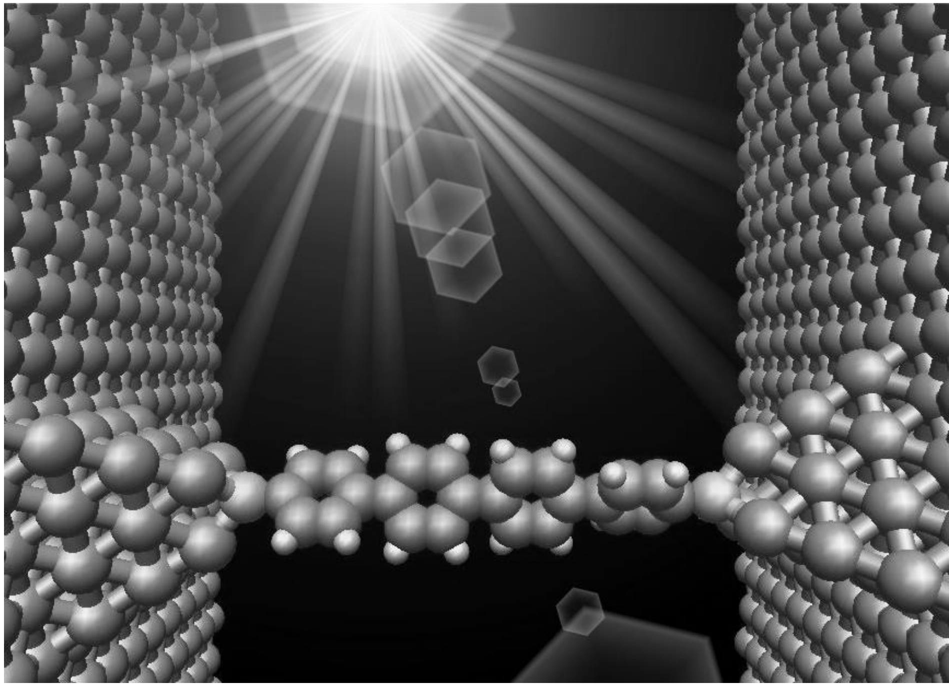
Quantum Coherent Transport



Elke Scheer,
University of Konstanz

Contents

- Reminder: Electrons in solids
- Length scales and transport regimes

- Ballistic transport in nano-sized conductors: Conductance quantization
  → Single atom and single molecule contacts

- Quantum interference effects in diffusive conductors

  → Aharonov Bohm effect, Universal conductance fluctuations,
  weak (anti)localization

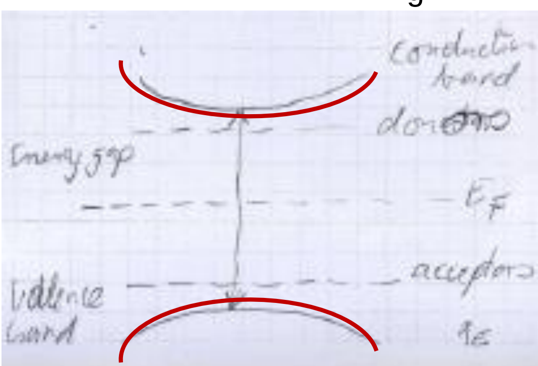
- Weak coupling: Coulomb Blockade
  → single molecule transistors

Reminder: Electrons in solids & reduced dimensions

- **Schrödinger Eq. with periodic potential:** $$\left(-\frac{\hbar^2}{2m}\Delta + V(\vec{r})\right)\Psi = E\Psi$$
- **Bloch states** $\Psi_{n,\vec{k}}$ **, energy bands** $E_n(\vec{k})$**, group veloc.** $$\vec{v}_n(\vec{k}) = \frac{\partial}{\partial \hbar \vec{k}} E_n(\vec{k})$$

Semiconductors

Energy gap E_g



parabolic approx. of $E_n(k)$

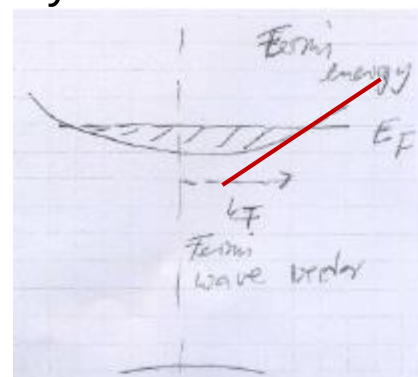
effective mass for 1 band

$$(m_n^*)^{-1} = \frac{\partial^2 E_n(k)}{\partial \hbar k^2}$$

may differ from free e^- mass

Metals

arbitrarily small excitations possible



linear approx. of $E_n(k)$

Fermi velocity

$$\vec{v}_F = \left.\frac{\partial E_n(\vec{k})}{\partial \hbar \vec{k}}\right|_{\vec{k}=\vec{k}_F}$$

$$(m^*)^{-1} = \frac{v_F}{\hbar k_F}$$

Effective mass approximation

- Electrons with one band behave like free particles with mass *m**:
- Hamiltonian $H = \sum \frac{1}{2m_n^*}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$
- Eigenstates $E_n(\vec{k}) = \frac{\hbar^2}{2m_n^*}\vec{k}^2$ plane waves $\Psi_{n\vec{k}} = e^{i\vec{k}\cdot\vec{r}}$
- Periodic boundary conditions in $\Omega = L^d$, *d* = 1,2,3: dimension
- 1d case: $\Psi(x) = \Psi(x+L) \rightarrow k_i = n_i \frac{2\pi}{L}$
- Density of states in *k*-space (fermions: 2 particles/state) $\rho_k = \frac{2}{(2\pi)^d}$
- Particle density $n(E_F) = \sum_{\text{all occupied states}} \frac{2}{(2\pi)^d} \underbrace{\rightarrow}_{\substack{\text{L big} \rightarrow \text{many states} \\ \text{k-states quasi} \\ \text{continuous}}} \frac{2}{(2\pi)^d}\int d^d k \rightarrow \int_0^{E_F} dE\,\rho_d(E)$
- Density of states (DOS) in *d* dimensions $\rho_d(E)$

Density of states $\rho(E) = \frac{d}{dE} n(E) \text{ with } E = E_n(\vec{k})$

- DOS denotes number of states per energy and per volume
- DOS used when going from momentum space to energy space
- DOS depends on dimension of the system
- "Sharp dimensions"

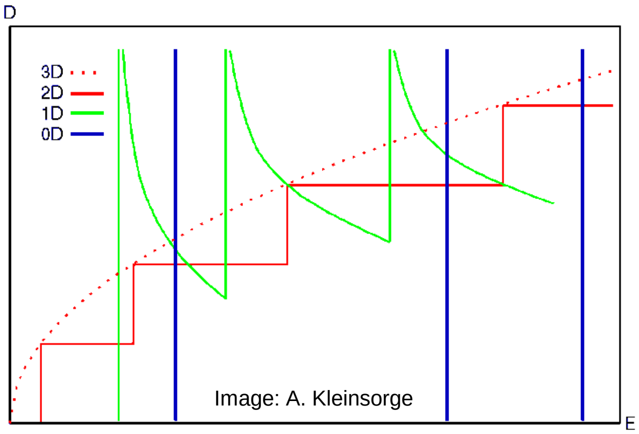
$$\rho_3(E) = \frac{(2m^*)^{3/2}}{2\pi^2\hbar^3}\sqrt{E} \qquad \rho_2(E) = \frac{m^*}{\pi\hbar} \qquad \rho_1(E) = \frac{1}{\pi\hbar}\sqrt{\frac{m^*}{2E}}$$

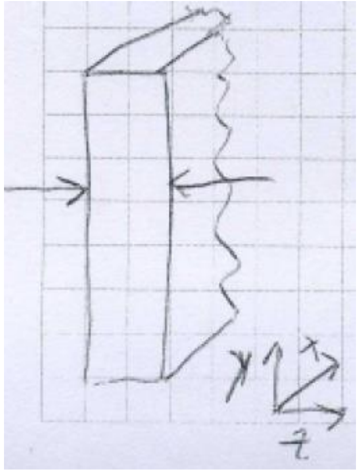
- Confinement $\Psi(\vec{r}) = \varphi(z) \cdot e^{i(k_x x + k_y y)}$ 2d subbands $E_n(k_x, k_y) = \mathcal{E}_n + \frac{\hbar^2(k_x^2 + k_y^2)}{2m^*}$
- Quasi 2d DOS $\rho_{2-3}(E) = \sum q_n^{(2)}\theta(E - \mathcal{E}_n)$
- Quasi 1d DOS

$$\rho(E) = \sum a_{nm}^1 (E - \mathcal{E}_{nm})^{-1/2}$$

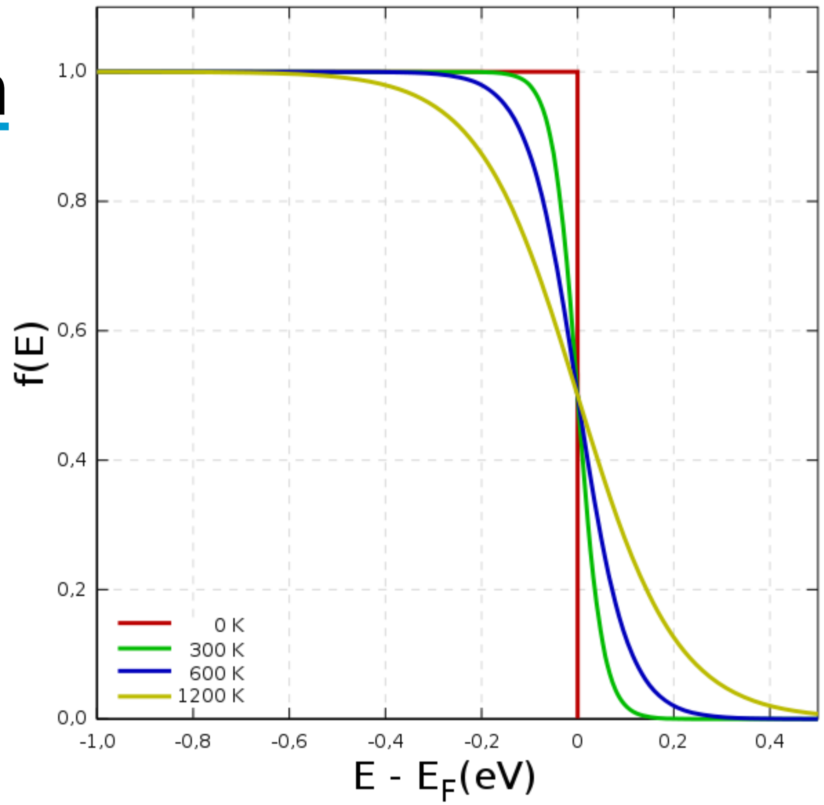
- Quasi 0d DOS: „artificial atoms"

$$\rho(E) = \sum_{n,m,l} \delta(E - \mathcal{E}_{n,m,l})$$





Fermi distribution function



Fermi distribution function at temperature *T* and with electrochemical potential *μ*, k_B : Boltzmann constant

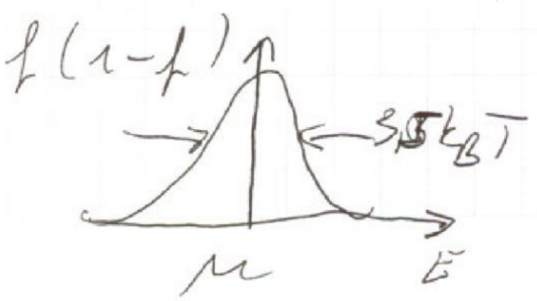
$$f(E,T,\mu) = \frac{1}{1+e^{(E-\mu)/k_B T}}$$

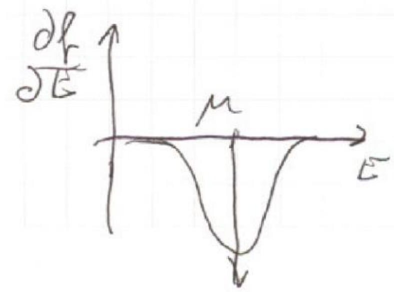
At *T* = 0 the „Fermi edge" is at $\mu = E_F$
Width of Fermi edge ~ 3.5 $k_B T$

Useful relations

$$f(E)(1-f(E)) = -k_B T\frac{\partial f}{\partial E} = \frac{1}{4\cosh^2\left(\frac{E-\mu}{2k_B T}\right)}$$

$$\lim_{T\to 0}\frac{\partial f}{\partial E} \to -\delta(E-\mu)$$





Charge transport in reduced dimensions

- Macroscopic conductor: Ohm's law

$$R = U/I$$

- Current density, potential, conductivity

$$j = \sigma \cdot \vec{E} = \sigma \cdot \mathrm{grad}\,\Phi = \sigma \cdot \mathrm{grad}\,\mu$$

- Resistance *R* and resistivity ρ

$$R = \rho \frac{L}{A}$$

- Drude-Sommerfeld formula

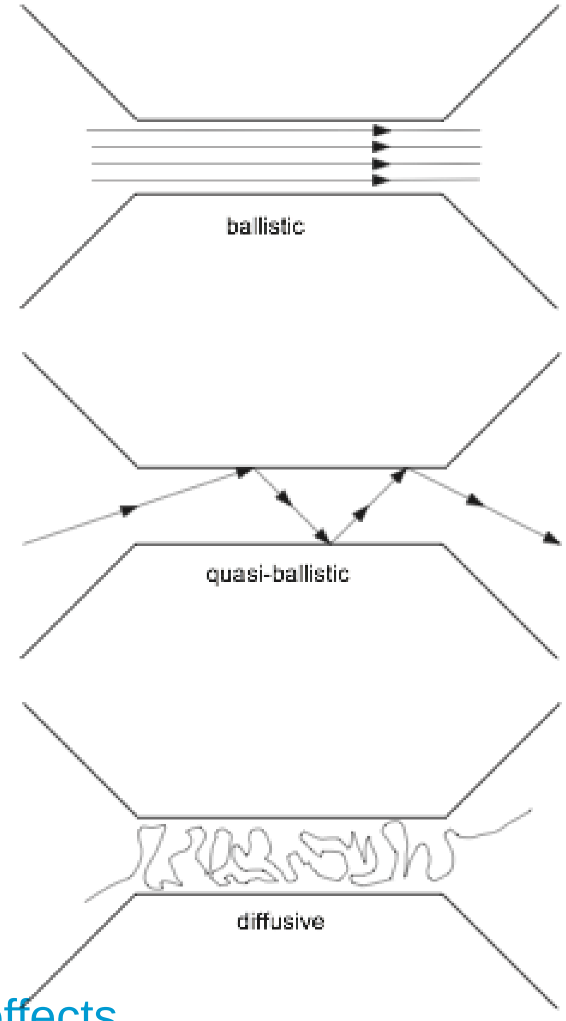
$$\rho = m/ne^2\tau$$

- Resistance caused by scattering with defects, phonons, surfaces

L : length of conductor
A : cross section
m : mass of charge carriers
e : charge
τ : scattering time

- Scaling sizes down:
  - *R* diverges
  - new phenomena on the nanoscale

Charge transport in reduced dimensions



- **Coherent transport regimes in conductors**
  - Ballistic transport
    - No scattering in the sample region
    - Geometry dependent transport
    - Conductance Quantization
    - Landauer-(Büttiker) transport
  - Quasi-ballistic transport
    - Scattering only at boundaries
    - Landauer approach valid
  - Diffusive transport
    - Multiple scattering
    - Random walk
    - Similar to macroscopic case but:
      phase coherence -> quantum interference effects
- **Weak-coupling transport: Coulomb Blockade**

Time, energy and length scales

Transport regime is determined by size relation between sample dimensions *L* and some intrinsic length scale and relative size of length scales:

e⁻ behaves like plane waves: $\Psi \sim e^{ikx} \quad k: \text{wave vector}$

Fermi wave vector:

$$k_\mathrm{F} = \sqrt{\frac{2 \cdot m^* \cdot E_\mathrm{F}}{\hbar^2}}$$

Fermi wavelength:

$$\lambda_\mathrm{F} = \frac{2\pi}{k_\mathrm{F}} = \begin{cases} 2/n_1 & ,\ 1\mathrm{D} \\ \sqrt{2\pi/n_2} & ,\ 2\mathrm{D} \\ 2\pi \cdot \left(3\pi^2 n\right)^{-1/3} & ,\ 3\mathrm{D} \end{cases}$$

Bulk metal: $\lambda_\mathrm{F} \approx 5\ \text{Å}$

GaAs 2DEG ($n = 5 \cdot 10^{11}\ \mathrm{cm}^{-2}$): $\lambda_\mathrm{F} \approx 35\ \mathrm{nm}$

Time, energy, and length scales

- Fermi velocity

$$v_F = \frac{\hbar k_F}{m^*} = \begin{cases} \frac{\hbar}{m^*} \cdot \pi n & , 1D \\ \frac{\hbar}{m^*} \cdot \sqrt{2\pi n} & , 2D \\ \frac{\hbar}{m^*} \cdot \left(3\pi^2 n\right)^{1/3} & , 3D \end{cases} \quad \begin{array}{l} \text{2DEG}: \; v_F \approx 3 \cdot 10^5 \text{ m/s} \\ \text{metal}: \; v_F \approx 10^6 \text{ m/s} \end{array}$$

- Elastic mean free path $l_{mfp} = l_{el} = l = v_F \cdot \tau$

  momentum relaxation length ~ distance between collisions with defects

  l ~ 10-20 nm in metals , l ~ 1-10 µm in 2DEGs

  → *Ballistic transport easily achieved in 2DEGs*

  → *Metallic nanostructures (L >~ 50 nm): mainly diffusive regime*

- Phase coherence length: mainly limited by inelastic scattering with phonons → similar to inelastic length ~ energy relaxation length l_{in}:

  ballistic: $l_\varphi = v_F \cdot \tau_\varphi$ diffusive: $l_\varphi = (D\tau_\varphi)^{1/2}$

  with diffusion constant $D = v_F l/d$ (*d* dimension) and dephasing rate τ_φ

  $l_\varphi \sim 1\mu\text{m at } T \sim 1\text{K in metals}$

- Level spacing: mean energy distance between electronic states $\delta = 1/(\rho(E)L^d)$

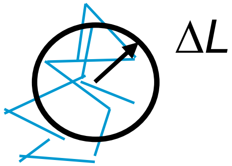
  Important for Coulomb blockade

Time, energy, and length scales

- Relation between time and energy scale via uncertainty relationship

$$\Delta E \cdot \Delta\tau \geq \hbar$$

- Relation between time and length depends on transport regime:



ballistic: $\Delta\tau = \frac{\Delta L}{v_F}$ diffusive: $\Delta\tau = \frac{\Delta L^2}{D}$

→ *distance* → *area increases lineary with time*

- Relation between length scale L_x and energy scale E_x via Thouless relation

ballistic: $E_x = \hbar v_F / L_x$ diffusive: $E_x = \hbar D / L_x^2$

Length scale L_x on which a wave package with width E_x diverges

$L_x = \hbar v_F / E_x$ $L_x = (\hbar D / E_x)^{1/2}$

- Finite sample size L defines Thouless energy E_{Thou}

ballistic: $E_{Thou} = \hbar v_F / L$ diffusive: $E_{Thou} = \hbar D / L^2$

Important for quantum interference effects and superconductivity

- Thermal (diffusion) length L_T

ballistic: $L_T = \hbar v_F / k_B T$ diffusive: $L_T = (\hbar D / k_B T)^{1/2}$

Electrons with energy spread $k_B T$ dephase over a distance L_T

Calculation of currents

Classical current formula:

$$\underbrace{\vec{j}}_{\text{current density}} = \underbrace{e}_{\text{charge}} \underbrace{n}_{\text{electron density}} \underbrace{\vec{v}}_{\text{velocity}}$$

Bulk solid state physics:

Requires local equilibrium
(grad *T* and grad *μ* small)

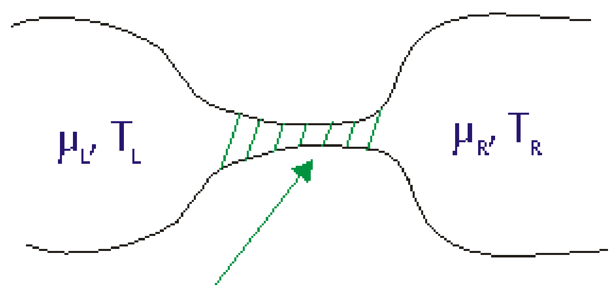
$$\vec{I}_n = \frac{2}{(2\pi)^d} \int d^d\vec{k}\, f(\vec{k})\vec{v}(\vec{k}) \qquad \text{particle current}$$

$$\vec{I}_E = \frac{2}{(2\pi)^d} \int d^d\vec{k}\, f(\vec{k})\vec{v}(\vec{k})E(\vec{k}) \quad \text{energy current}$$

$$\vec{I} = e\vec{I}_n \qquad \text{electrical (charge) current}$$

Mesoscopic physics:

Strong non-equilibrium
Conductor too small to
equilibrate: Ohm's law
not applicable:



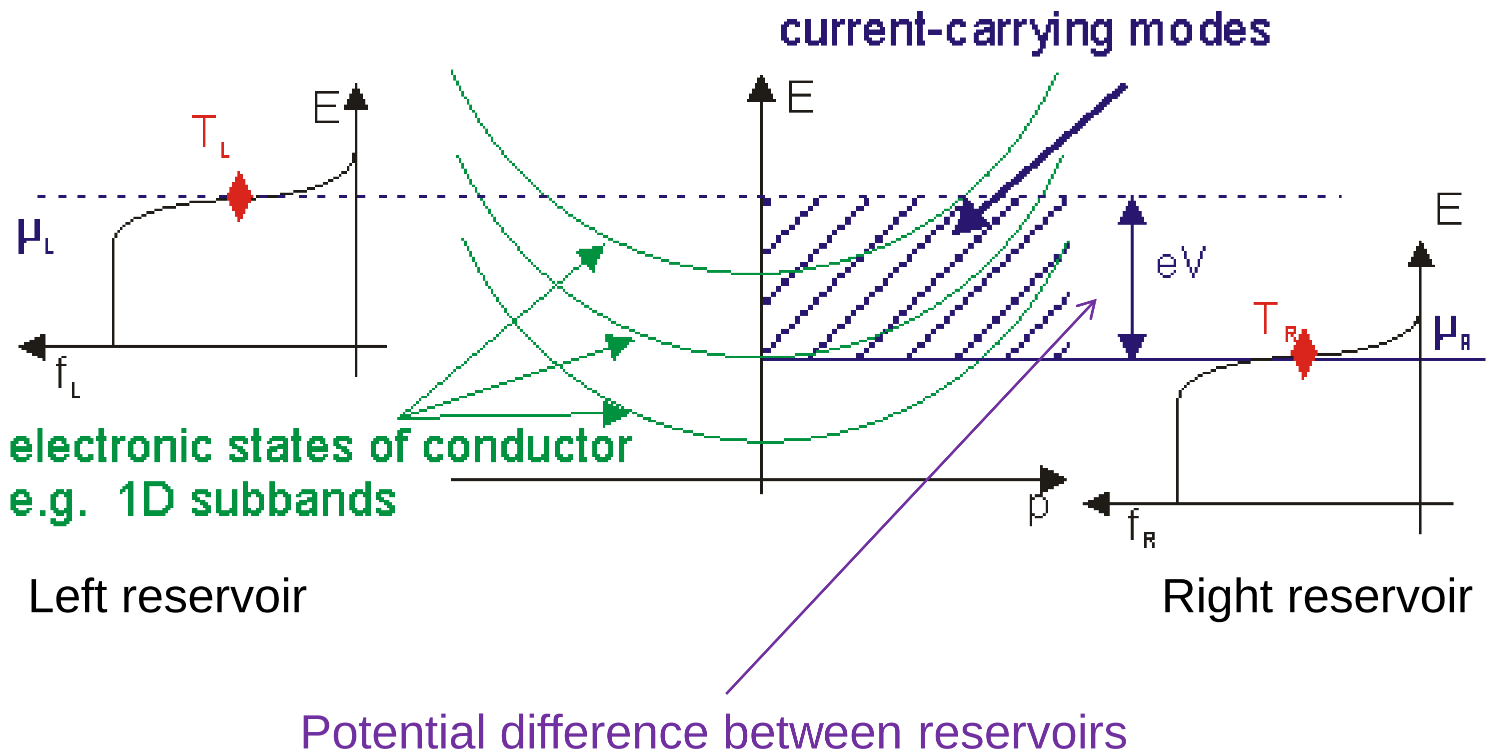
Reservoirs:
macroscop. objects,
in thermodyn. equilibrium

$j = \sigma E = \sigma \text{ grad } \mu_{local}$

not defined

Mesoscopic conductor: transport determined by electronic states and their local occupation

Ballistic and quasi-ballistic regime: Electronic transport as quantum mechanical wave-scattering: Landauer picture



Assumptions:

- Ideal transmission of incoming states (no elastic scattering) $T_n = 1$
- Ideal coupling between reservoirs and conductor: “reflectionless contacts”:

T_n: transmission probability of electron state n

Perfect 1d subbands: Conductance Quantization

Charge current
$$\vec{I} = \frac{2e}{2\pi}\int dk\vec{v}(\vec{k})\left[f^{+}(E,\mu_L,T_L) - f^{-}(E,\mu_R,T_R)\right]$$

$$= e\int dE\left(\rho_1^{+}(E)f^{+}(E) - \rho_1^{-}(E)f^{-}(E)\right)\vec{v}(E)$$

k-space -> *E*-space

with 1D DOS:
$$\rho_1^{\pm}(E) = \frac{1}{2}\sum_n \frac{1}{\pi\hbar}\sqrt{\frac{2m}{E-\varepsilon_n}}\Theta(E-\varepsilon_n)$$

and band energies
$$E_n = \varepsilon_n + \frac{\hbar^2 k^2}{2m} \longrightarrow v_n(E) = \frac{\hbar k_n(E)}{m} = \sqrt{\frac{2(E-\varepsilon_n)}{m}}$$

$$\vec{I} = e\sum_n \int dE \frac{1}{\pi\hbar}\Theta(E-\varepsilon_n)(f^{+} - f^{-})$$

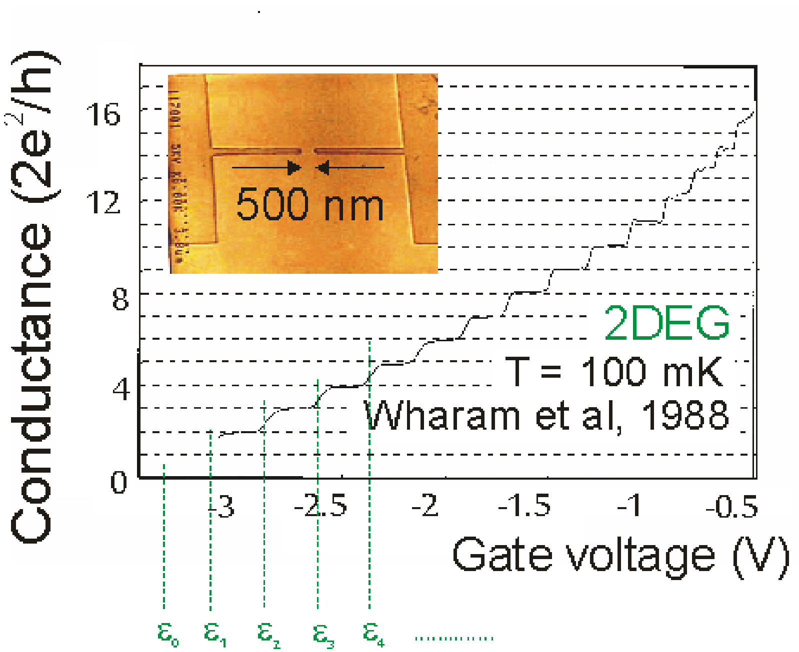
$$= \frac{2e}{h}\boxed{M(\mu)}\boxed{\int dE(f^{+} - f^{-})} = \frac{2e^2}{h}M(\mu)\quad V$$

Number of occupied subbands — $M(\mu)$; $\int dE(f^{+} - f^{-})$ = eV

$$eV = \mu_L - \mu_R << \mu$$
$$\mu := \frac{\mu_L + \mu_R}{2}$$

Conductance is quantized
$$G = \frac{2e^2}{h}M$$

Conductance quantization



Conductance is quantized

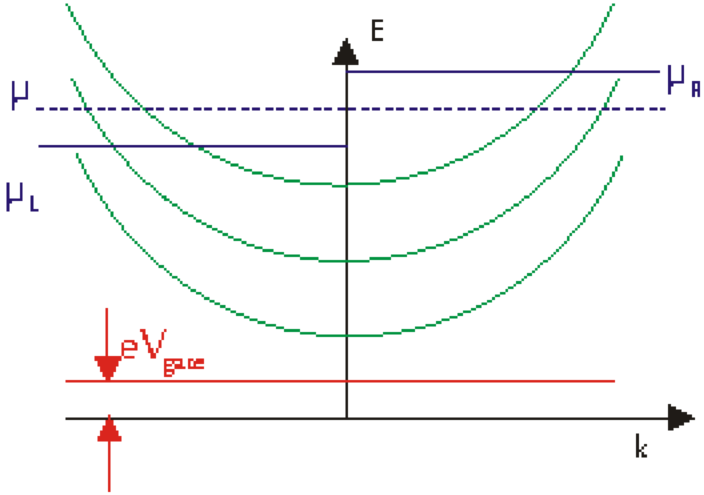
$$G = \frac{2e^2}{h} M(\mu)$$

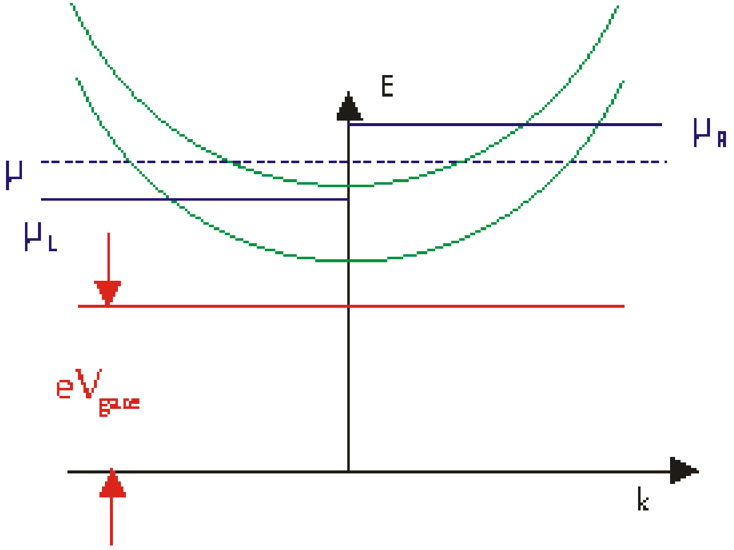
In multiples of the conductance quantum

$G_0 = 2e^2/h \sim 77.6\ \mu S = 1/12906\ \Omega$

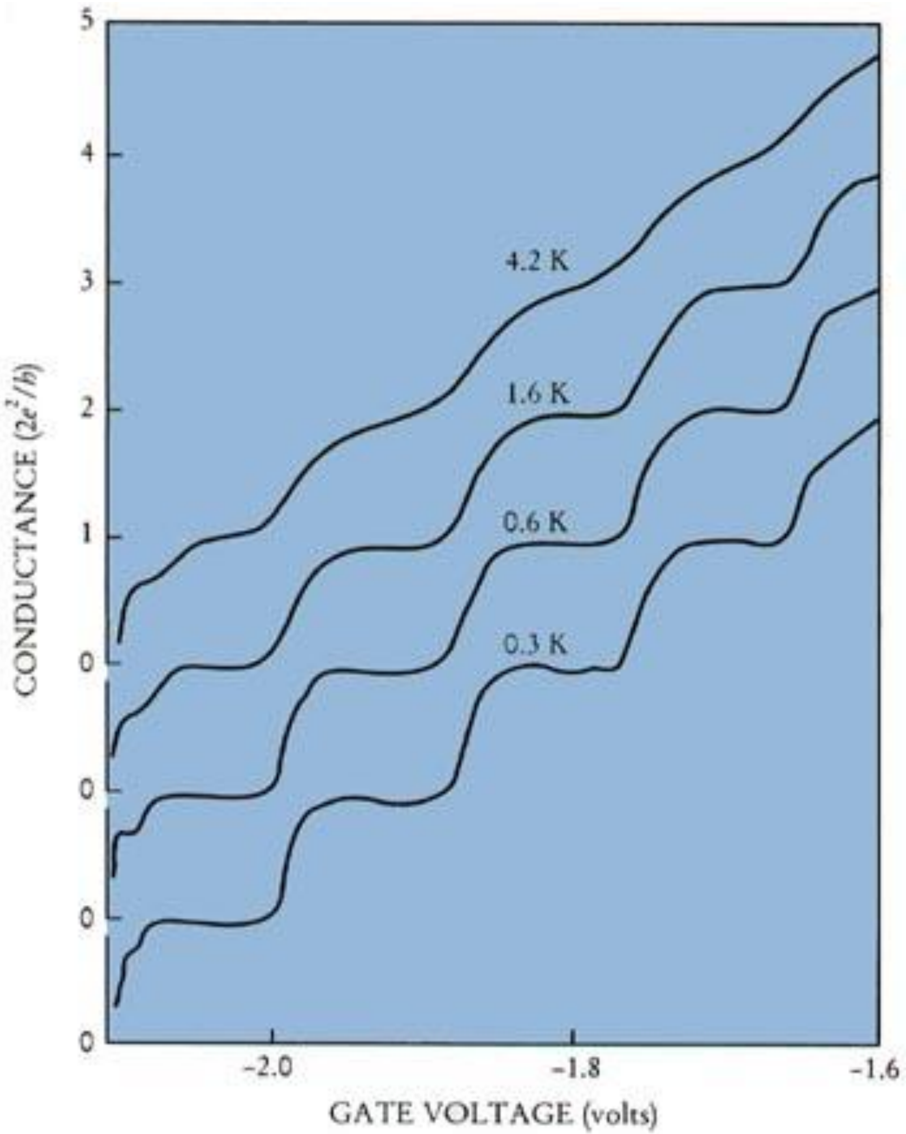
Reduction of V_{gate} corresponds to

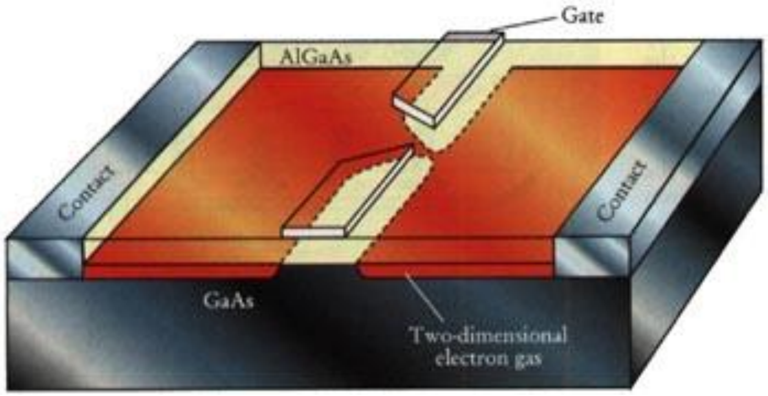
- Enhancement of potential
- Reduction of M(μ)
- Reduction of effective width w





Ballistic transport: Conductance quantization in a 2DEG



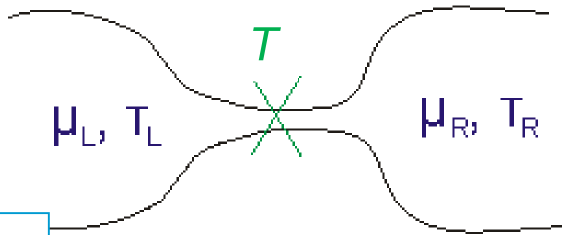


$$G = \frac{2e^2}{h}\sum_n T_n$$

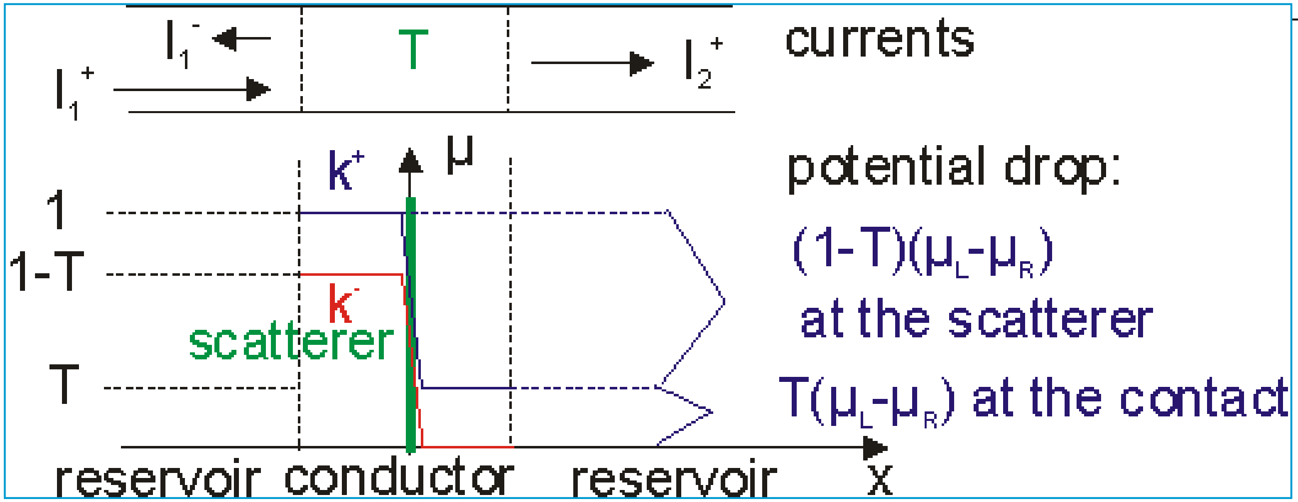
B. J. van Wees, H. van Houten, C. W. J. Beenakker, J. G. Williamson, L. P. Kouwenhoven, D. van der Marel, C. T. Foxon, Phys. Rev. Lett. **60**, 848 (1988); Phys. Rev. B **43**, 12431 (1991).

D. A. Wharam, T. J. Thornton, R. Newbury, M. Pepper, H. Ahmed, J. E. F. Frost, D. G. Hasko, D. C. Peacock, D. A. Ritchie, G. A. C. Jones, J. Phys. C **21**, L209 (1988).

With scattering: the Landauer formula



Finite transmission probability $0 < T < 1$



$$I_1^{\,+} = \frac{2e}{h} M(\mu_L - \mu_R)$$

$$I_2^{\,+} = T\, I_1^{\,+}$$

$$I_1^{\,-} = (1 - T\,) I_1^{\,+}$$

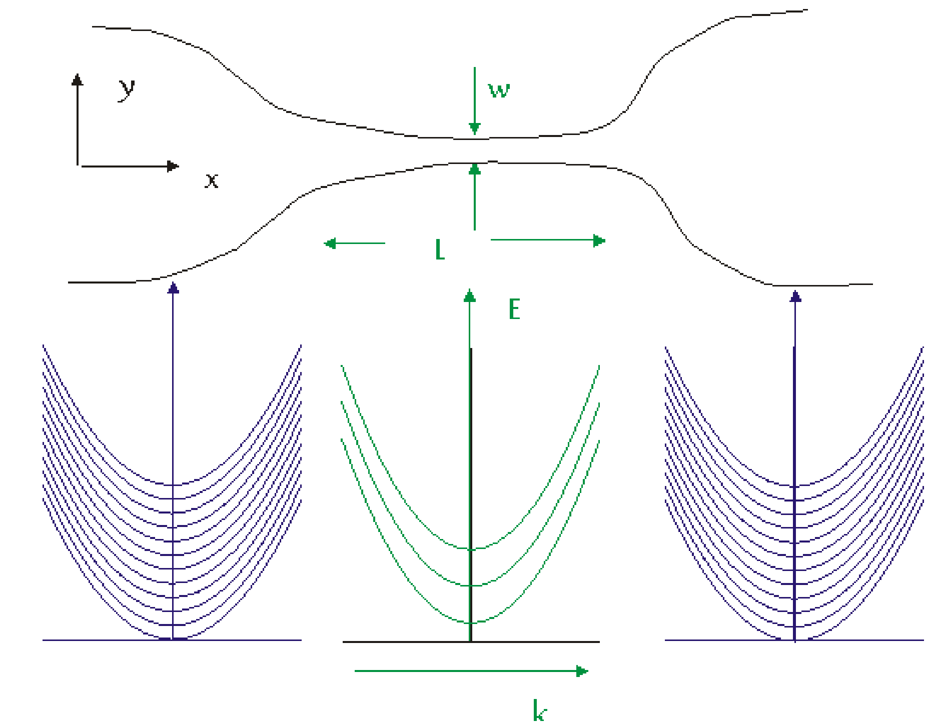
Current: $$I_{ges} = I_1^{\,+} - I_1^{\,-} = I_2^{\,+} = \frac{2e}{h} MT\,(\mu_L - \mu_R)$$

Conductance $G = I/V$ $$G = \frac{2e^2}{h} MT$$

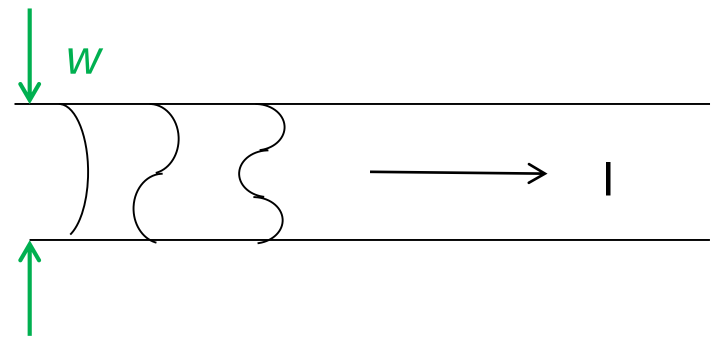
Landauer formula $$G = \frac{2e^2}{h} \sum_{n=1}^{M} T_n$$ Different T_n for different subbands ("channels"):

Contact resistance

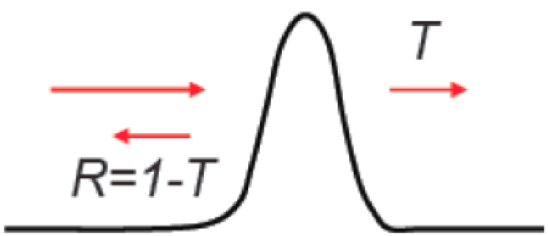
Origin of the resistance despite perfect transmission: Mode-filtering effect



Leads:
states densely packed
Conductor:
Finite level spacing due to confinement



$k_F\, w = M\, \pi \rightarrow M = [k_F W/\pi] = [W/(\lambda_F/2)]$



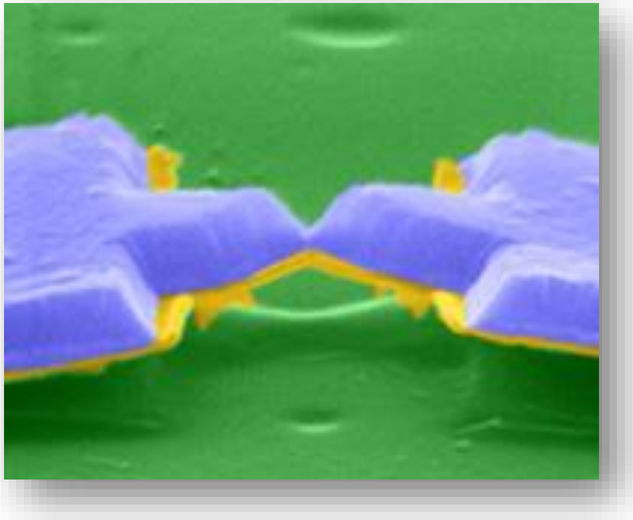
$$\text{Resistance} = \frac{h}{2e^2}\frac{1}{T} = \frac{h}{2e^2}\left(1 + \frac{1-T}{T}\right) = \boxed{\frac{h}{2e^2}} + \boxed{\frac{h}{2e^2}\frac{R}{T}} \quad (T + R = 1)$$

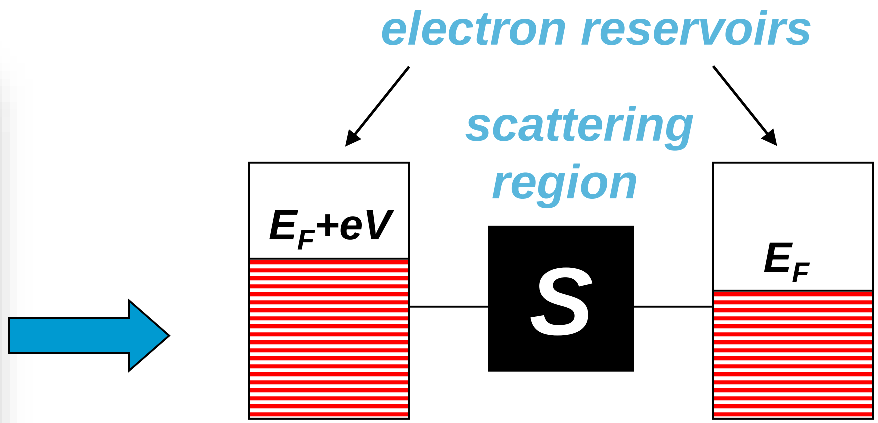
Contact resistance

Scattering resistance

Landauer approach to conductance

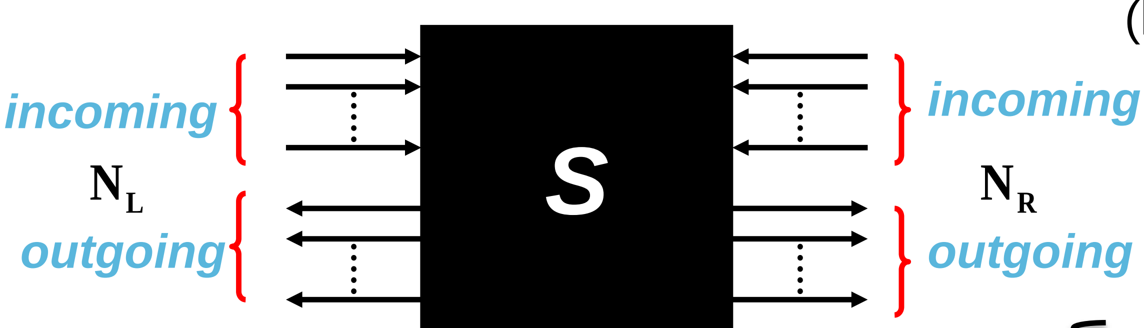
real system





Landauer formula

(low-temperature conductance)

