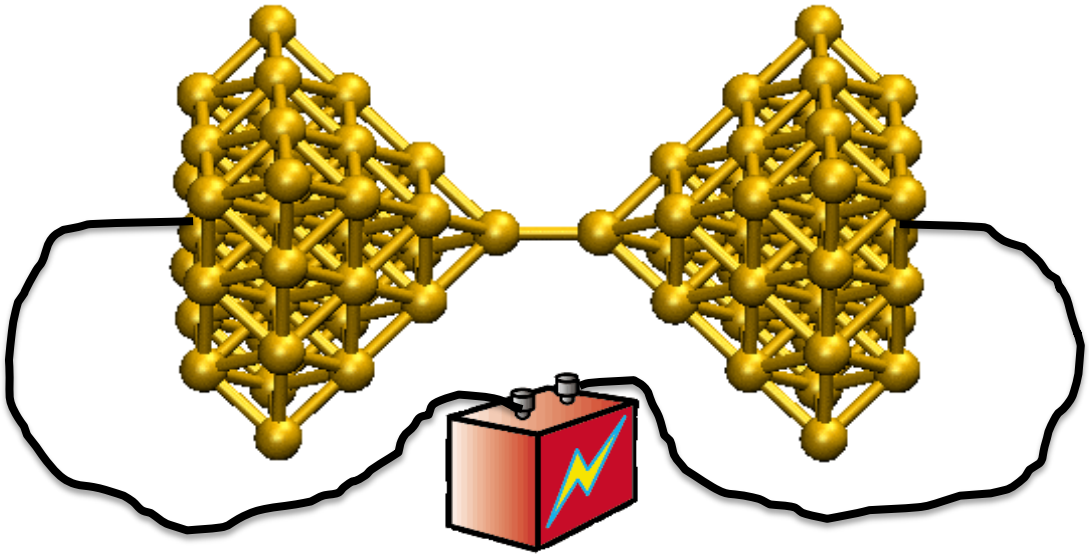
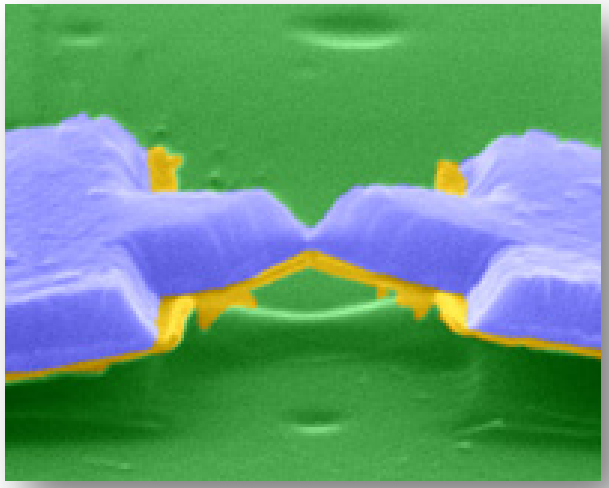
Chapter 7
I. The conductance of a single atom



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

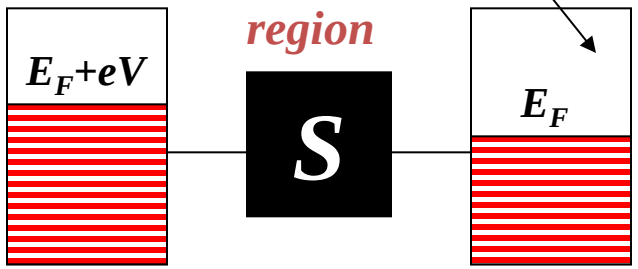
7.1.1 Landauer approach to conductance

real system



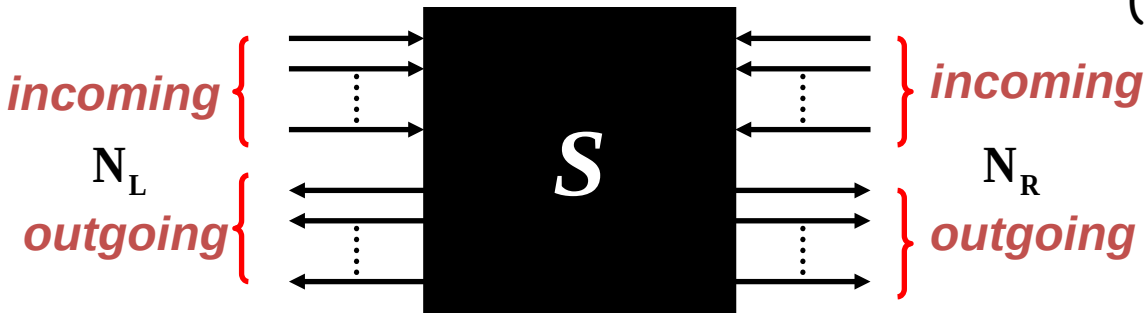
electron reservoirs

scattering region



Landauer formula

(low-temperature conductance)



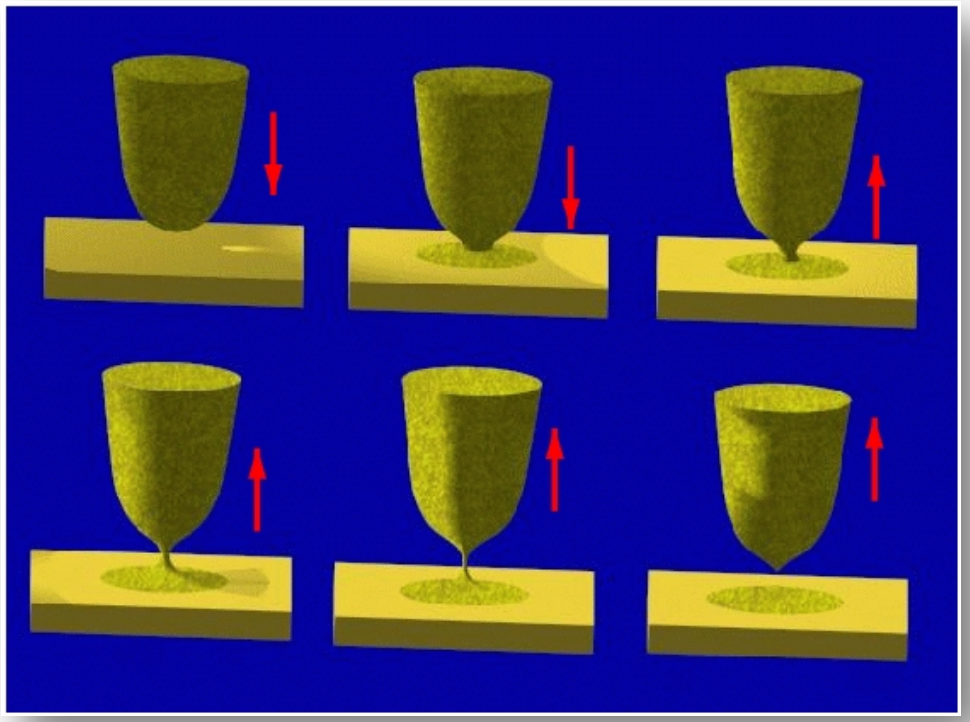
$$G = \frac{2e^2}{h} T(E_F) = G_0 \sum_n T_n$$

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

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

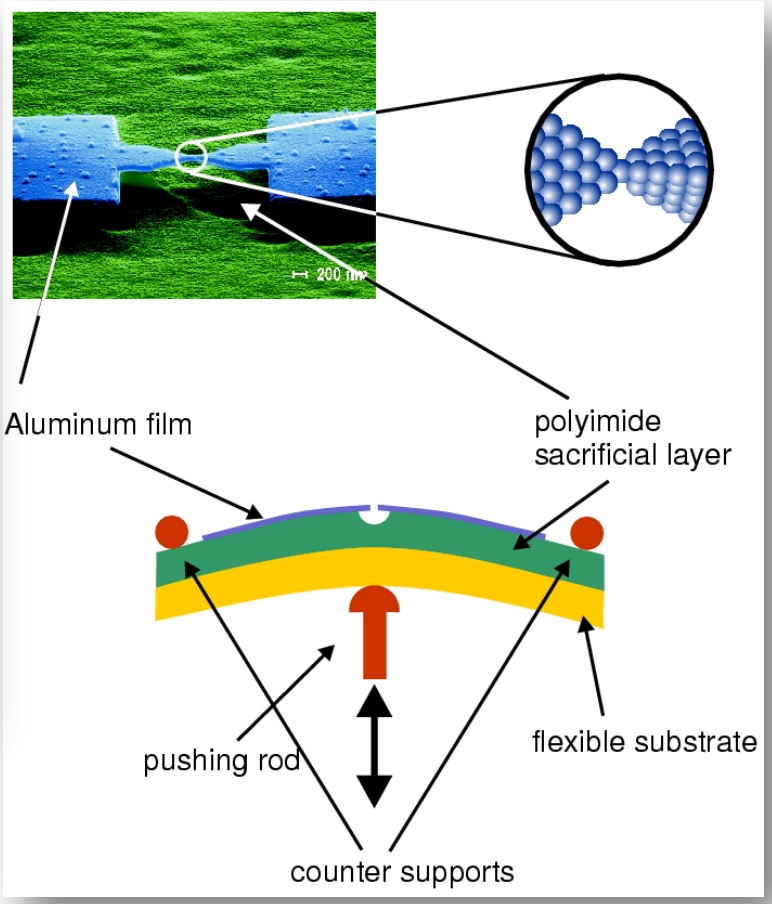
7.1.2 Conductance of atomic-scale contacts

1. Scanning tunneling microscope (STM)



Binning & Rohrer (1982)
Gimzewski & Möller (1987)
Agraït et al. (1992)
.....

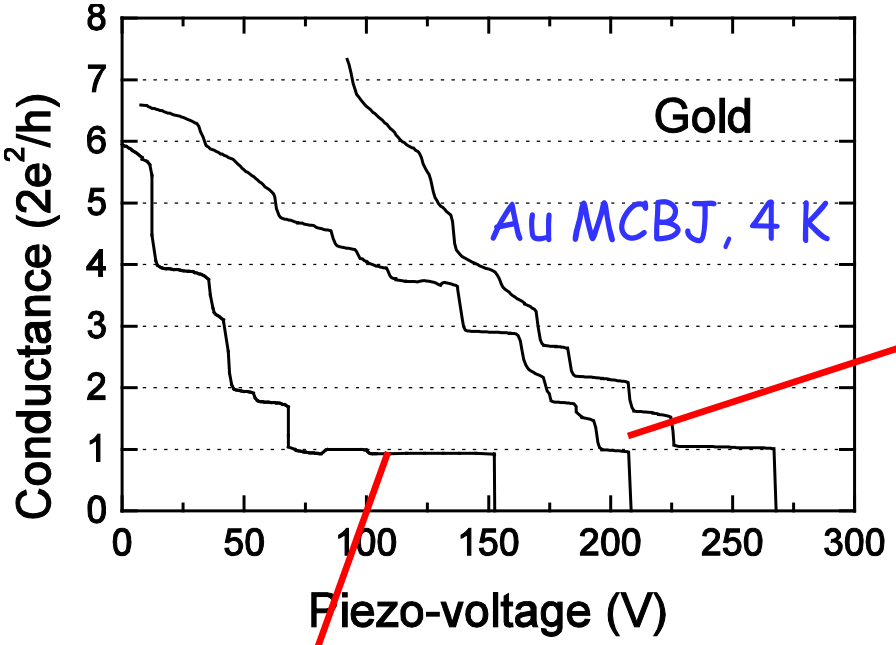
2. Break junctions (MCBJ)



