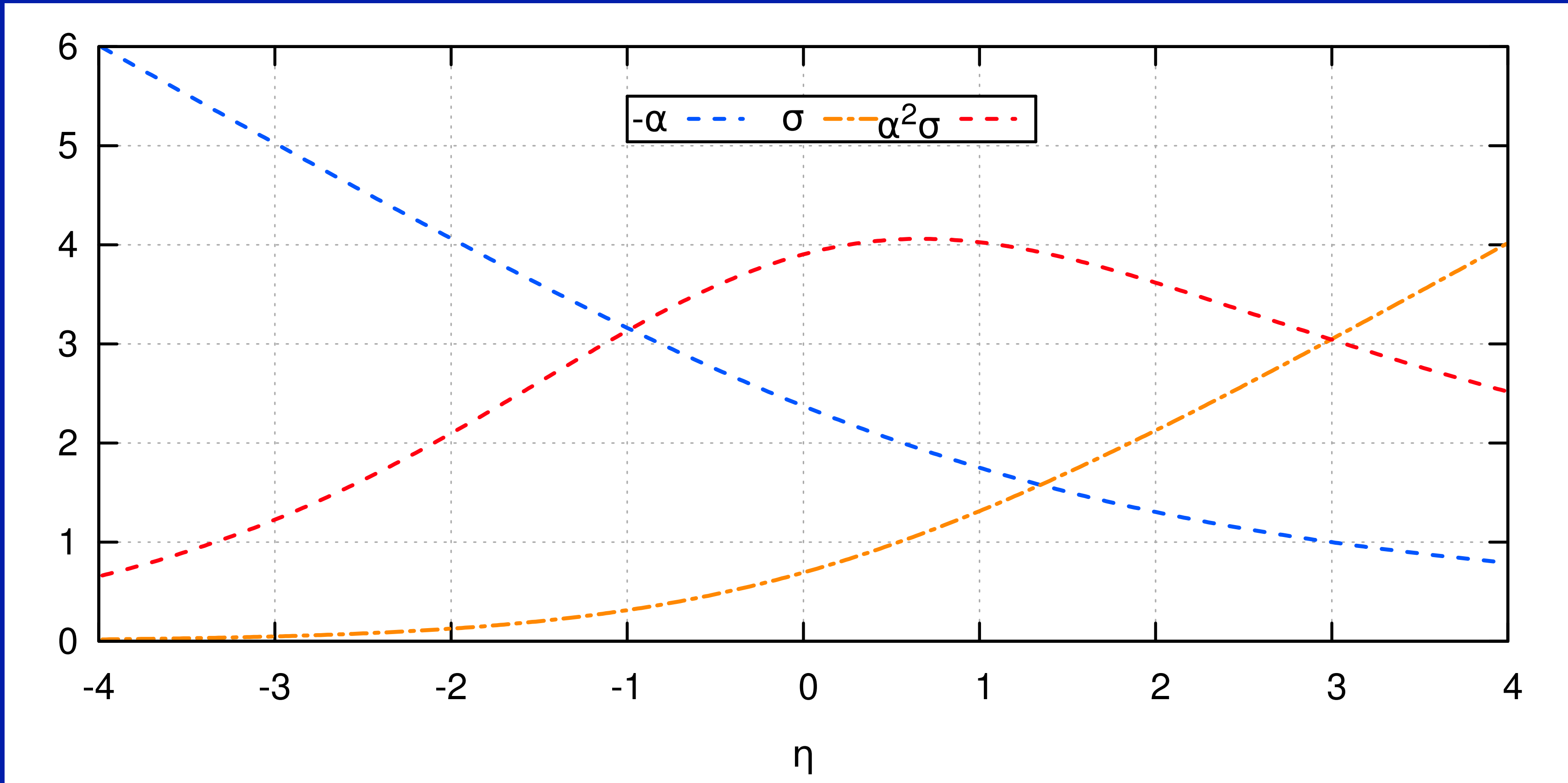
$$\boxed{\mu(T,\eta) \;=\; \frac{e\,\tau(T)}{m_c}\,\frac{2}{3}(r+\frac{3}{2})\,\frac{F_{r+1/2}(\eta)}{F_{1/2}(\eta)} \;\;,\;\; \tau(T) \equiv \tau(\varepsilon = k_B T) \simeq C_\tau (k_B T)^r}$$

- Conductivity (parabolic band):

$$\boxed{\sigma \;=\; n\,e\,\mu(T,\eta) \;=\; \sigma_0(T)\,\frac{F_{r+1/2}(\eta)}{\Gamma(r+3/2)} \;\;,}$$

$$\boxed{\sigma_0(T) = \frac{8\pi}{3}\Gamma(r+\frac{5}{2})\left(\frac{2m_c k_B T}{h^2}\right)^{3/2}\frac{e\,\tau(T)}{m_c}}$$

Power factor, conductivity and Seebeck vs. chemical potential:



Optimum for η ~ 0-1, corresponding to n ~ $10^{20}/cm^3$

Optimum ZT for η ~ -0.5, n~10^{19}

→ Optimum Seebeck around 200 μV/K

Acoustic phonon scattering r=-1/2 assumed in this plot