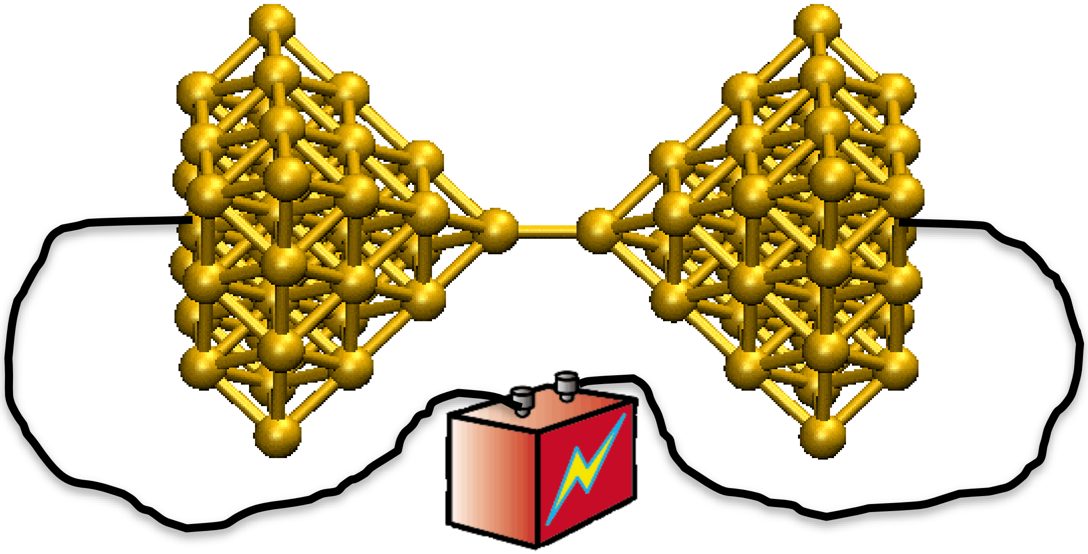


$$G = \frac{2e^2}{h} T(E_\mathrm{F}) = G_0 \sum_n T_n$$

$$G_0 = \frac{2e^2}{h} \approx (12.9\ \mathrm{k}\Omega)^{-1} = \text{ conductance quantum}$$

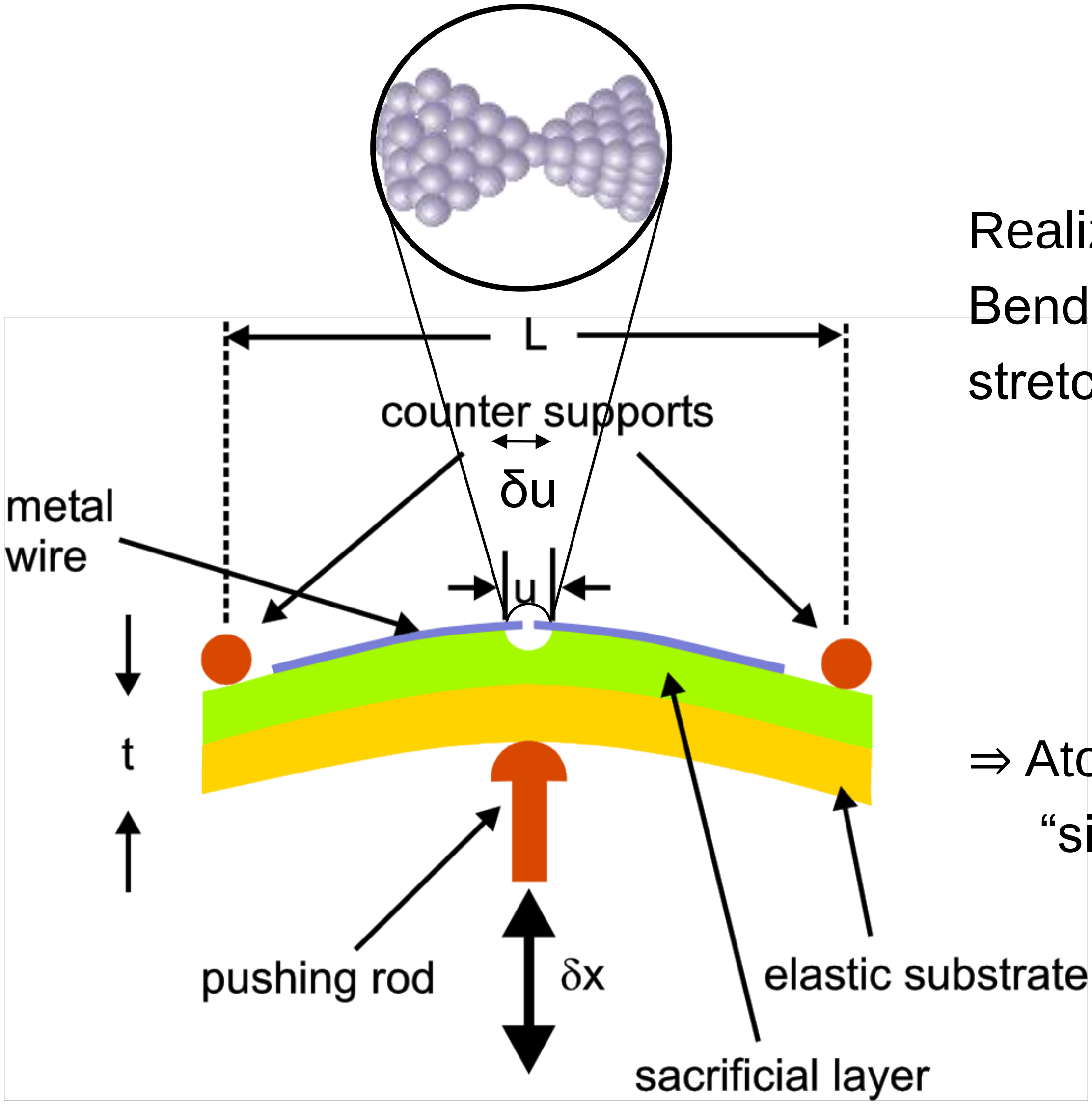
- $T(E_F)$ = total transmission at E_F
- T_n = transmission coefficients

1d Systems: The conductance of a single atom



Review: N. Agraït, A. Levy Yeyati, J.M. van Ruitenbeek, Phys. Rep. 377, 81 (2003).

Mechanically controllable break junctions (MCBJ)

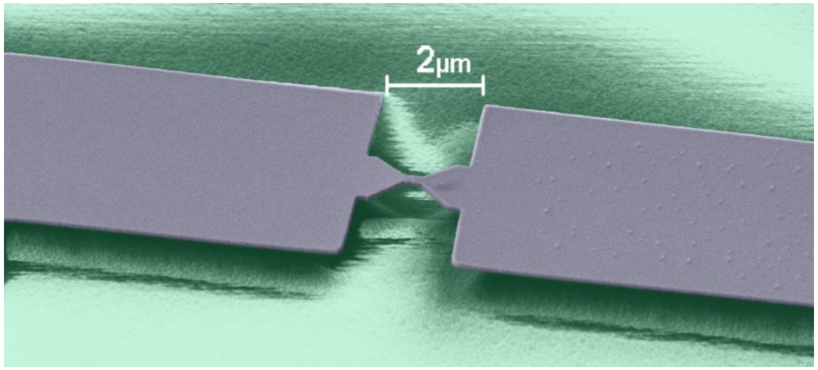


Realization of single-atom contact:
Bending by δx results in a lateral stretching of $\delta u = r\,\delta x$, where

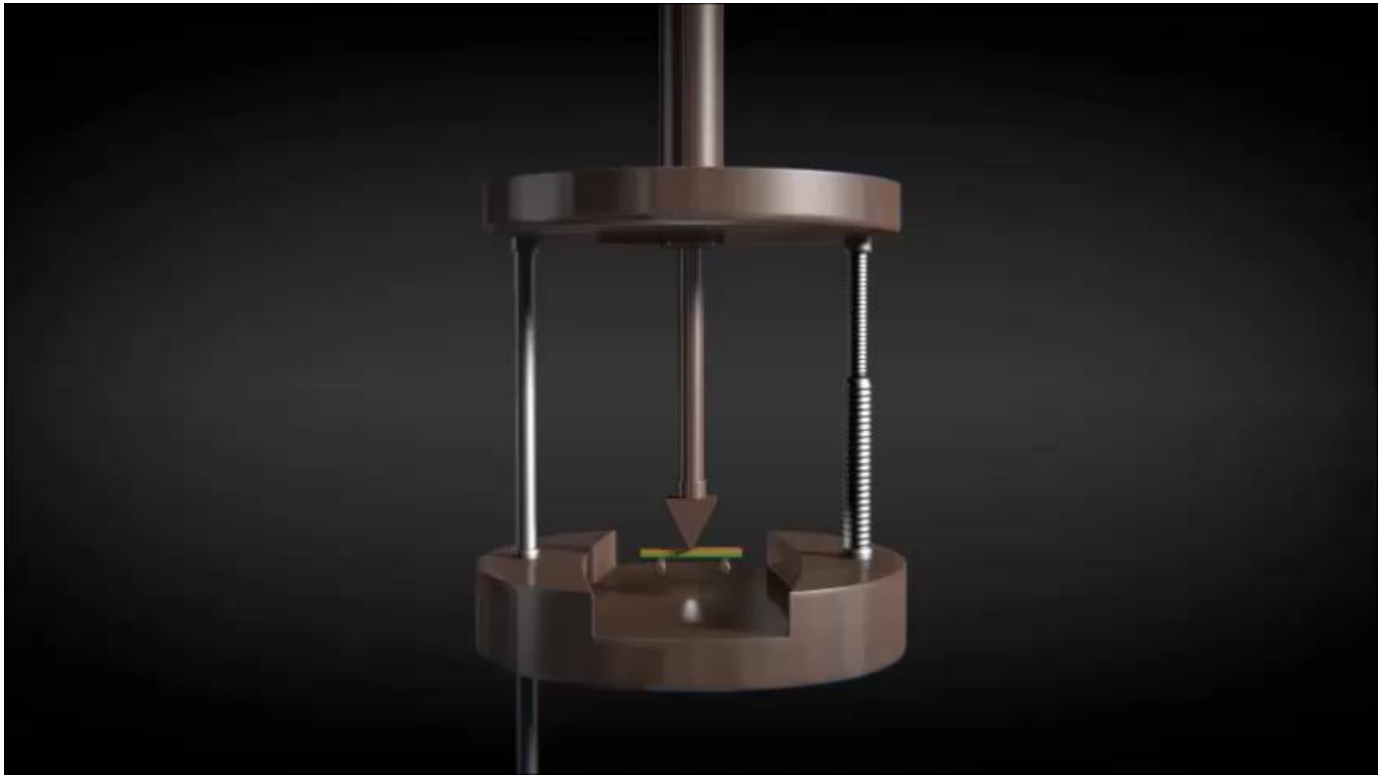
$$r = \frac{6tu}{L^2}$$

⇒ Atomic resolution possible with "simple" mechanics

MCBJ operation

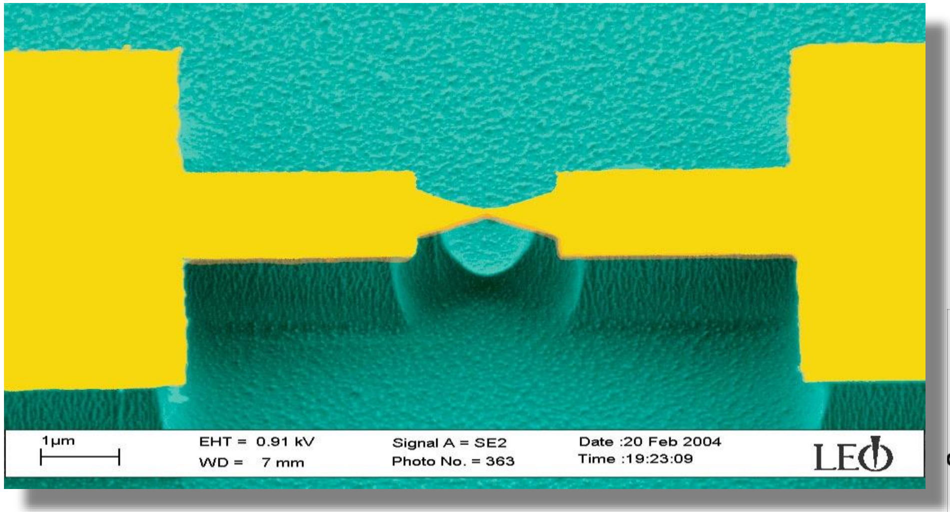


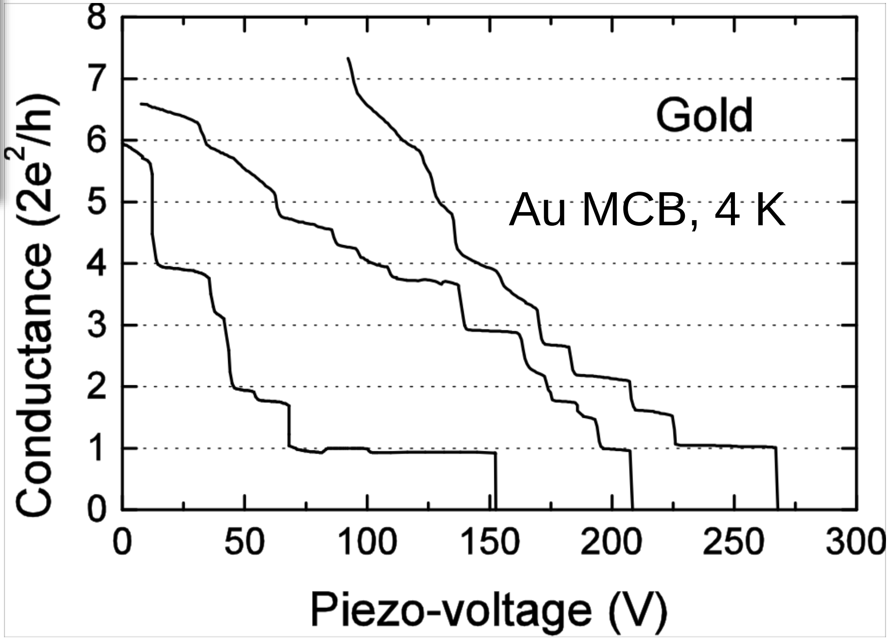
Sample design
Breaking mechanism



1d Systems: Single atom contacts

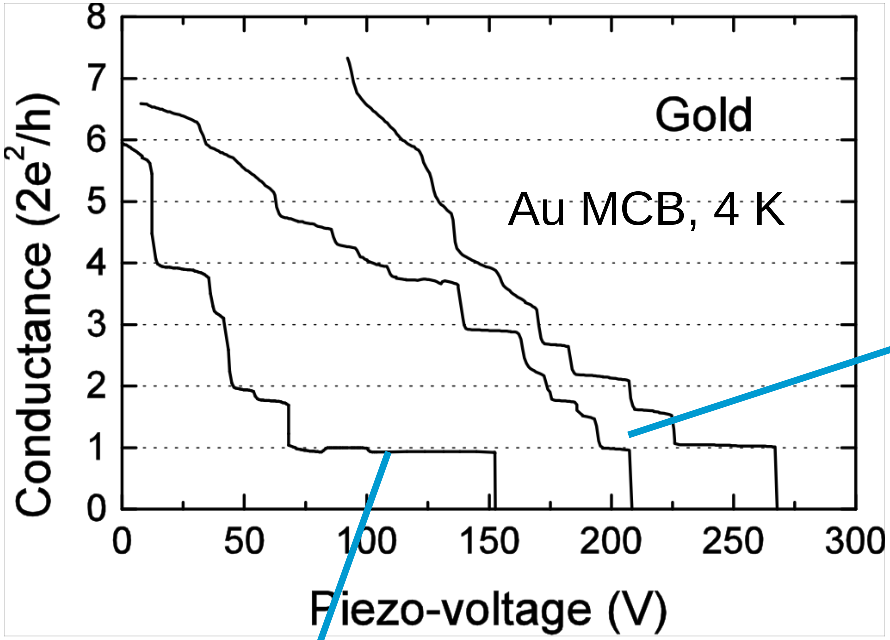
Review: N. Agraït, A. Levy Yeyati, J.M. van Ruitenbeek, Phys. Rep. 377, 81 (2003).



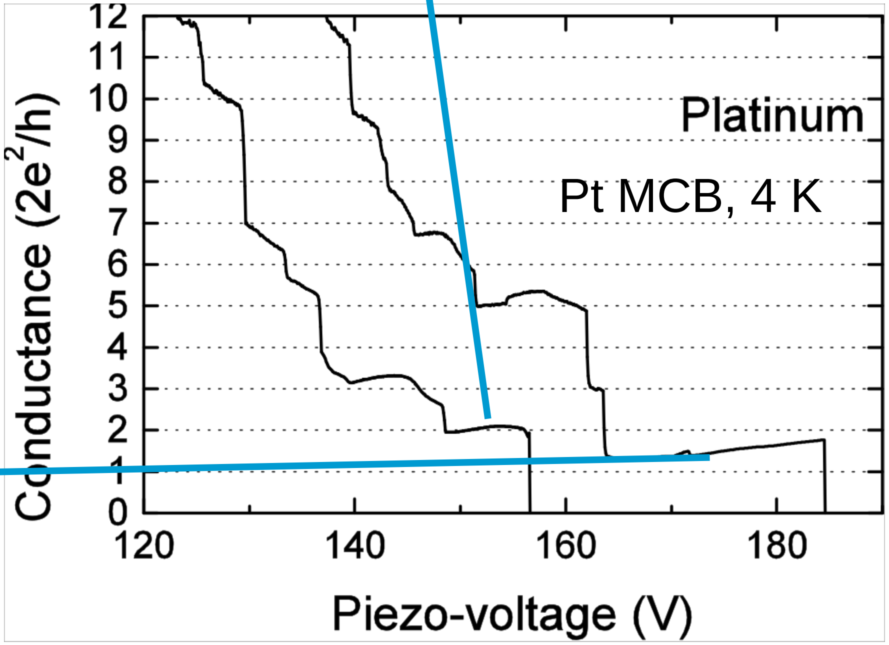


Conductance of atomic-scale contacts

Review: N. Agraït, A. Levy Yeyati, J.M. van Ruitenbeek, Phys. Rep. 377, 81 (2003).

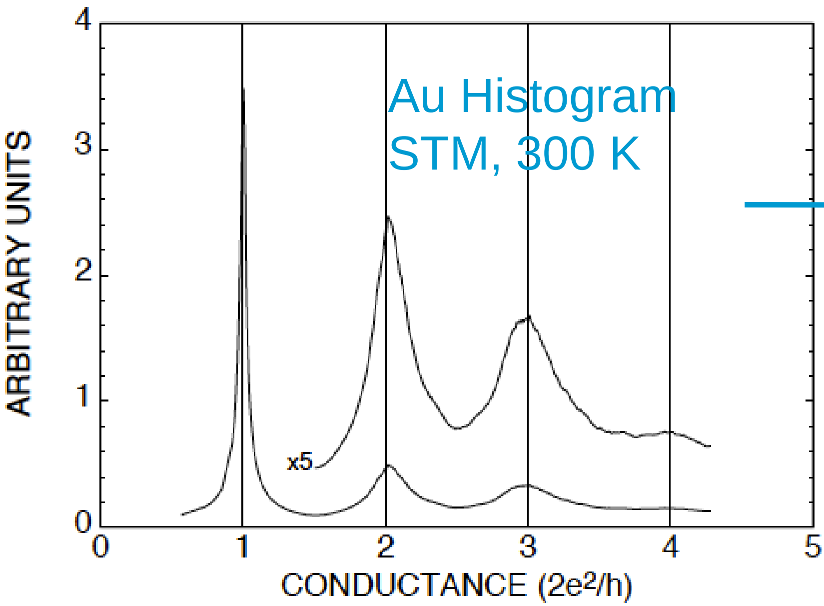


Single-atom contacts



Atomic chains

Conductance histograms

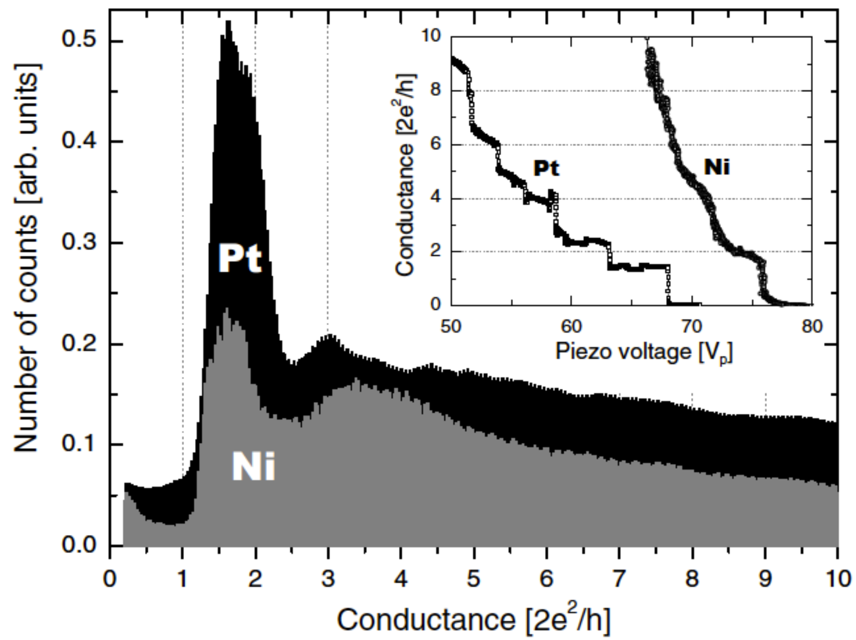


Au Histogram
STM, 300 K

M. Brandbyge et al., PRB 52, 8499 (1995).

Conductance quantization?

Pt and Ni Histograms
MCBJ, 4.2 K

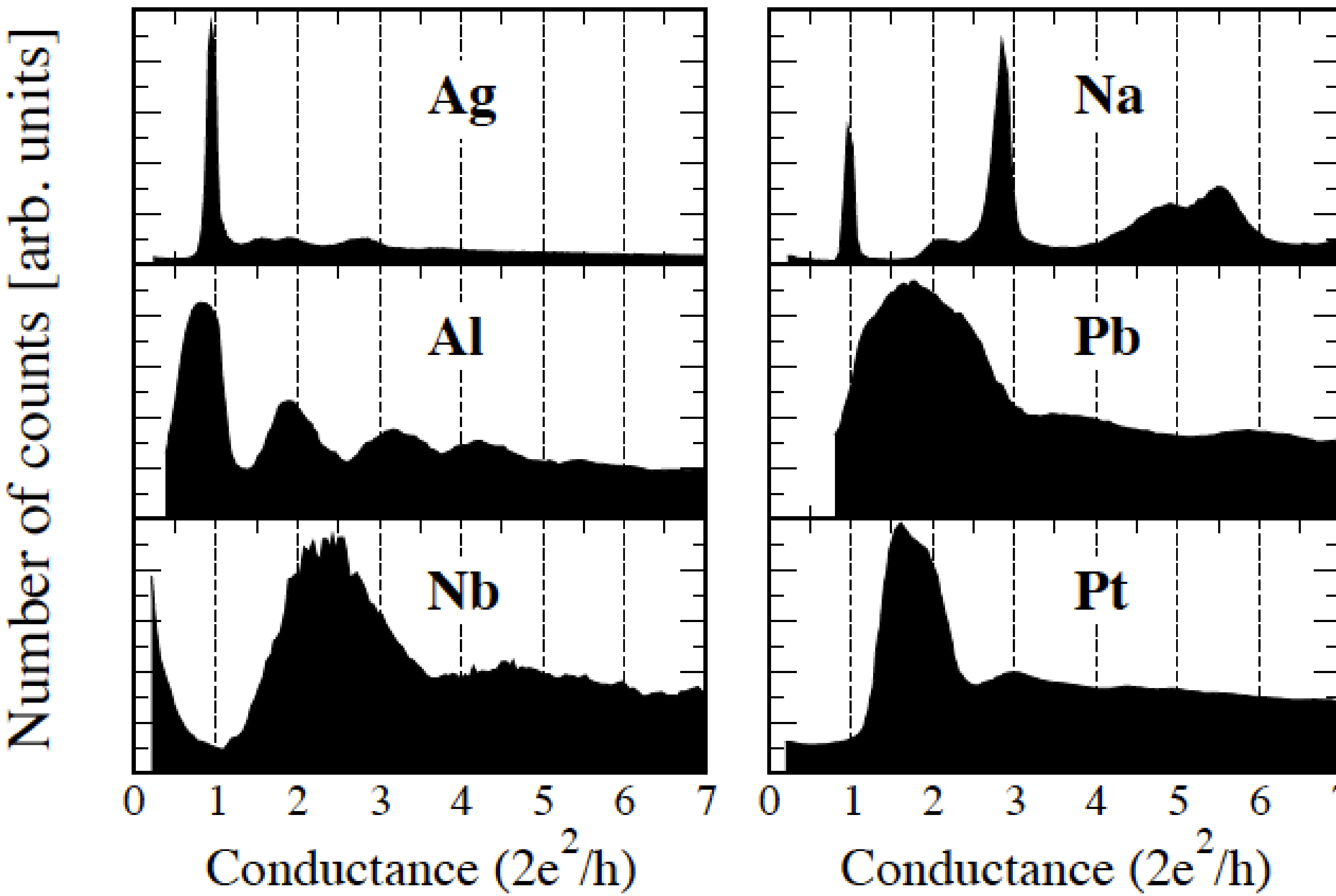


Not always!

A.I. Yanson, PhD thesis,
University of Leiden (2001).

Conductance histograms

A.I. Yanson, Ph.D. Thesis, Leiden (2001).

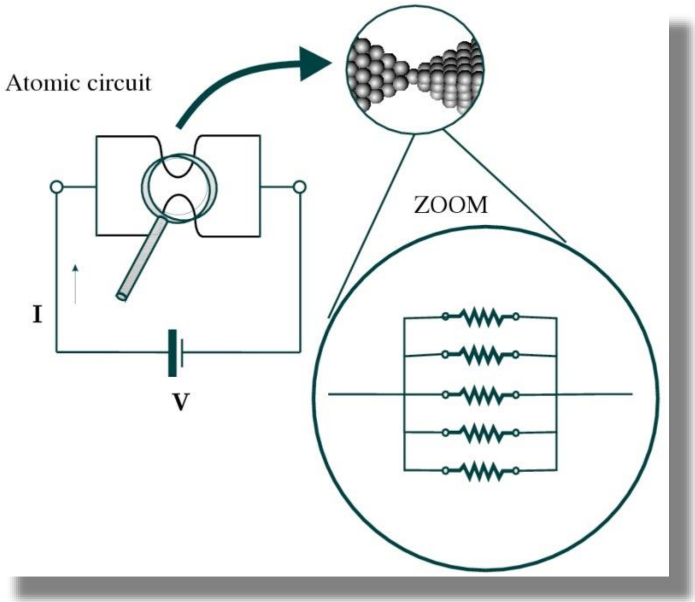


Conductance histograms

Summary of the findings concerning the conductance histograms:

- Highest peak at the lowest conductance value (exception: alkali).
- Position of first peak for all the elements between 0.7 and 2.3G_0. No structure in the histograms below the position of the first peak.
- For free electron-like metals (alkali and noble metals) the first peak is extremely sharp and located almost exactly at 1G_0.
- For divalent metals (Zn, Mg) and trivalent ones (Al) the first peak is rather sharp and located slightly below 1G_0.
- Other multivalent metals (transition metals): broad first peak located above 1G_0 , sometimes (e.g. Nb) above 2G_0.

Chemical nature of the conduction channels of one-atom contacts



Material	Conductance (G0)	Number channels	Orbitals
Alkali and nobel metals	~ 1	1	*s*
Al	0.6 – 1.1	3	*s* und *p*
Pb	2.0 - 2.8	3	*s* und *p*
Nb	2 - 3	5	*s* und *d*

Macroscopic wires: Resistivity (x 10^{-8} ∧m) at T = 300 K

Material	Ag	Cu	Au	Al	Na	Zn	Pt	Pb
Resistivity	1.61	1.72	2.27	2.73	4.93	6.01	10.8	21.3

Small is different!!

Comparison of Quantum Point Contact Realizations

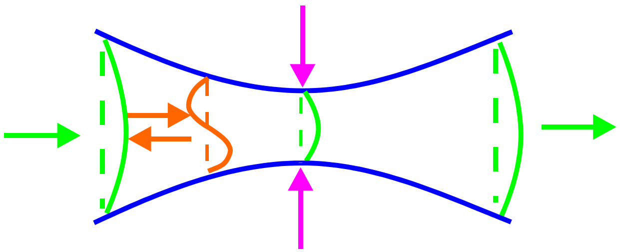
Low electron density metals

$\lambda_F \gg a_0$

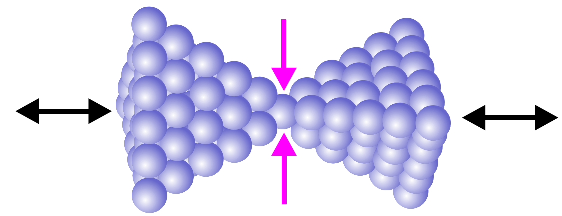
$W \sim \lambda_F$

High electron density metals

$\lambda_F \sim a_0$

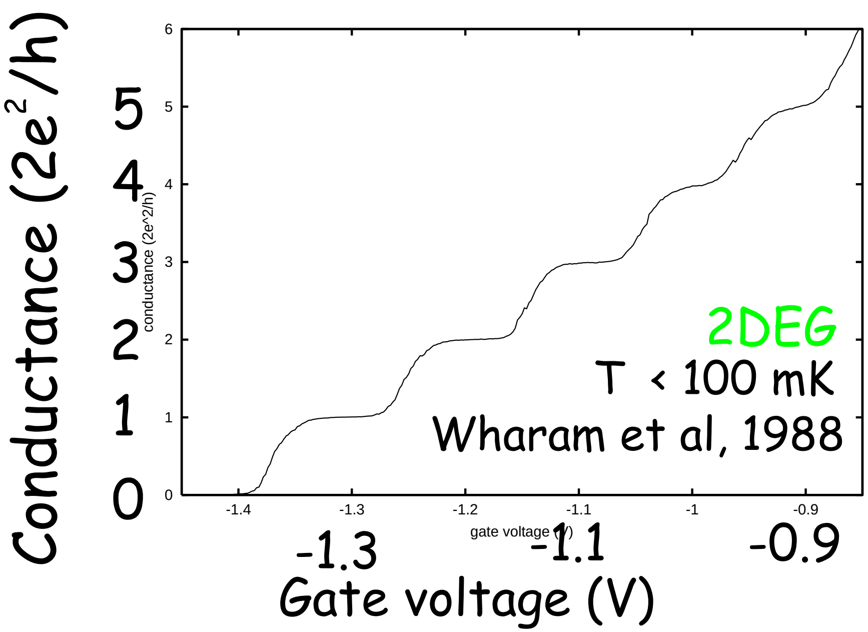


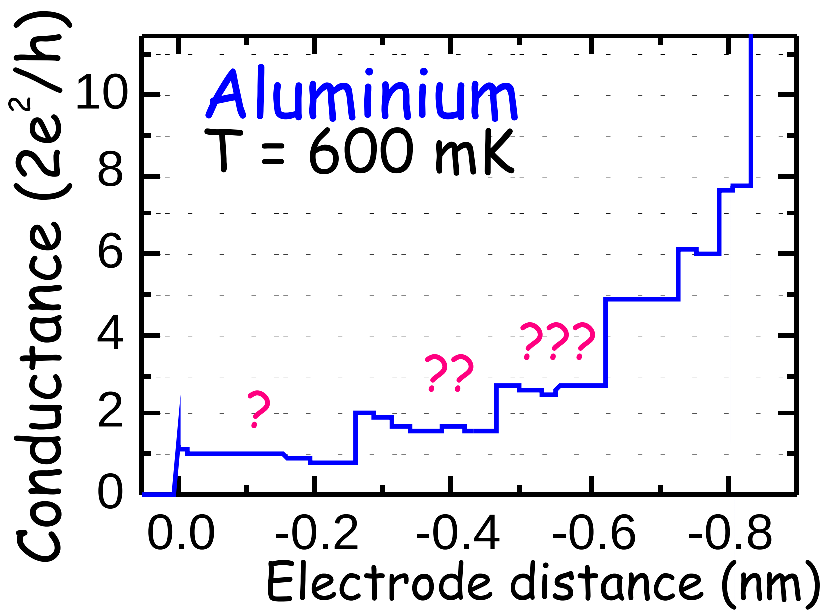
$$G = \frac{2e^2}{h}\sum_{i=1}^{N} T_i$$



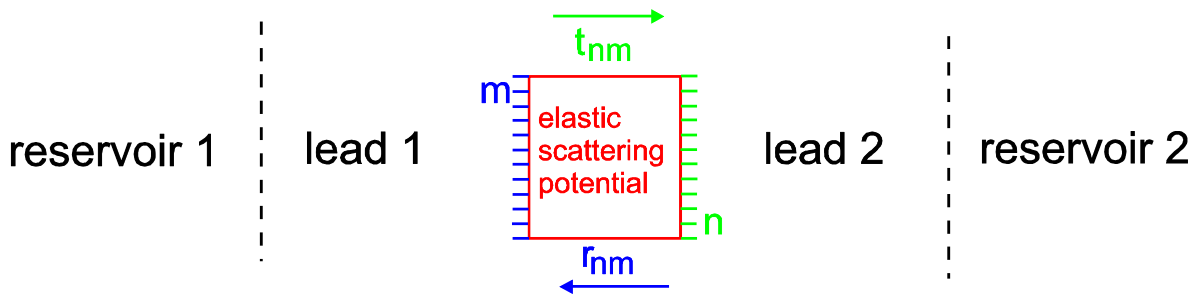
$T_1 = 1$, $T_2 = \ldots = T_N = 0$

$T_i = ?$





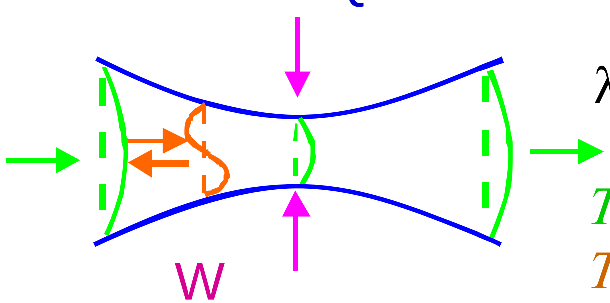
Calculation of transmission coefficients



Channels are eigenfunctions of scattering problem

Landauer formula: $G = \frac{2e^2}{h} T(E_F)$, $T(E_F) = \sum_{n=1}^{N} \sum_{m=1}^{N} |t_{nm}|^2 = Tr(t^+ t) = \sum_{i=1}^{N} \tau_i$

Adiabatic QPCs



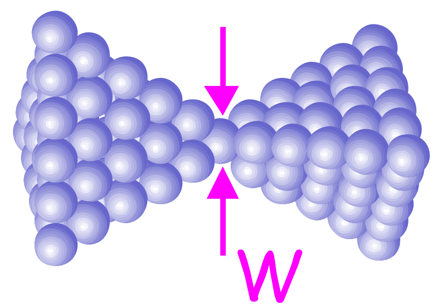
$\lambda_F \sim W >> a$

$T_1 = 1$,

$T_2 = \ldots = T_N = 0$

Wavefunctions in reservoirs, leads and QPC are of same kind, well matched: $\tau_i = 1$ for all modes with $n\lambda_F/2 < W$

Atomic QPCs in metals:



$\lambda_F \sim W \sim a$

$T_i = ?$

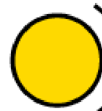
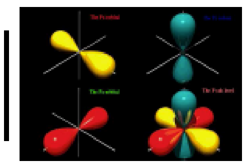
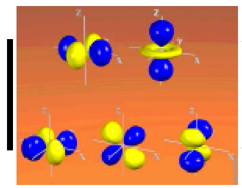
Wavefunctions in reservoirs and QPC are different: $\tau_i < 1$

Chemical nature of the conduction channels

- Transmission evaluated at the central atom: $\mathrm{Dim}(t^{+}t) = N_{orb}$

The number of channels is controlled by the number of valence orbitals in the central atom

- In the case of one-atom contacts the channels are linear combinations of the atomic orbitals of the central atom:

$|\mathrm{channel}\rangle_i = c_{is}\,|$  $\rangle + c_{ip}\,|$  $\rangle + c_{id}\,|$  $\rangle$

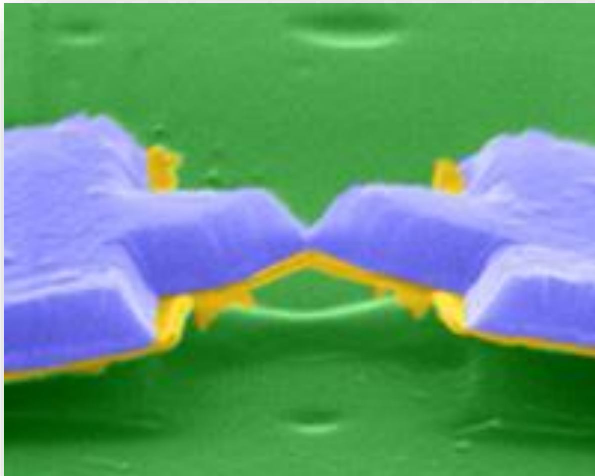
- Assuming that there is a single relevant orbital per atom, the transmission adopts the form:

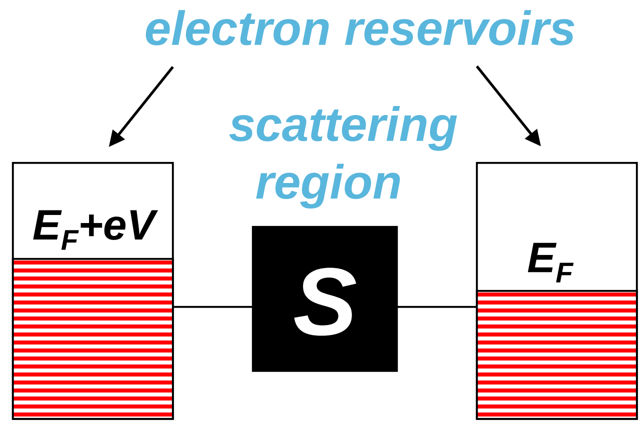
$$T(E) = \frac{4\Gamma_L(E)\Gamma_R(E)}{[E-\tilde{\varepsilon}_0]^2 + [\Gamma_L(E)+\Gamma_R(E)]^2}$$

- If there are several relevant orbitals per atom (sp-like metals, transition metals, etc.), then it is difficult to satisfy the “resonant” condition for all the channels at the same time. This implies that in multivalent metals there are often several channels with intermediate transmissions and therefore, there is **no conductance quantization!!!**

Landauer approach to conductance

real system





Landauer formula

Which values can *T*(*E*) adopt?
Models for the transmission function?

conductance)

$$G = \frac{2e^2}{h} T(E_F) = G_0 \sum_n T_n$$

$$G_0 = \frac{2e^2}{h} \approx (12.9\ \mathrm{k\Omega})^{-1} = \text{ conductance quantum}$$

- *T*(E_F) = total transmission at E_F
- T_n = transmission coefficients

Single-molecule junctions

Introduction

- Coherent transport models: Single level (resonant) tunneling

Basic experiments on testbed-molecules

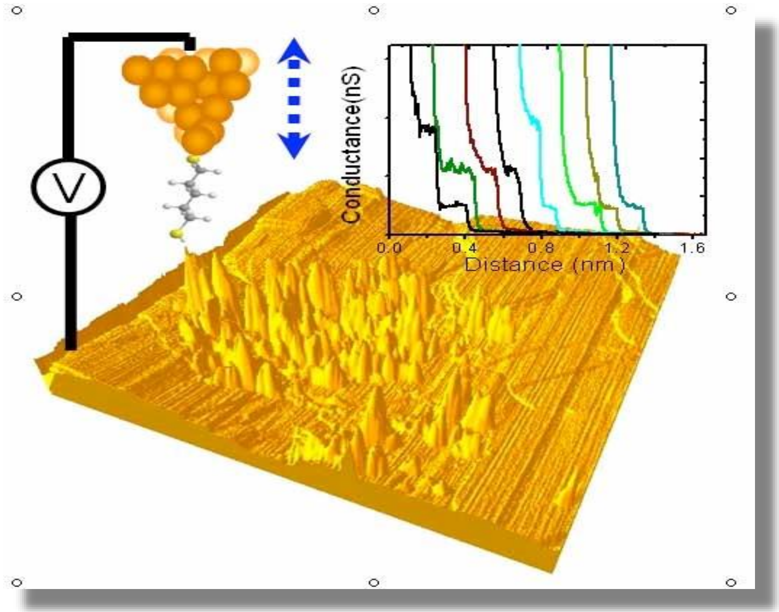
- Understanding current-voltage curves
- Bridging between metals and molecules: role of endgroup and role of metal

Functional molecular devices

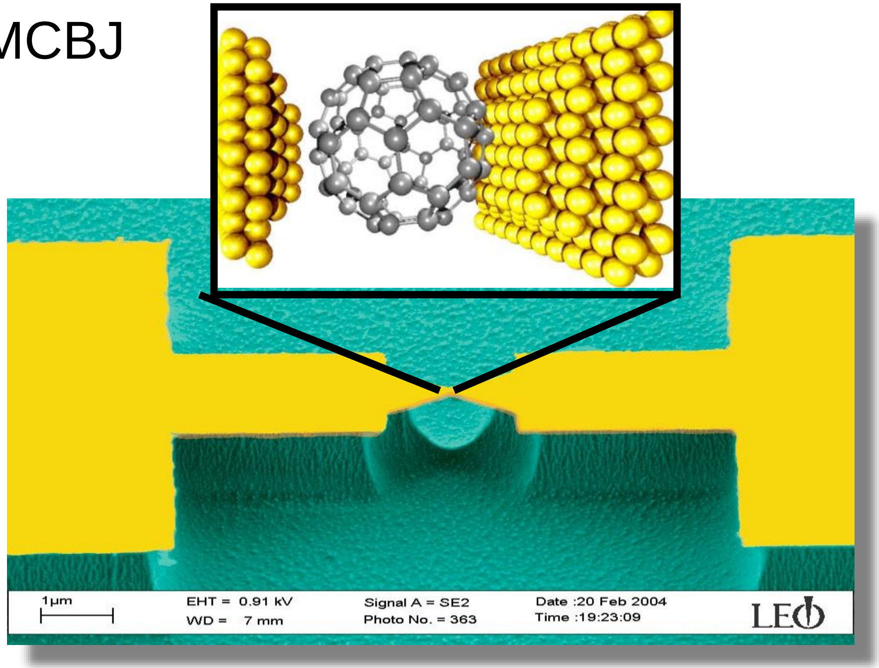
- Weak coupling regime: Single-electron transistor

Techniques providing single molecule contacts

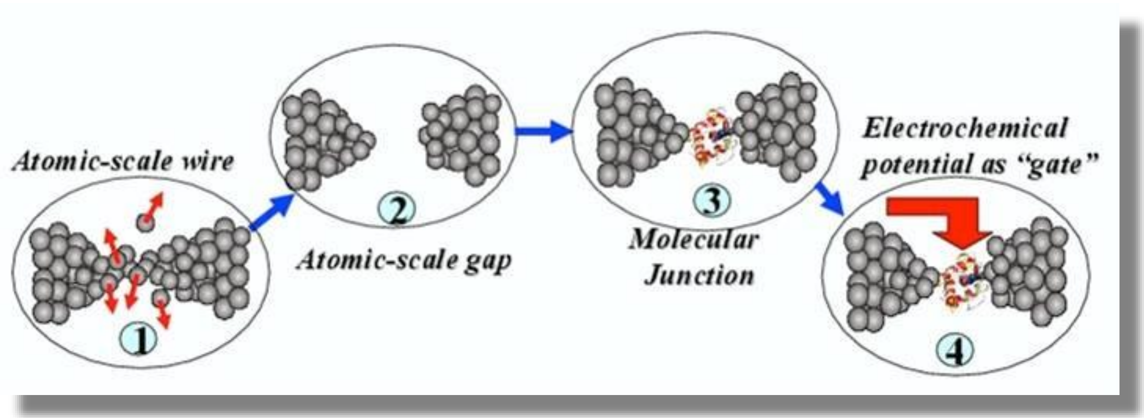
1. STM



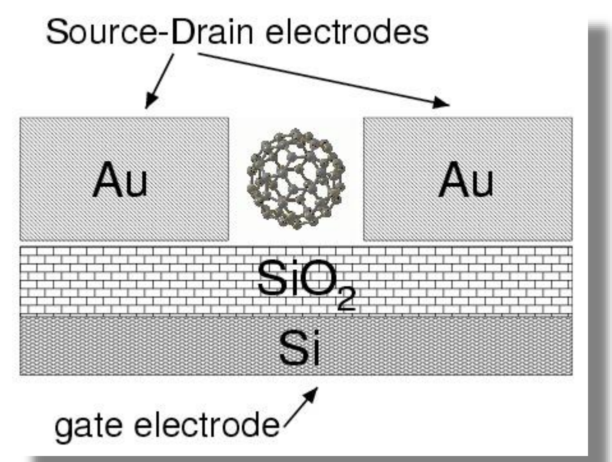
2. MCBJ



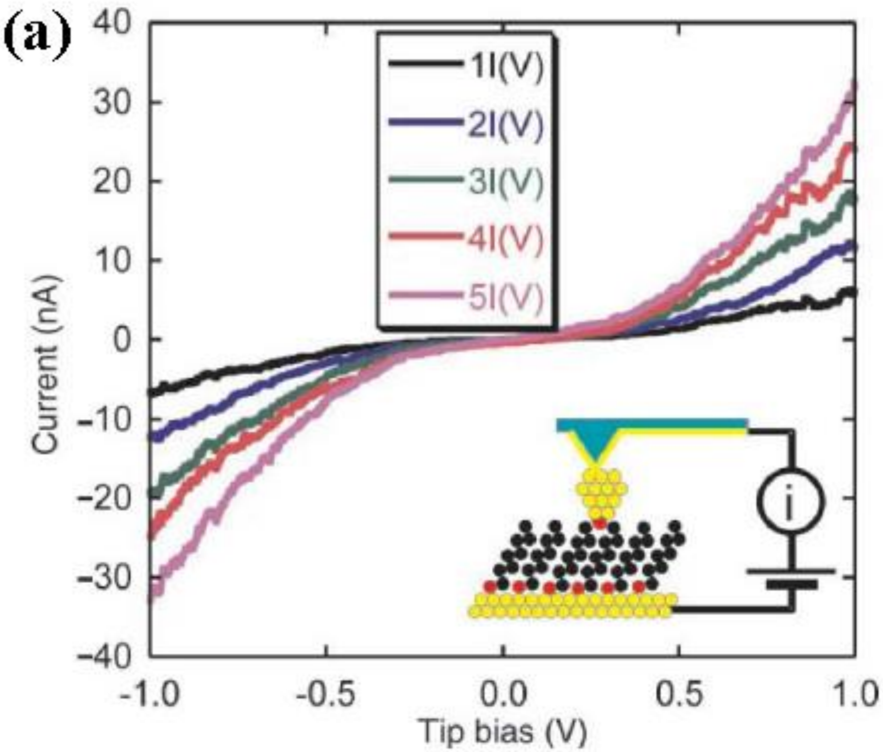
3. Electrochemical methods

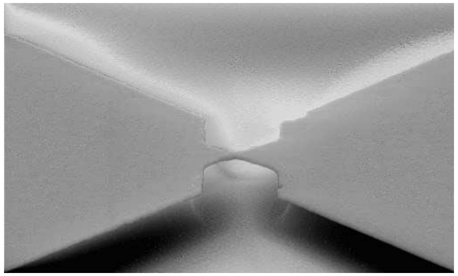


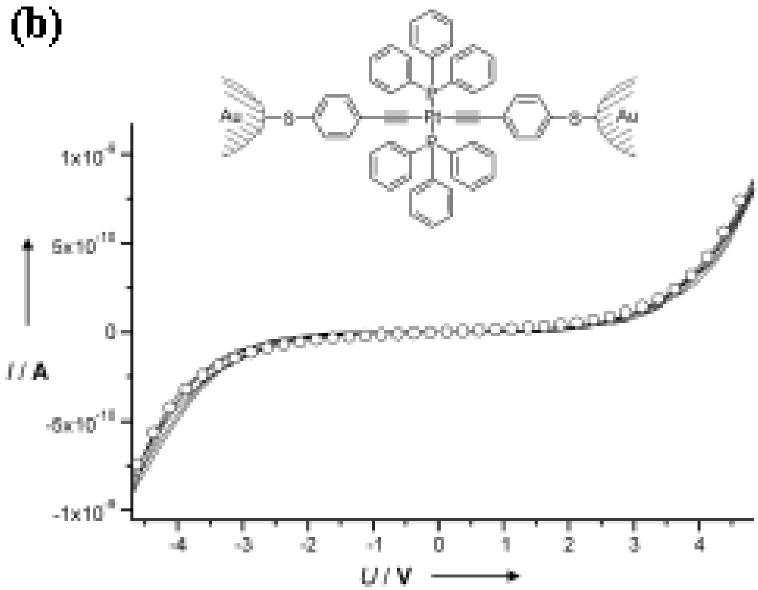
4. Electromigration



Current-voltage characteristics and the single-level model:





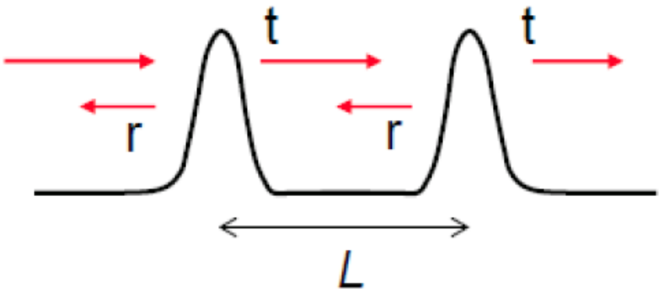


X.D. Cui et al, Science 294, 571 (2001).