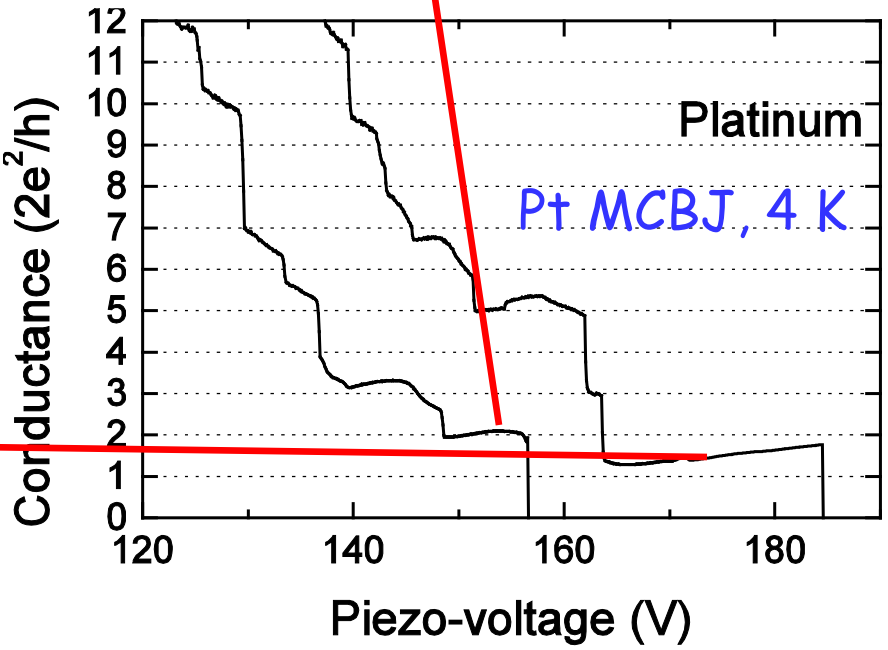
J.M. van Ruitenbeek et al. (1992,1996)

7.1.2 Conductance of atomic-scale contacts

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

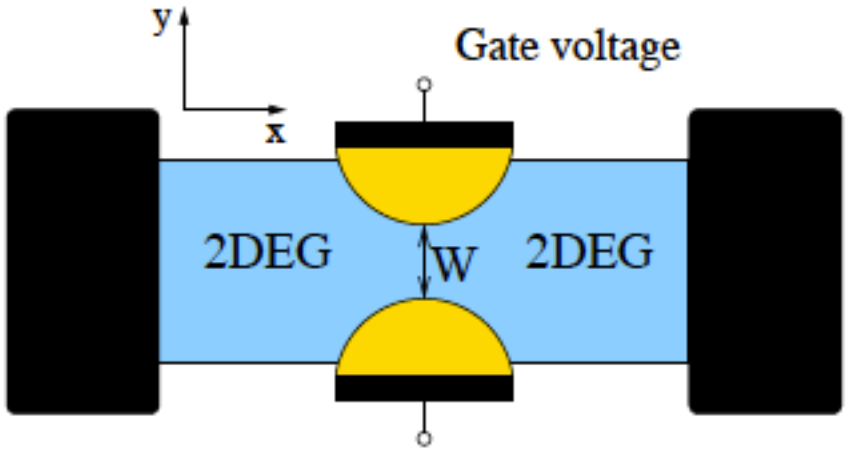


Single-atom contacts



Atomic chains

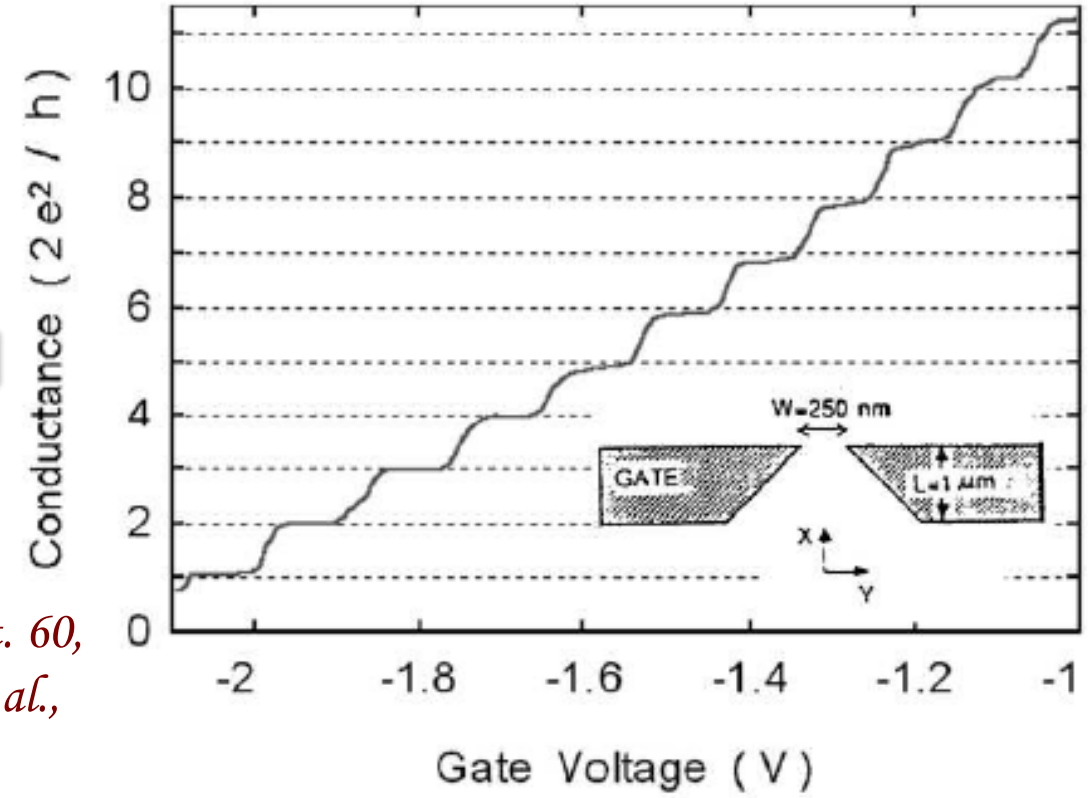
7.1.2 Conductance of atomic-scale contacts



Reminder: Conductance quantization in 2DEG point contacts

Point contact defined in a 2D electron gas by means of a split gate on top of a semiconductor heterostructure.

Point contact conductance as a function of gate voltage at 0.6 K. The constriction width increases with increasing voltage on the gate (see inset).

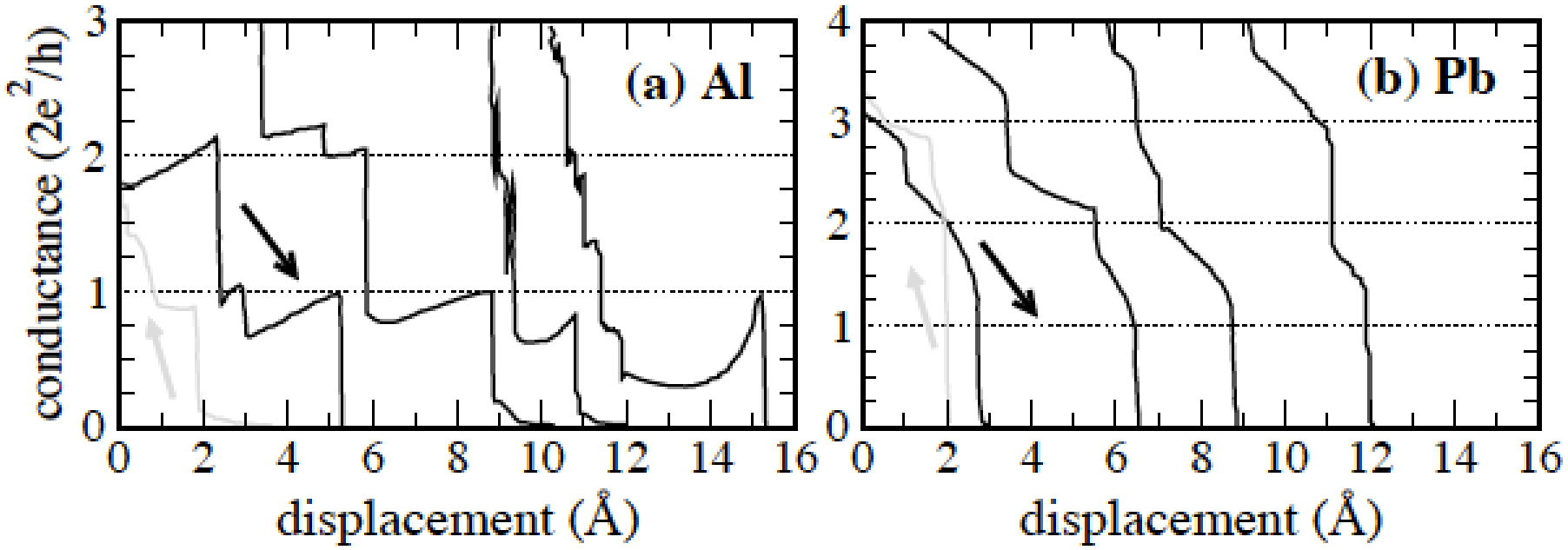


B.J. Van Wees et al., Phys. Rev. Lett. 60, 848 (1988); see also D.A. Wharam et al., J. Phys. C 21, L209 (1988).

7.1.2 Conductance of atomic-scale contacts

*J.C. Cuevas, A. Levy Yeyati, A. Martin-Rodero, G. Rubio-Bollinger, C. Untiedt, N. Agraït, Phys. Rev. Lett. **81**, 2990 (1998)*

STM experiments (4.2 K for Al and 1.5 K for Pb)



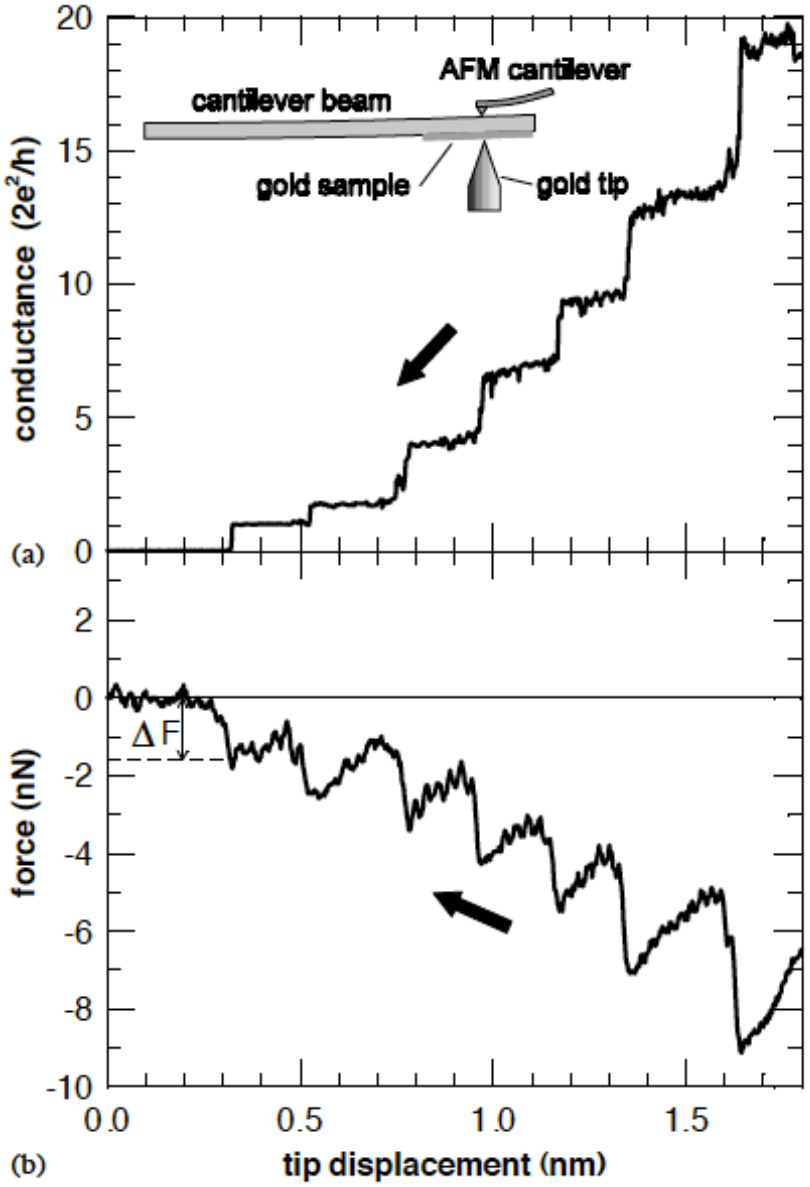
- The conductance traces differ significantly from metal to metal and, in the case of multivalent metals, there are no plateaus at multiples of the conductance quantum.