Mayor et al., Angew. Chem. Int Ed. **41** 1183 (2002)

Resonant tunneling – the Fabry-Perot problem

Coherent transport through two identical barriers in series



Complex transmission and reflection amplitudes

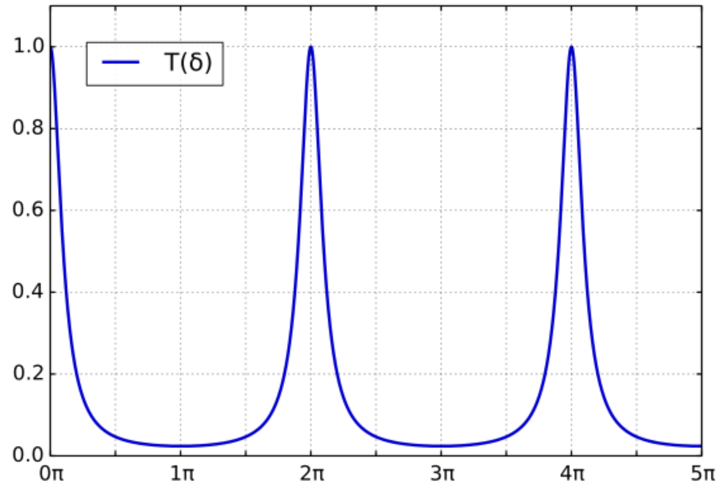
$$t = |t|e^{i\phi_t}$$

$$r = |r|e^{i\phi_r}$$

$$T_{\text{total}} = \frac{|t|^4}{1 + |r|^4 - 2|r|^2\cos(\phi)}$$

$$= \frac{T^2}{1 + R^2 - 2|R|\cos(\phi)}$$

$$\phi = 2kL + \phi_{r1} + \phi_{r2}$$



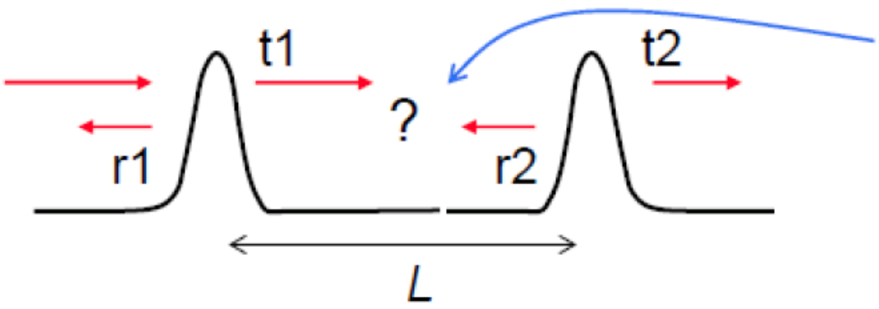
For $\phi = 2\pi n$:

$$T_{\text{total}} = \frac{|t|^4}{(1 - |r|^2)^2} = \frac{T^2}{(1 - R)^2} = \frac{T^2}{T^2} = 1$$

Perfect transmision possible

Outlook 2: Incoherent transport – transition to classical behavior

Distance L > L_φ



→ no interference term

$$T_{\text{total}} = \frac{|t_1|^2 |t_2|^2}{1 - |r_1|^2 |r_2|^2}$$

Classical addition of contributions from independent barriers as in Ohm's law

$$\text{Resistance} = \frac{h}{2e^2}\left(1 + \frac{|r_1|^2}{|t_1|^2} + \frac{|r_2|^2}{|t_2|^2}\right) = \frac{h}{2e^2} + \frac{h}{2e^2}\frac{R_1}{T_1} + \frac{h}{2e^2}\frac{R_2}{T_2}$$

$$\neq Res_1 + Res_2$$

Contact resistance becomes negligible for many channels (wide contacts, parallel resistors) only

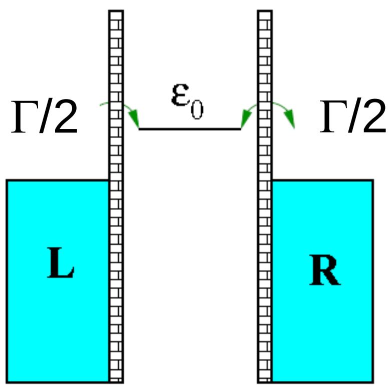
See e.g. Nazarov & Blanter, Quantum transport

Resonant tunneling – the single-level model

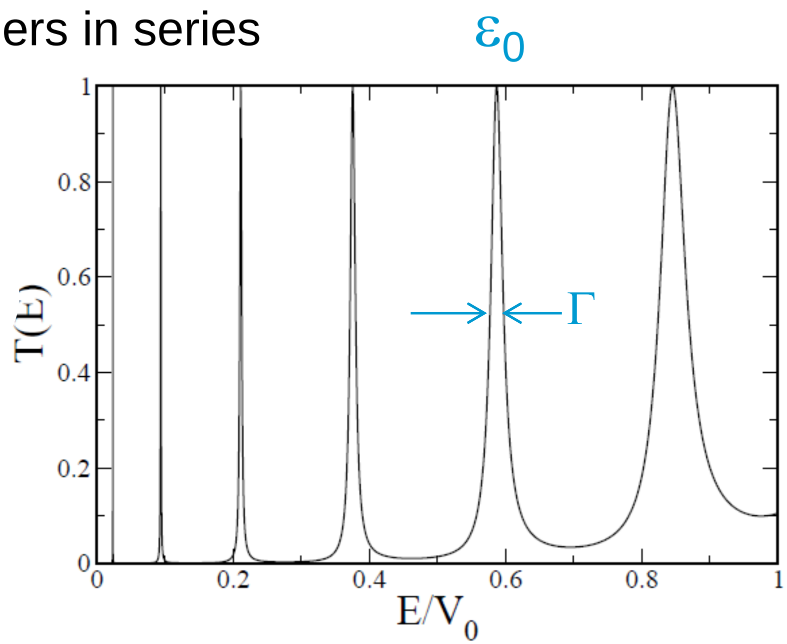
Coherent transport through two identical barriers in series

$$T = T_{total} = \frac{{T_B}^2}{1 + R^2 - 2|R|\cos(\phi)}$$

For electrons with $k = (2mE)^{1/2}/\hbar$ this can be expressed in energy space.



$\cos\phi = 1$ ($2kL = 2n\pi$) corresponds to particle-in-a-box states for potential well with width L



For rectangular barriers with V_0= 4 eV, spacing L = 2 nm and thickness d = 0.2nm

Approximation around resonance at $E = \varepsilon_0$ for $T_B \ll 1$ and $\varepsilon_0 \ll V_0$

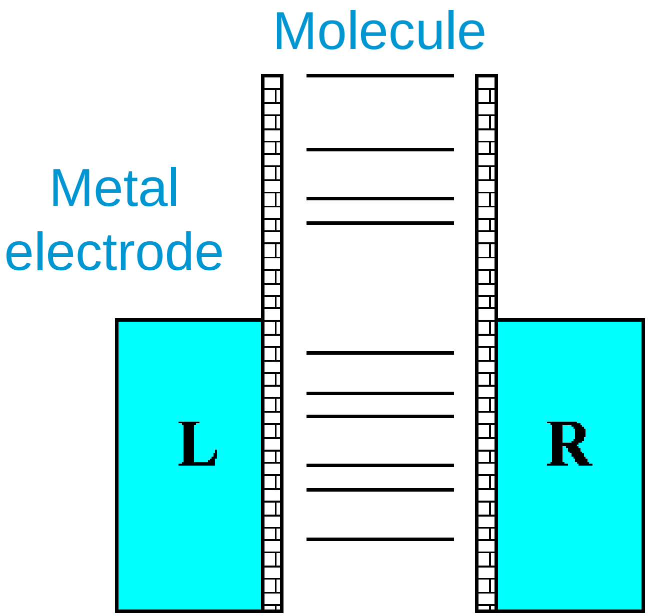
$$T(E) = \frac{4\Gamma^2}{(E-\epsilon_0)^2 + 4\Gamma^2}$$

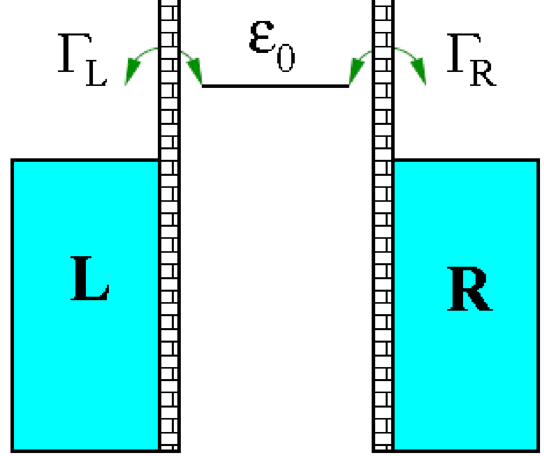
with $\Gamma = \frac{T}{2}\frac{d\phi}{dE}$ the width of the resonance

Lorentzian shape , “Breit-Wigner resonance“

Cuevas&Scheer: Introduction to Molecular Electronics, Ch 4 & 13

Understanding IVs: Single-Level Model





$$I(V) = \frac{2e}{h} \int_{-\infty}^{\infty} T(E,V)\left[f(E - eV/2) - f(E + eV/2)\right] dE$$

Landauer Formula (for current)

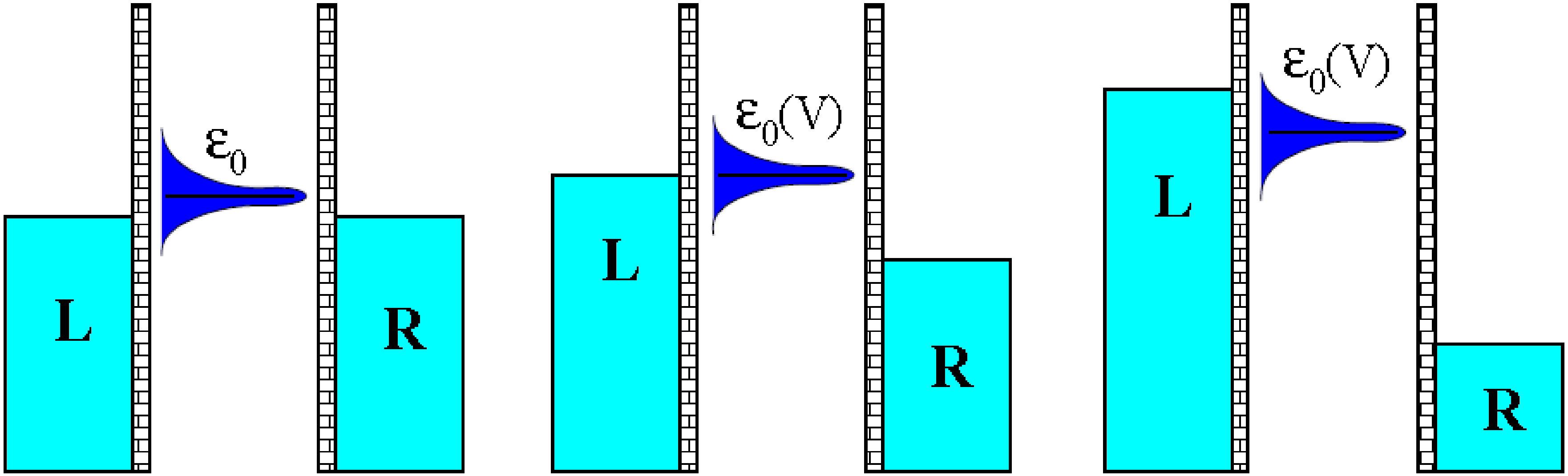
L. Zotti et al, Small 6, 1529 (2010)

$$T(E,V) = \frac{4\Gamma_L \Gamma_R}{[E - \varepsilon_0(V)]^2 + [\Gamma_L + \Gamma_R]^2}$$

See also: Thijssen& van der Zant, phys. stat. sol. (b) **245**, 1455 (2008)
Huisman et al., Nano Lett. **9**, 3909 (2009)

$$\Gamma = \Gamma_L + \Gamma_R$$

Understanding IVs: Single-Level Model



$$I(V) = \frac{2e}{h}\int_{-\infty}^{\infty} T(E,V)\left[f(E-eV/2) - f(E+eV/2)\right]dE$$

Landauer Formula (for current)

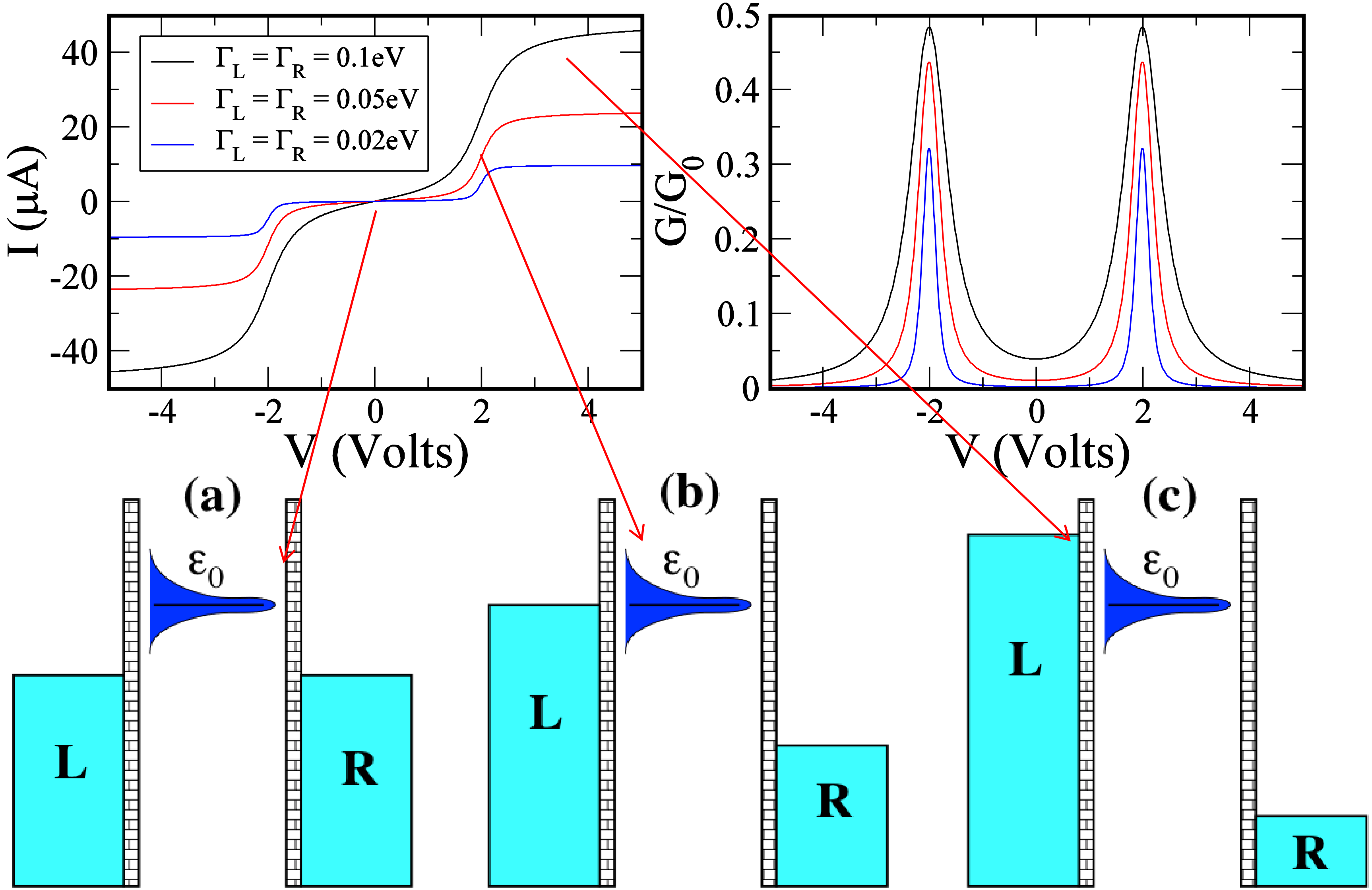
L. Zotti et al, Small 6, 1529 (2010)

$$T(E,V) = \frac{4\Gamma_L\Gamma_R}{[E-\varepsilon_0(V)]^2 + [\Gamma_L + \Gamma_R]^2}$$

See also: Thijssen& van der Zant, phys. stat. sol. (b) **245**, 1455 (2008)
Huisman et al., Nano Lett. **9**, 3909 (2009)

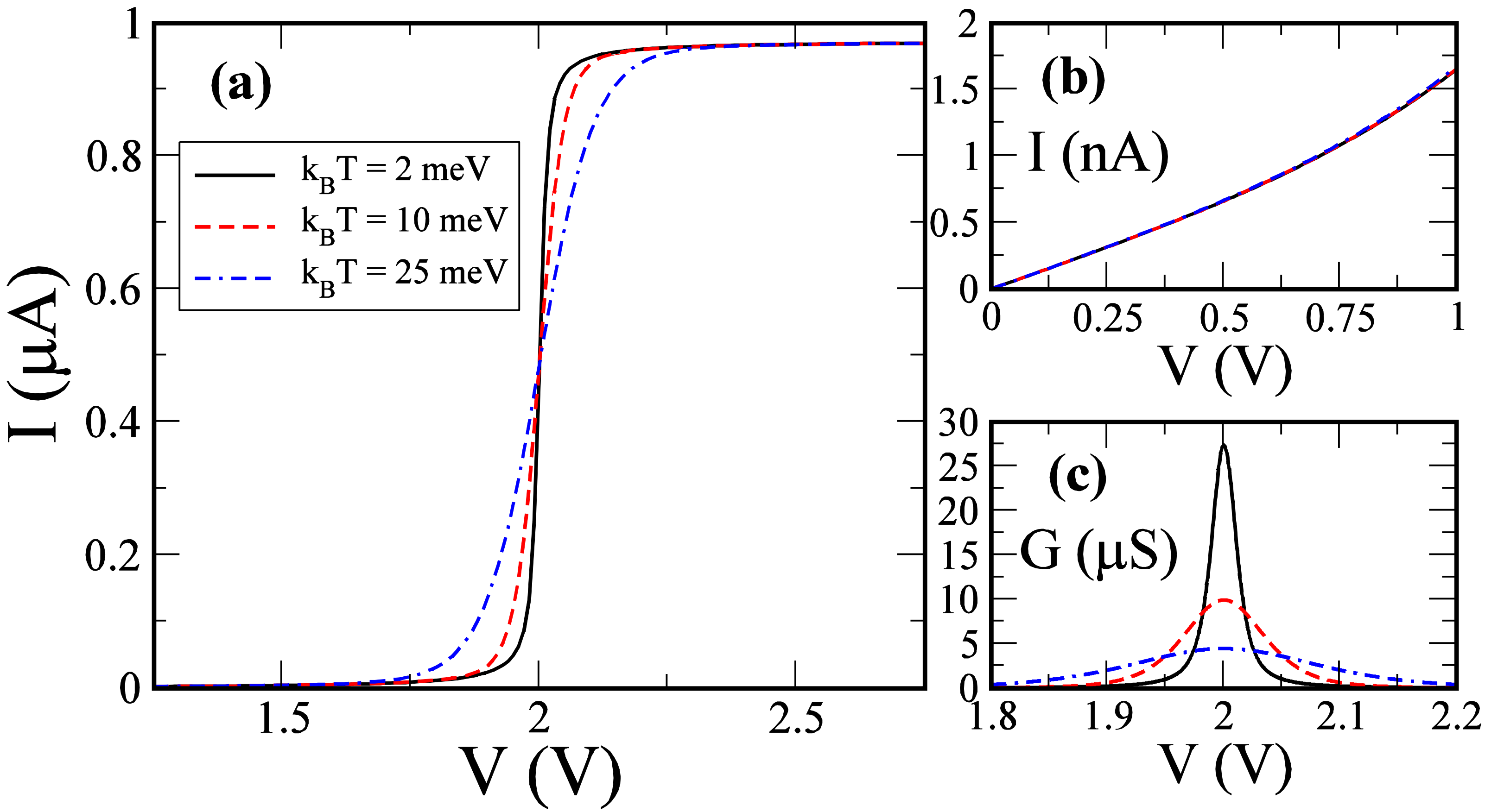
$$\Gamma = \Gamma_L + \Gamma_R$$

ε_0 = 1eV; $k_B T$ = 0.025 eV (room temperature)



Temperature dependence of the current

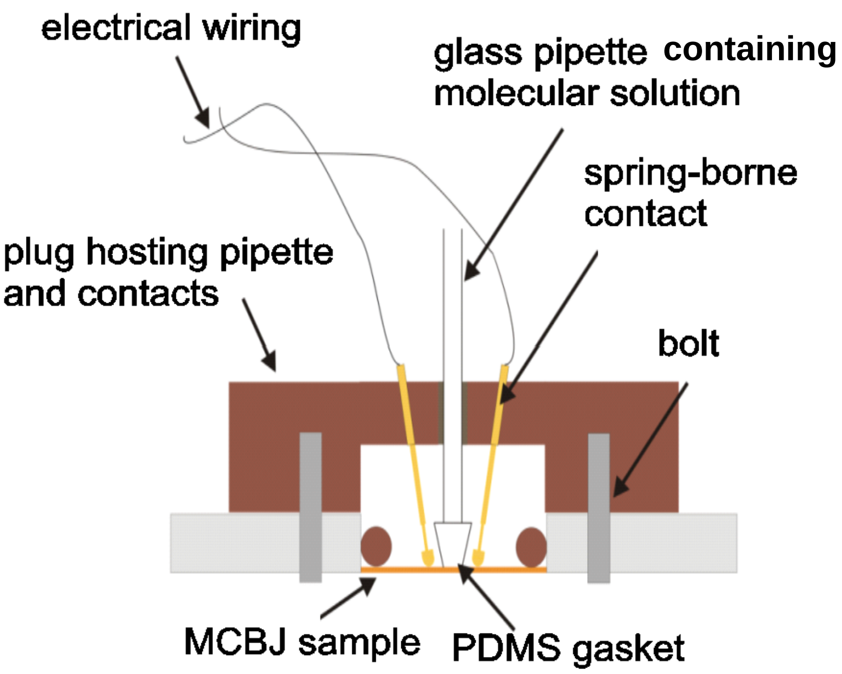
$$\varepsilon_0 = 1\,\mathrm{eV}; \Gamma_L = \Gamma_R = 2\,\mathrm{meV}$$

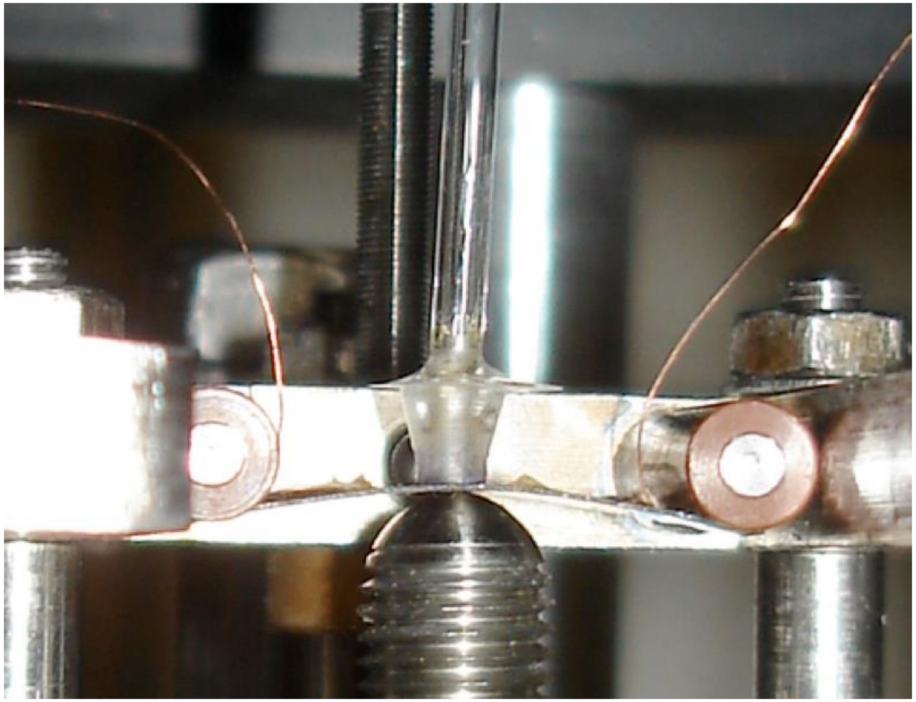


- **Off-resonant transport → *T* independent**
- **On-resonant transport → *T* dependent (as long as $k_BT > G$)**

Liquid MCBJ

Characterization of molecules in liquid environment

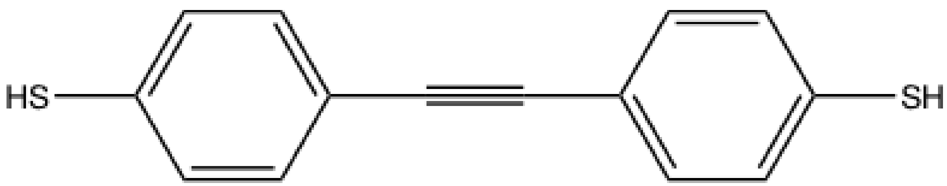




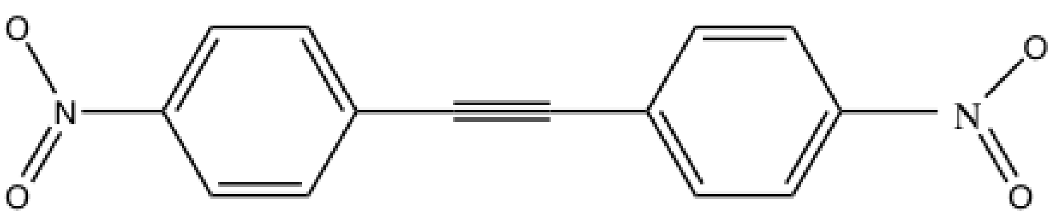
See also: L. Grüter et al., Small **1**, 1067 (2005)

Role of linker groups: Simple molecules

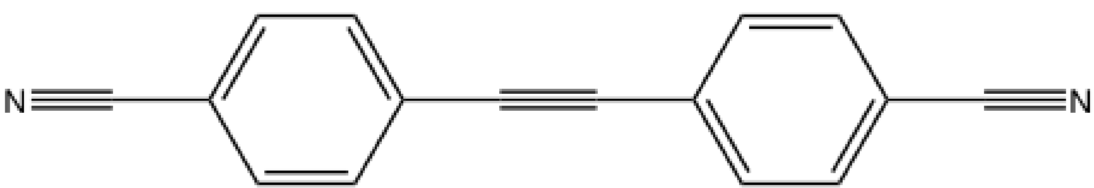
- Basic molecule: Bis-tolane
- Conjugated → conductive (wire)
- Change of linker groups



BTT: Bis-thiotolane



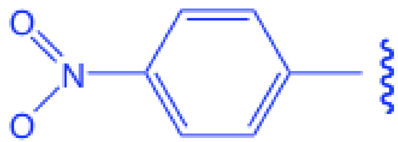
BNT: Bis-nitrotolane



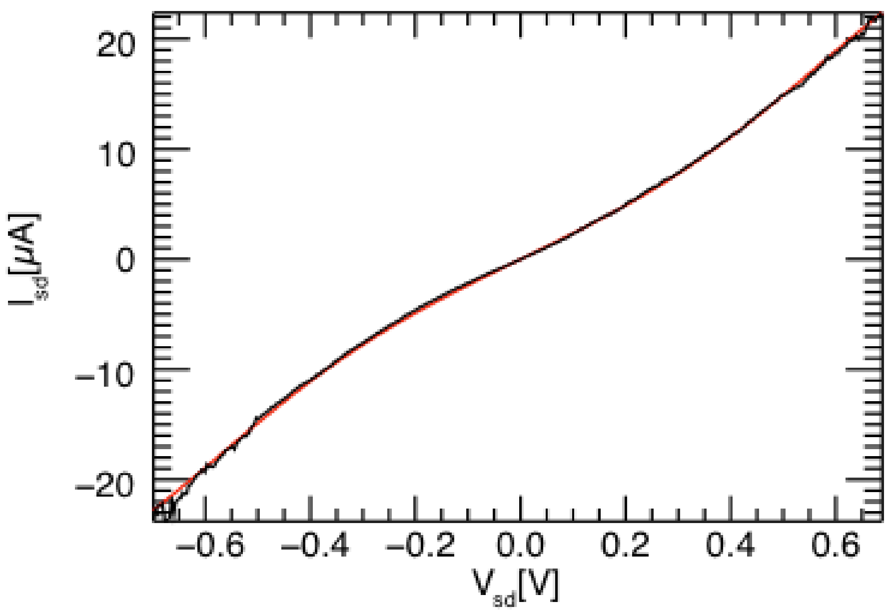
BCT: Bis-cyanotolane

IV curves with various linkers

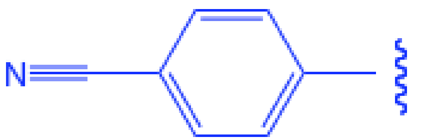
Nitro



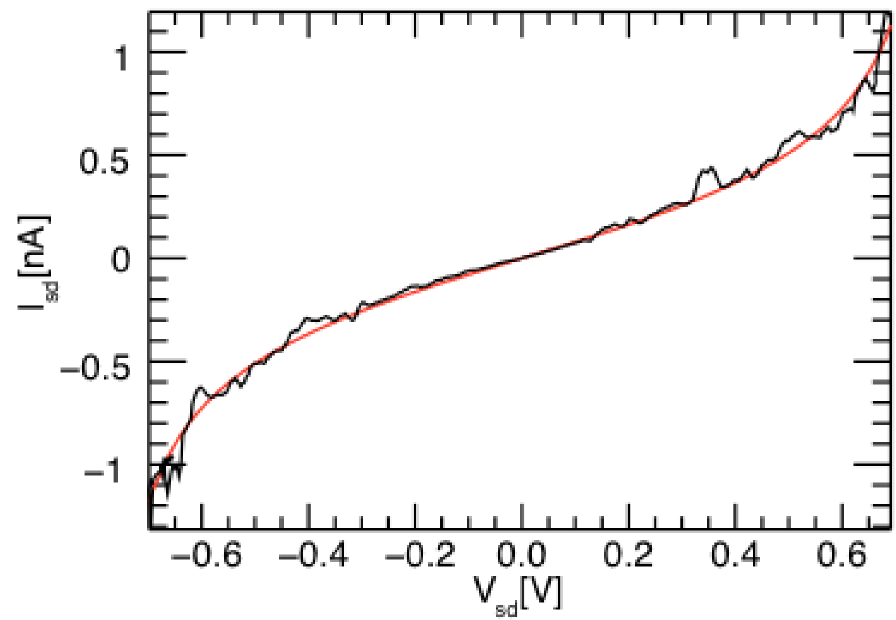
$$\Gamma_L = \Gamma_R = 0.094\mathrm{eV}$$
$$E_0 = 0.29\mathrm{eV}$$



Cyano

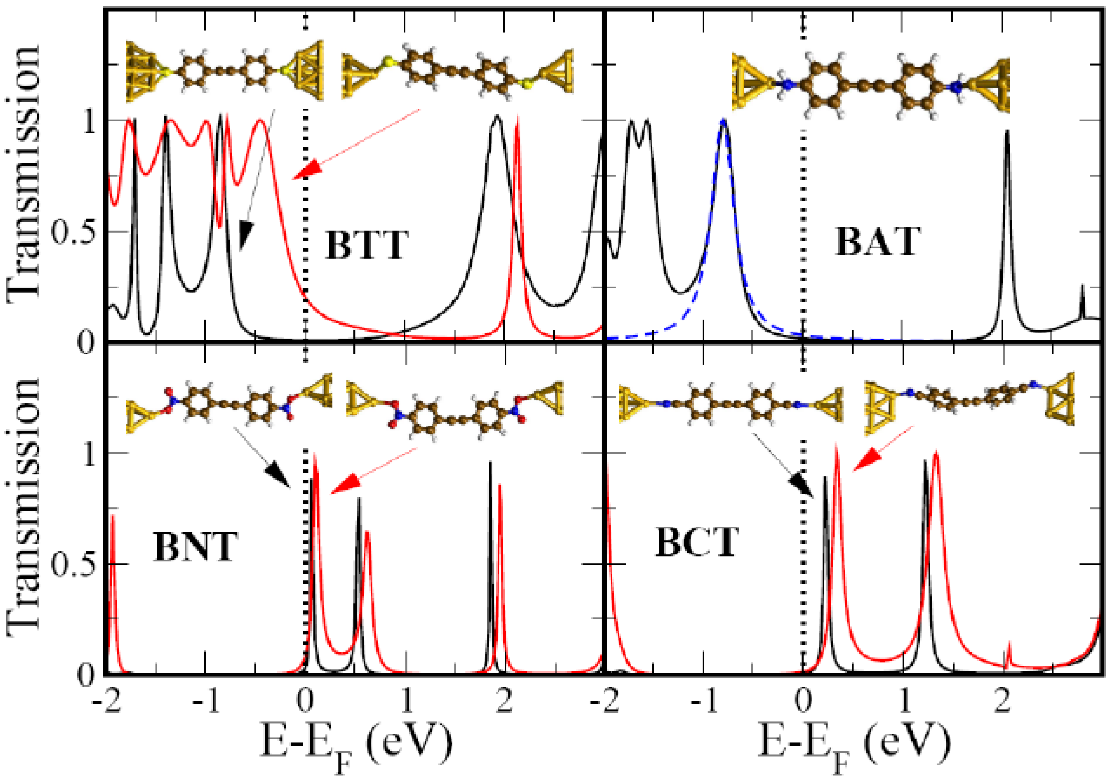


$$\Gamma_L = \Gamma_R = 0.85\mathrm{meV}$$
$$E_0 = 0.54\mathrm{eV}$$



Transmission function of molecular junctions

- Quantum chemistry & DFT
- Approximation to single Lorentzian valid
- Linkers determine nature of transport
- BTT & BAT: HOMO
- BNT & BCT: LUMO



Diffusive regime

- **Interference effects: Aharonov–Bohm Effect**
- **Contribution of the vector potential to the wave function**
- L: Lagrangian with field

$$L = L_0 + e \cdot \dot{\vec{r}} \cdot \vec{A}(\vec{r})$$

$$\Delta\phi_{A\to B} = \frac{e}{\hbar}\int_{r1,r2} \vec{A}\cdot d\vec{r} \quad r_1, r_2$$ 1-dimensional

$$\mathcal{T} = |t_1 \cdot \exp(i\phi_1) + t_2 \cdot \exp(i\phi_2)|^2$$

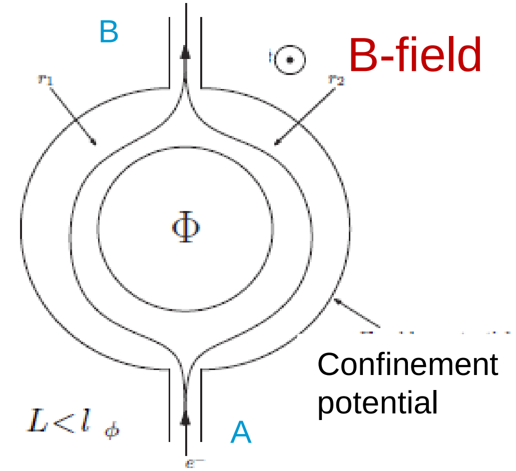
$$= 2 \cdot (1 + \cos(\Delta\phi))$$

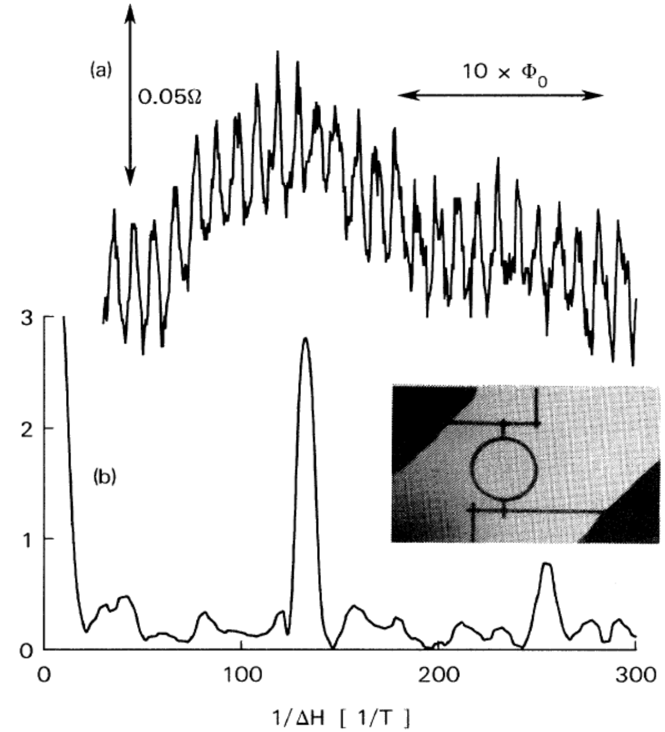
where

$$\phi = \frac{e}{\hbar}\int_{r_1} \vec{A}\cdot d\vec{r} - \frac{e}{\hbar}\int_{r_2} \vec{A} d\vec{r}$$

$$= \frac{e}{\hbar}\oint \vec{A}\cdot d\vec{r}$$

$$= \frac{e}{\hbar}\iint_F \mathrm{rot}\,\vec{A}\cdot d\vec{f} \overset{\text{Stokes}}{=} \frac{e}{\hbar}\iint \underbrace{\vec{B} d\vec{r}}_{\Phi}$$





R. A Webb et al., Phys. Rev. Lett. 54, 2696 (1985)

- **Periodic oscillation of the conductance with flux quantum $\Phi_0 = h/e$**

– **Universal conductance fluctuations:**

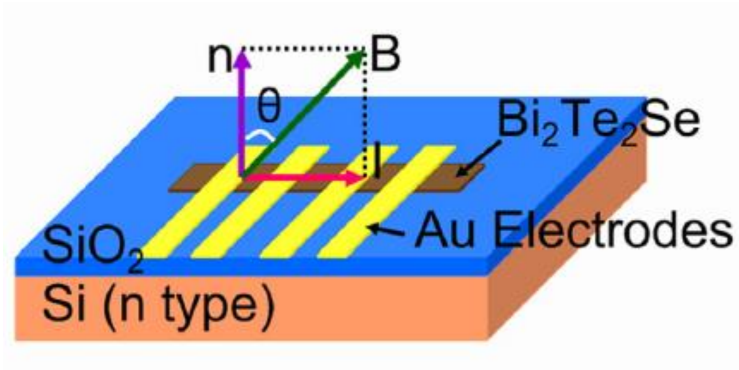
AB-effect in diffusive wires:

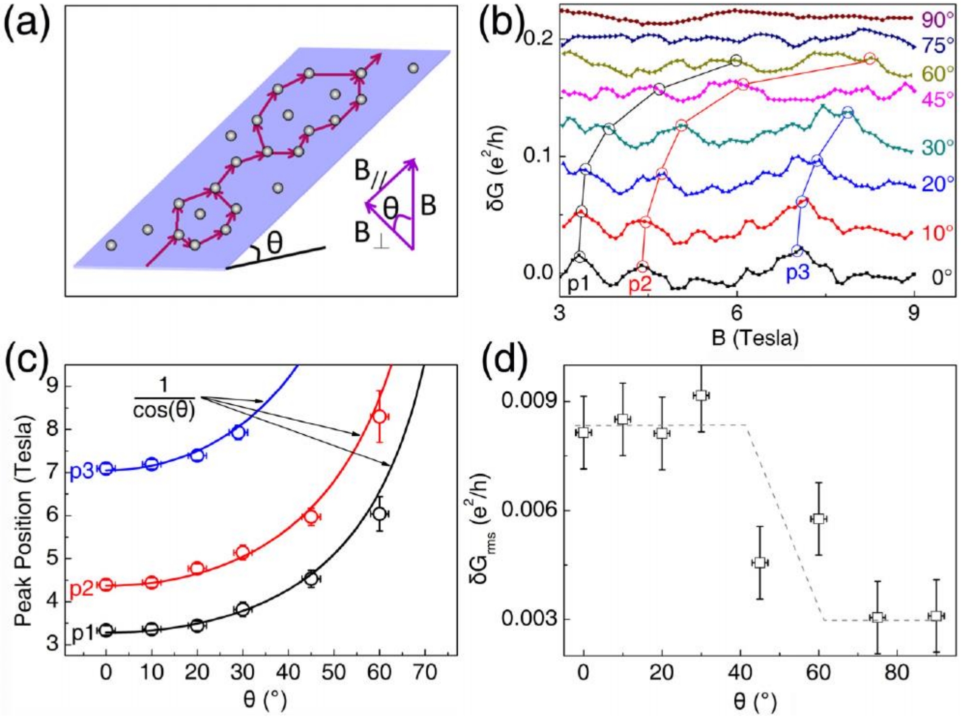
Wide distribution of areas defined by scattering paths

→ aperiodic fluctuations of conductance

- Interference along scattering path
- Fingerprint of impurities

Li, Z. et al. Sci. Rep. **2**, 595 (2012).



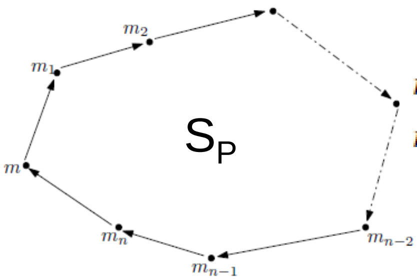


Review article: R. A. Webb and S. Washburn, Rev. Mod. Phys. 55, 1311 (1992)

– Weak localization

Bergmann 1982

- Two time-reversed paths



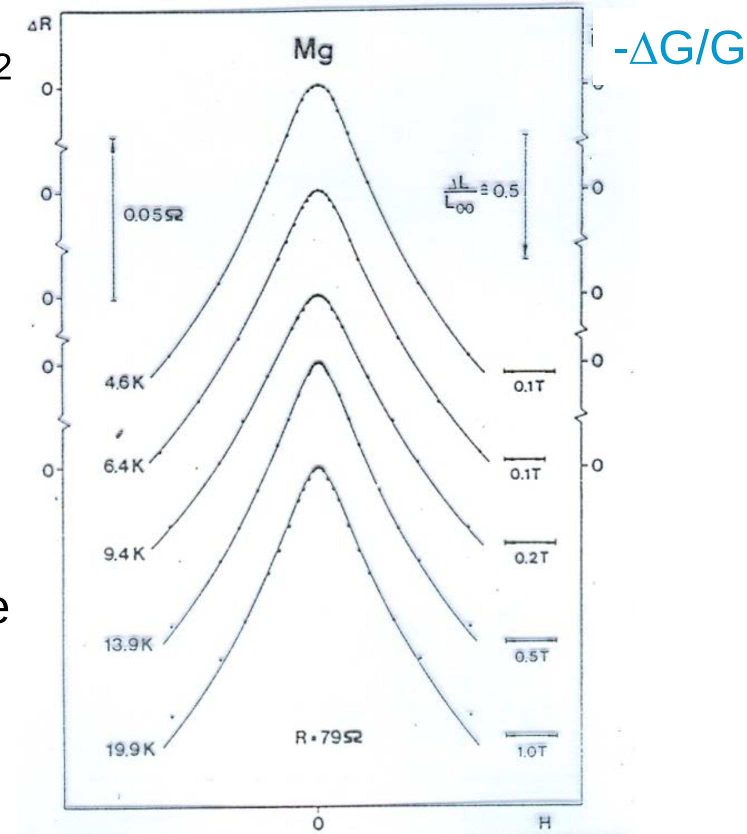
$$m \to m_1 \to m_2 \to \ldots m_{n-1} \to\to m_n \to m$$
$$m \to m_n \to m_{n-1} \to \ldots m_2 \to\to m_1 \to m$$

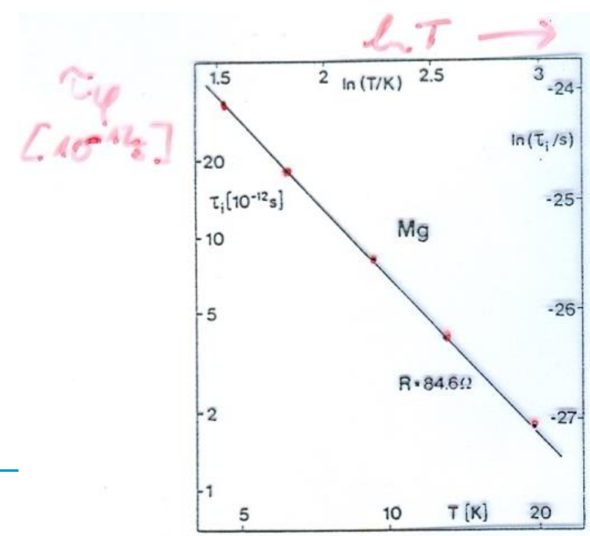
- Probability for “reverse” paths increased due constructive interference

$$R(m \to m) = |(A_1 + A_2 + \ldots) + (A_{1R} + A_{2R} + \ldots)|^2$$
$$= |A + A_R|^2$$
$$= 4 \cdot A^2 \qquad \text{w/o magnetic field}$$

- Minimum of conductance at $B = 0$
- B field breaks time-reversal symmetry –> destruction of interference on field scale limited by the phase coherence length: $B_p = \frac{h}{|e| \cdot S_p}$

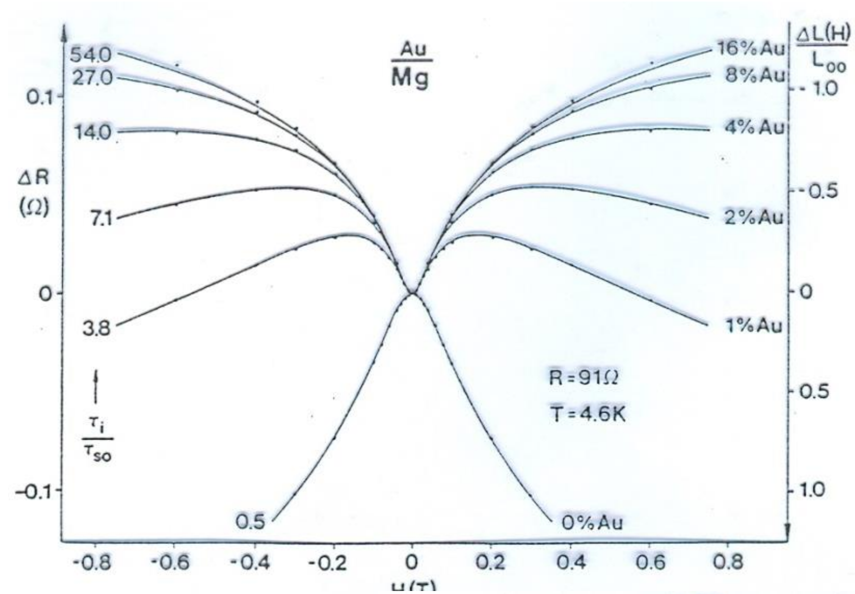
$$B_C = \frac{h}{|e| \cdot S_{max}} = \frac{h}{|e| \cdot L_\phi^2} \qquad \text{for a 2d layer}$$



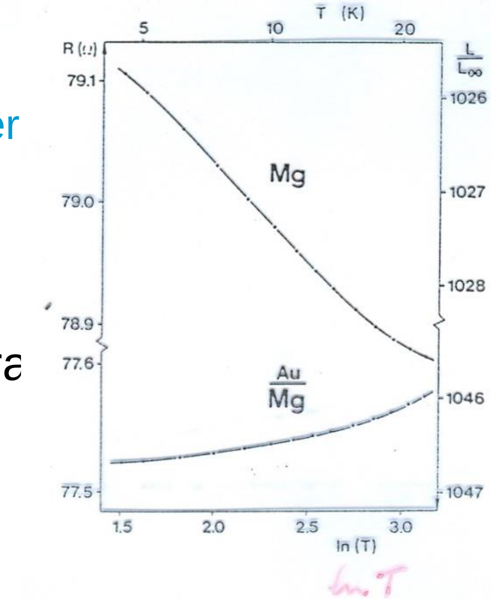


Weak antilocalization

- With strong **spin-orbit scattering**: Spin rotates with orbital wave function: Constructive interference only after rotation by 4 π.
- After return to origin: phase difference π
  → Reduced return probability: reduced resistance: Weak antiocalization
- Breaking time-reversal symmetry by *B*-field: Positive magnetoresistance



Adding submonolayer Au layers onto Mg



- New characteristic scale: spin orbit scattering length (or ra
- *T*-independent, but material dependent: $\tau_{SO}^{-1} \propto Z^4$
- Light elements: WL, Heavy elements: WAL
  Medium Z elements: WAL at low *T*, WL at higher *T*

Bergmann 1982

Weak coupling: Coulomb blockade

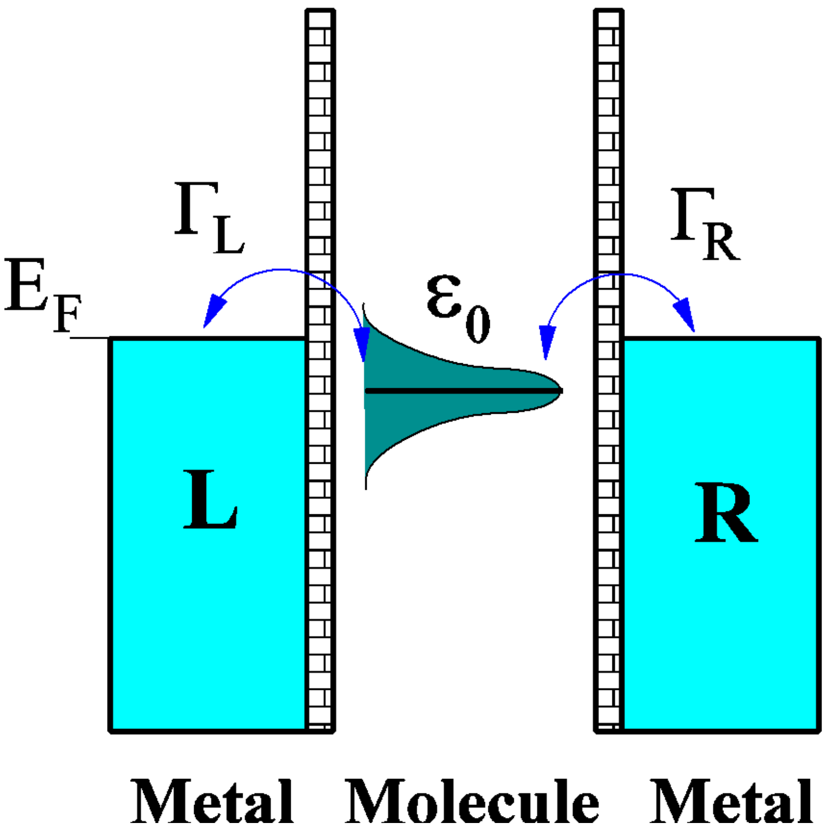
$\Delta E = |\varepsilon_0 - E_F| =$ injection energy

$\Gamma = \Gamma_L + \Gamma_R =$ level width

- Traversal time:

  $$\tau = \hbar / \sqrt{\Delta E^2 + \Gamma^2}$$

- Energy scale of the Coulomb interaction: U



In this section we focus on situations in which

$$\tau \gg \hbar / U$$

and therefore, the transport is dominated by the Coulomb repulsion of the electrons inside the QD/molecule.

This situation is realized when the metal-molecule coupling is relatively weak.

Charging effects in transport through nanoscale devices

How small and how cold should a conductor be so that adding or subtracting a single electron has a measurable effect?

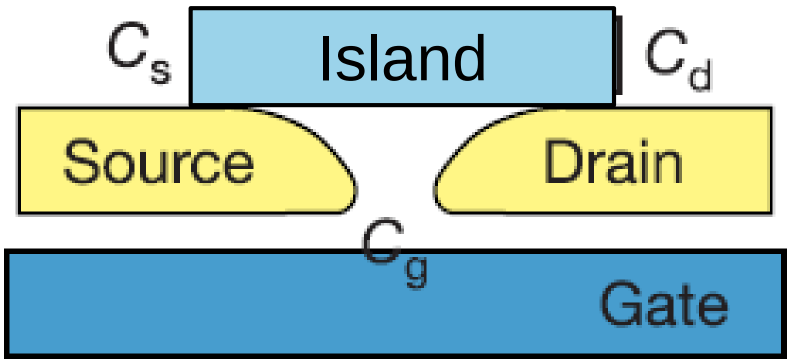
1. The capacitance C of the island (or dot) has to be such that the *charging energy* ($e^2/2C$) is larger than the thermal energy ($k_B T$):

$$E_C = e^2/2C >> k_B T$$

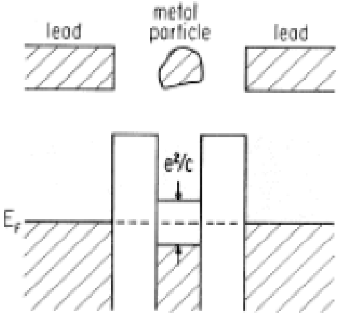
2. The barriers have to be sufficiently opaque such that the electrons are located on the dot:

$$\Delta E \Delta t = (e^2/C)(R_t C) > h \Rightarrow R_t > h/e^2$$

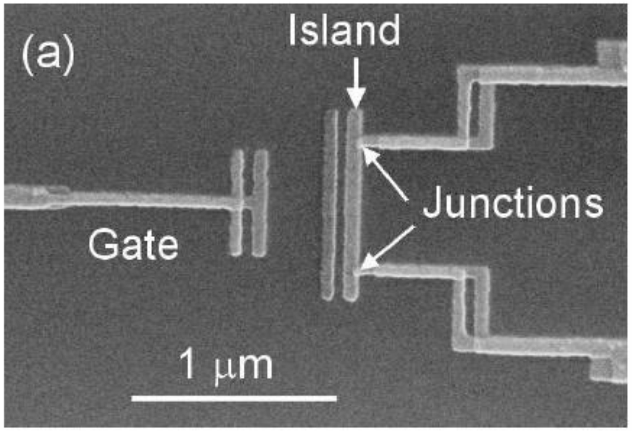
In molecular transistors these two requirements can be met.



Coulomb blockade phenomenology

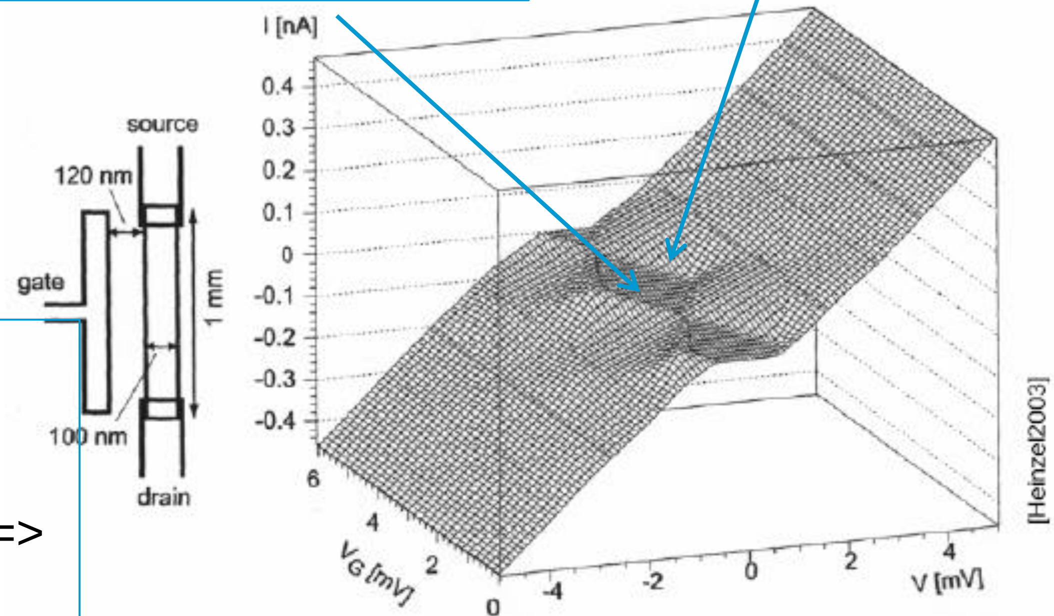


Metallic islands



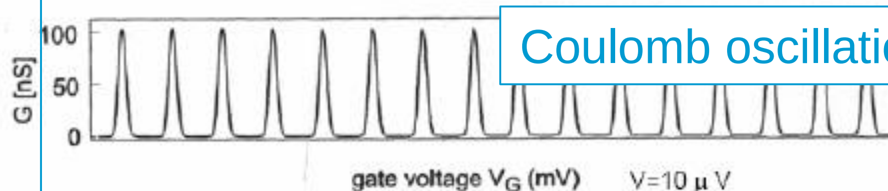
Gap in I-V characteristic
“Coulomb blockaded area“

Width is gate dependent



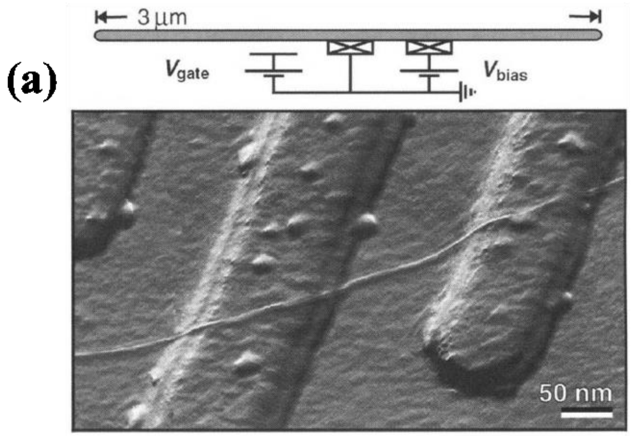
- if $E_C >> k_B T$ transport is blocked around zero bias
- higher bias: Coulomb blockade
- external gate tunes charge states => Coulomb Blockade diamond
- NO $\hbar$! Classical effect!
- Coulomb staircase if barriers to source and drain are different

Coulomb oscillations

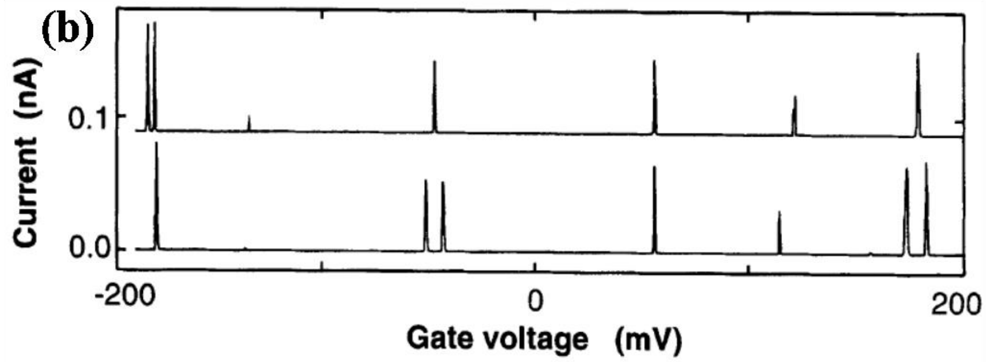


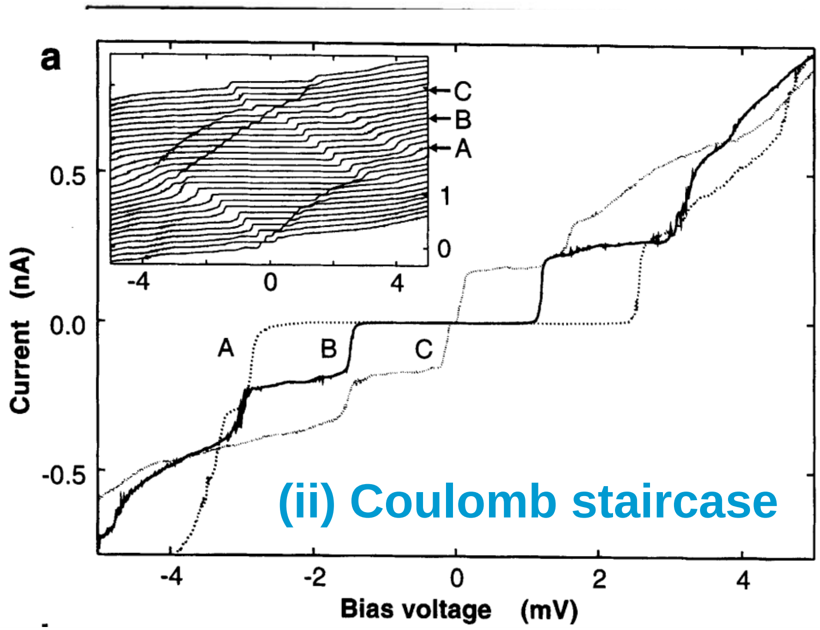
Coulomb blockade phenomenology in carbon nanotubes

S.J. Tans et al., Nature **386**, 474 (1997)

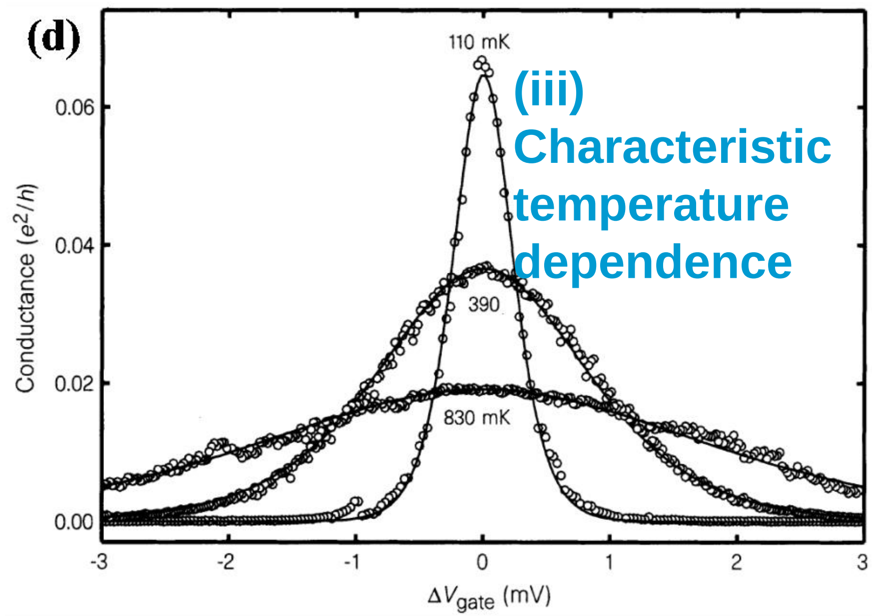


(i) Coulomb oscillations





(ii) Coulomb staircase



(iii) Characteristic temperature dependence

Quasi 0d systems: Charging effects in transport through nanoscale devices

Here the level spacing is denoted as ΔE

- To resolve the discrete electronic levels of a quantum dot: $\Delta E > k_B T$
- The level spacing at the Fermi energy for a box of size L depends on the dimensionality (N: electron density)

$$\Delta E = \frac{\hbar^2 \pi^2}{mL^2} \times \begin{cases} N/4 & \text{(1D)} \\ 1/\pi & \text{(2D)} \\ (3\pi^2 N)^{-1/3} & \text{(3D)} \end{cases}$$

- The level spacing of a 100 nm 2D dot is around 0.03 meV, which is large enough to be observable at dilution refrigerator temperatures (100 mK → 0.0086 meV).
- Using 3D metals to form a dot, one needs to choose a radius of around 5 nm in order to see the level spacing ("atom-like properties").
- In the case of molecular junctions, the level spacing is essentially the HOMO-LUMO gap and it is typically several electron volts. Therefore, the level quantization is easily observable in molecular transistors even at room temperature.

Coulomb blockade theory

- For small bias voltages, $V_{SD} \approx 0$:

$$\mu_{Dot}(N) = \left(N - \frac{1}{2}\right)\frac{e^2}{C} - e\alpha V_G + E_N; \qquad (\alpha = C_G / C = \text{ gate coupling})$$

- Thus, the addition energy is given by:

$$\Delta\mu(N) = \mu_{Dot}(N+1) - \mu_{Dot}(N) = \frac{e^2}{C} + E_{N+1} - E_N = \frac{e^2}{C} + \Delta E$$

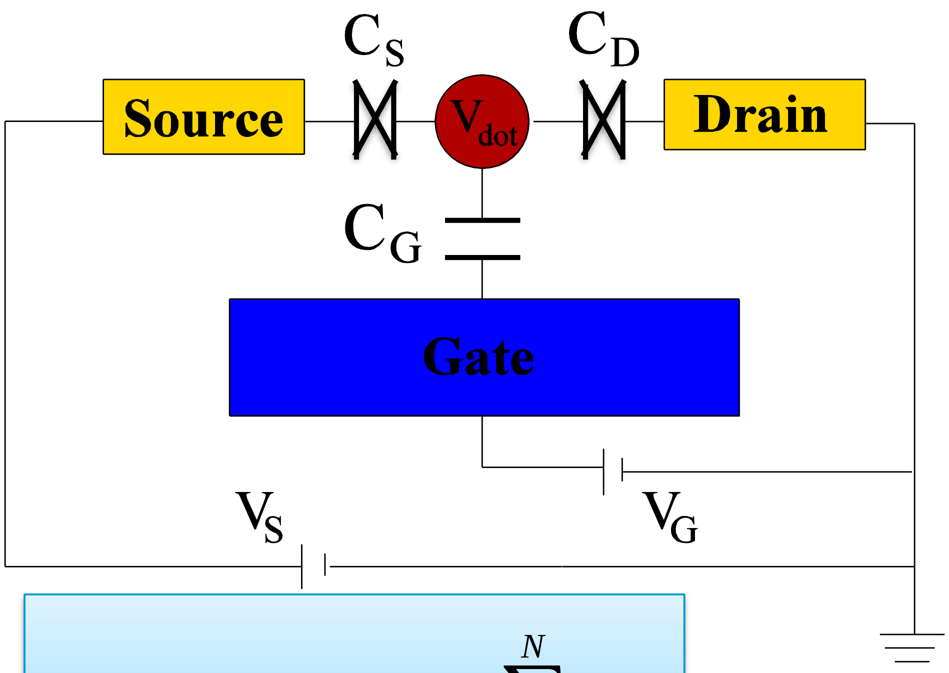
- In the absence of charging effects, the addition energy is determined by the irregular spacing ΔE of the single-electron levels. The charging energy e^2/C, in contrast, leads to a regular spacing. When it is much larger than the level spacing (as in metallic islands), it determines the periodicity of the Coulomb oscillations.

- From an experimental point of view, the Coulomb oscillations are measured as a function of the gate voltage and the peak spacing is given by:

$$\Delta V_G = \Delta\mu(N)/(e\alpha) = (e^2/C + \Delta E)/(e\alpha)$$

while the condition $e\alpha V_G^N = (N - 1/2)e^2/C + E_N$ gives the gate voltage of the *N*-th Coulomb peak.

Coulomb blockade theory: constant interaction model

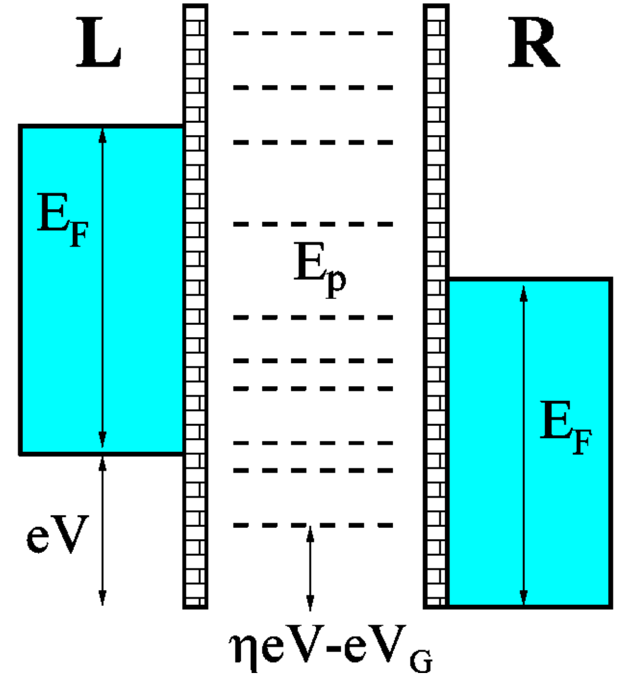


$$E_{Dot}(N) = U(N) + \sum_{p=1}^{N} E_p$$

$$U(N) = (Ne)^2/2C - NeV_{ext}$$

$$C = C_S + C_D + C_G$$

$$V_{ext} = \left(C_S V_S + C_G V_G + C_D V_D\right)/C$$



η: fraction of voltage dropping at the right barrier

$E_p \ (p = 1,2,\ldots) =$ single - electron energy levels

$\Gamma_L^{(p)}, \ \Gamma_R^{(p)} \Rightarrow$ tunneling rates

$$k_B T, \Delta E \gg h(\Gamma_L{}^{(p)} + \Gamma_R{}^{(p)})$$

(weak coupling)

Coulomb blockade theory

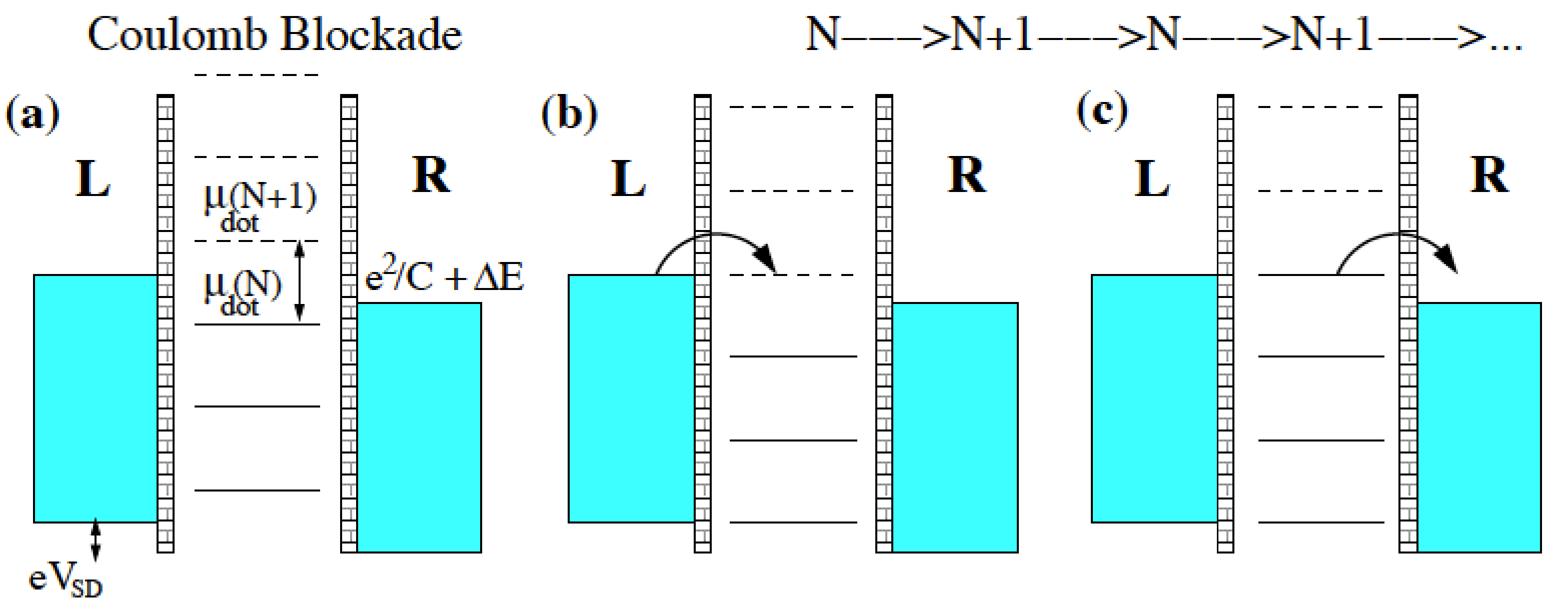
Periodicity of the oscillations

- Dot chemical potential:

$$\mu_{Dot}(N) = E_{Dot}(N) - E_{Dot}(N-1) = \left(N - \frac{1}{2}\right)\frac{e^2}{C} - eV_{ext} + E_N$$

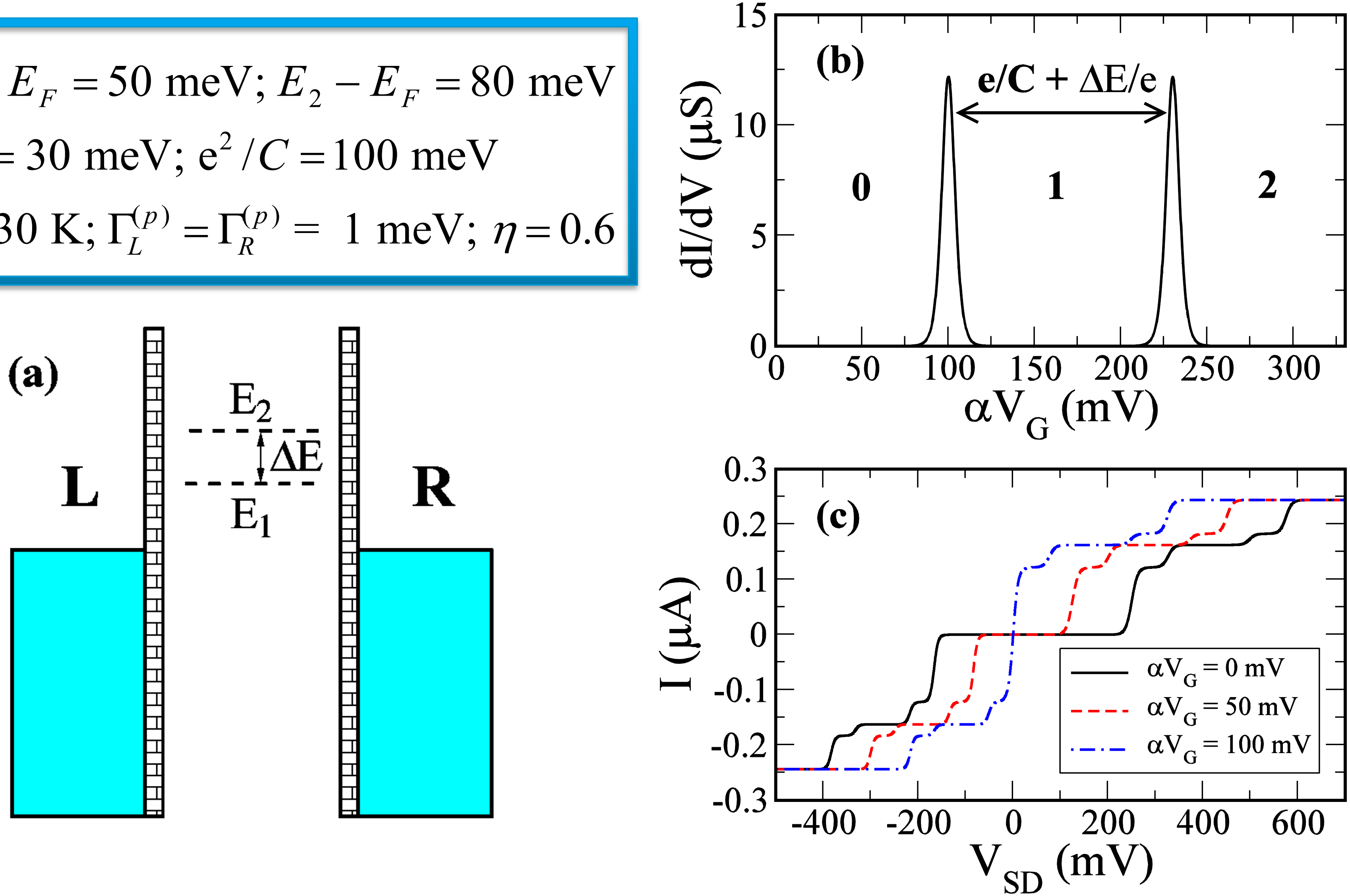
- Electrons can flow from left to right when:

$$\mu_L > \mu_{Dot} > \mu_R$$

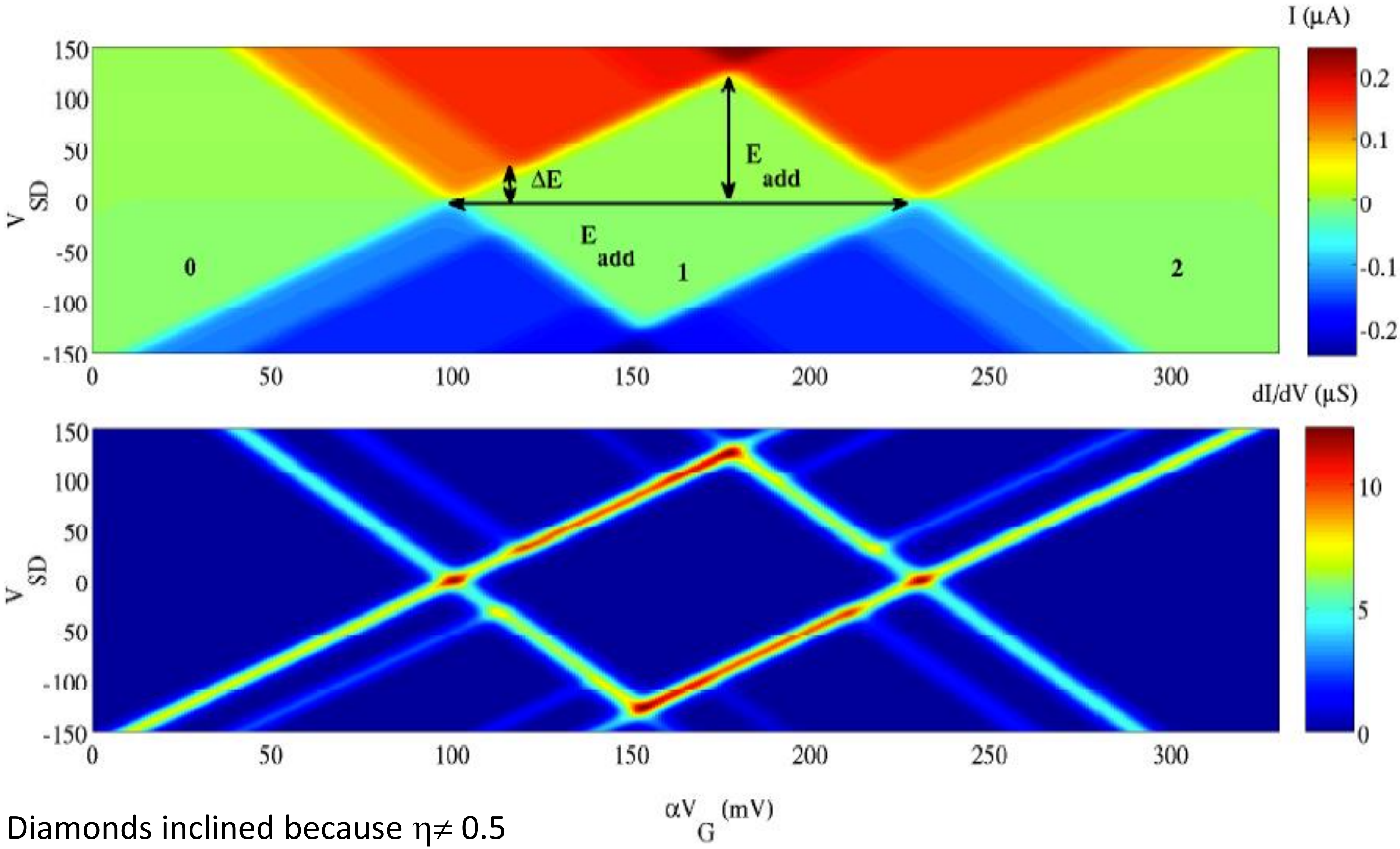


Coulomb oscillations and staircase

$$E_1 - E_F = 50 \text{ meV}; \; E_2 - E_F = 80 \text{ meV}$$
$$\Delta E = 30 \text{ meV}; \; e^2/C = 100 \text{ meV}$$
$$T = 30 \text{ K}; \; \Gamma_L^{(p)} = \Gamma_R^{(p)} = 1 \text{ meV}; \; \eta = 0.6$$



Stability diagrams and Coulomb diamonds



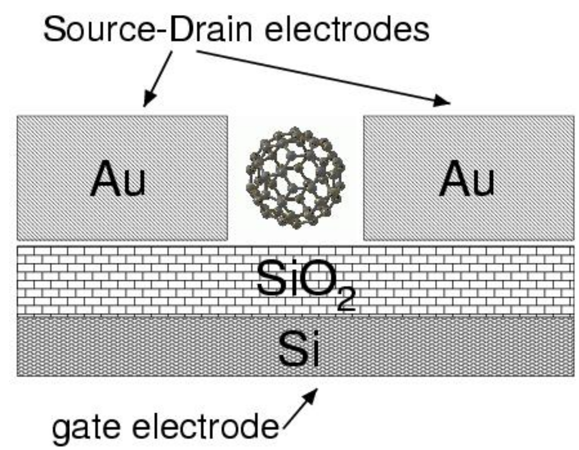
Diamonds inclined because $\eta \neq 0.5$

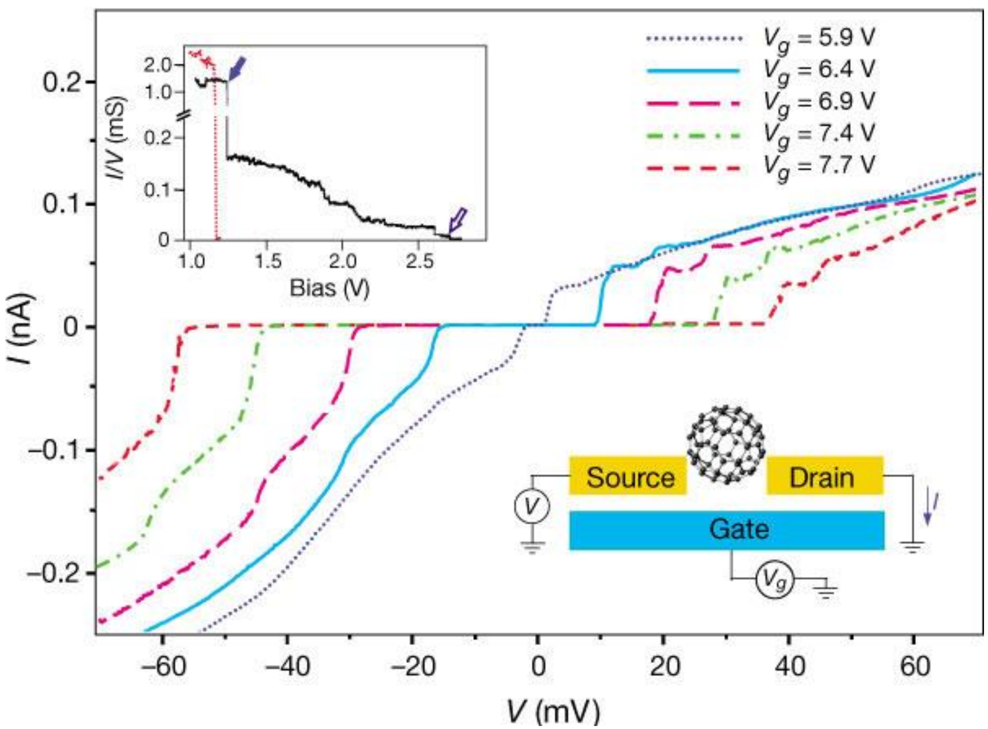
A molecular transistor

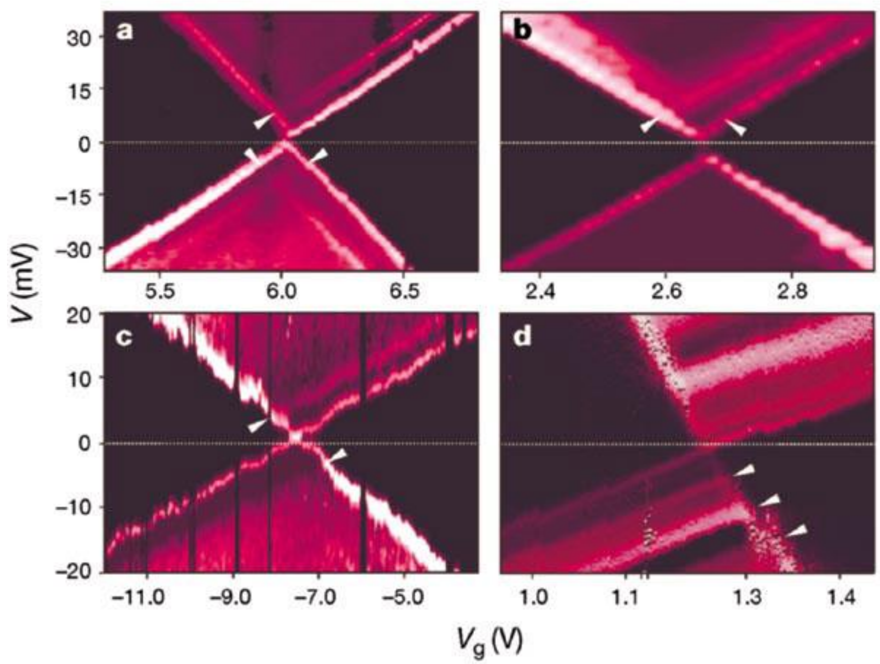
Nanomechanical oscillations in a single-C_{60} transistor