- Notice that the traces depend also on whether the contact is being opened or closed.

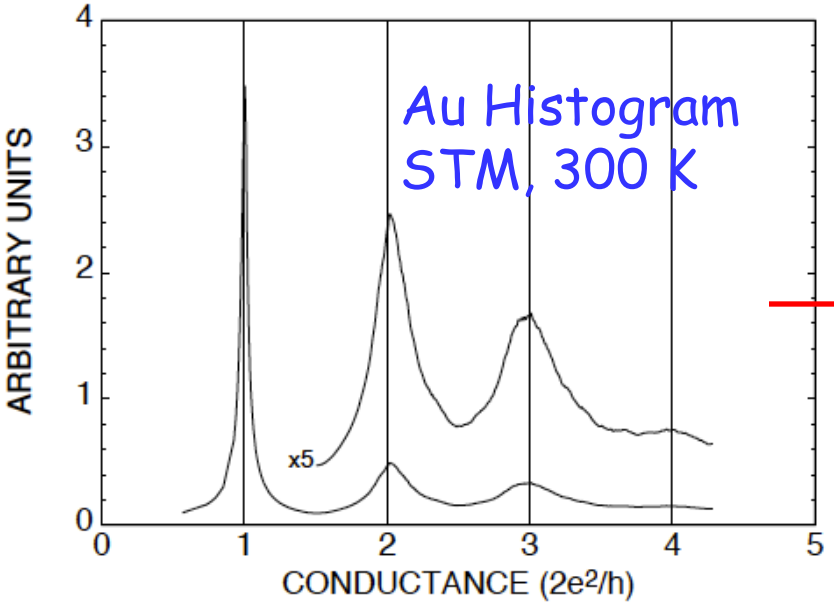
7.1.2 Conductance of atomic-scale contacts

G. Rubio, N. Agraït, S. Viera,
Phys. Rev. Lett. ***76****, 2302 (1996)*

- Simultaneous measurement of the conductance and force in a Au contact at room temperature.
- Notice the stress accumulation on the plateaus and the coincidence of the stress relief events with the jumps in the conductance.
- **Conclusion:** The conductance jumps correspond to sudden atomic rearrangements in which some atomic bonds are broken and the cross section of the contact varies in an abrupt manner.



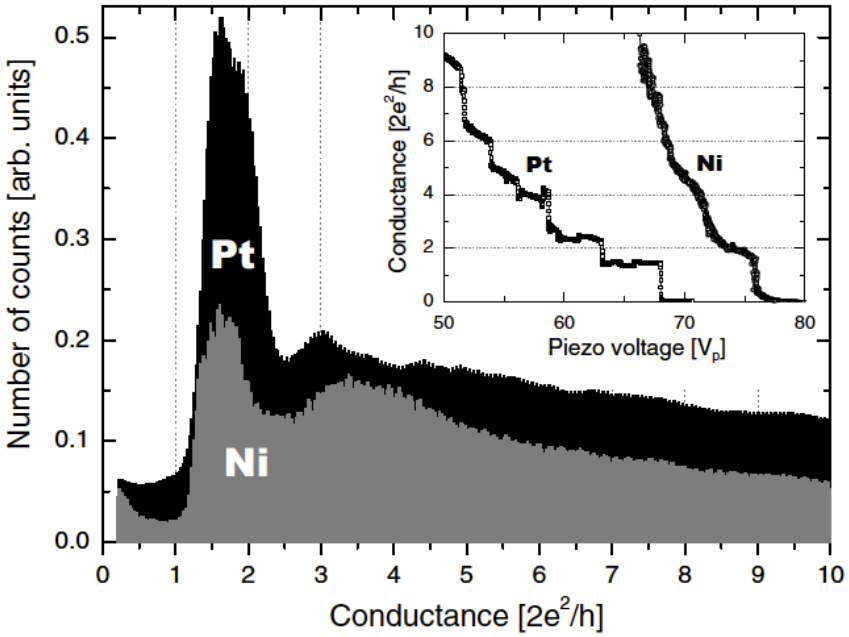
7.1.3 Conductance histograms



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

Conductance quantization?

Pt and Ni Histograms
MCBJ, 4.2 K

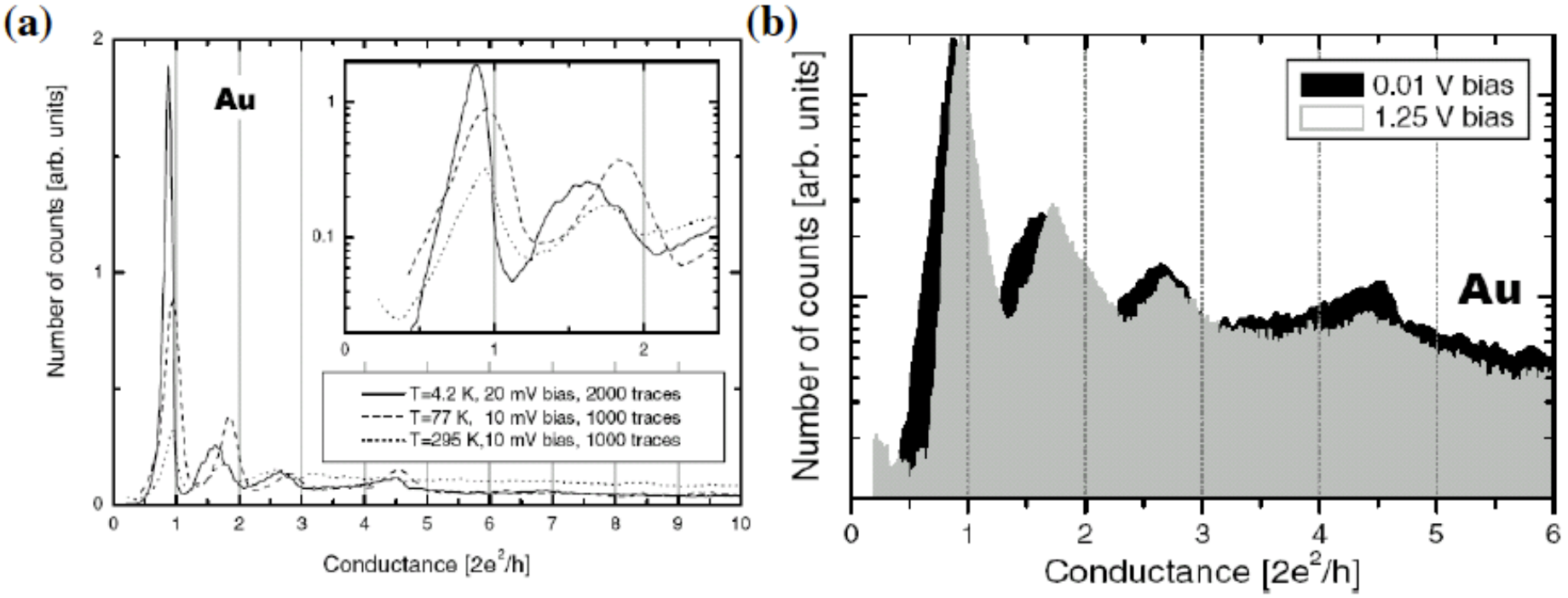


Not always!

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

7.1.3 Conductance histograms

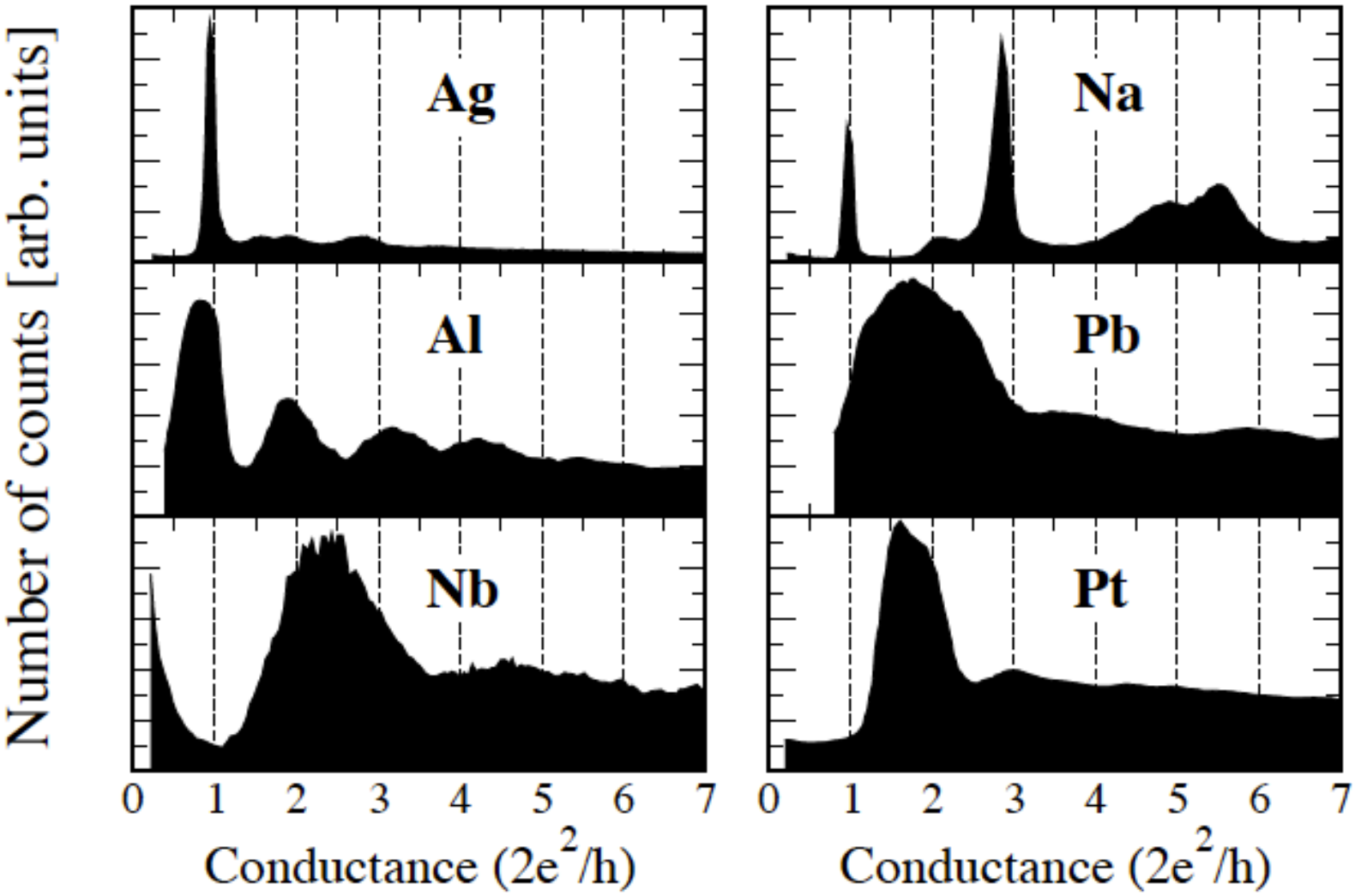
The conductance histograms are in general sensitive to experimental conditions such as temperature, voltage, breaking speed, environmental conditions, etc.