Park et al., Nature **407**, 57 (2000)

White arrows signal vibrations RIETS







Summary

- **Length & energy scales are important:**

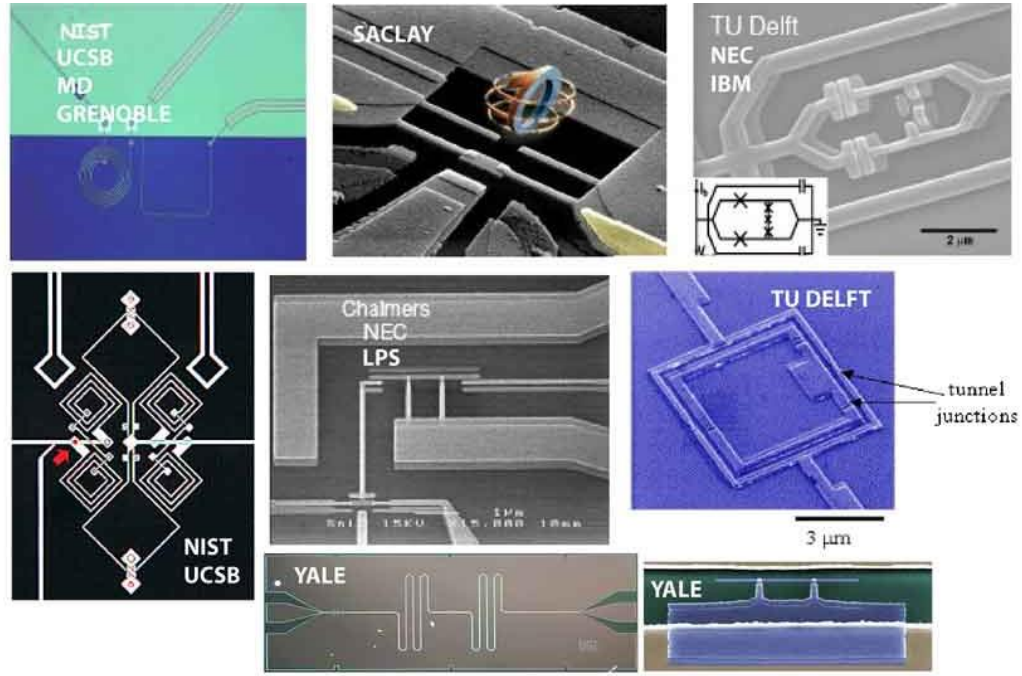
  ballistic: $E_x = \hbar v_F / L_x$ diffusive: $E_x = \hbar D / L_x^2$

- **Transport in ballistic and quasiballistic regime:**
  - Conductance determined by transmission channels
  - Description using Landauer approach
  - Single atom contacts: Conductance through atomic orbitals, no conductance quantization
  - Single molecule contacts: (Off-)resonant tunneling

- **Transport in diffusive regime**:
  - Quantum interference effects

- **Weak coupling regime:**
  - Coulomb Blockade
  - Molecular transistor

Phenomena of Superconductivity: Lossless electrical currents and macroscopic quantum physics



Perfect diamagnetism:

Superconducting coils

Magnetic field sensors

[Images: wikipedia.org, Nature, Science]

Superconducting circuits:

Definition of unit Volt (Josephson effect)

SQUID (Flux quantization)

Mesoscopic superconductivity:

SC phenomena in spatially confined SCs

SC phenomena at interfaces layer thickness ~ ξ

Spatially resolved investigation of SC

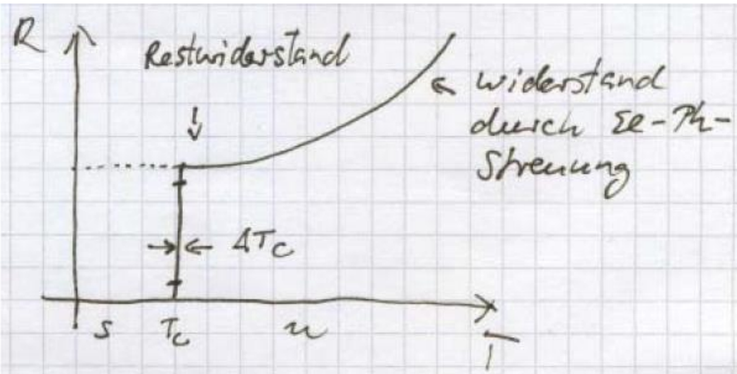
Mesoscopic Superconductivity

0. Superconductivity in a nutshell
1. Andreev reflection
1.1 Point contact spectroscopy on S-N-contacts
    - Experimental aspects
    - Examples
    - Outlook: Spin polarization in S-F contacts
1.2 Multiple Andreev reflection (MAR)
    - Point contact spectroscopy on S-S-contacts

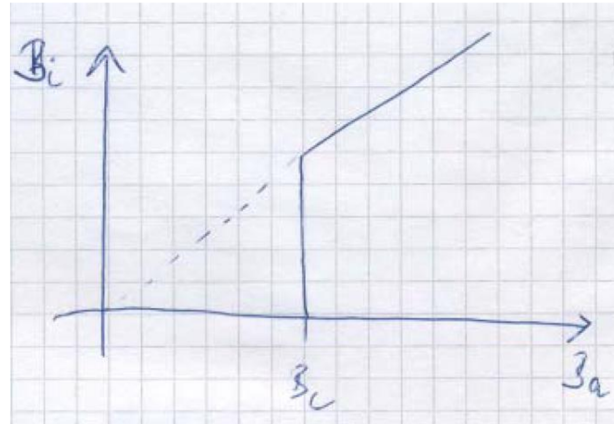
2 Proximity effect:
2.1 Scanning tunnelling spectroscopy on S-N bilayers
    - Outlook: Superconducting gold?
2.2 Phase dependence of proximity effect: Combined AFM/STM studies
    - Outlook: LDOS in S-F contacts
2.3 MAR in proximity superconductors
    - Point contact spectroscopy of S/N-N/S contacts
    - Outlook: Andreev Bound States (ABS):
        - Tunnel spectroscopy
        - Josephson effect by ABS

0. Superconductivity in a nutshell

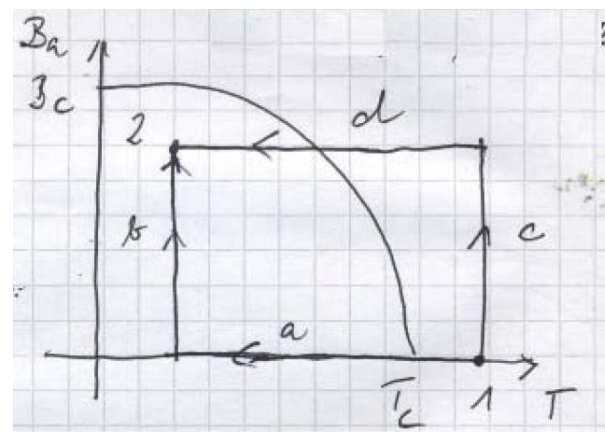
Perfect conductors with zero resistance



Perfect inductors with magnetic susceptibility χ = -1
SC expells magnetic field

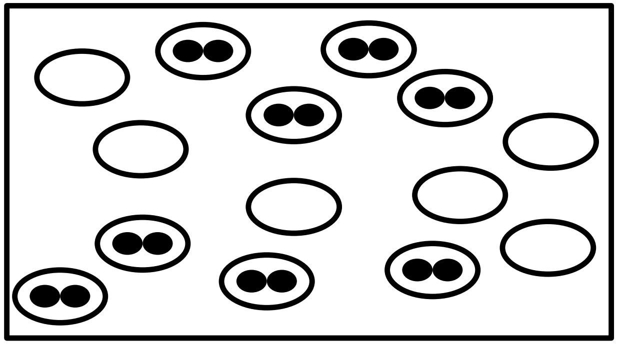


Superconductivity is thermodynamic ground state.
Phase transition: Ginzburg-Landau theory
Critical temperature Critical field B_c (T)



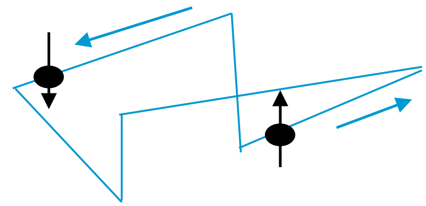
Microscopic theory: Bardeen Cooper Schrieffer (BCS)
Supercurrent I_S carried by pairs of electrons (Cooper pairs) coupled by electron-phonon interaction
$T_c = 1.14\ \theta_D \cdot \exp(-1/\rho_F V_0)$
CPs form “condensate“ with macroscopic phase
I_S driven by phase difference, not by voltage

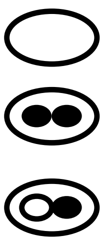
0. Superconductivity in a nutshell



Superconductor in its ground state:

- electroncs are paired to Cooper pairs.
- ground state: superposition of empty pair states and doubly occupied pair states
- no singly occupied states





Pair of time and spin reversed states

Cooper pair (CP): double occupancy

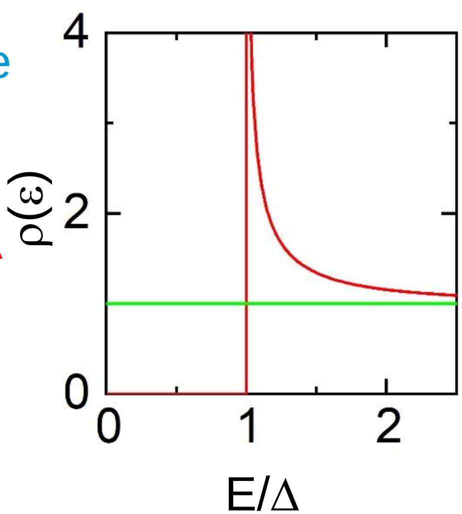
Quasiparticle (qp): single occupancy of a pair state, excitation with energy *E*

Quasiparticle density of state

Superconducting state

Minimum excitation energy Δ

Normal conducting state



$$\frac{\rho_S(E)}{\rho_N(E_F)} = \begin{cases} \dfrac{E}{\sqrt{E^2 - \Delta^2}} & (E > \Delta) \\ 0 & (E < \Delta) \end{cases}$$

BCS theory (Bardeen, Cooper, Schrieffer)

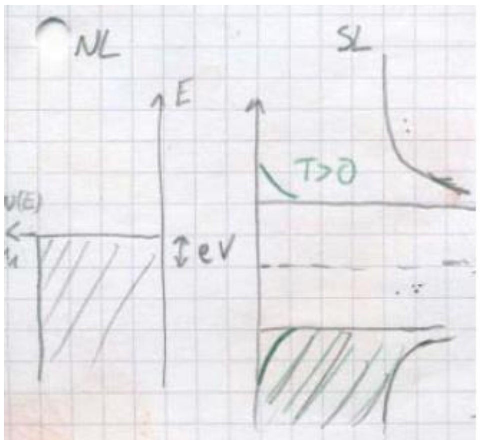
0. Tunnel spectroscopy of superconductors and normal metals

Consider tunnel contact beween superconductor (S) and normal metal (N)

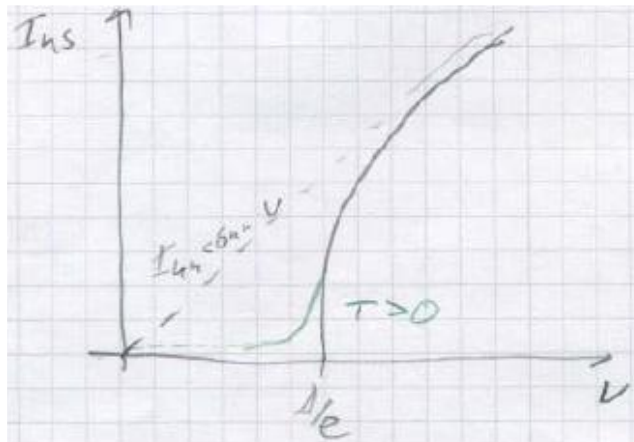
Normal metal superconductor (NS) contact

|eV| < Δ: no qp states in SC available --> no qp transport possible

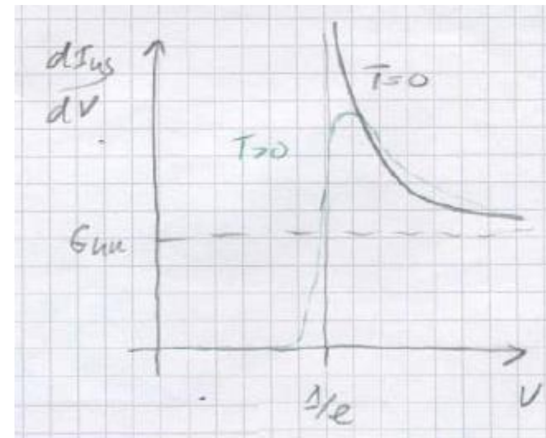
DOS



Current-voltage characteristics



Differential conductance

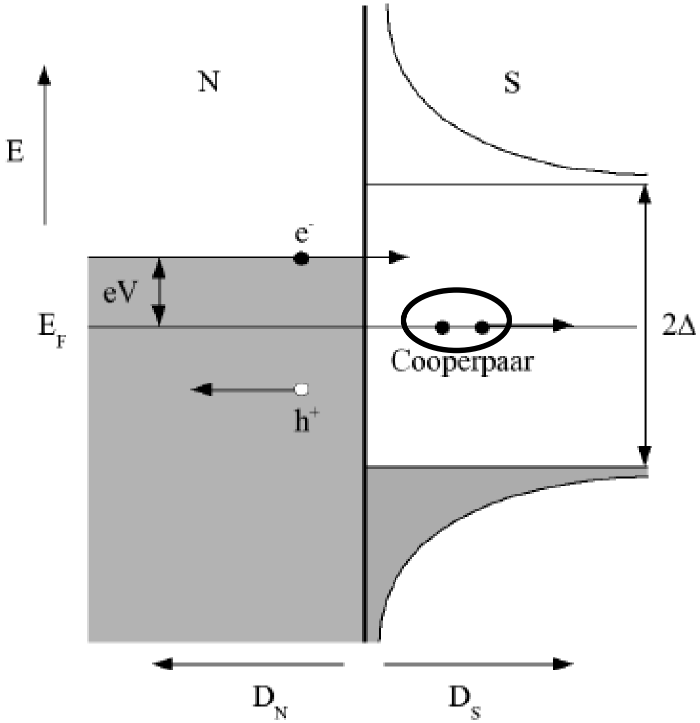


- No current for |e*V*| < Δ
- I_{NS} approaches normal conducting I-V ($I_{NN} = G_{NN} V$) for large eV
- Tunnel spectroscopy used for determining Δ
- Differential conductance at low temperature dI_{NS}/dV measures DOS

1 Andreev reflection

Consider spatially confined good contact beween SC and normal metal.
Good contact: no oxide barrier, no tunnel barrier,
but finite transmission probability $0 < \tau \leq 1$ is possible.

Normal metal superconductor (NS) contact



$|eV| < \Delta$: no qp states in SC available
→ no qp transport possible

2qp from N may form CP in S and travel simultaneously.

Conductance $G_{NS} = 2\ G_{NN}$ possible
Probability $P_{AR} \propto \tau^2$

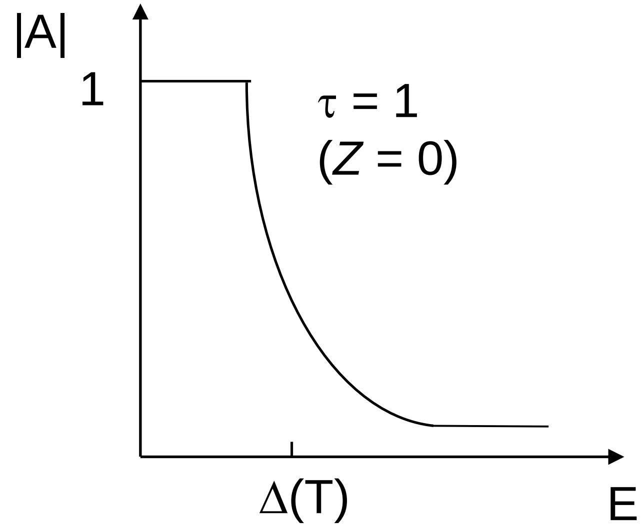
Analogous formulation:
Electron is reflected as hole on time-reversed Trajectory → "Andreev reflection"

1 Andreev reflection

Description by Andreev reflection amplitude $A(E)$

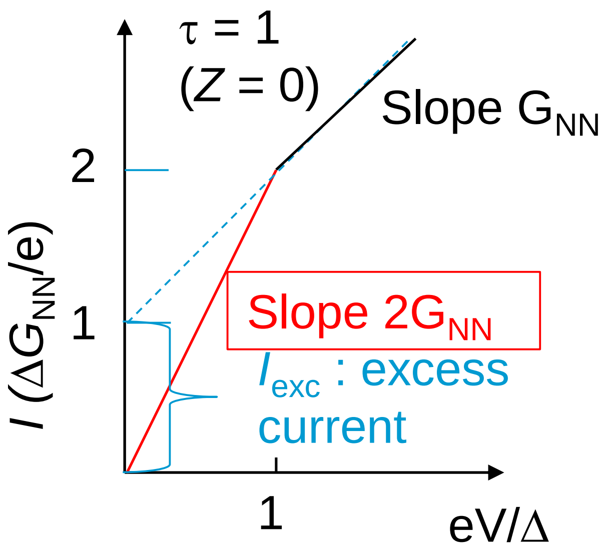
Perfect transmission $\tau = 1$

$$A(E) = \frac{1}{\Delta} \cdot \begin{cases} E - \mathrm{sign}(E)\sqrt{E^2 - \Delta^2} & \text{für } |E| > \Delta \\ E - i\sqrt{\Delta^2 - E^2} & \text{für } |E| < \Delta \end{cases}$$

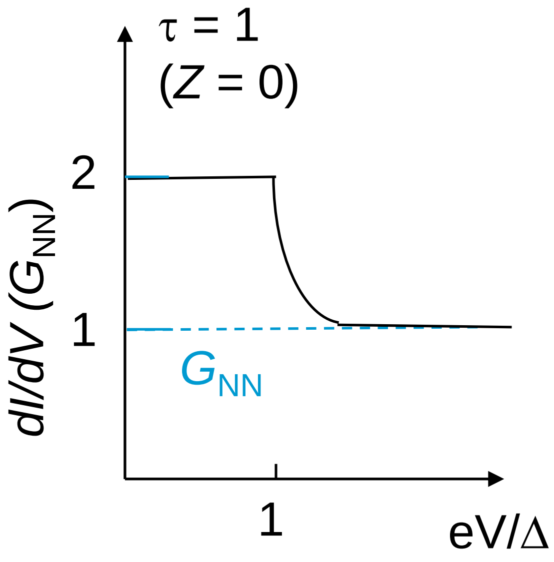


Transport properties

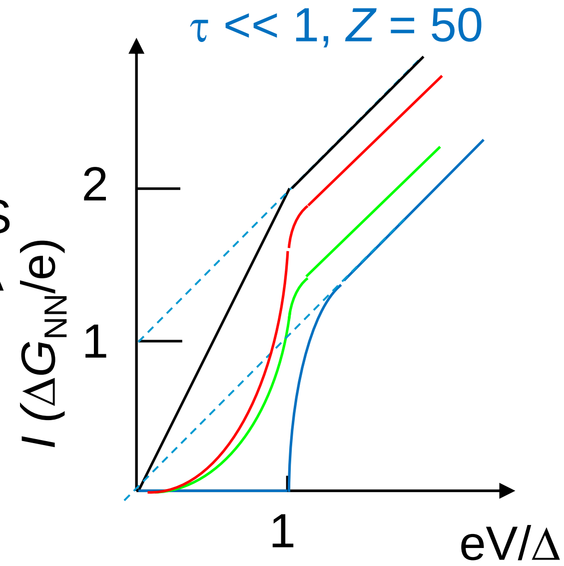
Current-voltage characteristics



Differential conductance

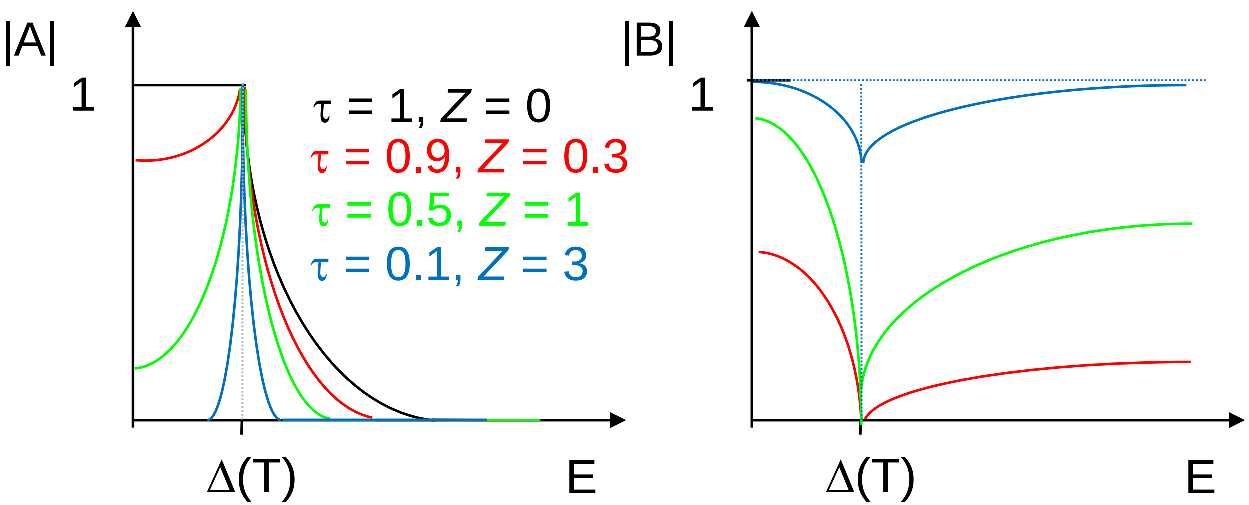


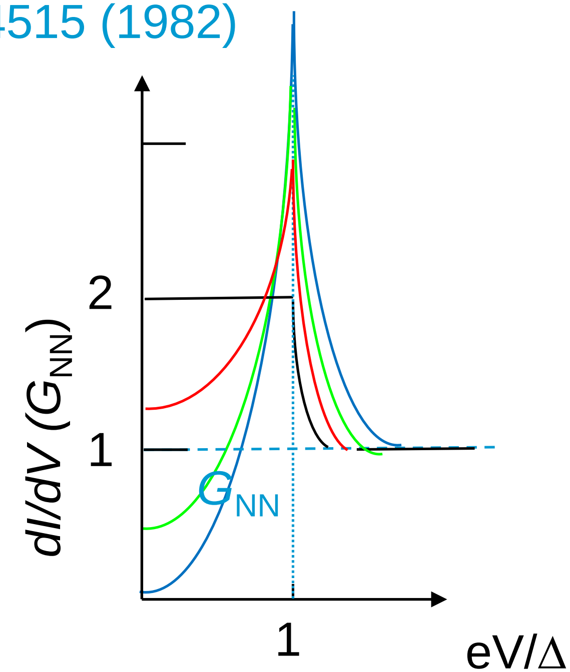
1 Andreev reflection for finite transmission $\tau < 1$



Imperfect interface, mismatch of Fermi velocities of N and S
Finite back reflection $B(E)$ with $|A(E)| + |B(E)| = 1$ for $|E| < \Delta$
$B(E)$ depends on τ or barrier parameter Z with $\tau = 1/(1+Z^2)$
$\tau = 1 \Leftrightarrow Z = 0$ perfect contact
$\tau << 1 \Leftrightarrow Z = \infty$ tunnel contact

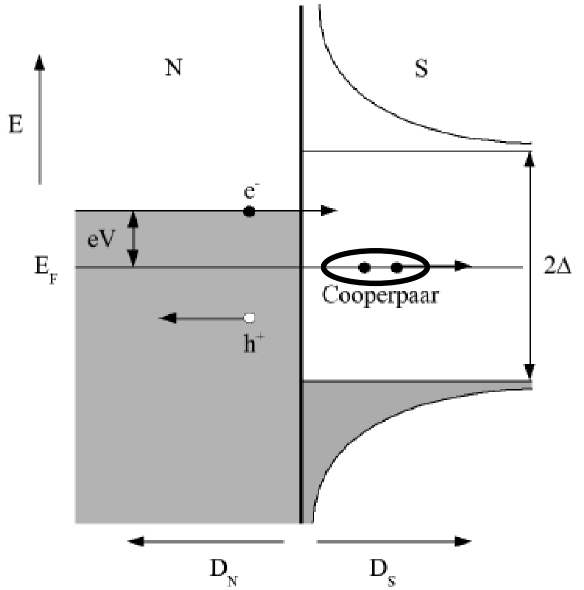
BTK model: Blonder, Tinkham, Klapwijk, Phys Rev. B 25, 4515 (1982)

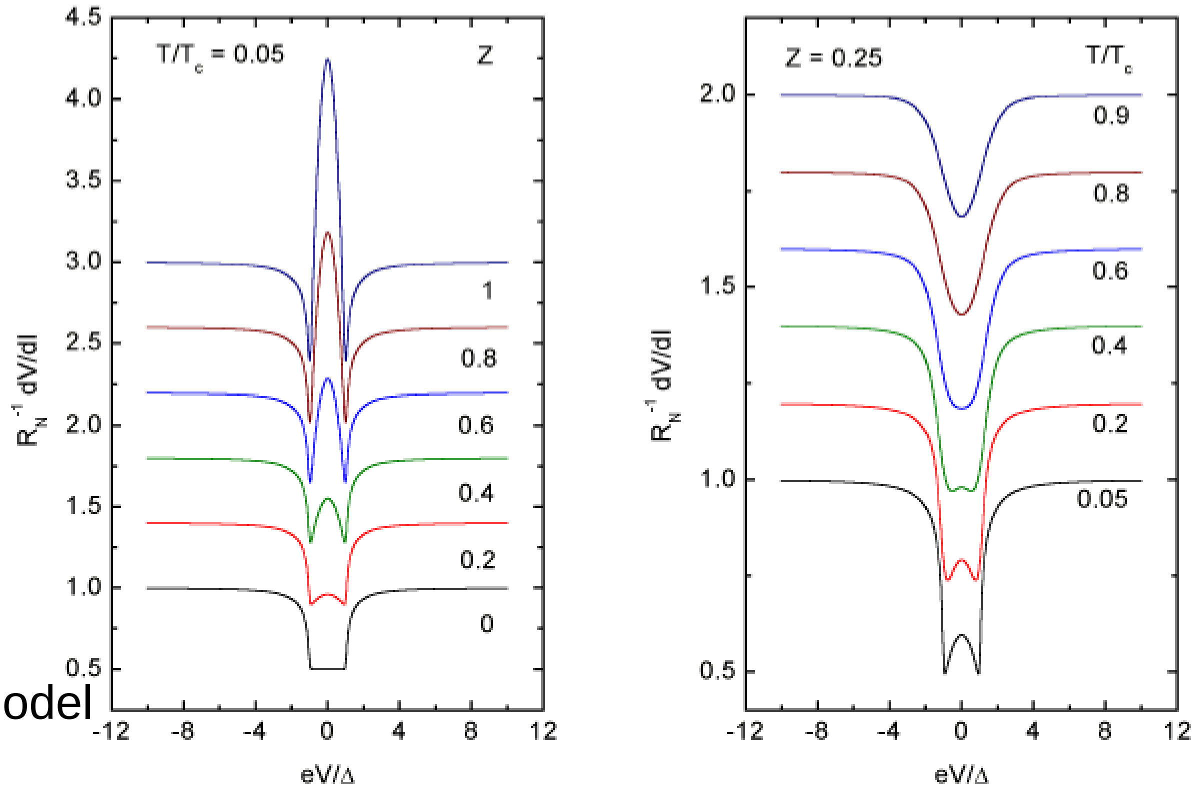




1.1 Point contact spectroscopy (PCS) of N-S contacts:

dV/dI* instead of *dI/dV





Spectra calculated with BTK model

Deviations from BCS spectrum described by phenomenological Γ parameter

$$N(E,\ ) = RE\left\{\frac{E-i\Gamma}{\sqrt{(E-i\Gamma)^2-\Delta^2}}\right\}$$

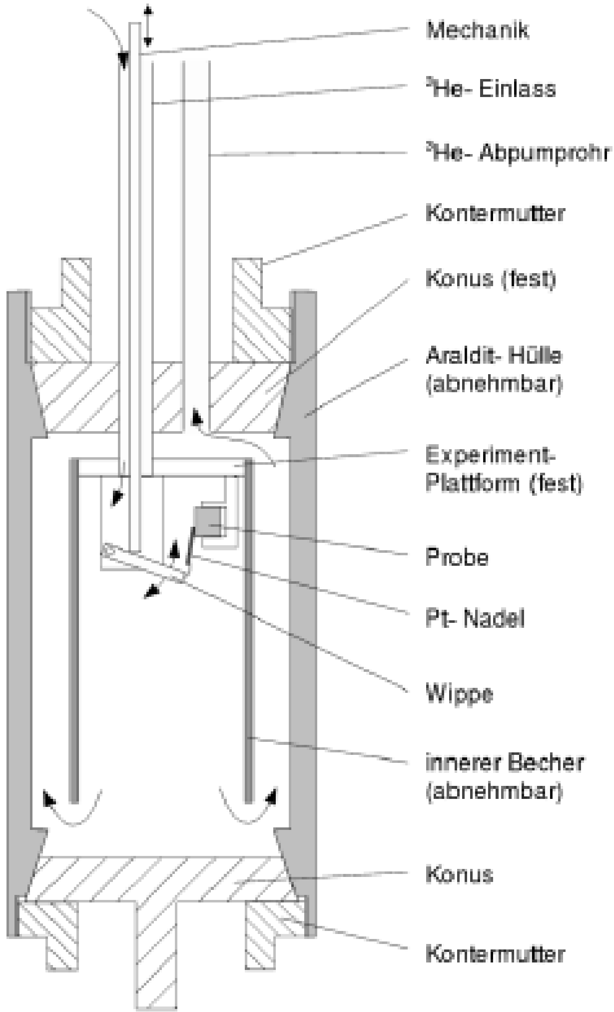
May account for:

- Pair breaking (magnetic field, spin flips)
- Broadening by external influences
- Microscopic origins (transmission coefficients)
- Complex pairing mechanisms

Brugger, Diploma Thesis, KIT, 2006

1.1 Point contact spectroscopy of N-S contacts: Needle-Anvil method

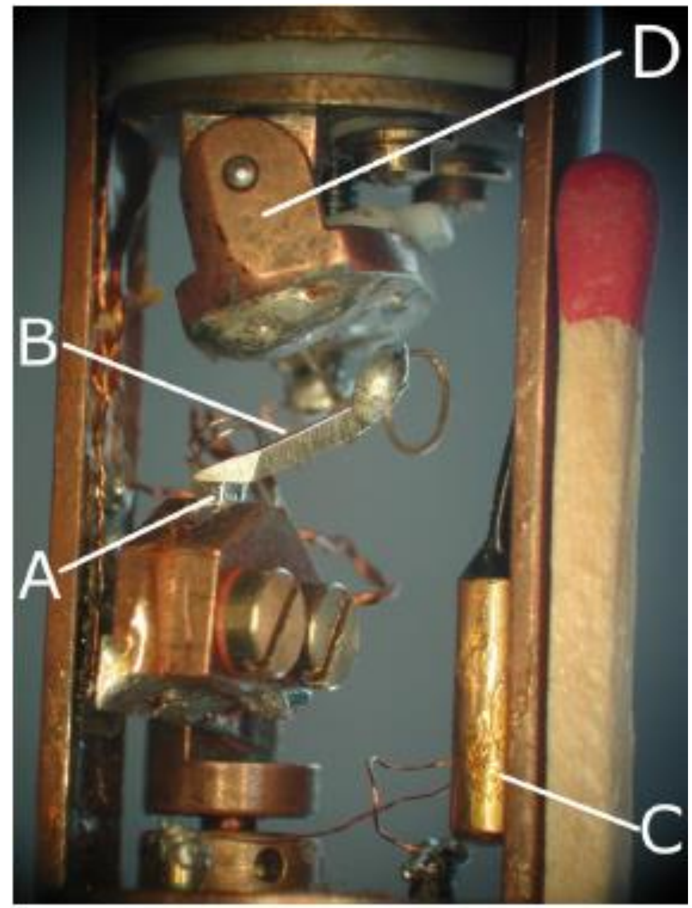
T = 50 mK: inside mixing chamber of dil-fridge



Goll, PhD Thesis, KIT 1993, Brugger, Diploma Thesis, KIT, 2006

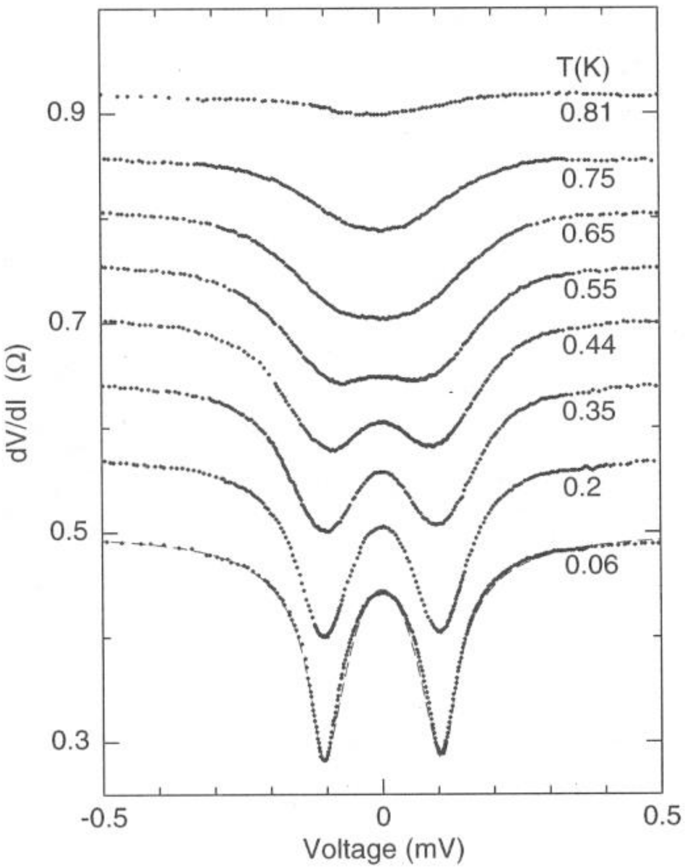
A: SC sample (Anvil)
B: N metal (Needle)
C: Thermometer
D: „Wippe" ("seesaw")

T = 4.2 K

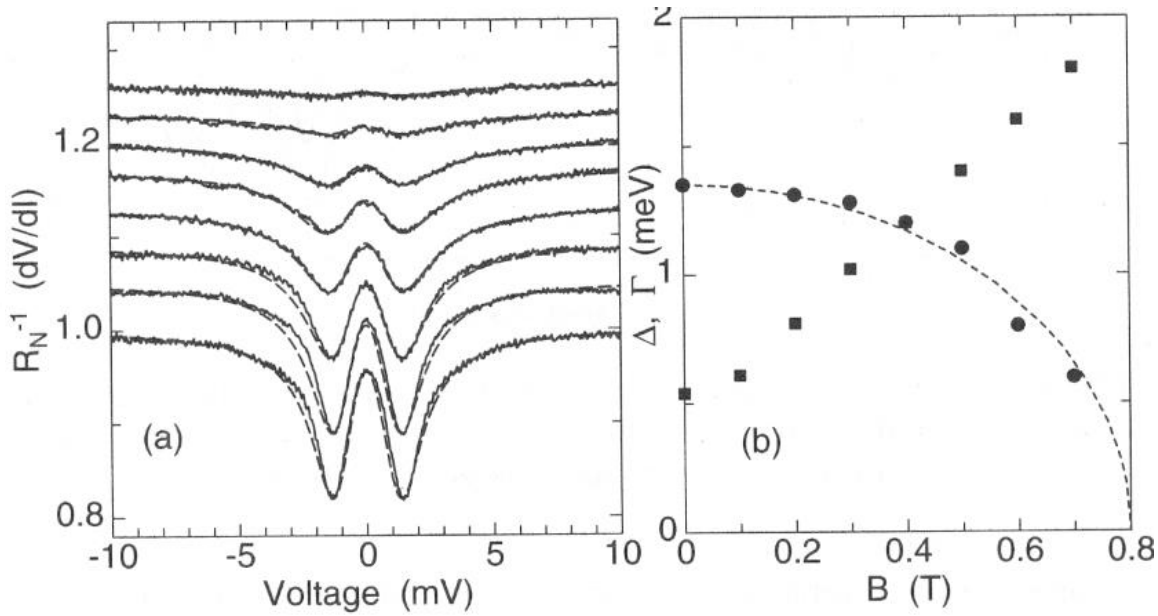


1.1 Point contact spectroscopy (PCS) of S-N contacts

Temperature Dependence



Magnetic field dependence



Nb-Ag, R = 4.9Ω, T = 1.5 K,
B = 0, 0.1, …0.7 T (bottom to top)
Dotted line: $\propto (1-(B/B_c)^2)^{1/2}$

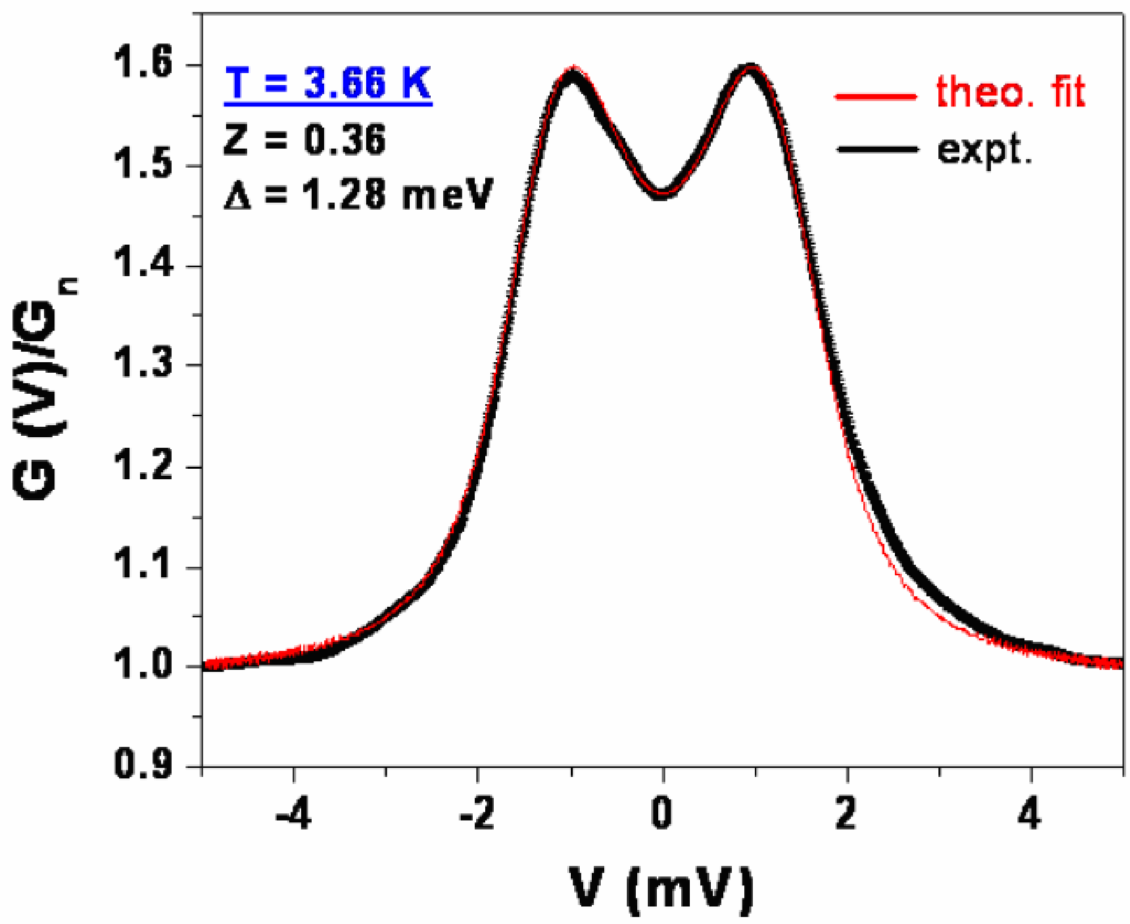
Zn-Ag, R = 0.5Ω, T_c = 0.82 K, T = 0.06 K
Fit parameters: Δ = 110 μeV, Z = 0.5, Γ = 6 μeV

Naidyuk & Yanson, PCS, 2005

1.1 Modern plotting of PC spectra: dI/dV instead of dV/dI

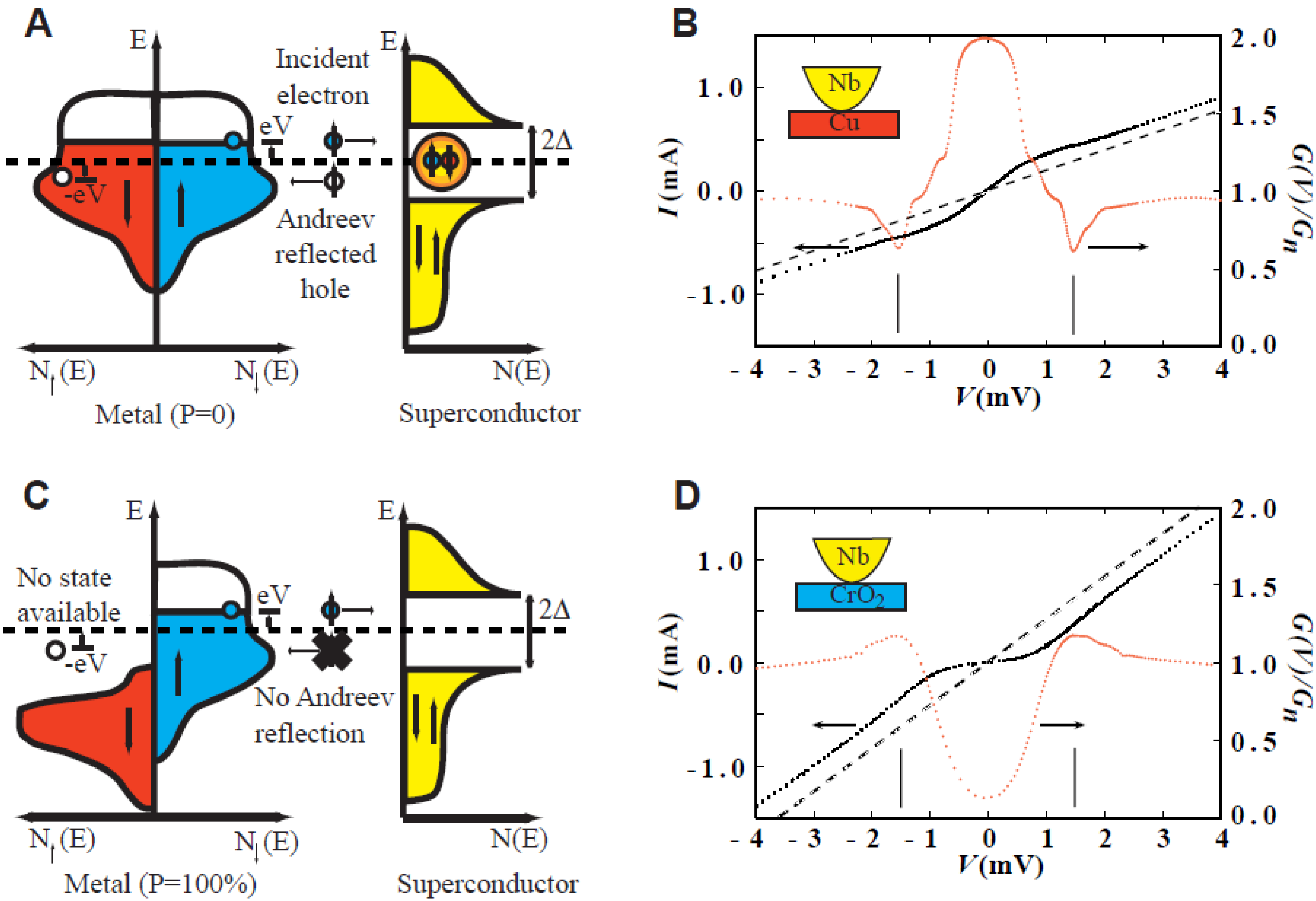
Differential conductance $G = dI/dV$

S = Pb, N = Au



G. Sheet, PhD Thesis, Tata Institute, 2006

Outlook: Determination of Spin Polarization in F-S contacts: Suppression of Andreev Reflection



Soulen et al, Science 282, 85 (1999)