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

7.1.3 Conductance histograms

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



7.1.3 Conductance histograms

Summary of the findings regarding the conductance histograms:

- With exception of alkali metals, the highest peak is always lying at the lowest frequently occurring conductance value.

- The position of this peak for all the elements falls in the range between 0.7 and 2.3G_0. There is no structure related to metallic conductance in the histograms below the position of the first peak.

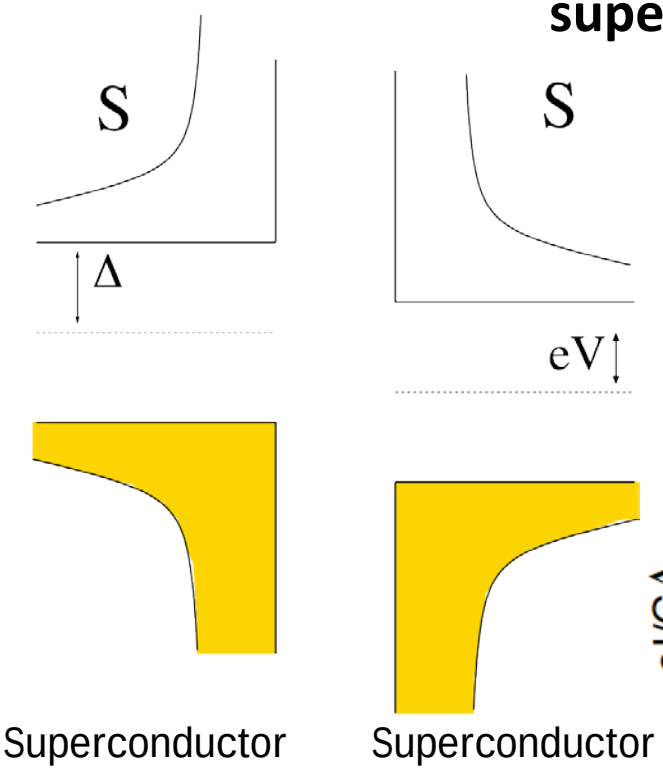
- For free electron-like alkali metals the first peak is extremely sharp and is located almost exactly at 1G_0. This statement also extends to the noble metals.

- For divalent metals (zinc, magnesium) and trivalent ones (aluminum) the first peak is rather sharp and located slightly below 1G_0. Other multivalent metals, and in particular transition metals, exhibit a broad first peak located well above 1G_0 and in some cases like niobium it lies even above 2G_0.

7.1.4 Determining the conduction channels

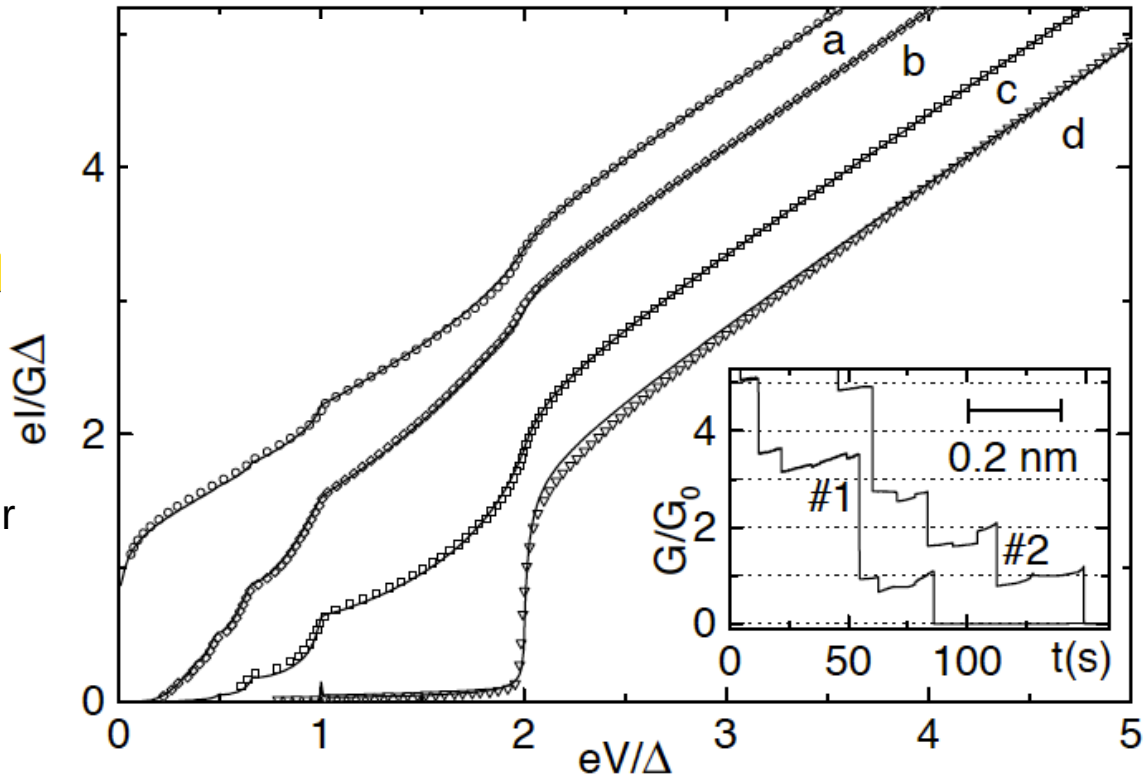
E. Scheer, P. Joyez, D. Esteve, C. Urbina, M.H. Devoret, Phys. Rev. Lett. ***78****, 3535 (1997)*

One can determine experimentally the transmission coefficients in superconducting materials.



V = voltage
Δ = energy gap

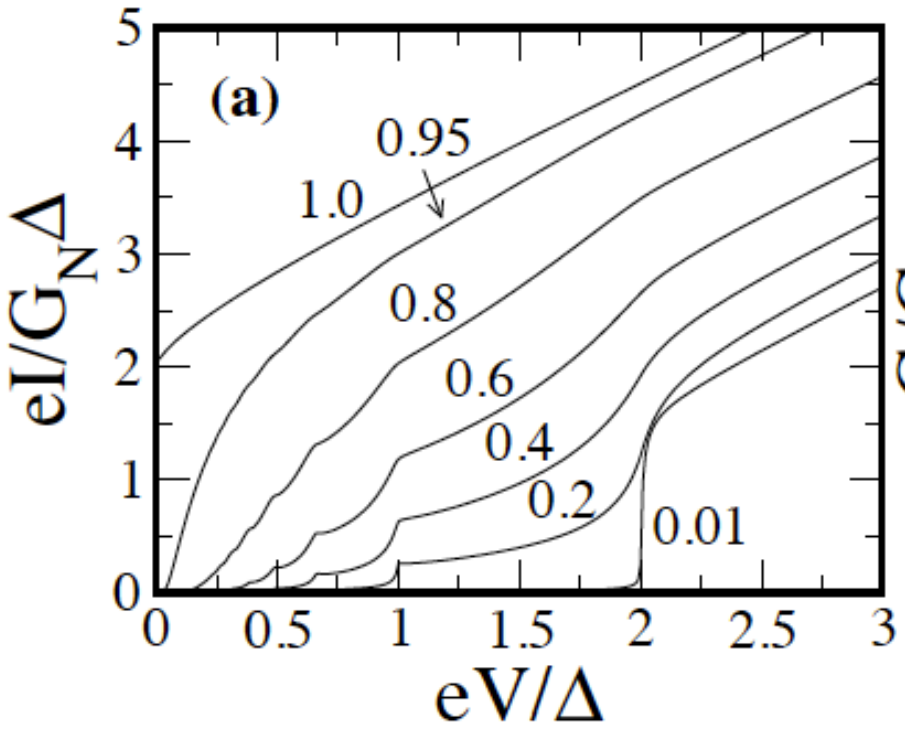
Break junctions: Al single-atom contacts (30 mK)



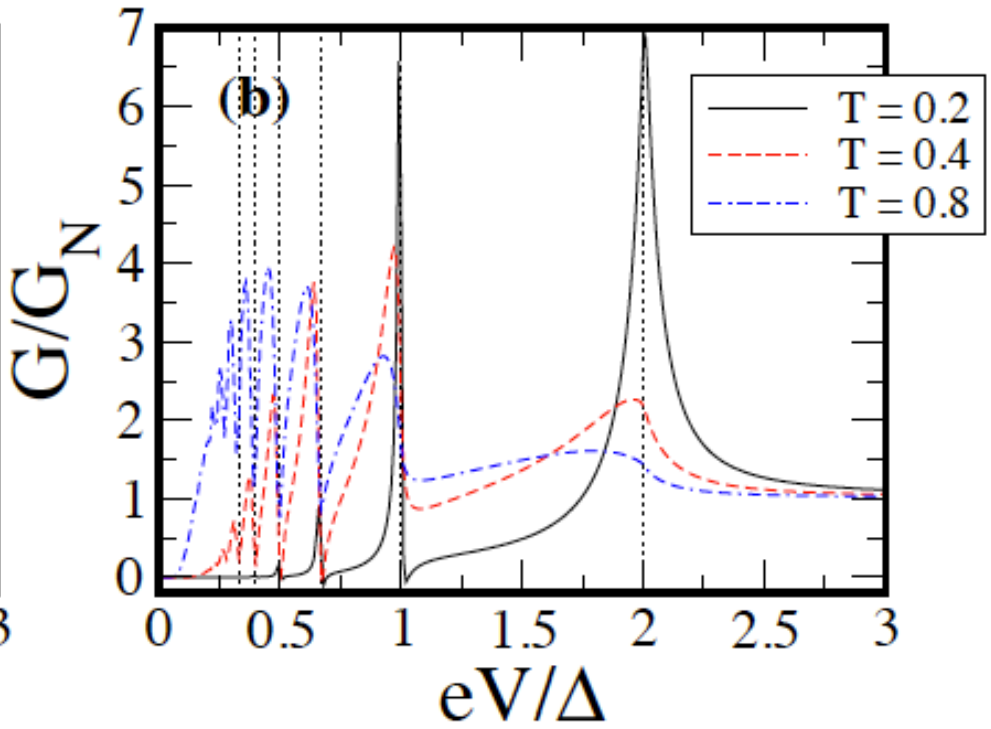
7.1.4 Determining the conduction channels

Theoretical results for the I-V curves of a single-channel superconducting quantum point contact.