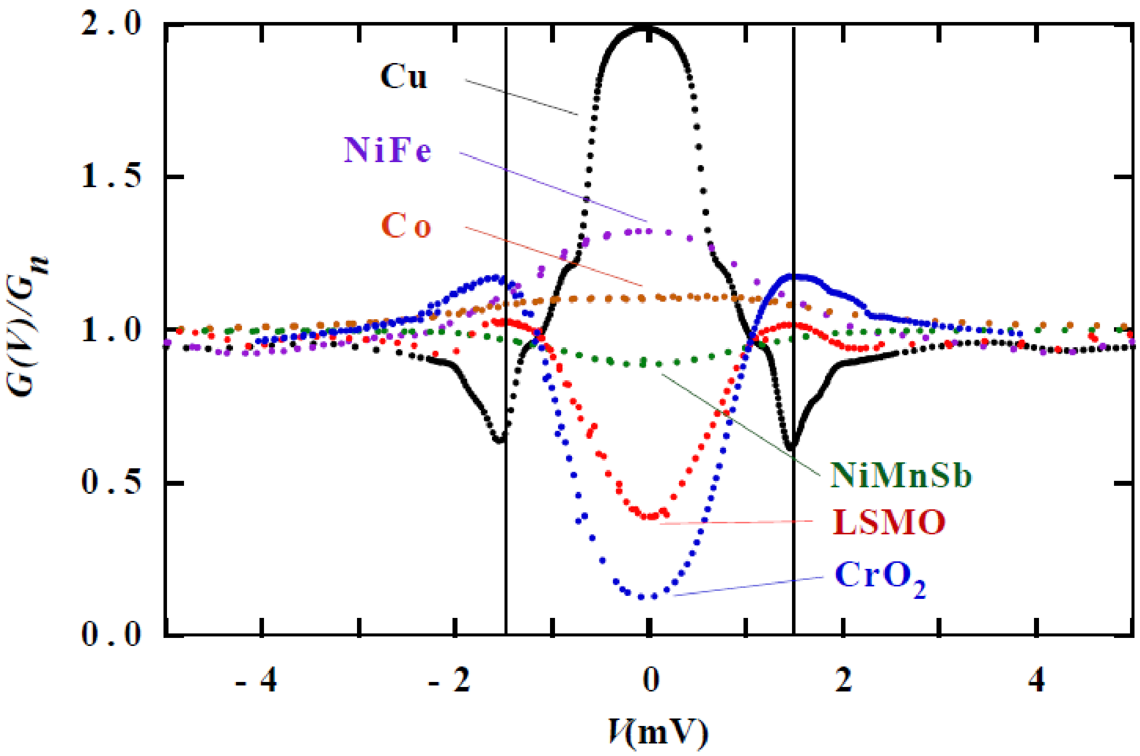
Outlook: Determination of Spin Polarization in F-S contacts: Suppression of Andreev Reflection

$$P_C = \frac{N_\uparrow(E_F)v_{F\uparrow} - N_\downarrow(E_F)v_{F\downarrow}}{N_\uparrow(E_F)v_{F\uparrow} + N_\downarrow(E_F)v_{F\downarrow}}$$

Here: S = Nb
T = 1.4 – 4.2 K

P_C: Spin polarization of a contact can be determined from the PC spectra by

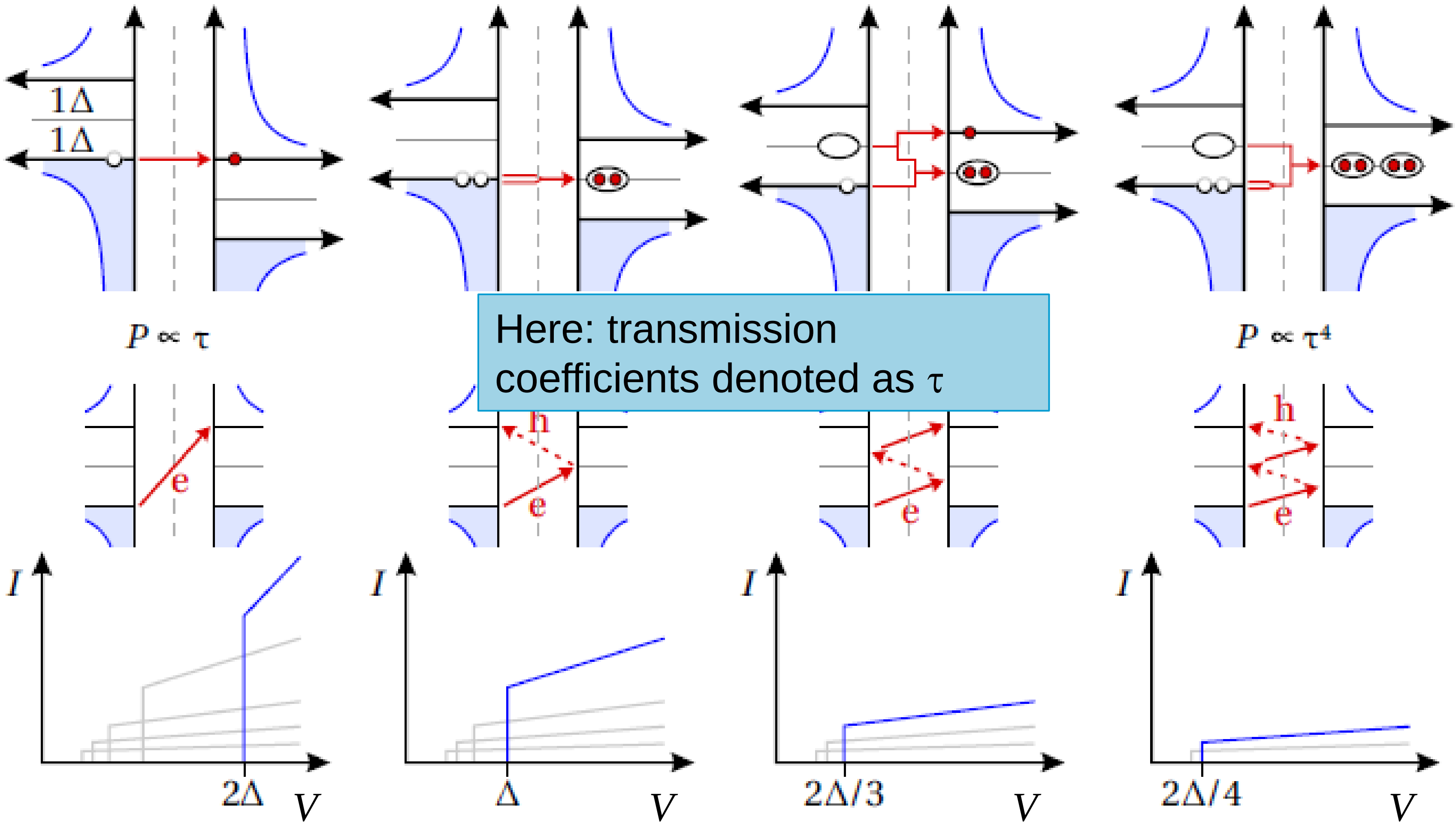
$$\frac{1}{G_n}\frac{dI}{dV}(eV \to 0, T \to 0; P_C, Z = 0) = 2(1 - P_C)$$



Fitting procedure required for finite T and Z

Soulen et al, Science 282, 85 (1999)

1.2 S-S contacts: Multiple Andreev Reflections (MAR) with *m* charges



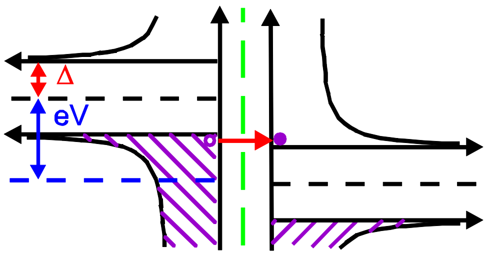
Here: transmission coefficients denoted as τ

$|eV| < 2\Delta$: no single qp transport possible, $0 < |eV| < \Delta$: Andreev reflection (AR)
$|eV| < \Delta$: multiple AR (MAR) with $m \geq 3$: $|eV| > 2\Delta/m$, $P \propto \tau^m$
CPs in both electrodes are involved !

PhD Thesis, C. Schirm, Konstanz 2008

1.2 I-Vs by MAR: „subharmonic gap structure“

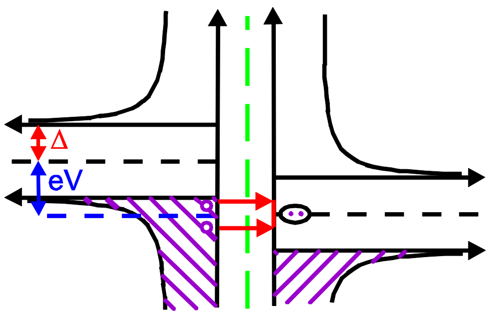
single-electron transport



eV ≥ 2Δ/1

P ∝ τ[1]

2 electrons:

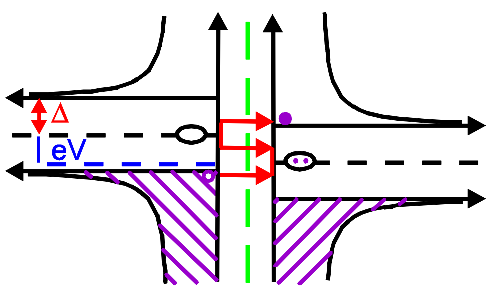


eV ≥ 2Δ/2

P ∝ τ[2]

Andreev reflection

3 electrons:



eV ≥ 2Δ/3

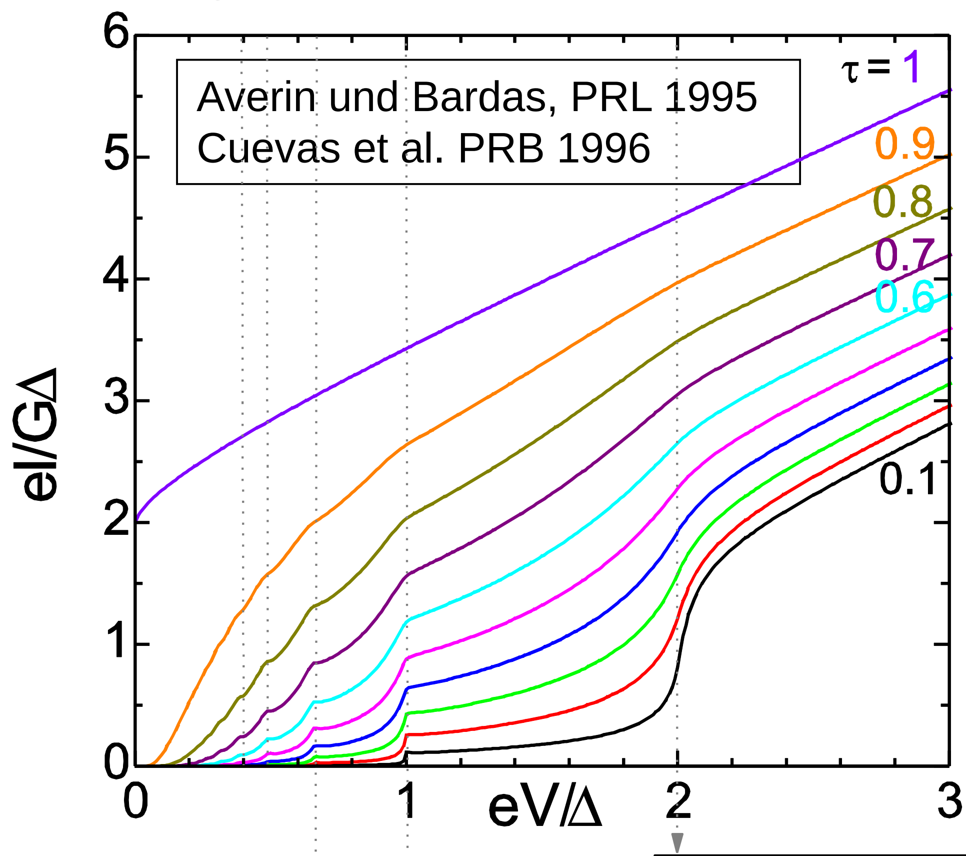
P ∝ τ[3]

multiple Andreev reflection (MAR)

m electrons:

eV ≥ 2Δ/m

P ∝ τ[m]

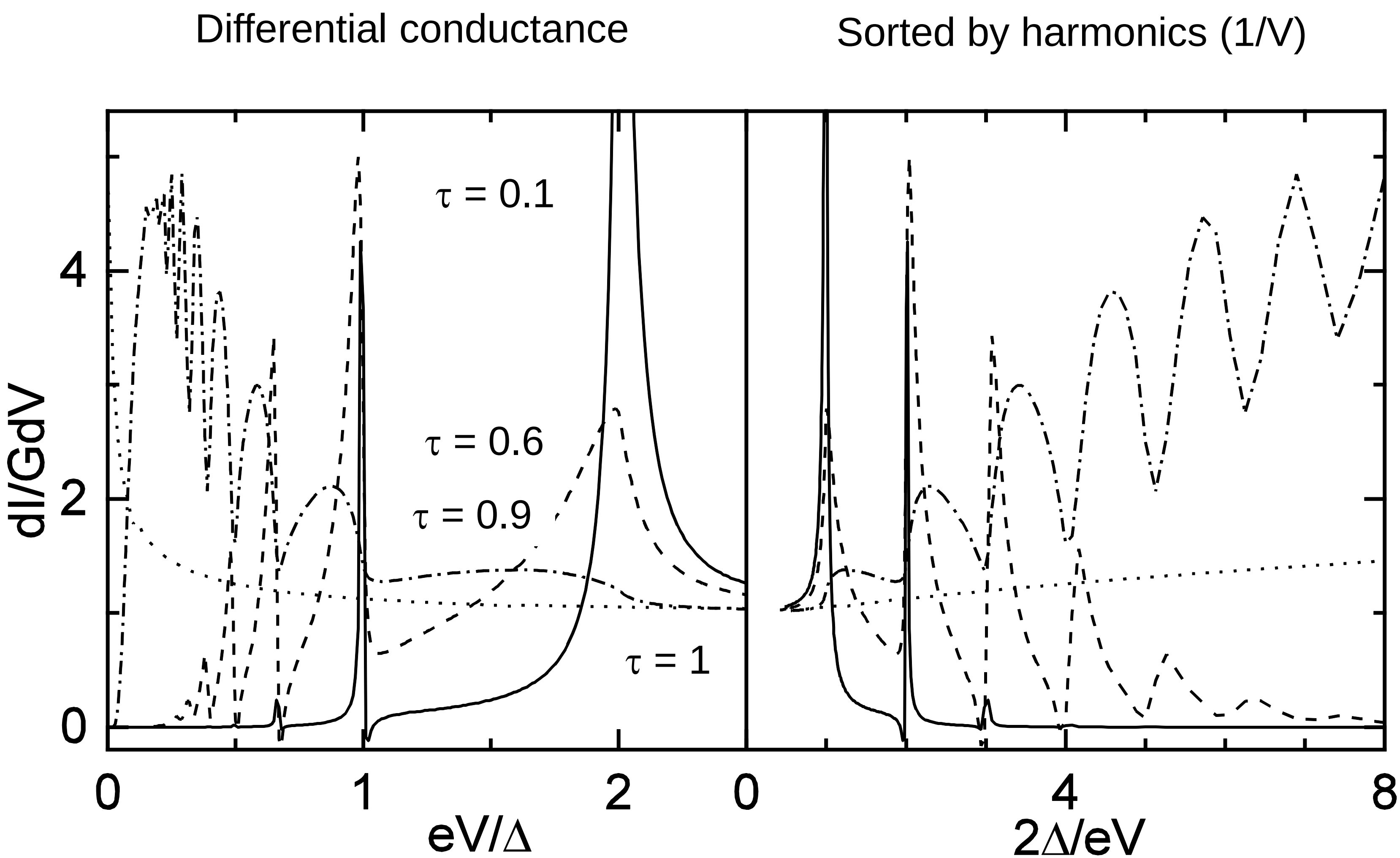


3 e⁻ transfered
2 qp created
eV > 2Δ/3
P ∝ τ[3]

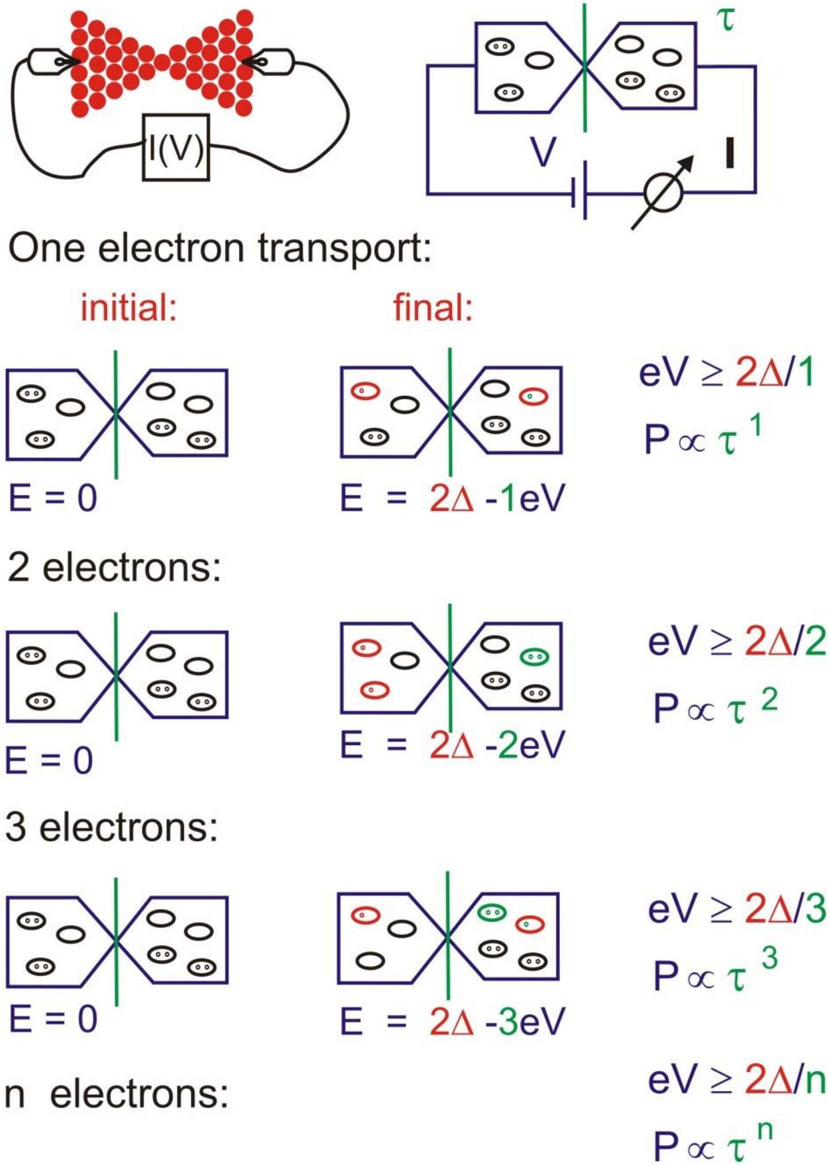
2 e⁻ transfered
2 qp created
eV > 2Δ/2
P ∝ τ[2]

1 e⁻ transfered
2 qp created
eV > 2Δ/1
P ∝ τ

1.2 I-V characteristics by MAR: “Subharmonic gap structure“

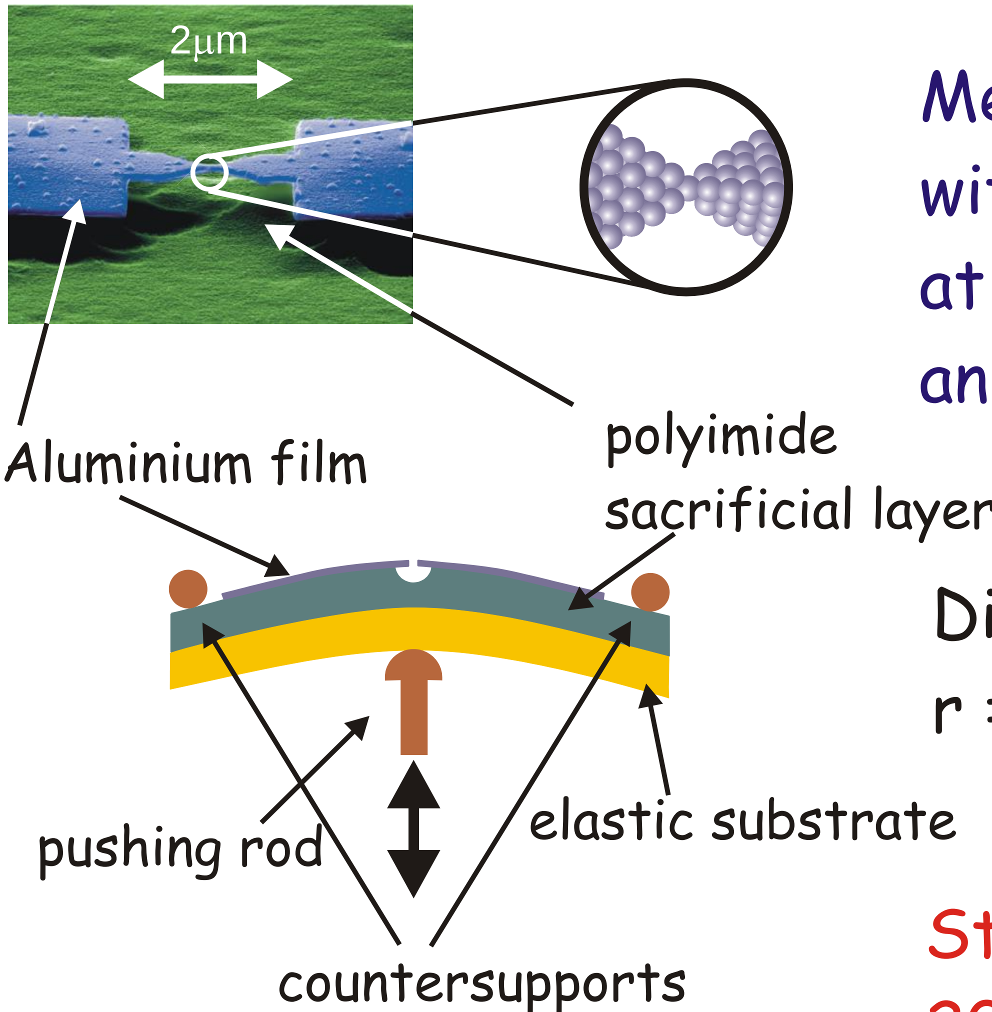


1.2 Nonlinear IV characteristics by MAR



P: Probability of MAR process to occur
Indicated proportionalities hold for small Transmission coefficients τ

Suspended nanobridge for adjusting ScS contacts



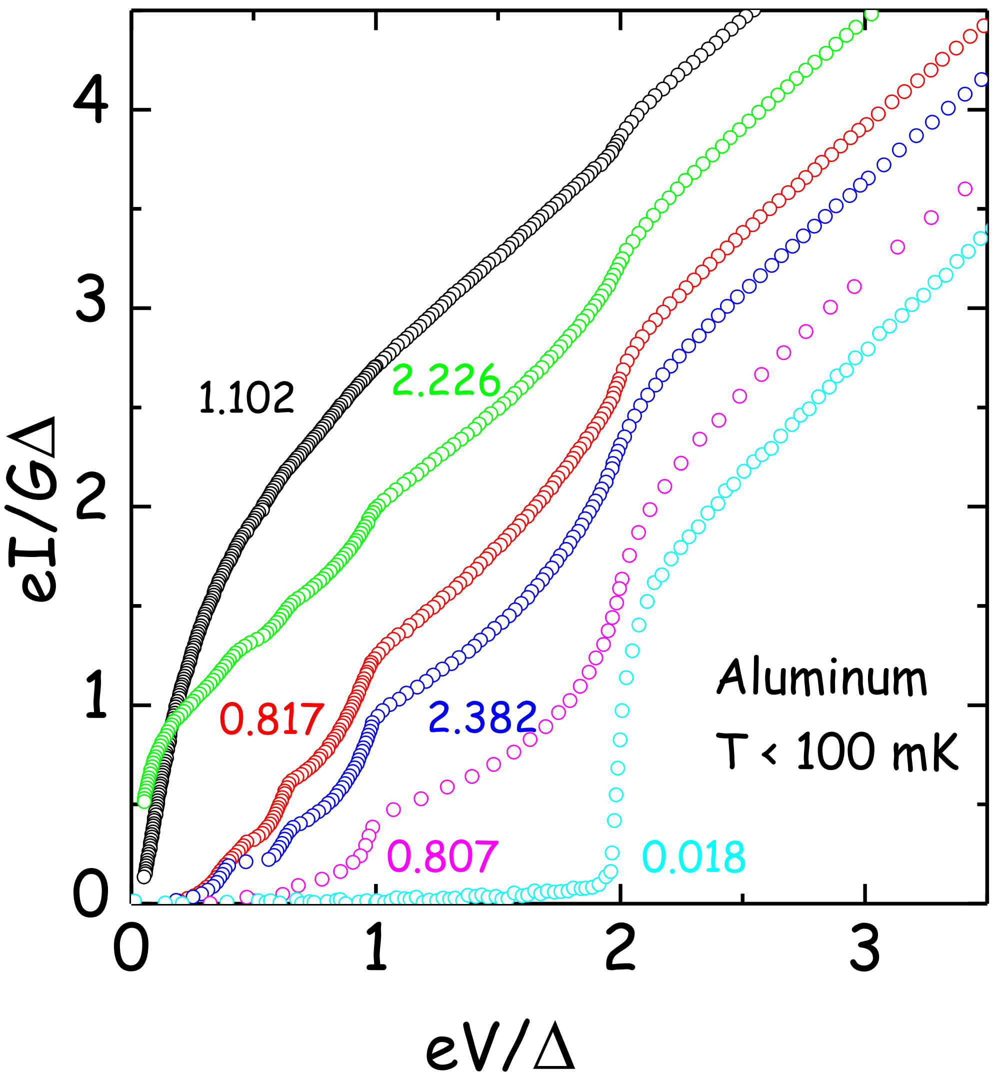
Mechanical adjustment with atomic precision at low temperatures and in UHV

Displacement ratio:
$r = 10^{-4}$ to 10^{-5}

Stability better than 200 fm/h (at 4.2 K)

J.v.Ruitenbeek et al, Rev. Sci. Instrum., 1995

1.2 Examples of experimental I-V curves



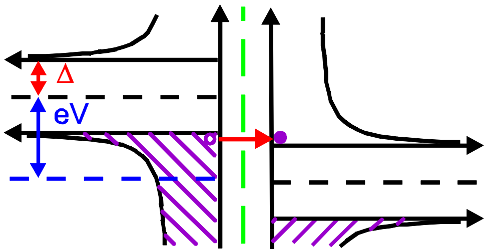
Δ : superconducting gap energy

G : conductance at eV » 2Δ

Nonlinear IV characteristics of superconducting atomic contacts:

1.2 Superconductivity: Nonlinear IV characteristics by MAR

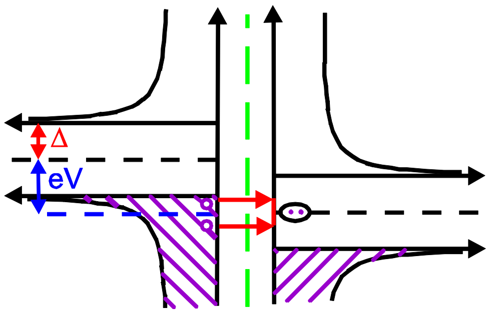
single-electron transport



$eV \geq 2\Delta/1$

$P \propto \tau^1$

2 electrons:

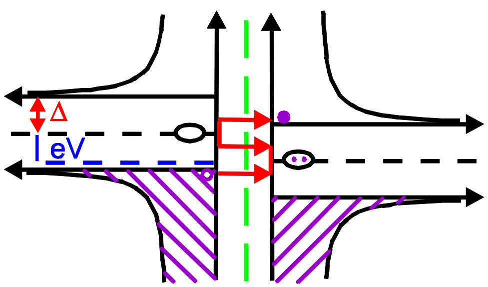


$eV \geq 2\Delta/2$

$P \propto \tau^2$

Andreev reflection

3 electrons:



$eV \geq 2\Delta/3$

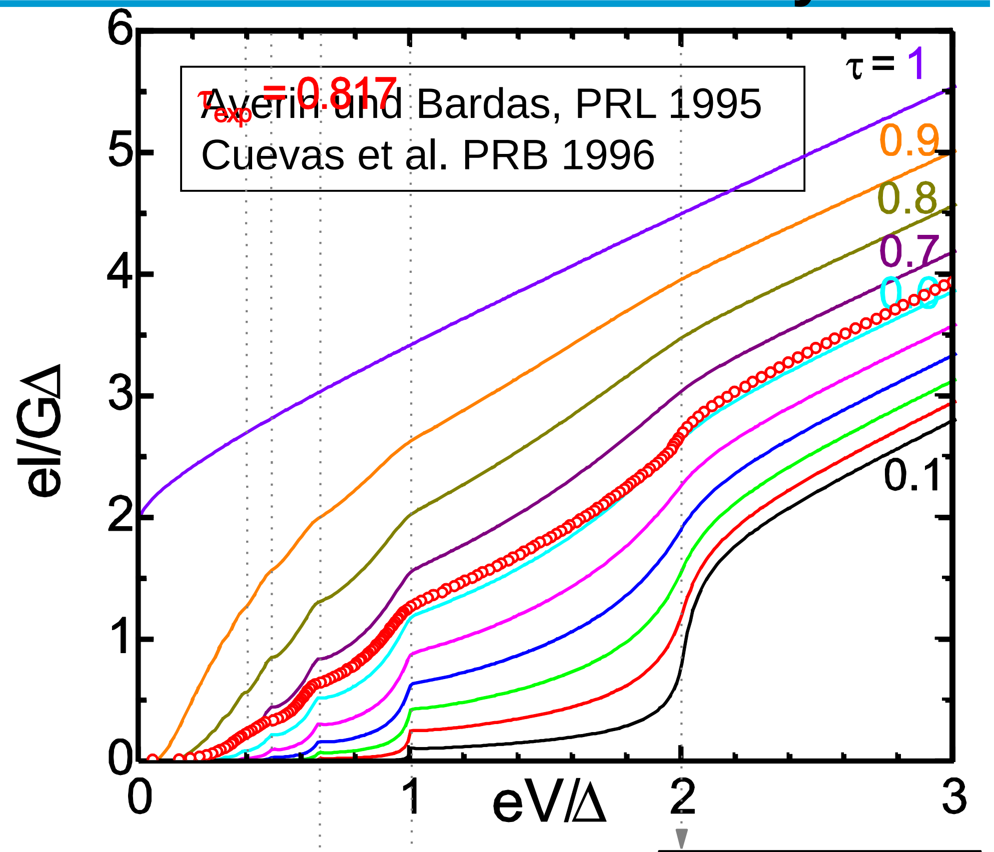
$P \propto \tau^3$

multiple Andreev reflection (MAR)

m electrons:

$eV \geq 2\Delta/m$

$P \propto \tau^m$



3 e⁻ transfered
2 qp created
$eV > 2\Delta/3$
$P \propto \tau^3$

2 e⁻ transfered
2 qp created
$eV > 2\Delta/2$
$P \propto \tau^2$

1 e⁻ transfered
2 qp created
$eV > 2\Delta/1$
$P \propto \tau$

SPECTROSCOPY OF THE CHANNEL ENSEMBLE

Decomposition of exp. IVs into contributions of *N* channels with transmission coefficients $\{\tau_1, \tau_2, \tau_3, \ldots\ldots, \tau_N\}$

$$I_{exp} = \sum_{i=1}^{N} i(V, \tau_i)$$

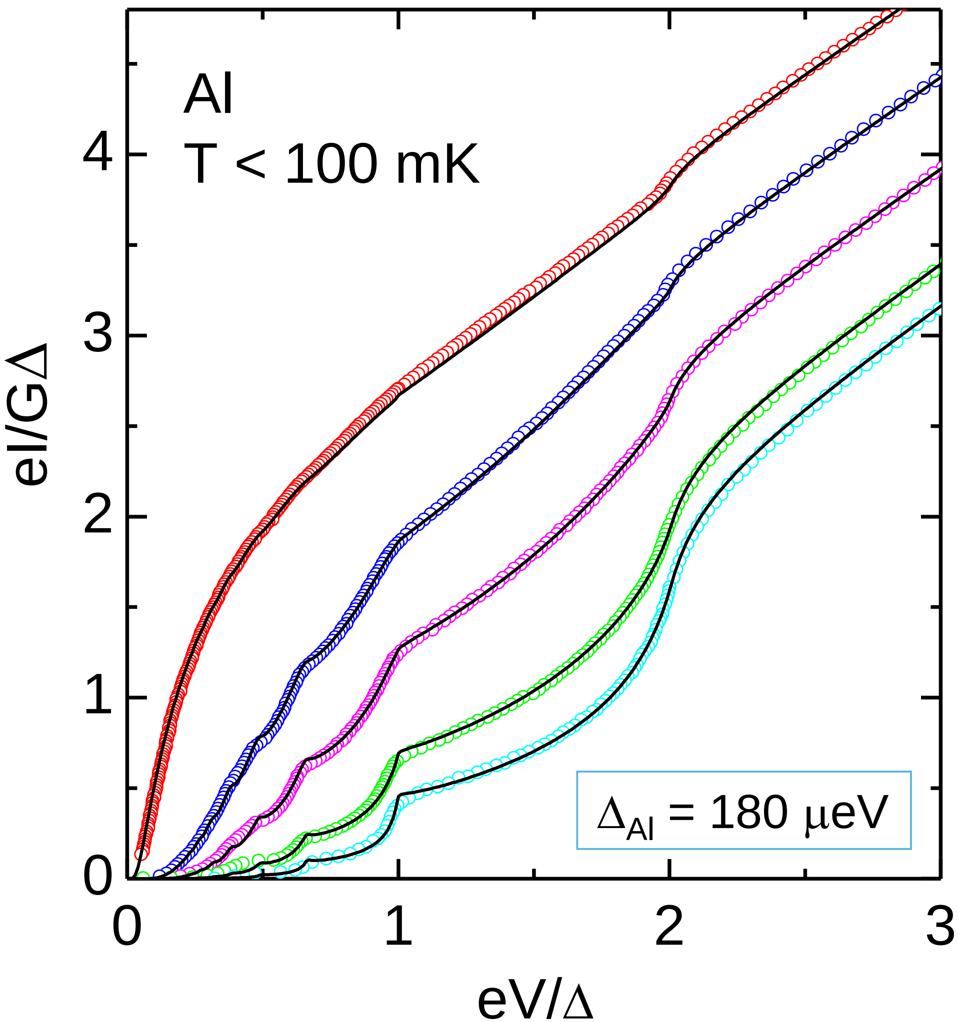
$i(V, \tau_i)$: current contribution of channel with τ_i

- (total) conductance *G*: $G = G_0 \sum_{i=1}^{N} \tau_i = G_0 T$

- total transmission *T*: $T = \sum_{i=1}^{N} \tau_i$

E. Scheer et al., PRL 1997

Single-atom contacts of aluminum



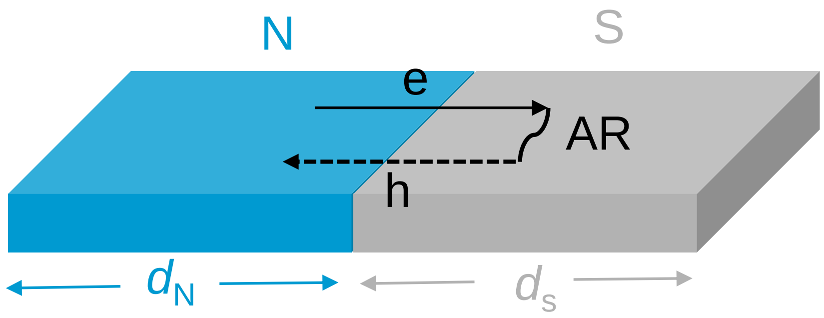
G_N/G_0, $\{\tau_i\}$	N
○ (red) 1.095 {0.956,0.139}	2
○ (blue) 0.875 {0.800,0.075}	2
○ (magenta) 0.816 {0.682,0.120,0.014}	3
○ (green) 0.898 {0.535,0.244,0.119}	3
○ (cyan) 0.808 {0.400,0.254,0.154}	3

E. Scheer et al., Phys Rev Lett. 78, 3535 (1997)

2 Proximity Effect

- **Mutual influence** between SC and NC in good contact with each other
- Phase coherent superposition of Andreev reflection

Proximity effect (PE) = Andreev reflection (AR) + Phase coherence (PC)



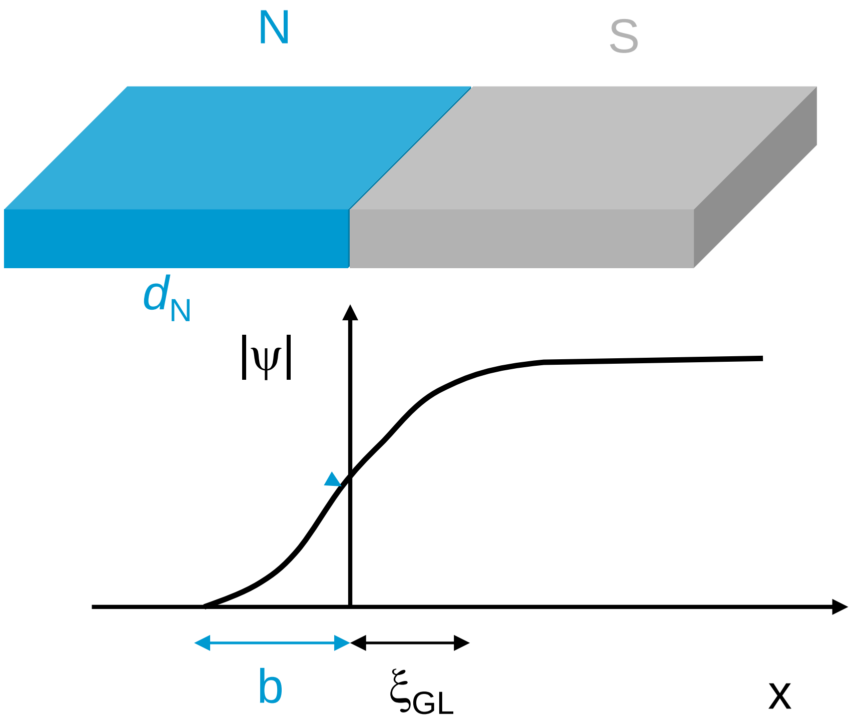
Good contact, no oxide barrier, planar interface
Transformation of quasiparticles into Cooper pairs by Andreev reflection

What are the electronic spectroscopic properties on either side of the interface?

2 Classical model of PE (1960s, de Gennes et al.)

Description by Ginzburg Landau theory with boundary conditions

$$(-i\hbar\nabla + 2e\vec{A})\Psi|_n = \frac{i\hbar}{b}\Psi$$



ψ: order parameter

$|\psi|: = (n_{CP})^{1/2}$

n_{CP} : Cooper pair density

ξ_{GL}: GL coherence length, "stiffness" of ψ

b: "penetration depth" of n_{CP} into N

$b \leq \xi_{GL}$ required

b = 0: vacuum, magnetic metal

$b \neq 0$: normal metal

How large is *b*?

"clean limit" $b << l_N$ ballistic transport, momentum direction conserved

$$b = \frac{\hbar v_F}{2\pi k_B T} = L_T \propto \frac{1}{T}$$

"dirty limit" $b >> l_N$ diffusive transport

$$b = \sqrt{\frac{\hbar D}{2\pi k_B T}} := L_T \propto \frac{1}{\sqrt{T}} \text{ with } D = \frac{1}{3} v_F l_N$$

Outlook: Bogoliubov-de Gennes (BdG) equations

Generalization of Hartree-Fock eqs. with spatially dependent pair potential $\Delta(\vec{r})$

$$\mathcal{H}_0 u(\vec{r}) + \Delta(\vec{r})v(\vec{r}) = Eu(\vec{r})$$
$$-\mathcal{H}_0^* v(\vec{r}) + \Delta^*(\vec{r})u(\vec{r}) = Ev(\vec{r})$$

where $\mathcal{H}_0 = \frac{1}{2m}(-i\hbar\nabla + 2e\vec{A})^2 + \mathcal{U}(\vec{r}) - \mu$

with
$\mathcal{U}(\vec{r})$ Hartree term (Coulomb interaction)
Pair amplitude $F(\vec{r}) = \langle\Psi_\uparrow(\vec{r})\Psi_\downarrow(\vec{r})\rangle$
Pair potential $\Delta(\vec{r}) = V(\vec{r})\langle\Psi_\uparrow(\vec{r})\Psi_\downarrow(\vec{r})\rangle = V(\vec{r})\sum_n v_n^*(\vec{r})u_n(\vec{r})(1-2f_n)$

Simple test: $\Delta = 0$: $\mathcal{H}_0 u = Eu$, $\mathcal{H}_0^* v = -Ev$ → bdG eqs decoupled

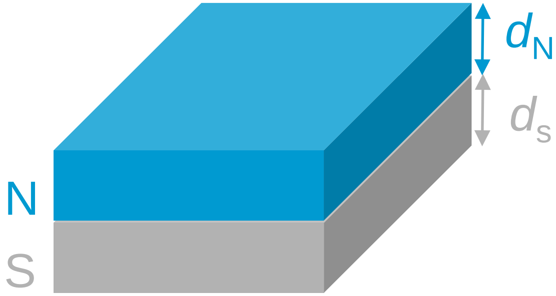
u,*v* are conventional electron and hole states with energy $\pm E$ above $E_F = \mu$

In general BdG eqs: coupled differential equations
→ *self consistent solution* $\Delta(\vec{r})$ for $u(\vec{r})$ and $v(\vec{r})$.

Result:

N adopts sc properties and vice versa: sc in S is weakened (Δ, n_{CP}, T_c, B_c, …) (inverse proximity effect)

2 Classical example: Cooper approximation, inverse proximity effect



Consider double layer with:

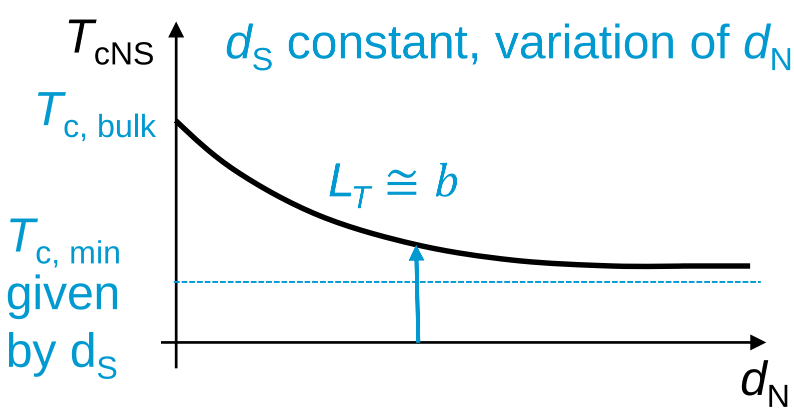
- $L_T > d_N$, $\xi_S > d_S$
- $v_{F,N} = v_{F,S}$
- Perfect interface

Probability for a qp to be in S or N given by the ratio of the volumes of S and N

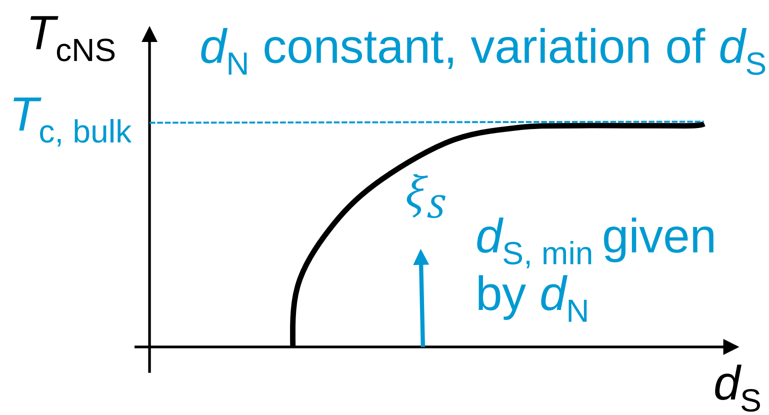
→ Effective pair interaction $\rho_F V_{eff}$ by averaging

→ $(\rho_F V)_{\text{eff}} = \frac{\rho_{F,N} V_N d_N + \rho_{F,S} V_S d_S}{\rho_{F,N} d_N + \rho_{F,S} d_S}$ → $T_{cNS} = 1.14\Theta_D e^{-\frac{1}{(\rho_F V)_{\text{eff}}}}$

→ Reduction of T_{cNS} compared to $T_{c,bulk}$ ("**Inverse PE**")



T_{cNS} saturates for $d_N \sim L_T$



T_{cNS} saturates for $d_S \sim \xi_S$

2 Interface resistance

Imperfect interface: qp cannot move freely between S and N

→ weaker PE, weaker T_c reduction

Origins of interface resistance

- Roughness, oxide /insulator/contamination layer: γ_B
- Mismatch of v_F and mfp (in normal-conducting state) expressed by conductivities and diffusion constants:

Interface parameter ("dirty limit"):

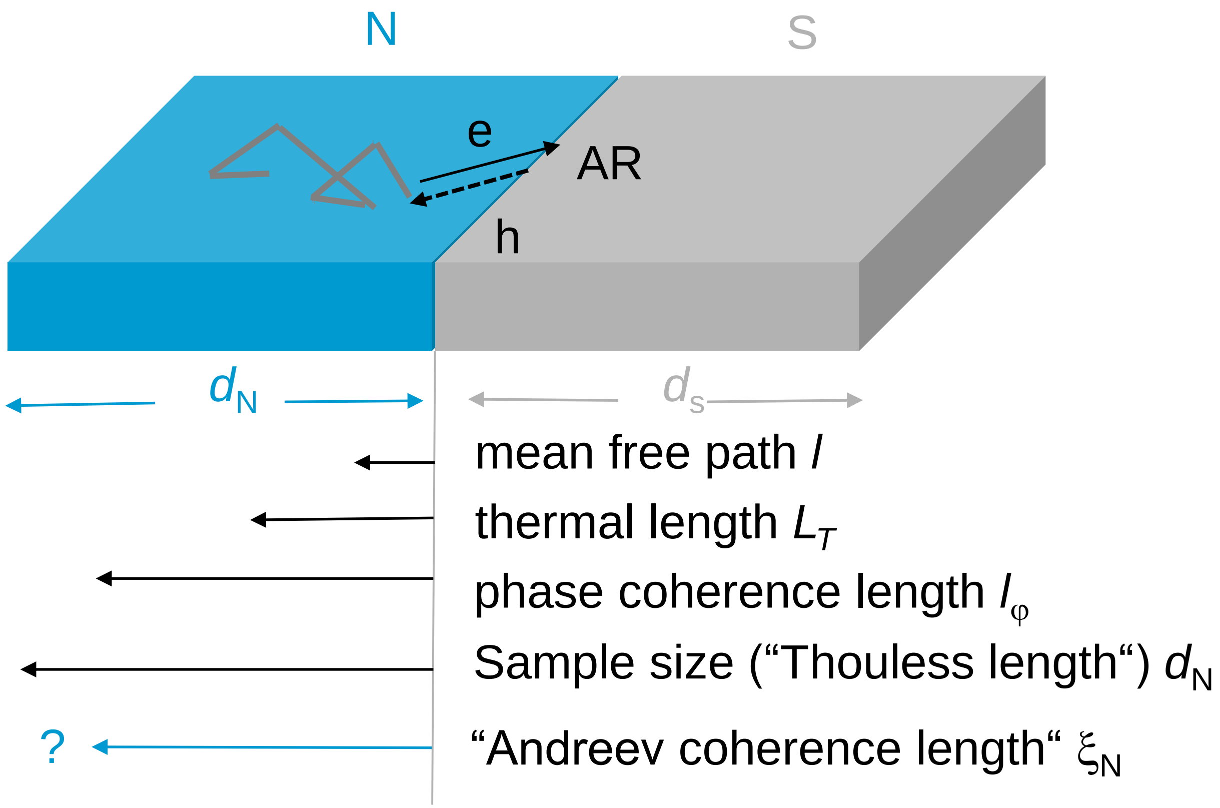
$$\gamma = \frac{\sigma_N}{\sigma_S} \cdot \sqrt{\frac{D_S}{D_N}}$$

($\sigma = \sigma(v_F, l)$ and $D = D\,(v_F, l)$)

Examples follow in section 2.1…..