I-V curves (zero temperature)



Differentical conductance vs. voltage

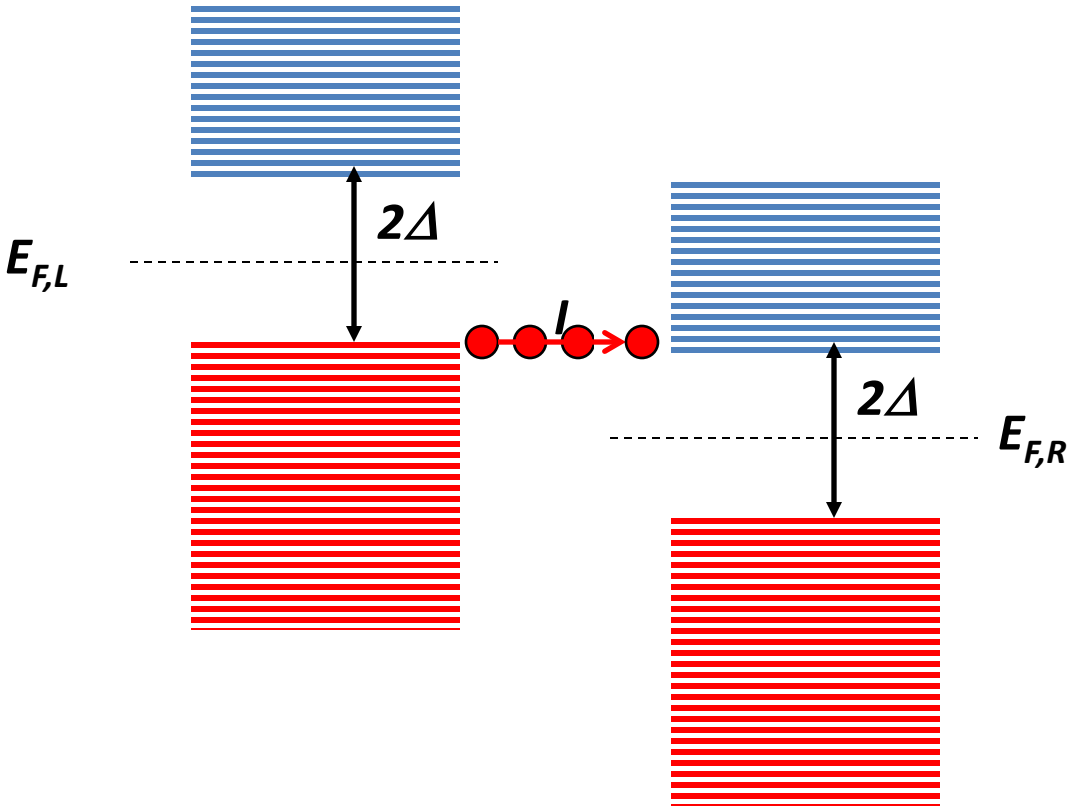


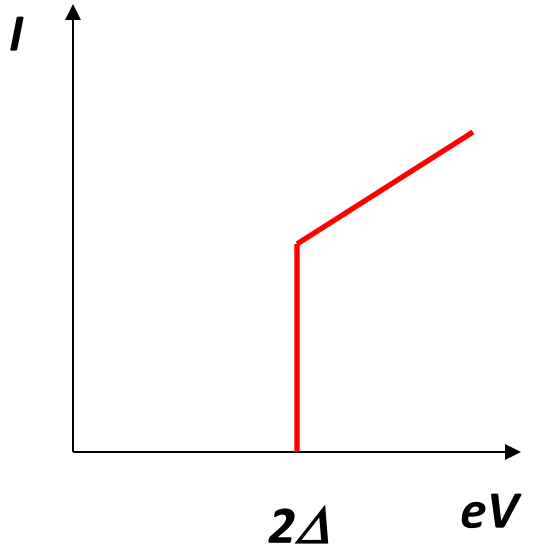
*J.C. Cuevas, A. Martín-Rodero and A. Levy Yeyati, PRB **54**, 7366 (1996).*

The same results with different methods: Averin & Bardas (95), Shumeiko et al. (97).

7.1.4 Determining the conduction channels

Transport between superconducting electrodes:
tunnel regime → single-particle processes





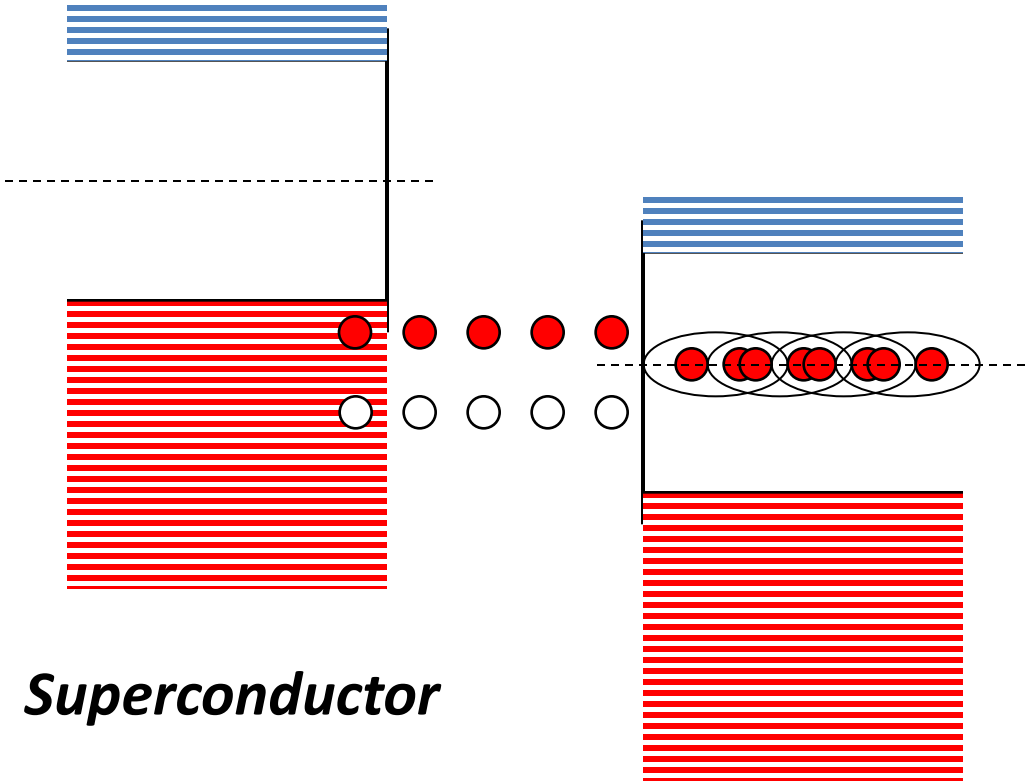
$E_{F,L} - E_{F,R} = eV > 2\Delta$

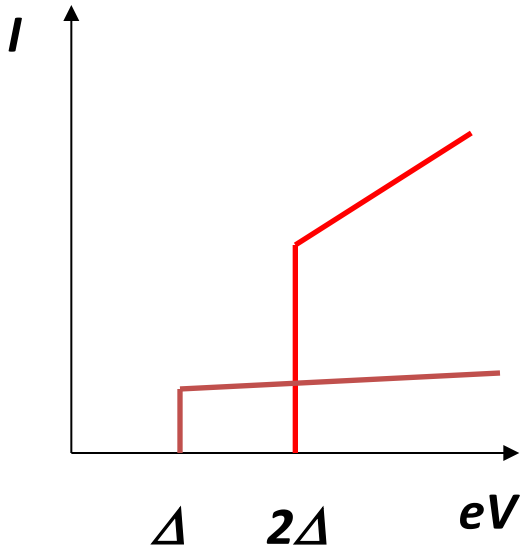
Probability: T

Charge transfer: $1e$

7.1.4 Determining the conduction channels

Andreev reflection: a two-particle tunneling process





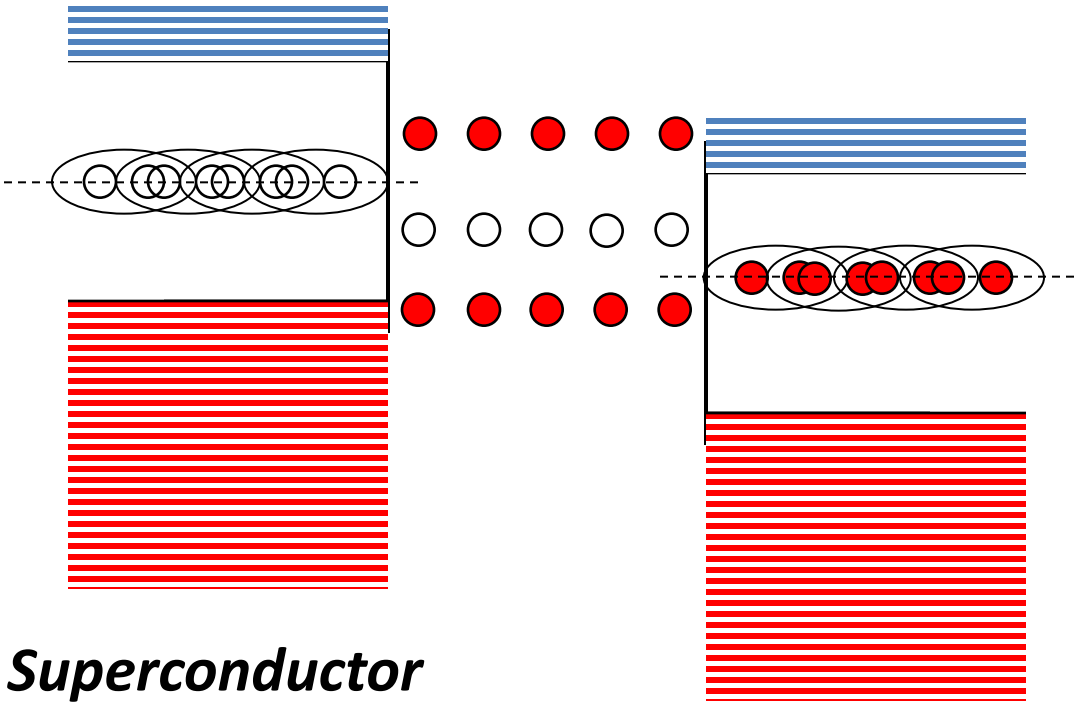
$eV>\Delta$

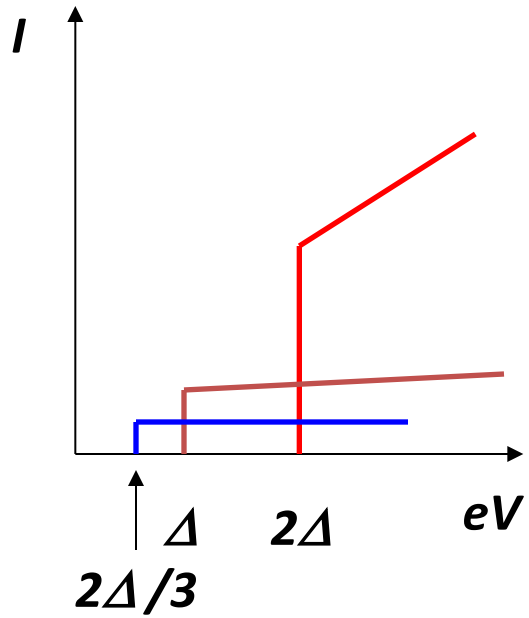
Probability: T^2

Charge transfer: $2e$

7.1.4 Determining the conduction channels

Multiple Andreev reflection: a multi-particle tunneling process





$eV > 2\Delta/3$

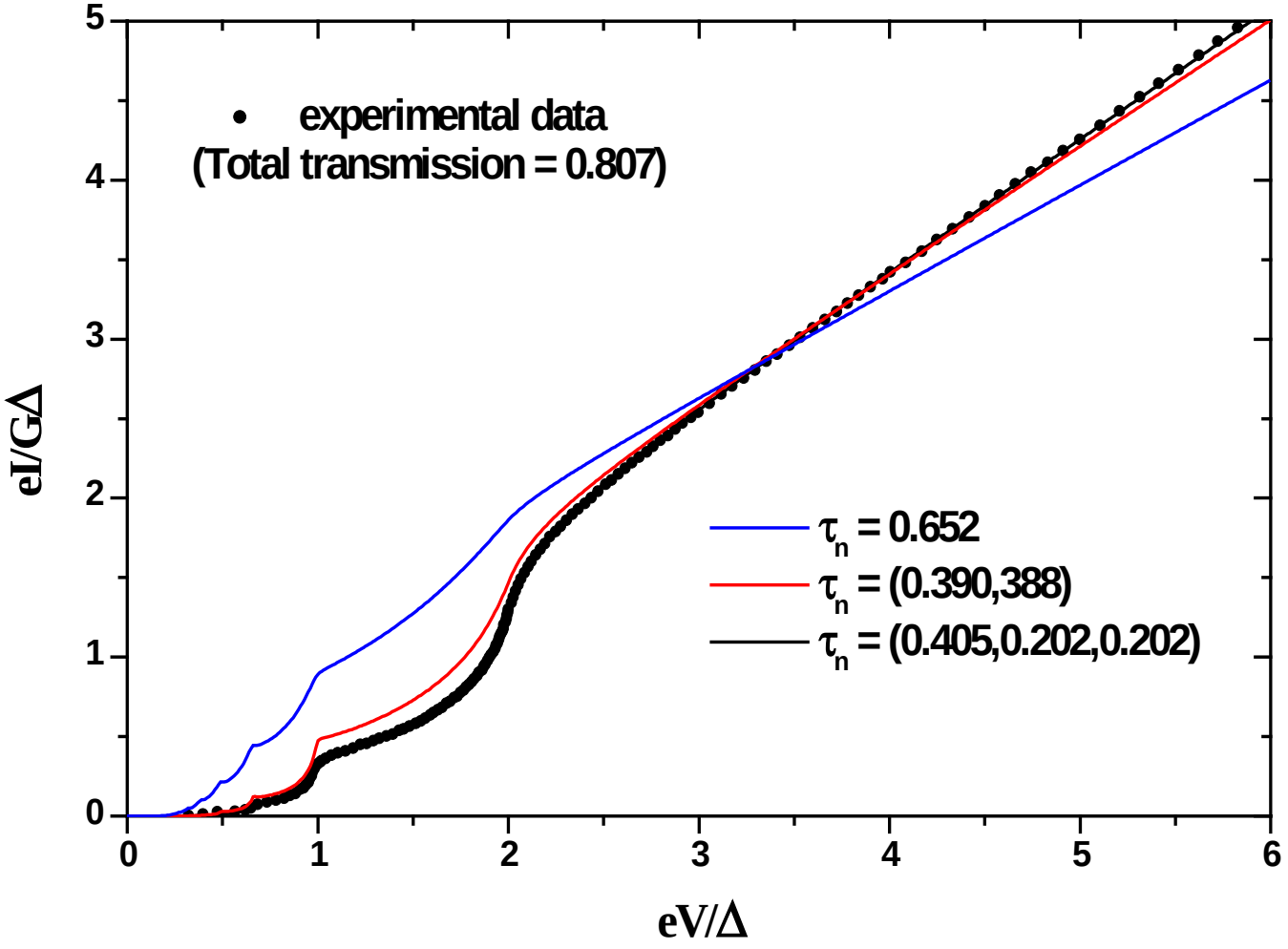
Probability: T^3

Charge transfer: $3e$

7.1.4 Determining the conduction channels

Fitting the experimental I-V curves

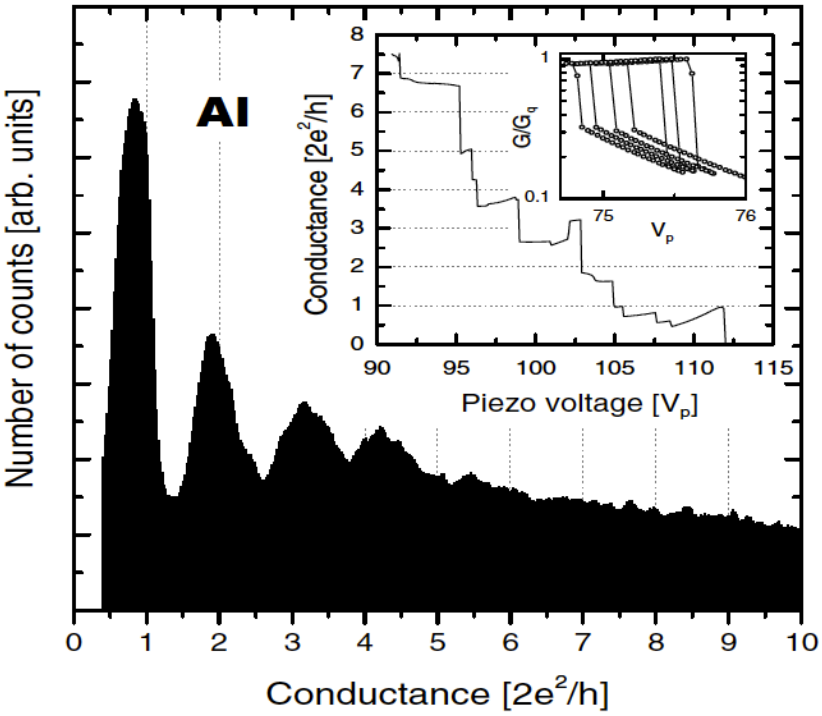
(Al MCJB, 30 mK, last conductance plateau)



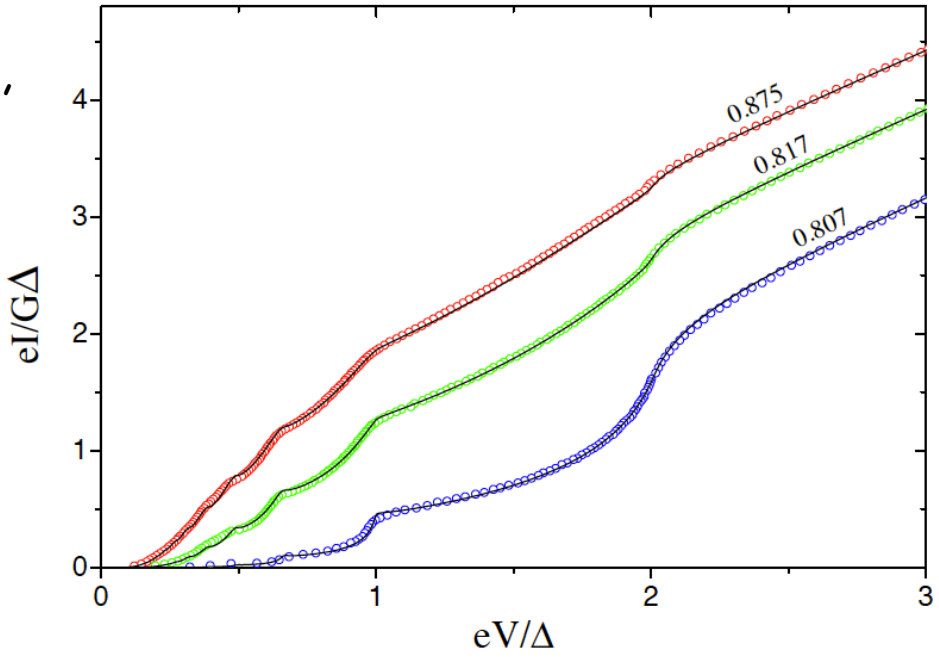
7.1.4 Determining the conduction channels

*E. Scheer, P. Joyez, D. Esteve, C. Urbina, M.H. Devoret, Phys. Rev. Lett. **78**, 3535 (1997).*

- In the last plateau of an Al contact, where $G < G_0$, two or three channels contribute to the transport.



[Yanson and van Ruitenbeek PRL (1997)]



T_{total}=0.875	T_{total}=0.817	T_{total}=0.807
0.80	0.682	0.399
0.075	0.12	0.254
	0.015	0.154

7.1.5 Chemical nature of the conduction channels of one-atom contacts

J.C. Cuevas, A. Levy Yeyati, and A. Martín-Rodero, Phys. Rev. Lett. ***80****, 1066 (1998)*

$$\hat{H} = \sum_{i\alpha,\sigma} \varepsilon_{i\alpha} \hat{c}^{+}_{i\alpha,\sigma} \hat{c}_{i\alpha,\sigma} + \sum_{i \neq j,\alpha\beta,\sigma} t_{i\alpha,\, j\beta} \hat{c}^{+}_{i\alpha,\sigma} \hat{c}_{j\beta,\sigma}$$

$$\begin{cases} i, j \rightarrow \text{atoms} \\ \alpha, \beta \rightarrow \text{orbitals} \end{cases}$$

- $t_{i\alpha,\, j\beta} \rightarrow$ (nearest neighbors) bulk parameterization (Papaconstantopoulos, 1986).
- Orthogonal basis and Slater-Koster two-center approximation.

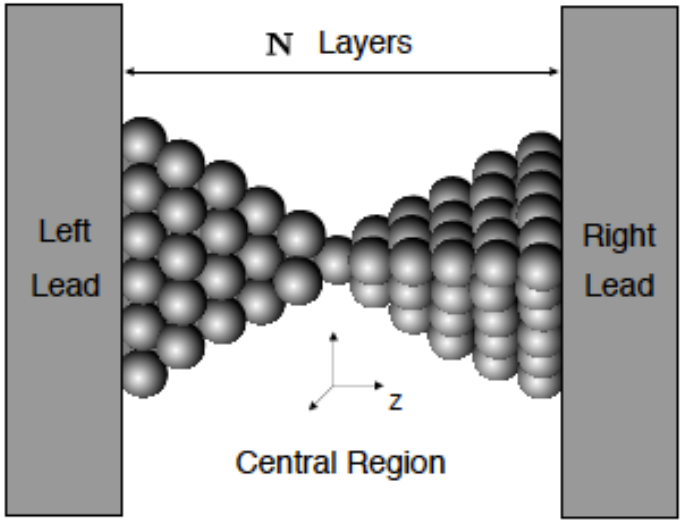
Ingredients

- **Chemistry:** minimum basis → valence orbitals.

Material	Orbitals
Alkali and noble metals: Li, Na, K, …, Cu, Au, and Ag	*s*
sp-like metals: Al, Pb, Zn, Cd, Mg, etc.	*s* and *p*
Transition metals: Nb, Pt, Pd, Ti, Fe, Co, etc.	*s* and *d*

- **Geometry:** importance of the local environment.
- **Charge neutrality:** self-consistent determination of the on-site energies.