2 Microscopic mechanism of PE: Length scales and Andreev pairs

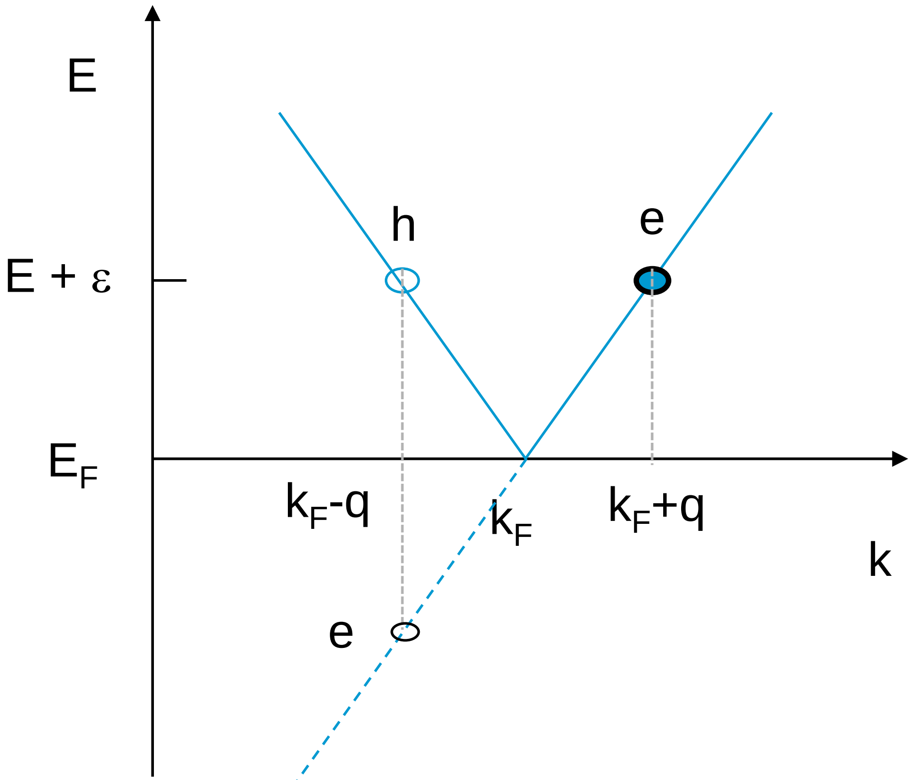
Neglected so far: energy dependence of AR
Which energy scale rules the PE?
“Coherence length“ in N?



H. Courtois et al., J. Low Temp Phys. 116, 187 (1999)

2 Microscopic mechanism of PE: Length scales and Andreev pairs

Andreev reflection in E(k) diagram (linear approximation)



In S:

- CP formed by time-reversed states ($E_F \pm \varepsilon$, $|\varepsilon| < \Delta$)
- Phase fixed by pair interaction (macroscopic phase)

In N:

$E = E_F$: e and h have same $k = k_F$, inverse v → time reversed paths, diffuse together, like CP : "Andreev pair"

Here: phase not fixed!

$E \neq E_F$: different k: $k_e = k_F + q$, $k_h = k_F - q$

→ $\delta k = 2q \cong k_F \cdot \varepsilon / E_F = 2\varepsilon / \hbar v_F$

Time evolution:

Andreev pair consists of 2 electrons with $E_1 = E_F + \varepsilon$ and $E_2 = E_F - \varepsilon$ → $\delta E = 2\varepsilon$

→ Acquire phase difference $\delta\varphi = 2\varepsilon t/\hbar$ within time interval t after entering N

H. Courtois et al., J. Low Temp Phys. 116, 187 (1999)

2 Microscopic mechanism of PE: Length scales and Andreev pairs

	Clean limit (ballistic)	Dirty limit (diffusive)
Travel distance in time *t*	$L = v_F \cdot t$	$L^2 = D \cdot t$
Destruction of phase coherence if $\delta\varphi \sim 2\pi$	$L_\varepsilon = 2\pi\hbar v_F/\varepsilon$	$L_\varepsilon = (2\pi\hbar D/\varepsilon)^{1/2}$

→ for $E = E_F$: $L_\varepsilon \to \infty$ non physical

→ L_ε limited by other mechanisms: thermal smearing (L_T), phase coherence of electrons (l_φ), Cooper pair coherence length/gap $\xi_{CP} = \hbar v_F/2\Delta$, sample size L

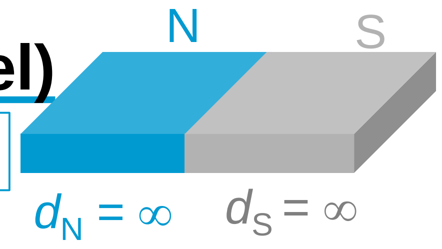
→ Effective "coherence length" ξ_N of Andreev pairs varies between L_T (high energy) and l_φ (low energy)

→ Small samples: Thouless energy is relevant energy scale for PE on length scale *L*. For given *L* only Andreev pairs with $\varepsilon < E_{thou}$ contribute to PE.

→ Consider particular combinations of d_N (= L) and d_S (> and < ξ_S)

H. Courtois et al., J. Low Temp Phys. 116, 187 (1999)

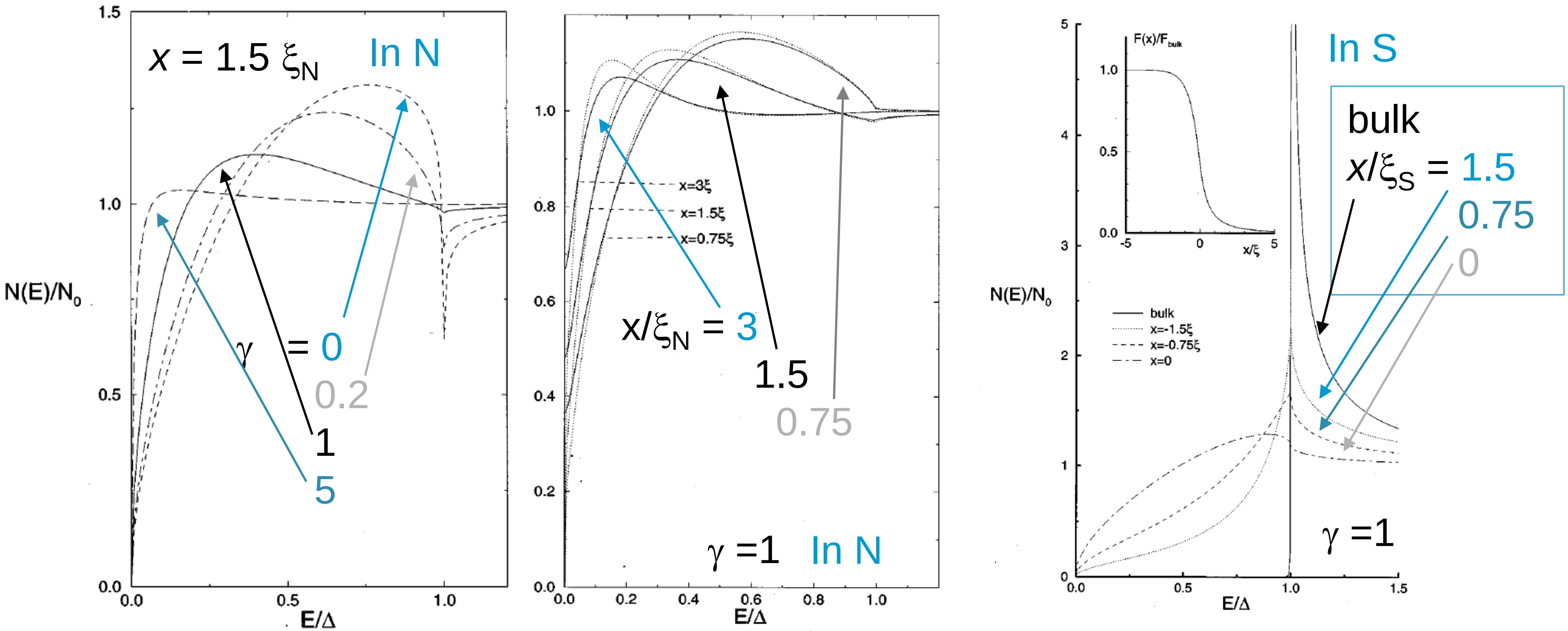
Proximity effect in diffusive metals (BBS model)



Infinite system (d_N and d_s much larger $\xi_{N,S}$):
DOS spatially dependent, DOS in N reduced, no gap in N, singularity in S weakened

Interface parameter

Distance dependence

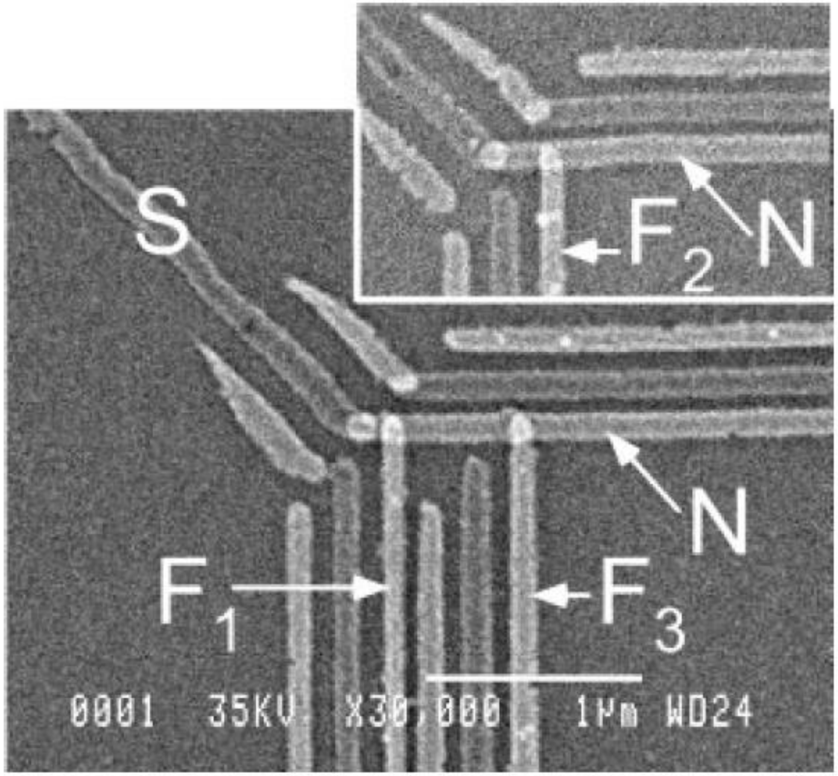


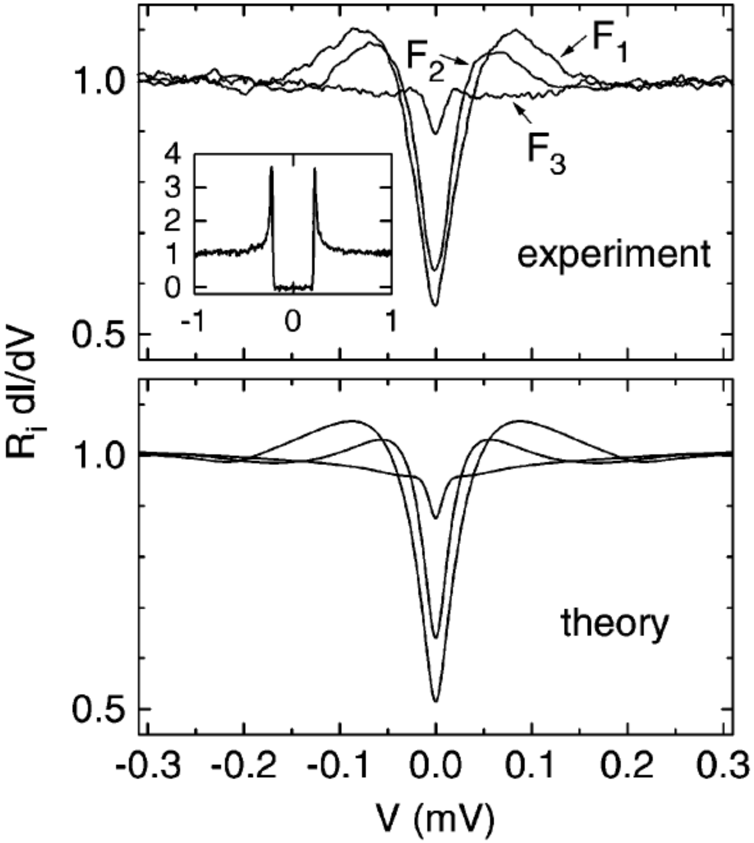
γ = 0, 0.2: bad N metal, Andreev pairs short ranged, influence up to Δ
γ = 5: Andreedv pairs long range, influence at small *E*

Belzig, Bruder, Schön, PRB **54,** 9443 (1996)

Experimental verification of distance dependence

Tunnel spectroscopy with fixed “finger“ probes



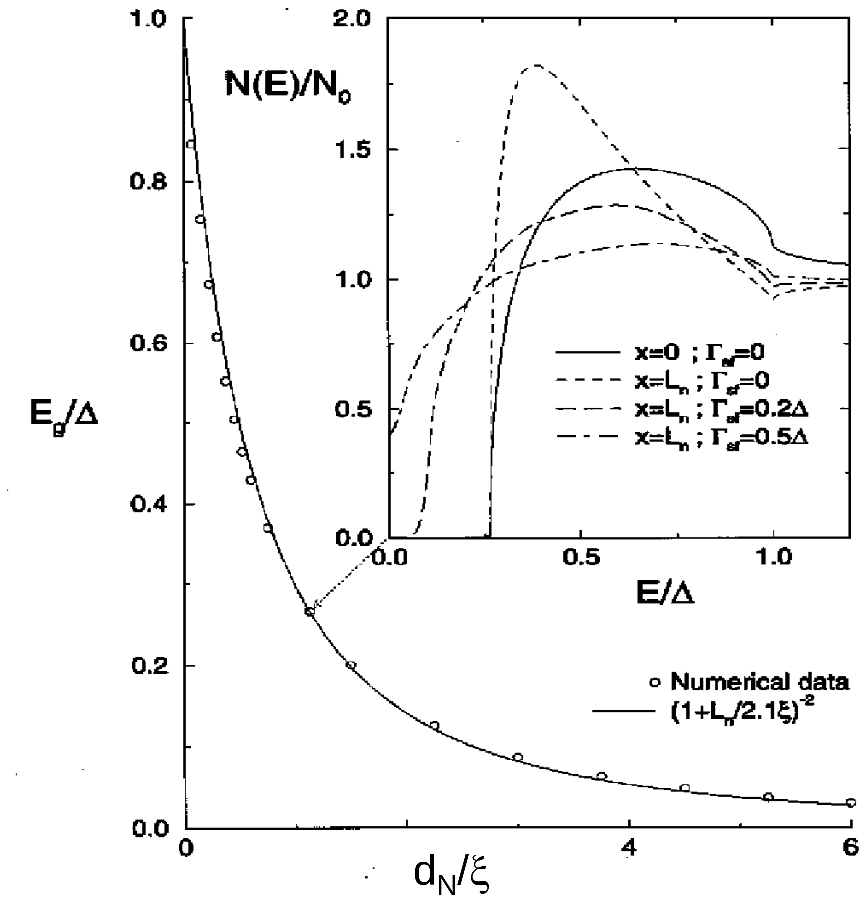


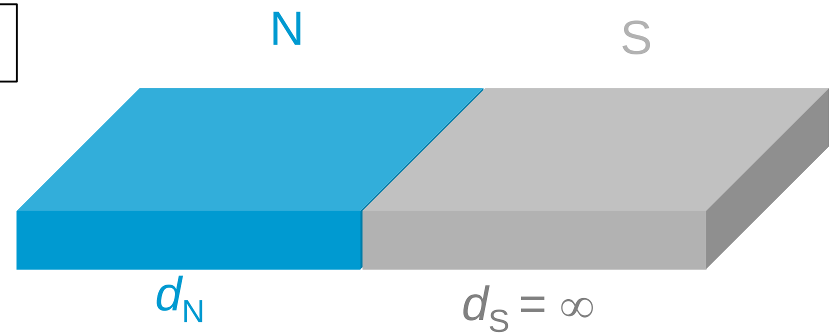
Gueron et al., PRL77 3025 (1996)

Proximity effect in diffusive metals (BBS model)

Semi-infinite system (finite d_N): DOS of the finite normal metal reveals minigap E_g

In this section the DOS is denoted as $N(E)$





BCS and Usadel eq. in the diffusive limit

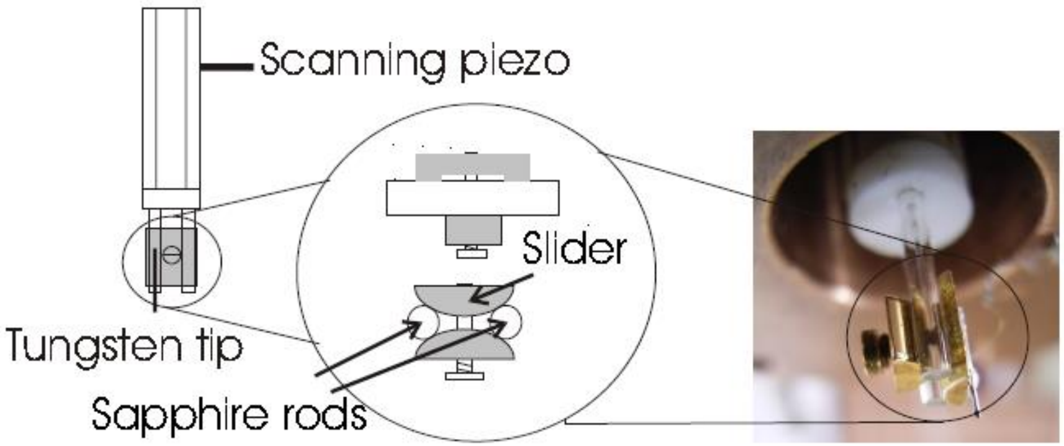
- Elastic mfp $l << \xi_S = (\hbar D/2\Delta)^{1/2}$
- Interface parameter $\gamma = \frac{\sigma_N}{\sigma_S}\sqrt{\frac{D_S}{D_N}}$
- Pair-breaking by spin-flip γ_s
- Finite interface transmission

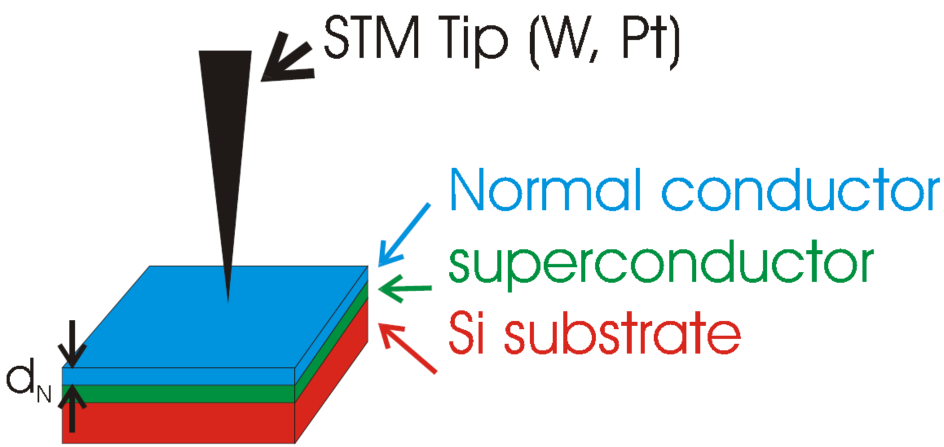
  yields barrier parameter $\gamma_B = \frac{R_B \sigma_N}{\xi_n}$

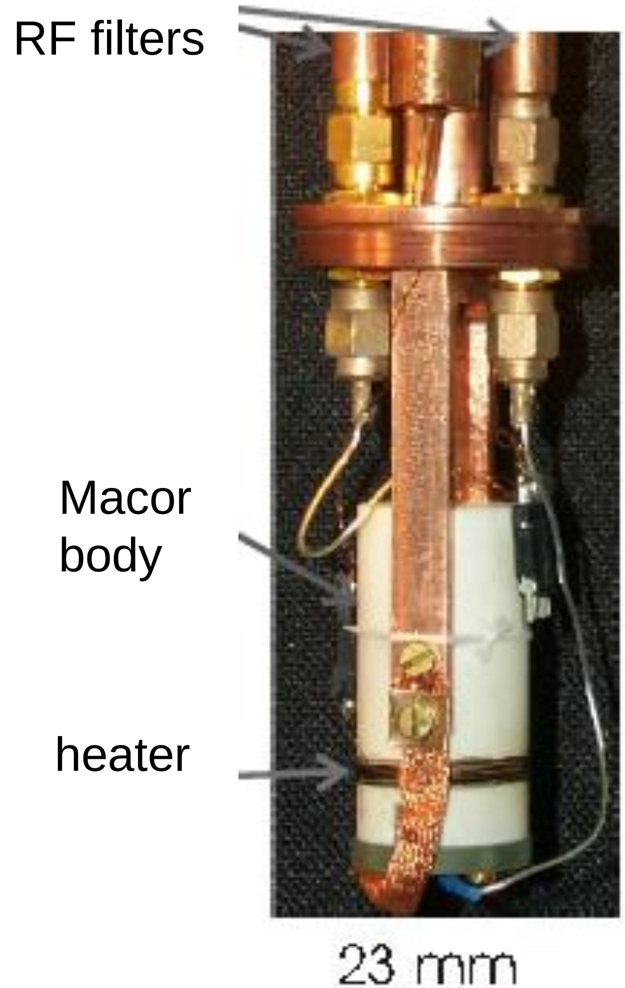
  > determine T_c and minigap E_g

Belzig, Bruder, Schön, PRB **54,** 9443 (1996)

2.1 Scanning Tunneling spectroscopy on SN bilayers







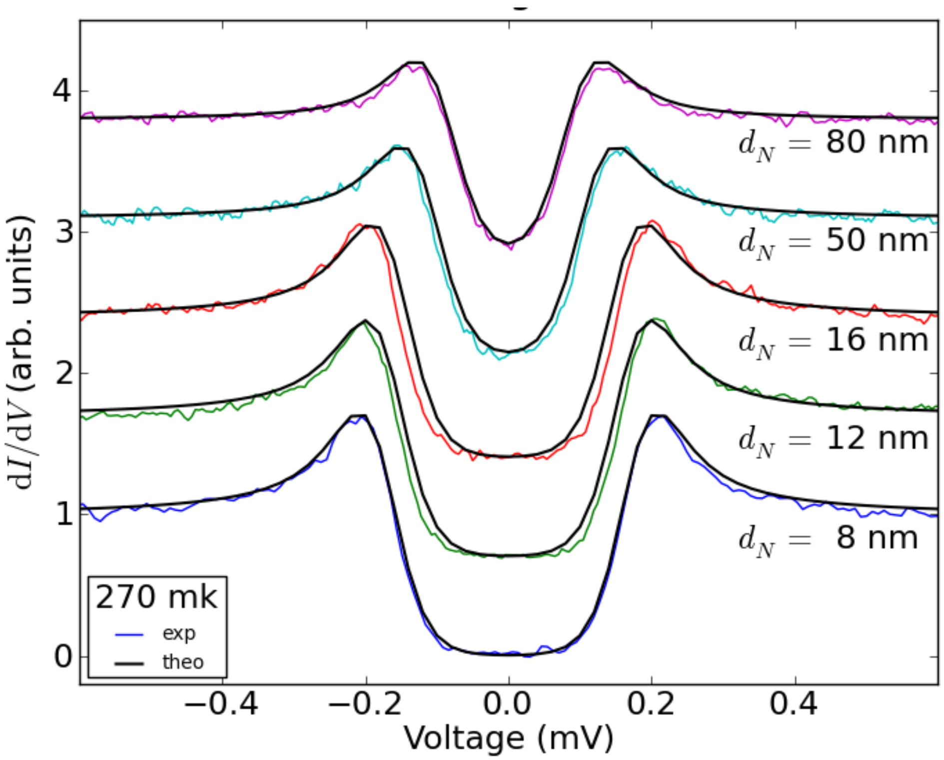
F. Mugele et al. Rev. Sci. Instrum. **67,** 2557 (1996)
N. Moussy et al. Rev. Sci. Instrum. **72,** 128 (2001)
C. Debuschewitz et al, J. Low Temp. Phys. **147**, 525 (2007)

Requirements:
- High energy resolution
- Non-magnetic

2.1 Proximity Effect in diffusive SN Bilayers

S = Al, T_c= 1.2 K, ξ_S = 250 nm, d_S = 350 nm

N = Ag



Calculation with γ_B = 0, γ_S = 0

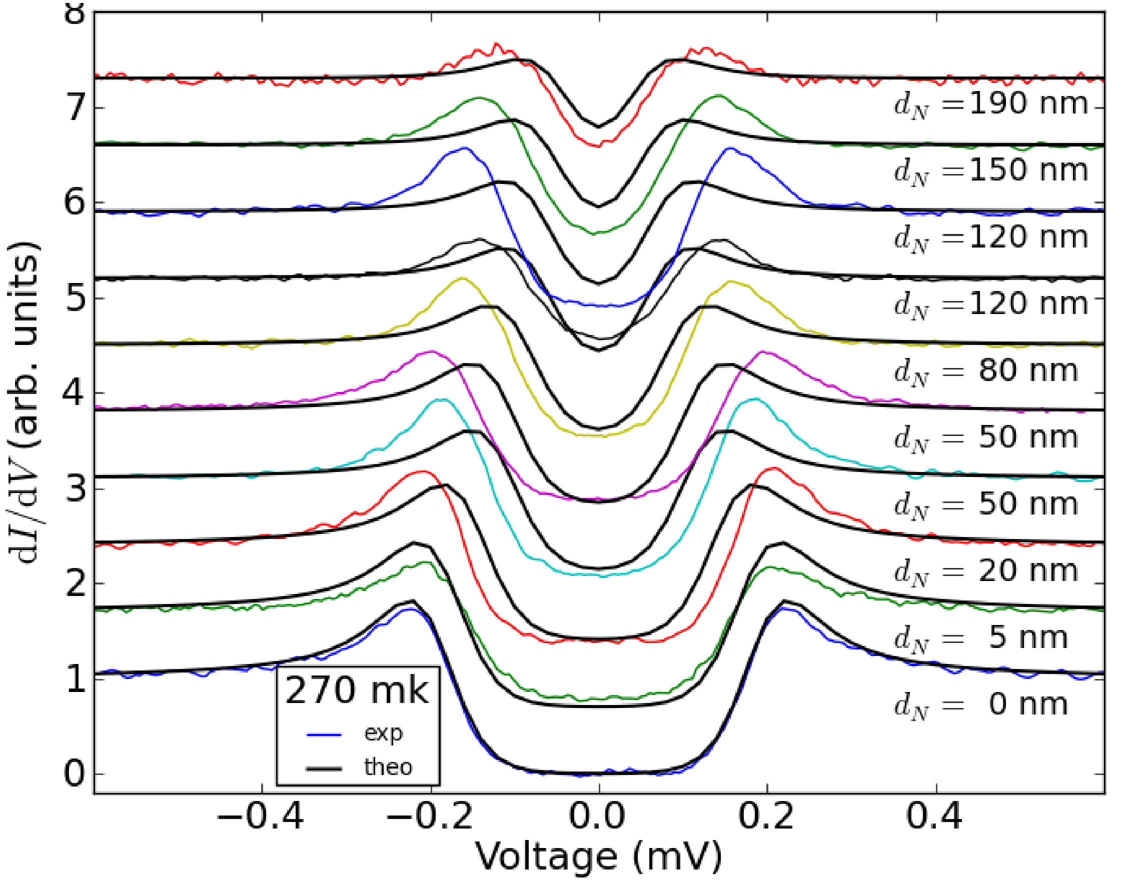
M. Wolz, C. Debuschewitz, W. Belzig, E. Scheer, PRB 84, 104516 (2011)

Outlook: Superconducting gold?

Results on bilayers of Al/Au

N = Au
l , *D*, σ almost identical with Ag
-> same interface parameter γ
-> same PE expected,
if γ_B and γ_S are equal

- Apparent minigap too large for theory!
- Cannot be described with finite γ_B and/or γ_S



Calculation with $\gamma_B = 0$, $\gamma_S = 0$

M. Wolz, C. Debuschewitz, W. Belzig, E. Scheer, PRB 84, 104516 (2011)

Outlook: Superconducting gold?

Attractive pair interaction in Au

Mc Millan formula

$$T_c = \frac{\Theta}{1.45} \exp\left[-\frac{1+\lambda}{\lambda - \mu^*(1+0.62\lambda)} \right]$$

weak coupling →

BCS formula

$$T_c = 1.13 \frac{\hbar\omega_c}{k_B} \exp(-\frac{1}{N_0 V})$$

$$N_0 V = \lambda - \mu^*$$

Band structure calculations: $(N_0 V)$ = 0.07-0.11, λ_{Au} = 0.12-0.17 Bauer, PRB 57 (1998) 11276

State of the art: no measurable T_c in Au down to 200µK: Buchal et al., 1982 , Solid State Comm. 42, 43, R. F. Hoyt et al. 1981, Phys. Lett. A 84 ,145

Extrapolation from Au-containing alloys: Mota et al. 1976, Sol. St. Comm 18, 139; Nishida et al.,1982, Solid State Comm. 44, 305

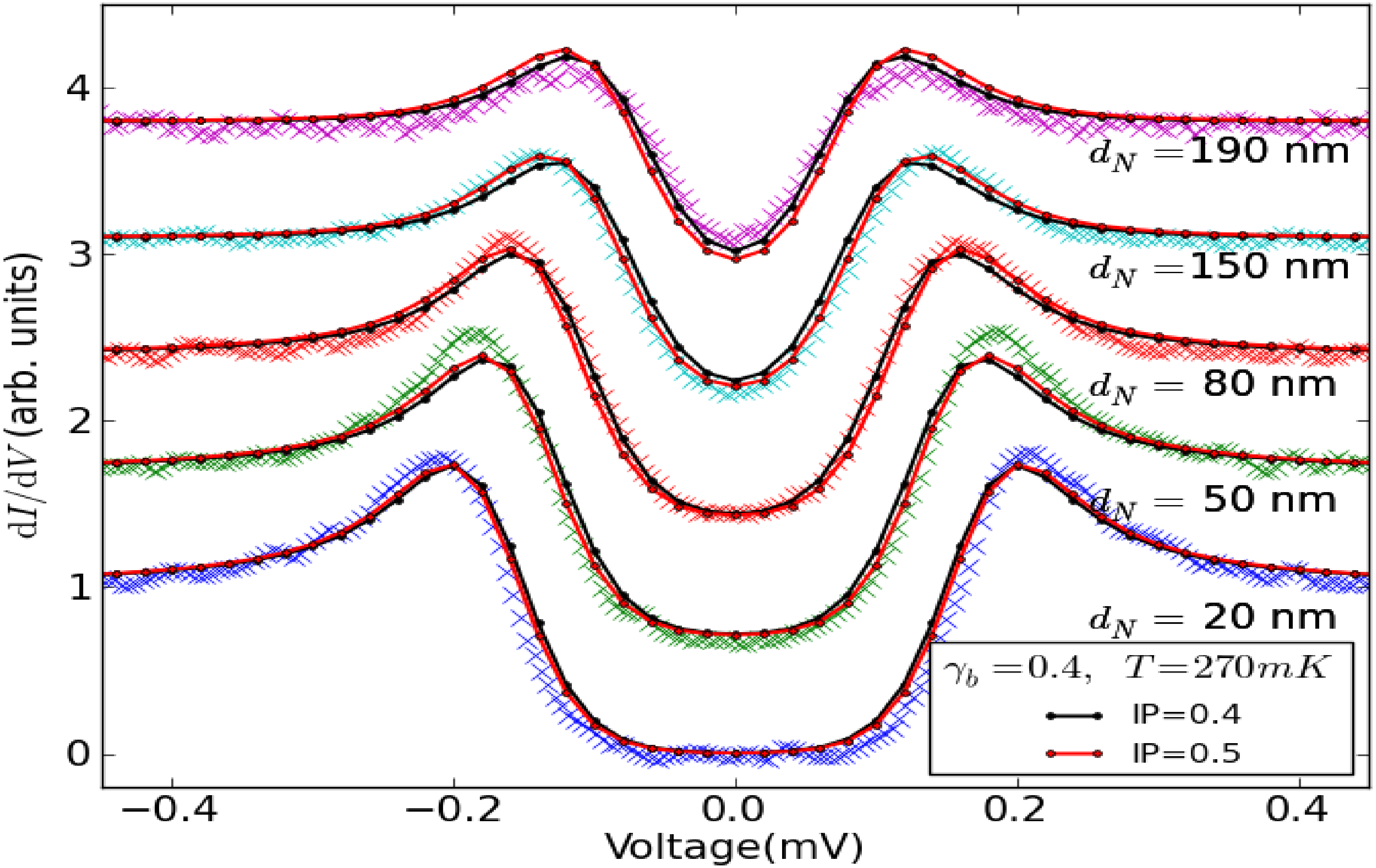
Proximity Effect with $(N_0V)_N \neq 0$

- Usadel eq
- $$\frac{D_{N,S}}{2}\frac{\partial^2\theta(x)}{\partial x^2} = -iE\sin\theta(x) - \Delta_{N,S}(x)\cos\theta(x)$$ where $$G_R(E,x) = \cos\Theta(x)$$ $$F_R(E,x) = \sin\Theta(x)$$
- Self consistency $$\Delta_{N/S}(x) = \frac{(N_0V)_{N/S}}{2}\int dE\sin\left[\theta(E,x)\right]\tanh\left(\frac{E}{2k_BT}\right)$$
- DOS in N $$N(E,x) = \mathrm{Re}\cos\left[\theta(E,x)\right]$$
- Interface parameter γ, barrier parameter γ_B, spin-flip γ_s

- $(N_0V)_N$ enters linearly in contribution to spectral gap
- **Interaction parameter IP = $(N_0V)_N/(N_0V)_S$**

measures relative strength of attractive pair interaction in normal metal

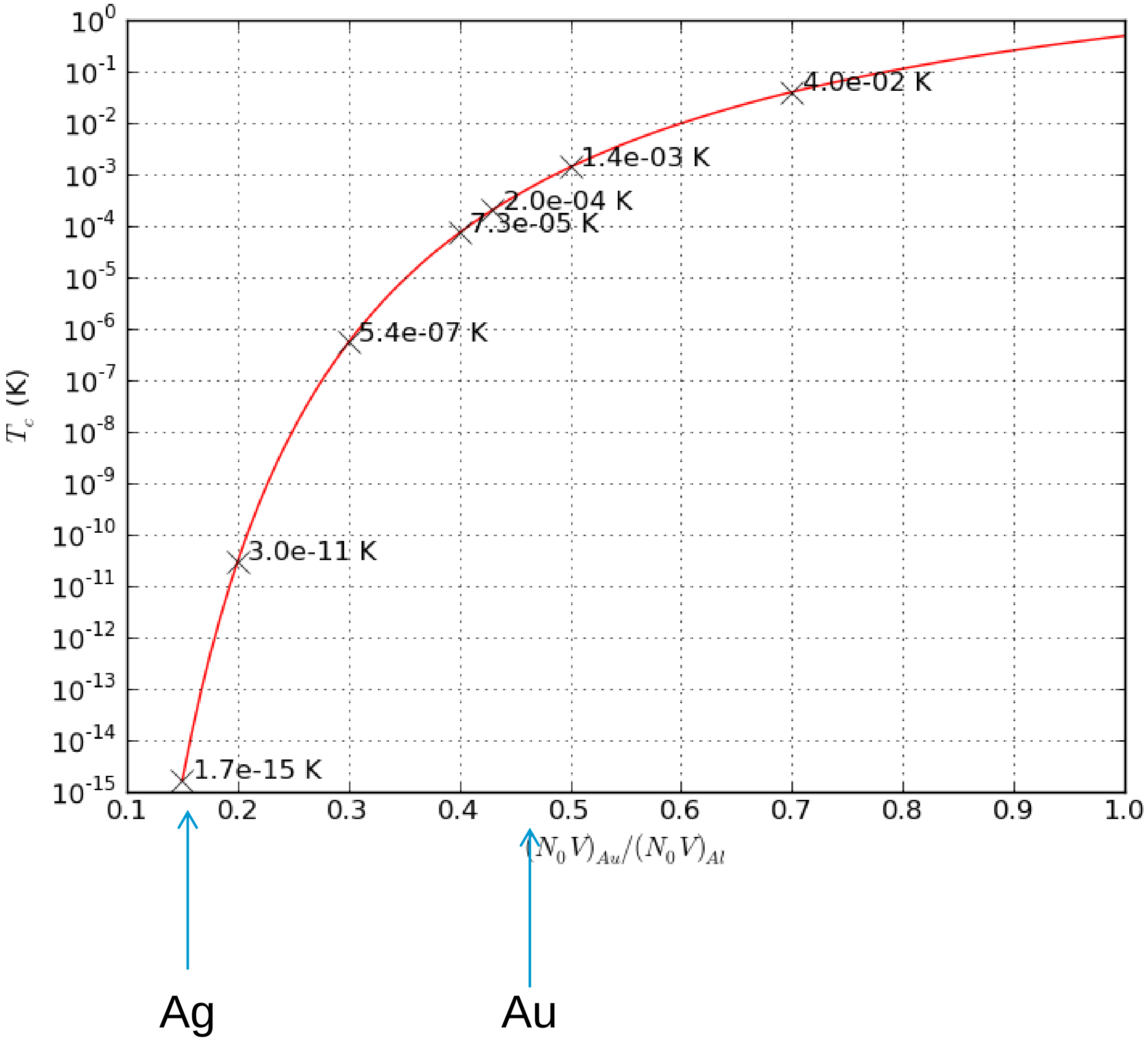
Analysis Al/Au with IP



IP = $(N_0V)_N/(N_0V)_S$

M. Wolz, C. Debuschewitz, W. Belzig, E. Scheer, PRB 84, 104516 (2011)

Intrinsic critical temperature of Au or Ag



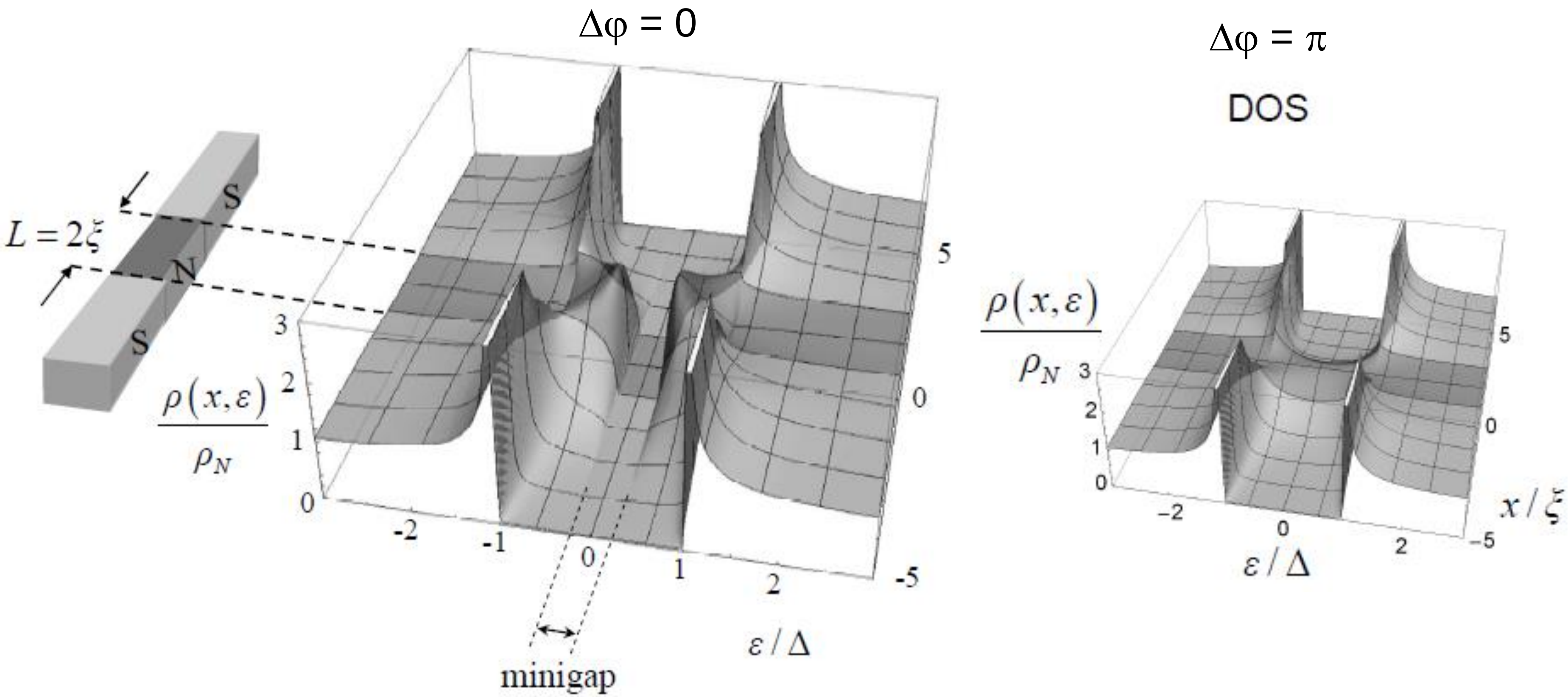
Ag: unmeasurably low T_c

Au: T_c ~ 70µK-1.4 mK expected,

No T_c observed (> 200 µK)
-> Presumably suppressed by magnetic impurities and other external influences