7.1.5 Chemical nature of the conduction channels of one-atom contacts



Electrical current (Landauer formula):

$$I = \frac{2e}{h}\int_{-\infty}^{\infty} dE \mathrm{Tr}\left\{t^{+}t\right\}\left[f_L - f_R\right]$$

Transmission matrix expressed via Green's functions:

$$t(E,V) = 2\Gamma_L^{1/2}(E,V)G_{CC}^{r}(E,V)\Gamma_R^{1/2}(E,V)$$

- Scattering rates: $\Gamma_X = \mathrm{Im}\left\{\Sigma_X^a\right\}$, where $\Sigma_X^a = t_{CX}\, g_{XX}^a\, t_{XC} \quad (X = L, R)$
- The central Green's functions are given by: $G_{CC}^{r,a} = \left[(E \pm i\eta)1 - H_{CC} - \Sigma_L^{r,a} - \Sigma_R^{r,a}\right]^{-1}$
- $\mathrm{Dim}(t^{+}t) = N_C \rightarrow$ number of orbitals in the first layer (due to nearest neighbor couplings).

Linear regime:

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

T_i = eigenvalues of $t^{+}t$ at the Fermi energy.

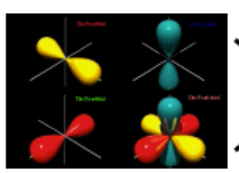
7.1.5 Chemical nature of the conduction channels of one-atom contacts

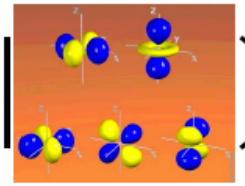
➢ Transmission evaluated at the central atom: $\mathrm{Dim}(t^{+}t) = N_{orb}$

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:

$$|\text{channel}\rangle_i = c_{is}\,|\,\bigcirc\rangle + c_{ip}\,|\,\text{p-orbitals}\rangle + c_{id}\,|\,\text{d-orbitals}\rangle$$





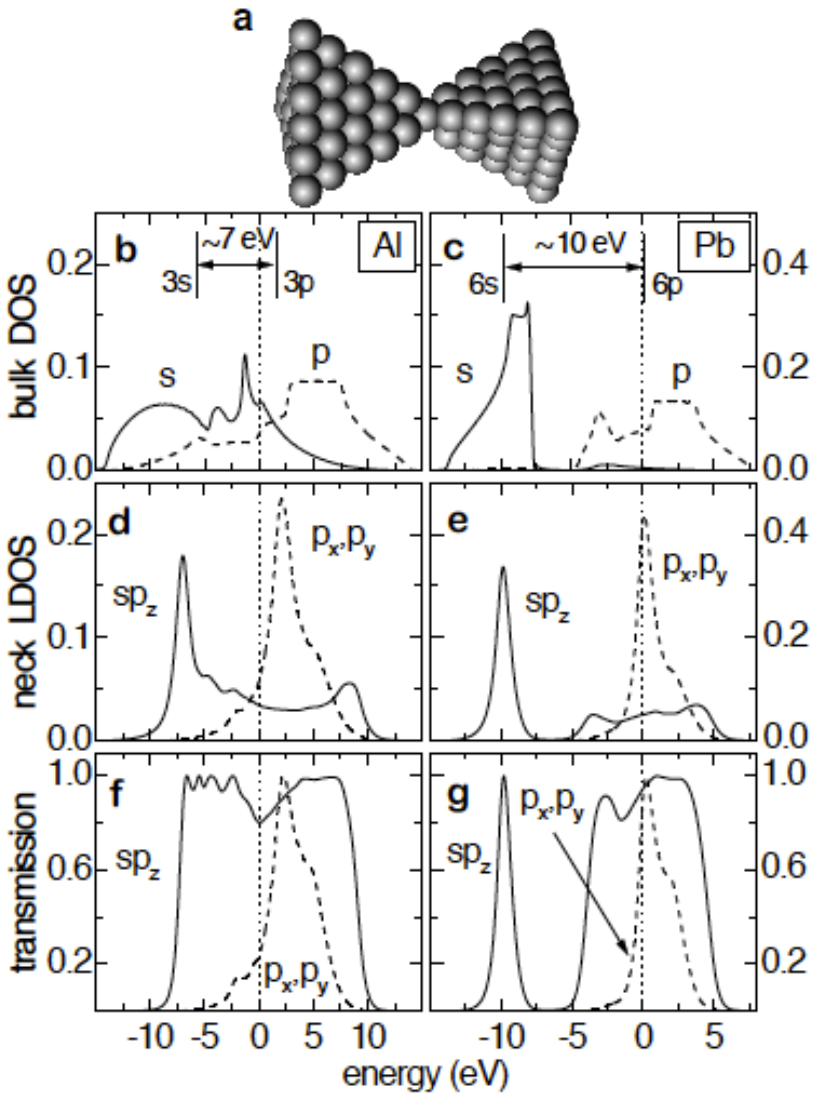
➢ Assuming that there is a single relevant orbital per atom, the transmission adopts the form:

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

➢ 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!!!**

7.1.5 Chemical nature of the conduction channels of one-atom contacts

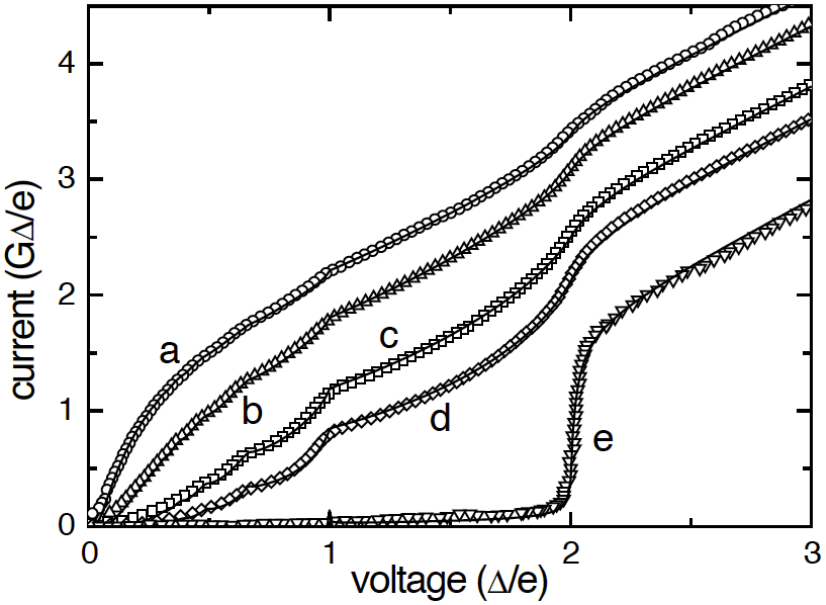
Aluminum: $[Ne]3s^2 3p^1$ Lead: $[Xe]6s^2 6p^2$



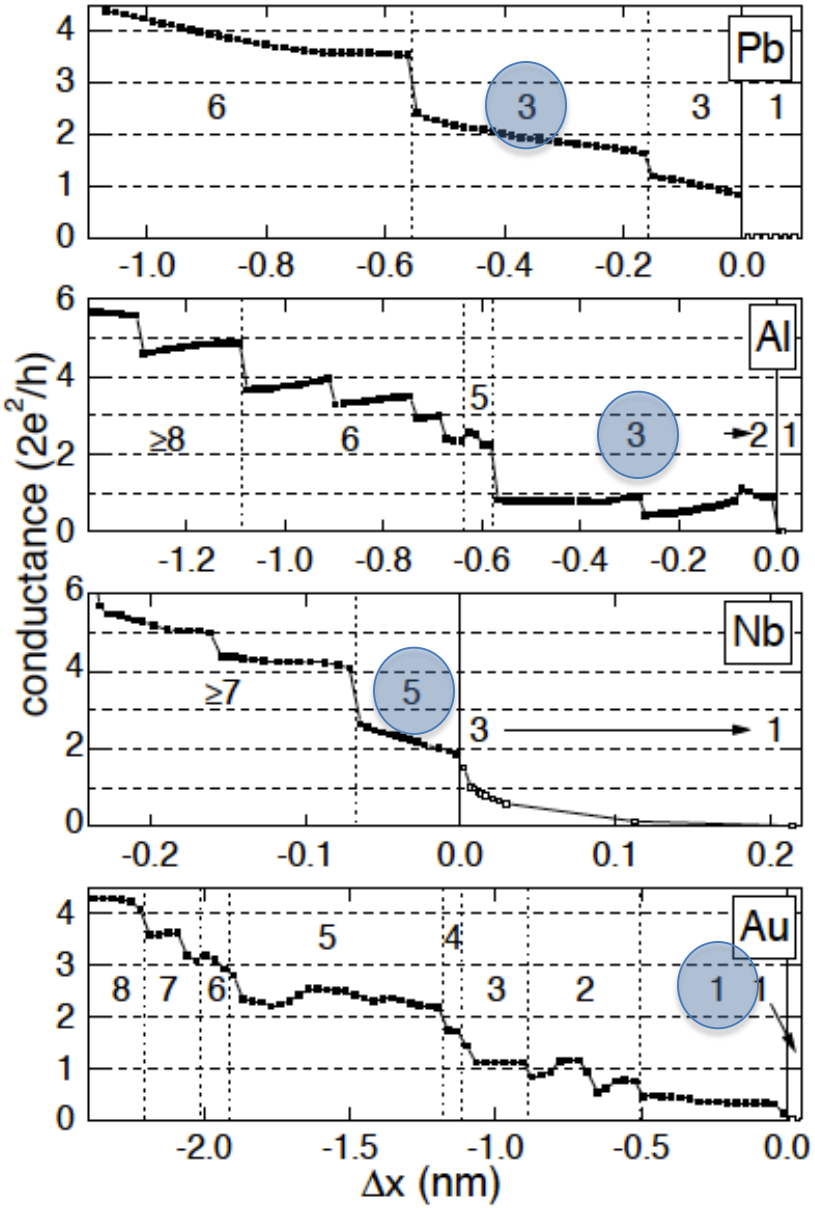
7.1.5 Chemical nature of the conduction channels of one-atom contacts

*E. Scheer, N. Agrait, J.C. Cuevas, B. Ludoph, A. Levy Yeyati, A. Martín-Rodero, G. Rubio, J. van Ruitenbeek, C. Urbina, Nature **394**, 154 (1998).*

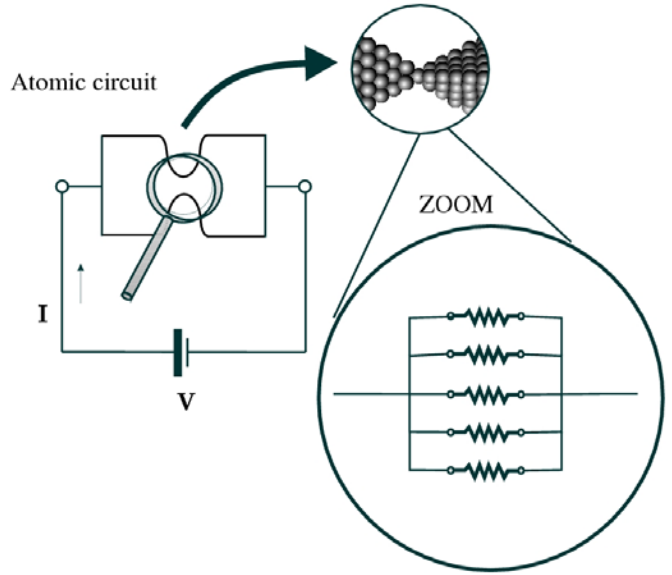
Experimental confirmation that the chemical valence determines the number of channels of one-atom contacts.