2.2 Phase (flux) dependence of proximity effect

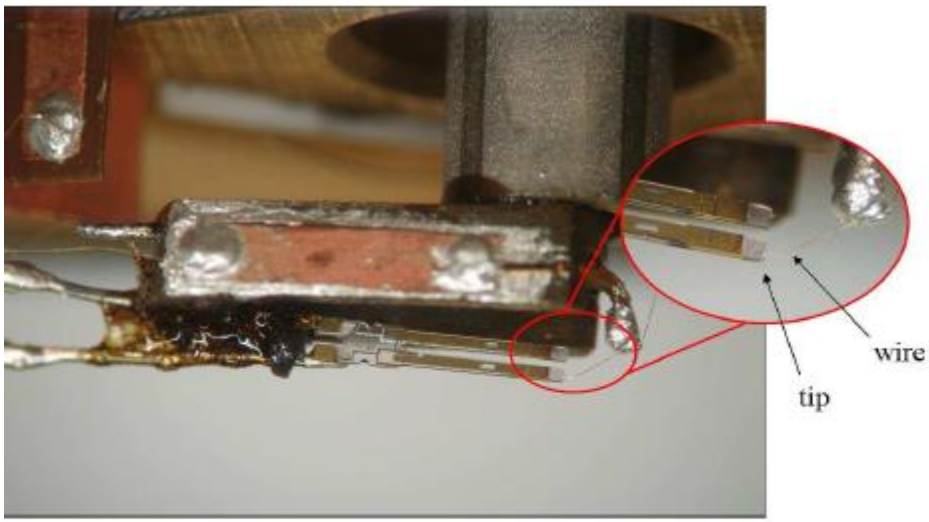
Goal: Local spectroscopy on mesoscopic hybrid structure
Challenge: Devices are placed on insulating device

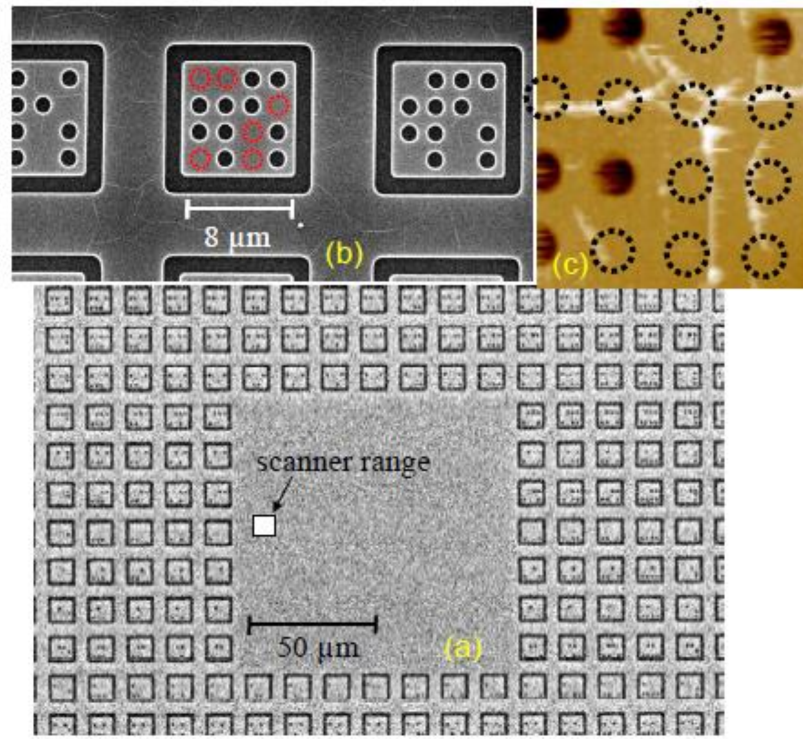


Le Sueur, PhD Thesis, Univ Paris VI, 2007

STM/AFM for spectroscopy on laterally patterned devices

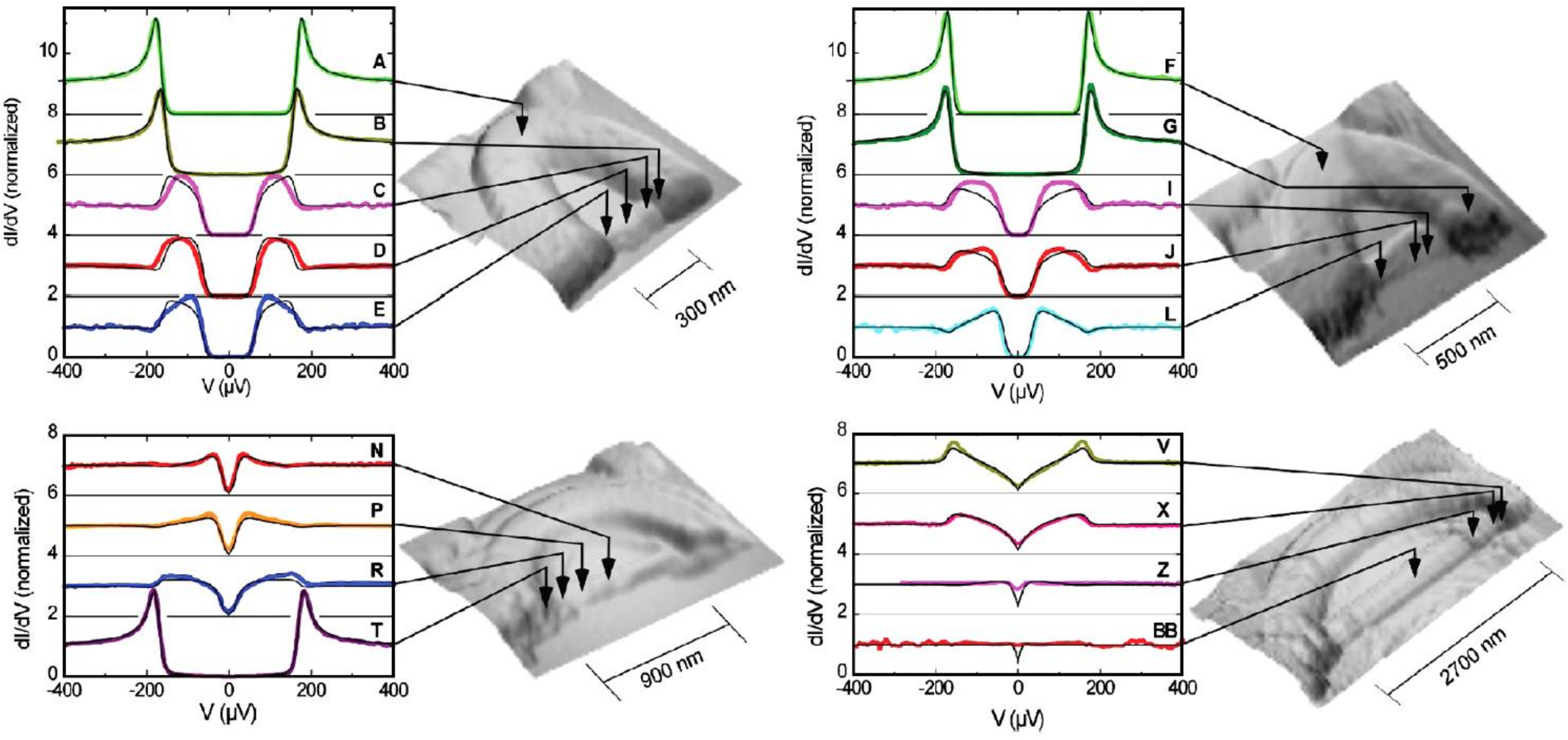
Goal: Local spectroscopy on mesoscopic hybrid structure on insulating device
-> STM on substrate not possible -> combine STM with AFM
Challenges: Localization of device with limited scan area
-> binary code map for coars approach





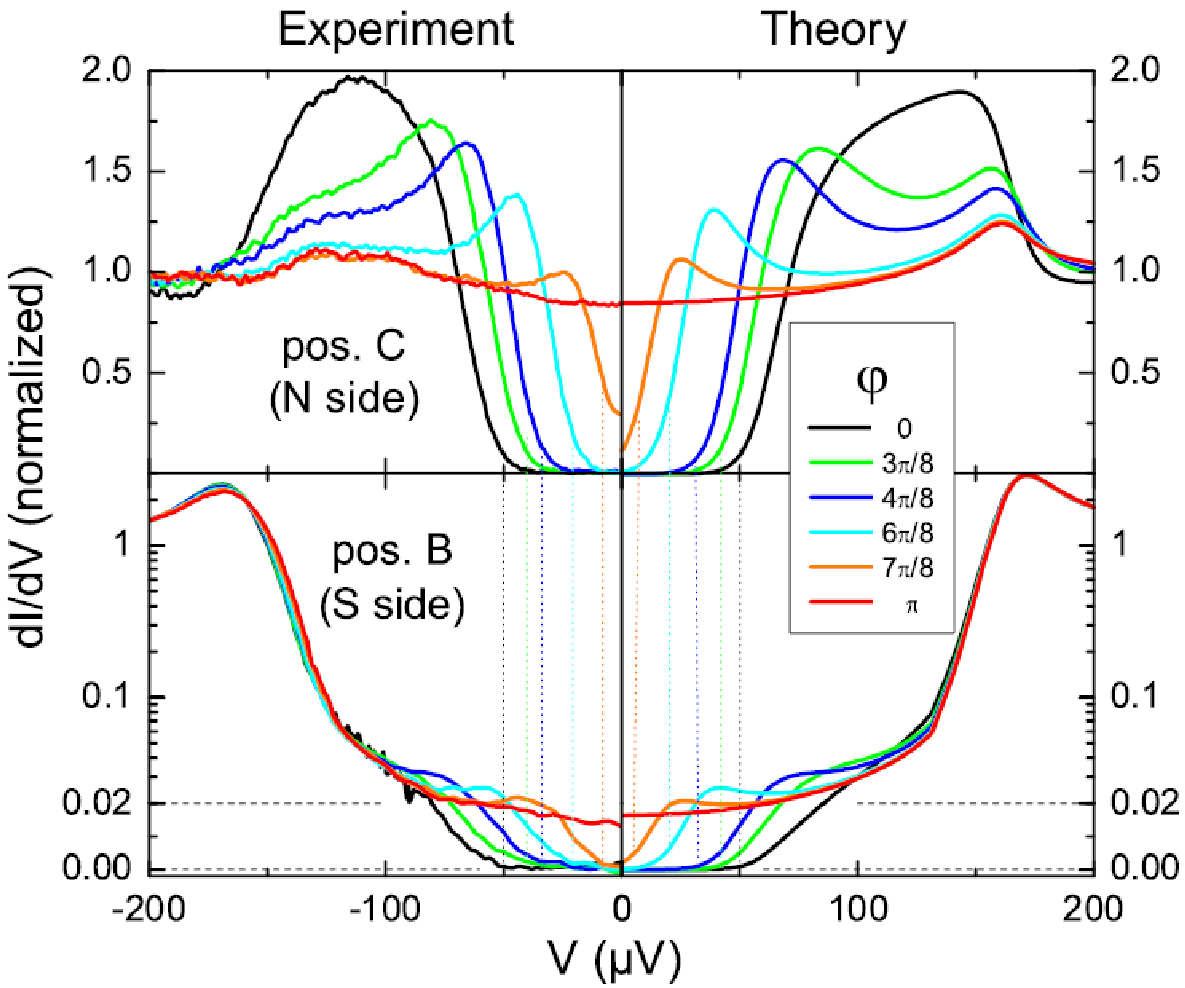
Le Sueur, PhD Thesis, Univ Paris VI, 2007

Spatial and length dependence of DOS



Le Sueur et al., Phys. Rev. Lett. 100, 197002 (2008)

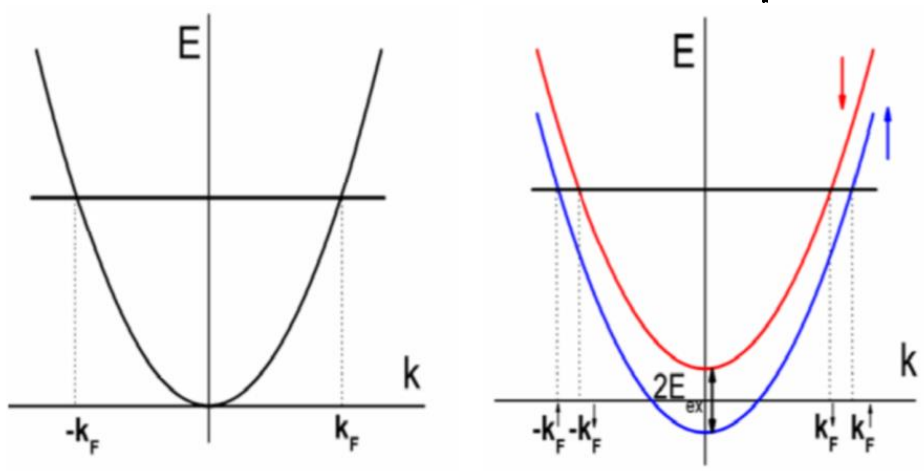
Phase dependence at both sides of the interface



Le Sueur et al., Phys. Rev. Lett. 100, 197002 (2008)

Outlook: Proximity effect with ferromagnets

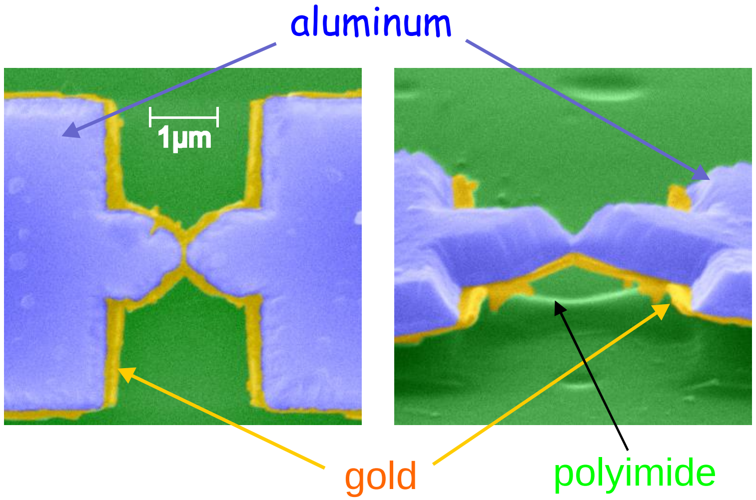
- BCS superconductivity: Cooper pairs of electrons with opposite momentum and spin bound together by electron-phonon interaction V_{ph}
- Spin-singlet Cooper pairs: $|0{,}0\rangle = \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow)$
  (odd spin function & even orbital function to fullfil Pauli's principle)
- Proximity effect with normal metal (S-N): no net V_{ph}, but "leakage" of pair amplitude into normal metal over a distance $\xi_N \approx \sqrt{\frac{\hbar D}{2\pi k_B T}}$

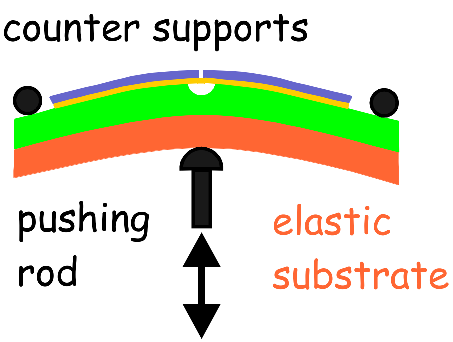


Superconductor-ferromagnet (S-F) proximity effect:
Spin splitting results in spin-dependent
k vectors -> $Q = k_\uparrow - k_\downarrow \approx 2E_{ex} / \hbar v_F$
Fast decay of spin-singlet pair amplitude ~ nm

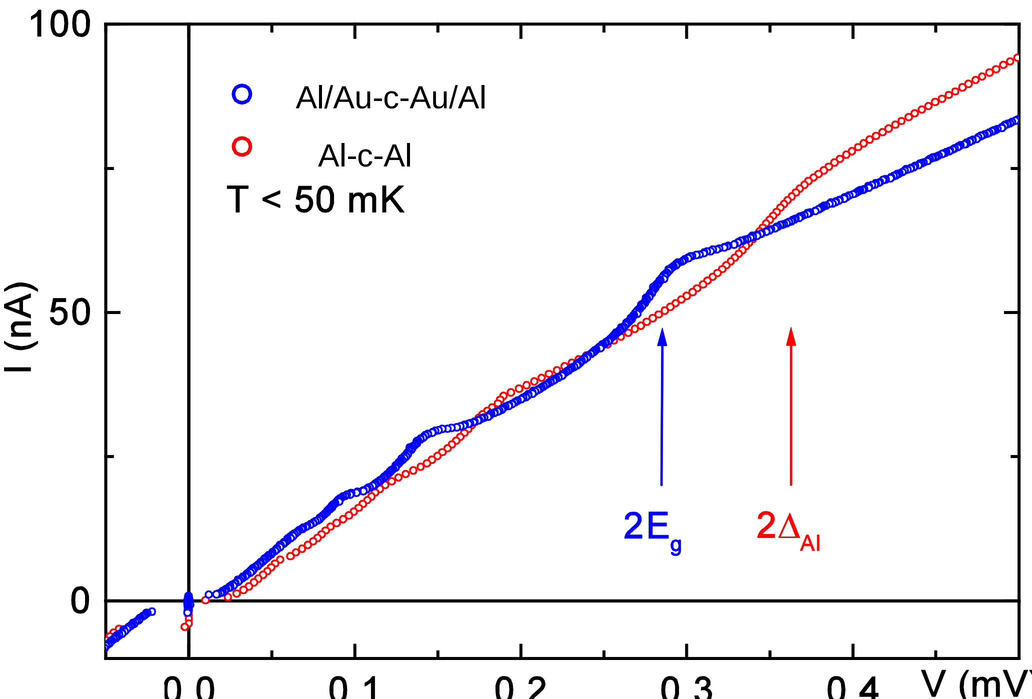
Image source: T.S. Khaire, PhD Thesis 2010

2.3 MAR / Point contacts of proximity superconductors





thickness of aluminum leads ~ 400 nm
thickness of gold layer ~ 30 nm
gap width between leads ~ 50 nm



E. Scheer, W. Belzig et al., Phys Rev Lett. 86, 284 (2001)

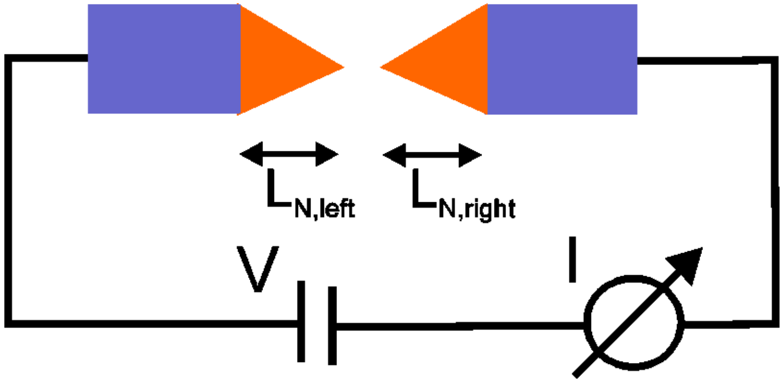
2.3 MAR in proximity superconductors

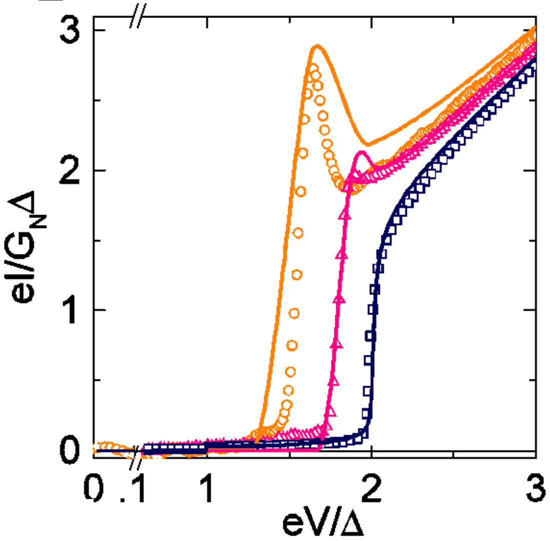
Here $d_N = L_N$

1. Extract N(E) from tunnel IVs with the assumption:

$$L_{N,left} = L_{N,right} \quad => \quad N(E)_{left} = N(E)_{right} = N(E)$$

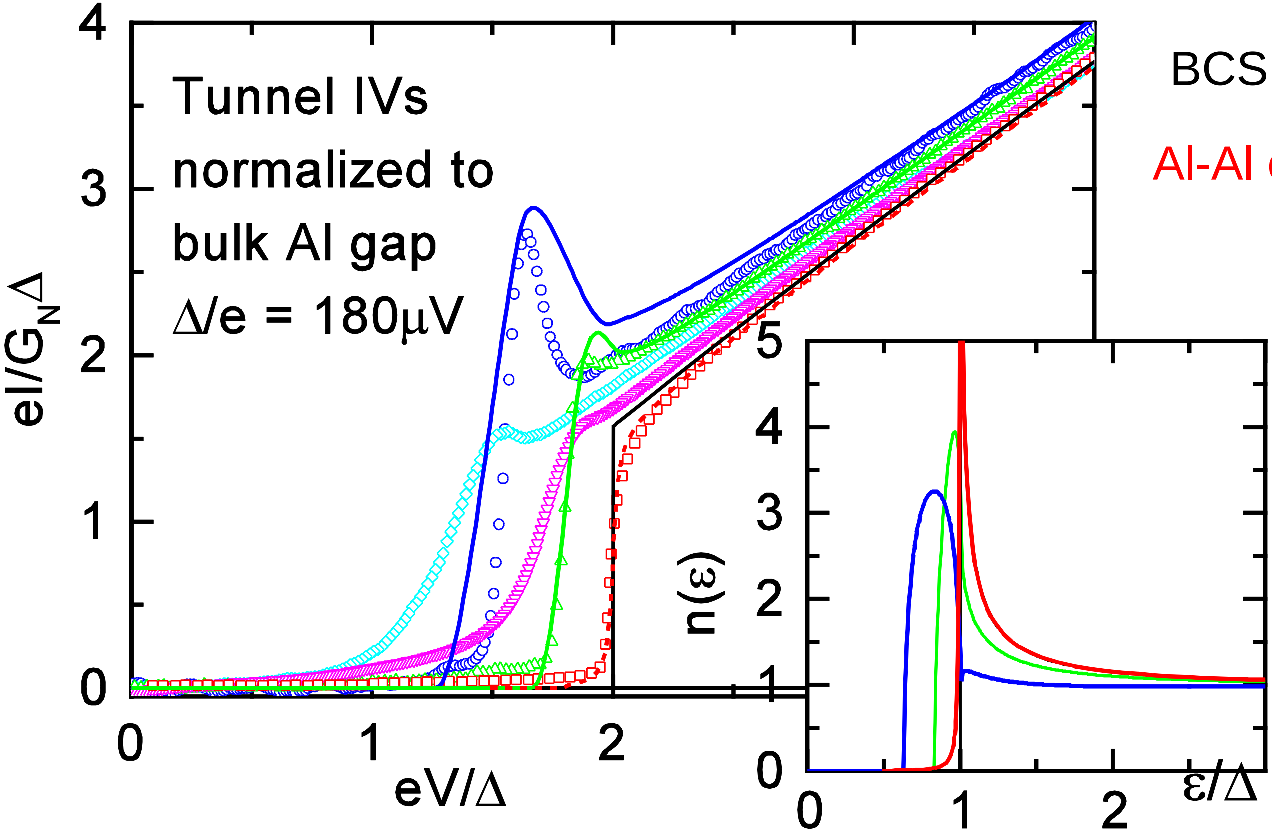
$$I \propto \int N(E)N(E-eV)[f(E-eV)-f(E)]\, dE$$





Al-Al contact, T = 30 mK

2.3 Point contacts of proximity superconductors



BCS , T = 0

Al-Al contact, T = 30 mK

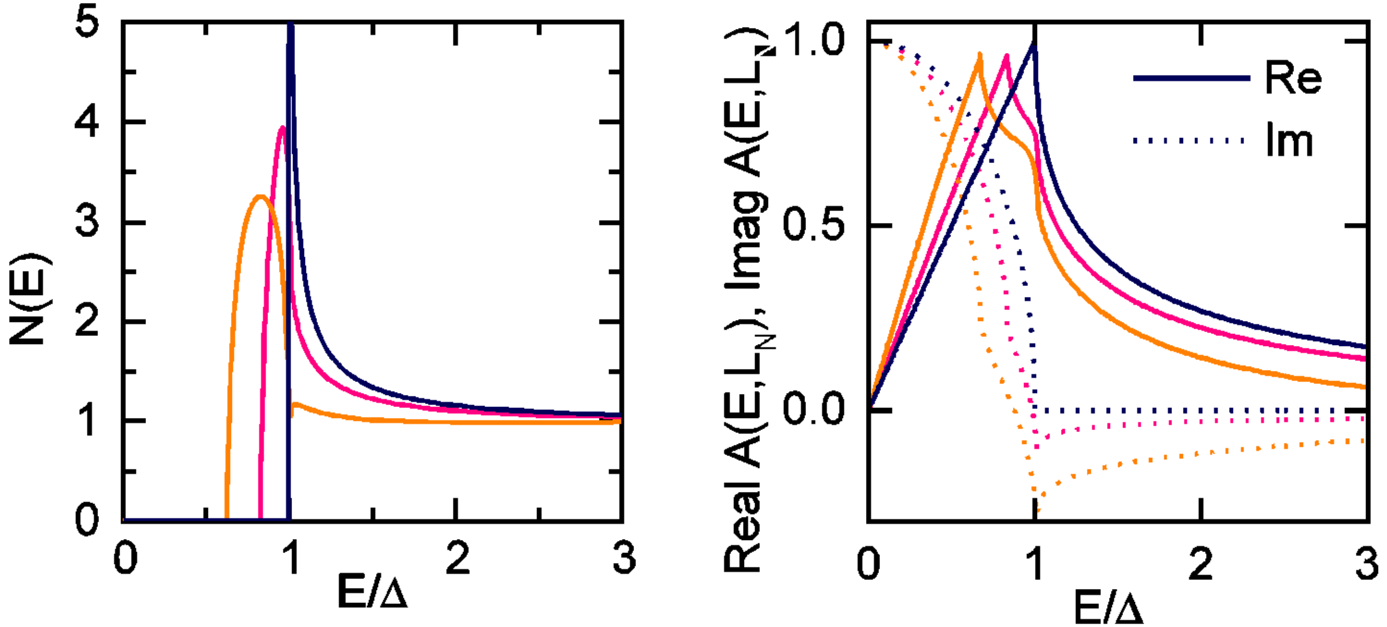
Blue, green, magenta cyano for different L_n and interface parameter γ

Remarkable observation:

d*I*/d*V* shows “overshoot“ although DOS is rounded

2.3 MAR in proximity superconductors

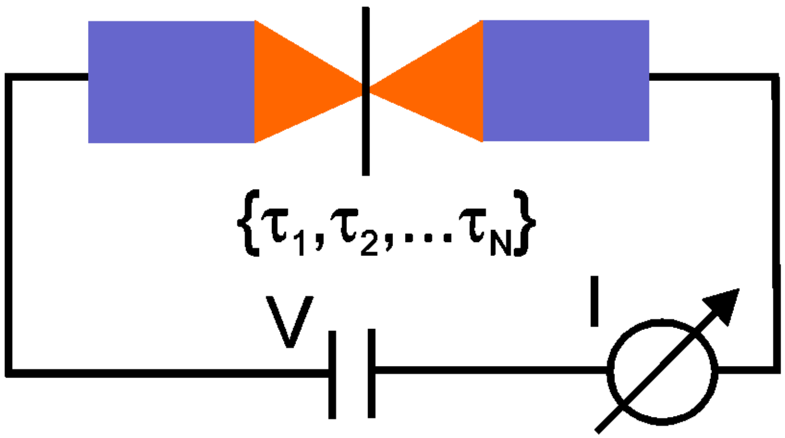
2. Compute $A(E,L_N)$ with PE model

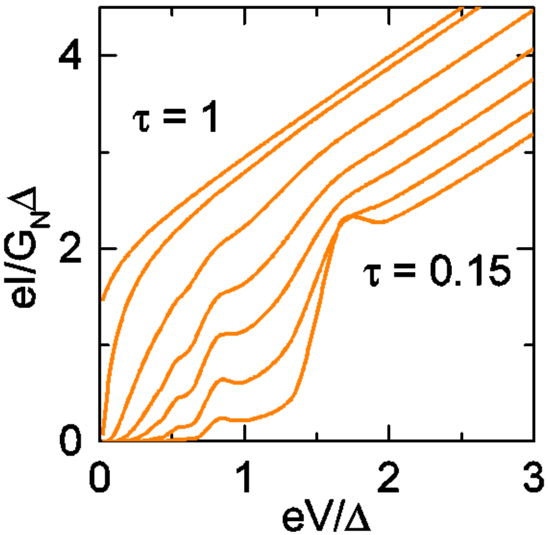


$A\ (E,L_N)$: Andreev reflection amplitude

2.3 MAR in proximity superconductors

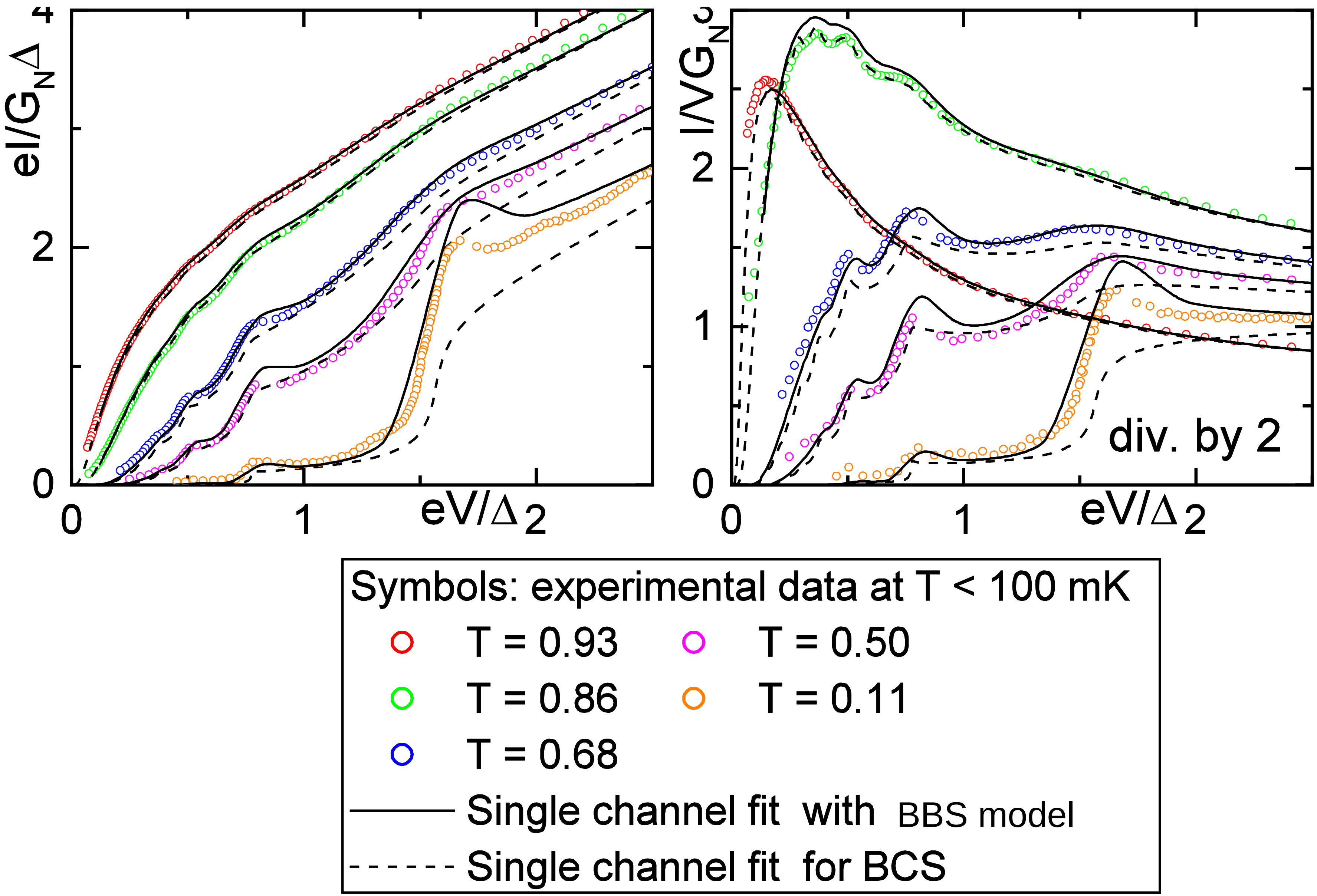
3. Compute IVs for arbitrary transmission with $A(E,L_N)$



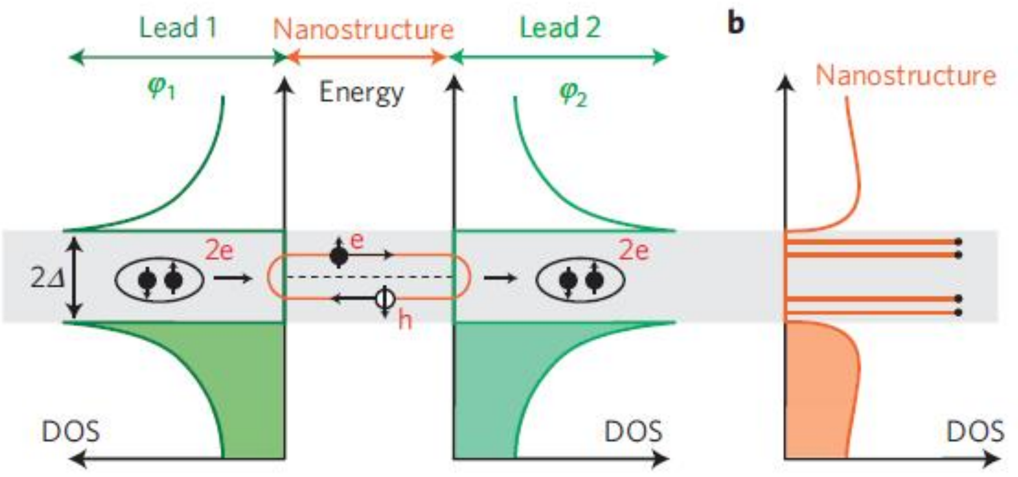


Assumption: $A(E,L_N)$ is not affected by the coupling

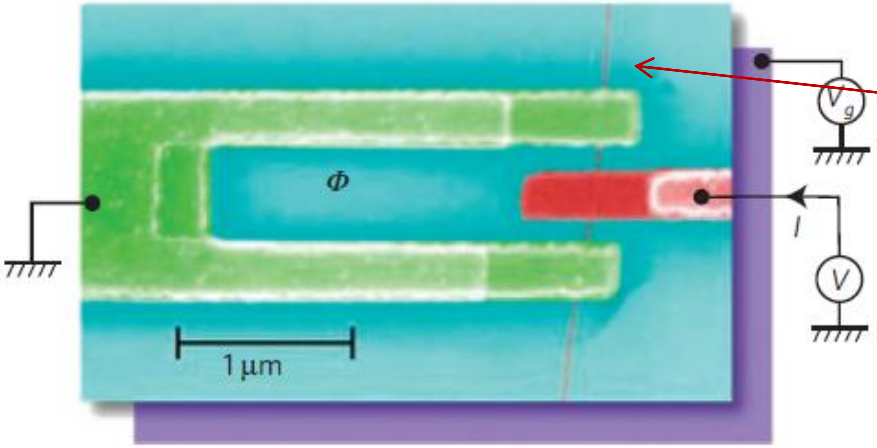
2.3 MAR in single-atom Al/Au-c-Au/Al



Outlook: Andreev Bound States (ABS)



ABS

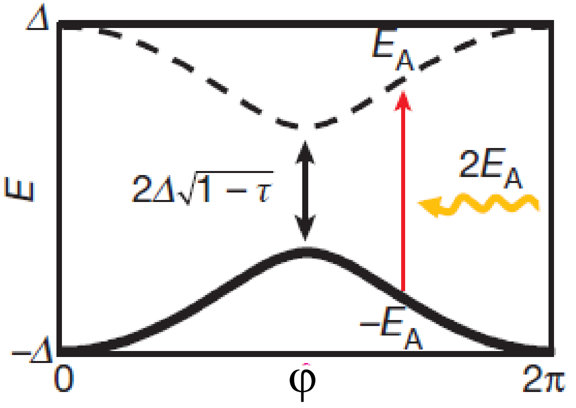


Carbon Nanotube (CNT)

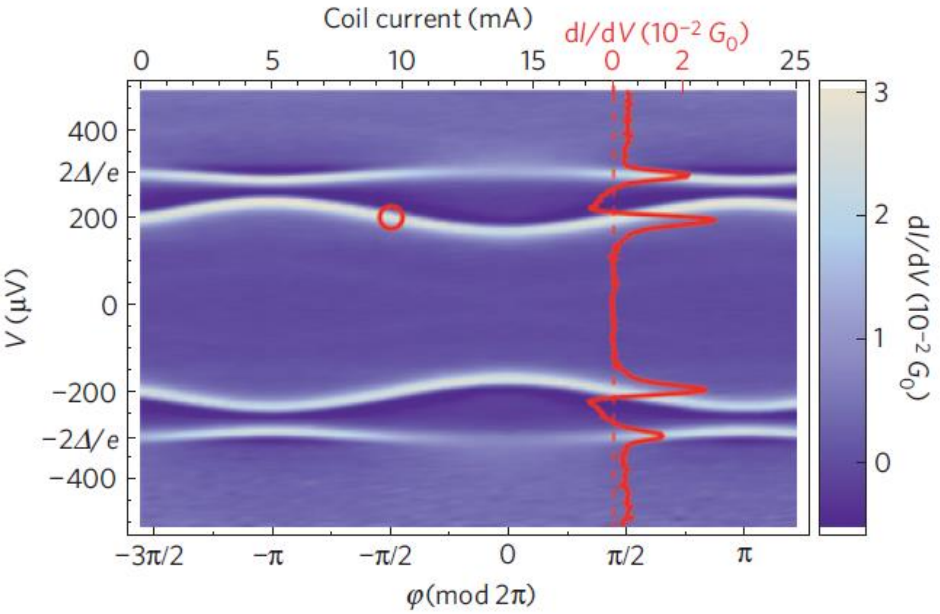
SC tunnel contact (Al)
to probe local DOS

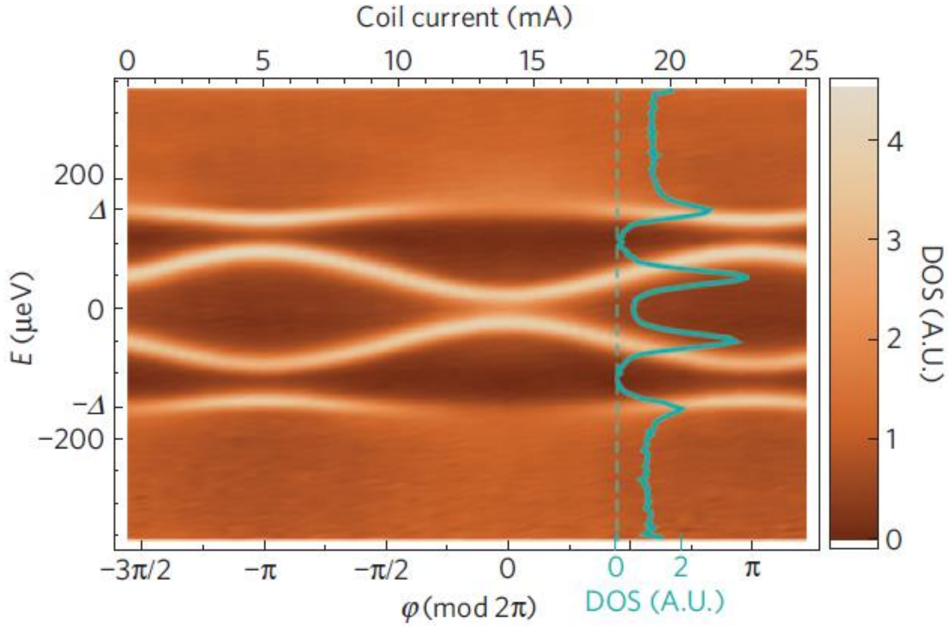
Pillet et al, Nature Physics 6, 965 (2010)

[Outlook:]() Spectroscopy of Andreev Bound States



Differential tunnel conductance



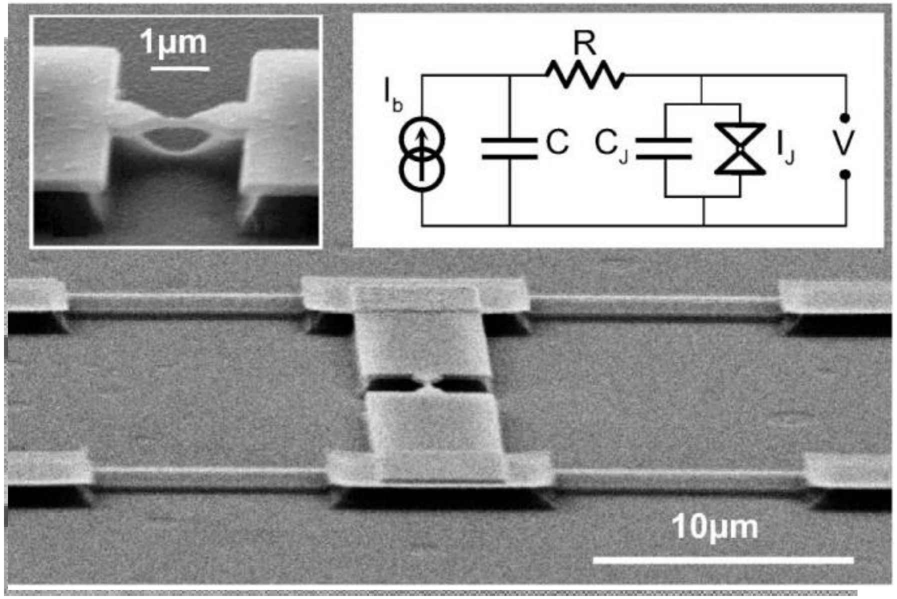


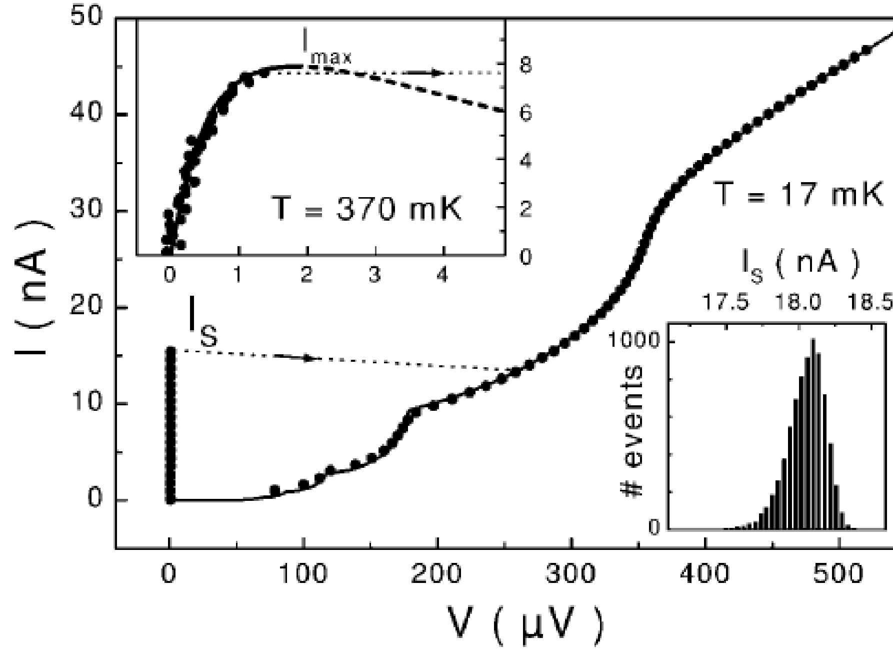
DOS in CNT (by deconvolution assuming BCS DOS in probe)

Pillet et al, Nature Physics 6, 965 (2010)

Outlook: Josephson effect by ABS

M.F. Goffman et al., PRL 85, 170 (2000)





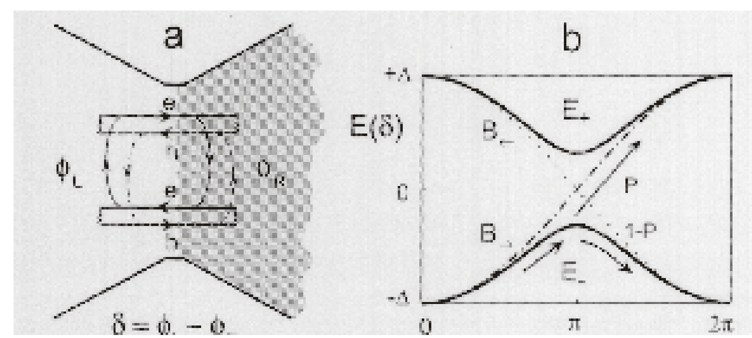
Current phase relation: $I_J(\delta,\{\tau_i\}),\{n_{i\pm}\}) = \sum_{i=1}^{N} (n_{i-} - n_{i+}) \cdot I_-(\delta,\tau_i)$

with $I_\pm(\delta,\tau) = \varphi_0^{-1} dE_\pm(\delta,\tau) / d\delta$

where $\delta = \Phi_L - \Phi_R$ and $\varphi_0 = \hbar / 2e$

$n_\pm$: occupation number of Andreev bound states

Supercurrent: $I_0(\{\tau_i\}) = \max_\delta [I_J(\delta,\{\tau_i\}, n_{i+} = 0, n_{i-} = 1)]$



Summary

- Andreev reflection is the mechansim converting Cooper pairs into quasiparticles and vice versa
- Proximity effect = Andreev reflection + phase coherence
- Many length scales /energy scales involved
- Experiments: Point contact spectroscopy / tunnel spectroscopy
- Andreev Bound States (ABS): carry supercurrent (Josephson effect)