(Pb STM contact, 1.5 K)



7.1.5 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	1.5 - 2.5	3	*s* und *p*
Nb	2 - 3	5	*s* und *d*

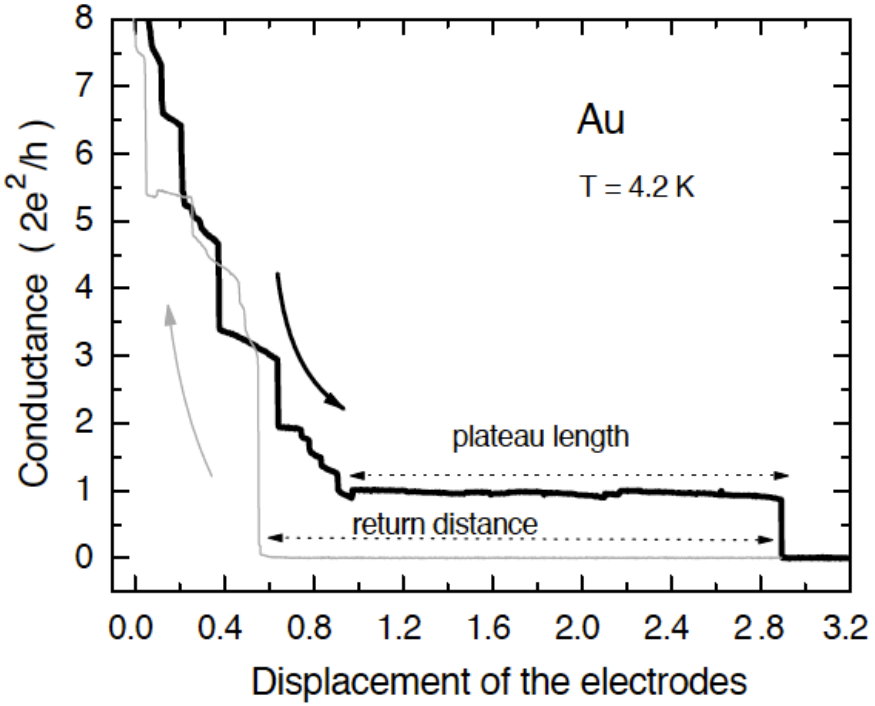
Macroscopic wires: Resistivity (x 10^{-8} Ωm) at T = 300 K

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

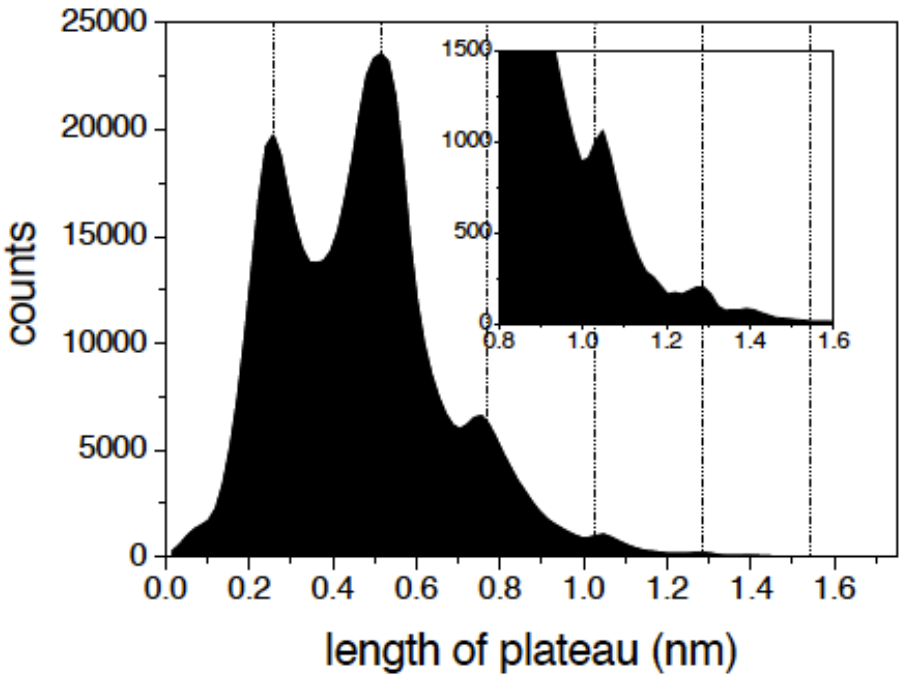
Small is different!!

7.1.6 Atomic chains: discovery

*A.I. Yanson, G. Rubio Bollinger, H.E. van den Brom, N. Agraït, J.M. van Ruitenbeek, Nature **395**, 783 (1998)*



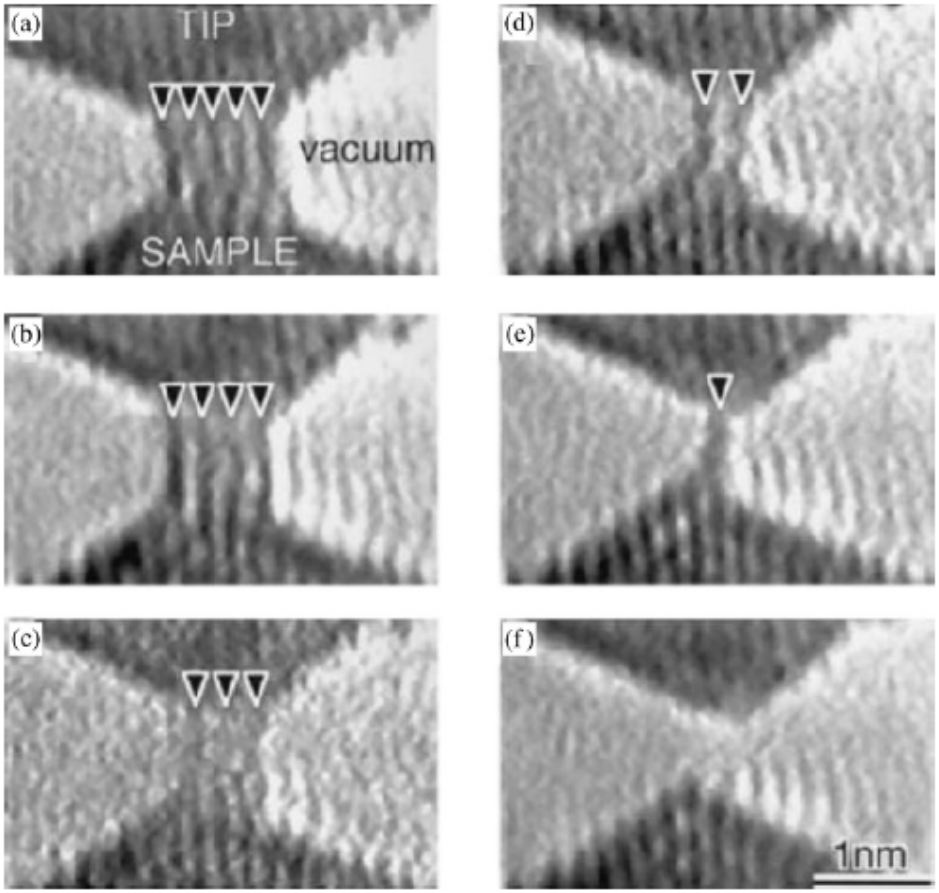
Conductance as a function of the displacement of the two gold electrodes with respect to each other in a MCBJ experiment at 4.2 K.



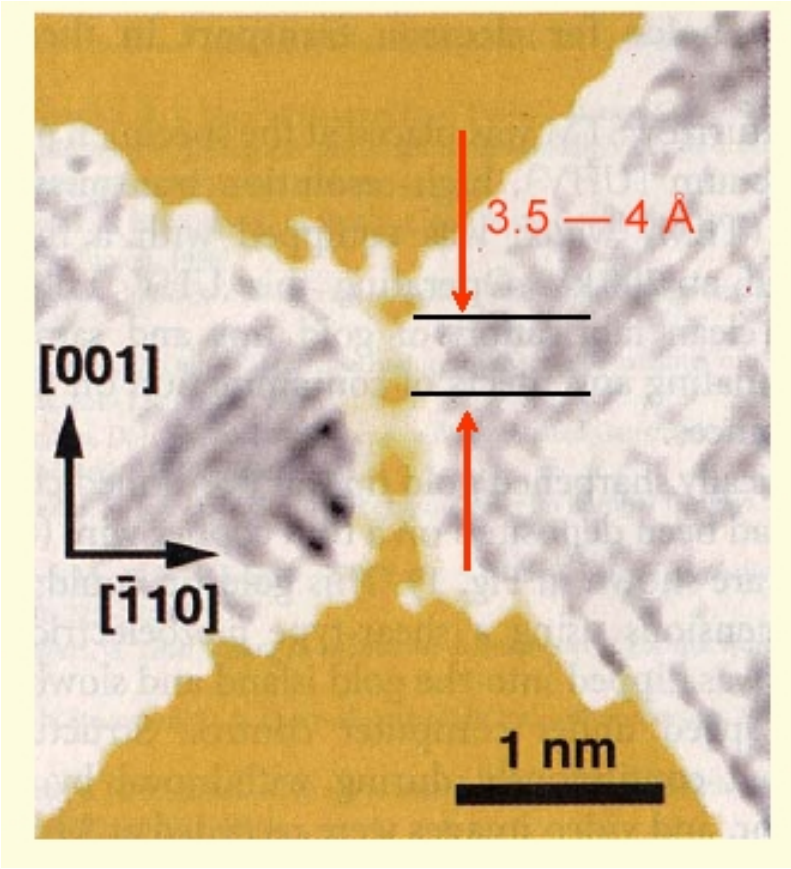
Distribution of lengths for the last conductance plateau for Au, obtained from 10000 experiments.

7.1.6 Atomic chains: discovery

*H. Ohnishi, Y. Kondo, K. Takayanagi, Nature **395**, 780 (1999)*



TEM images of a gold contact recorded while withdrawing the tip from the sample.

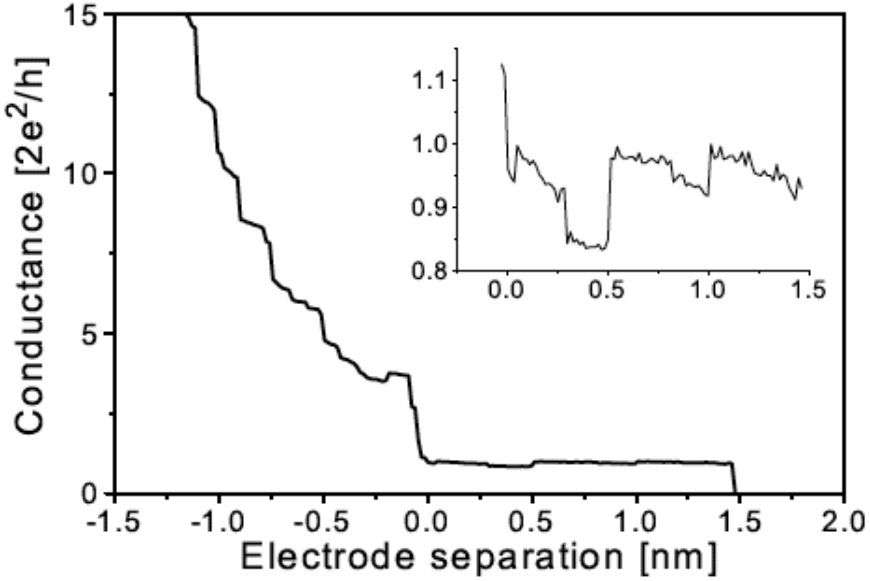


TEM image of a gold atomic chain (four yellow dots) forming a bridge between two gold banks (yellow areas above and below).

7.1.6 Atomic chains: discovery

R.H.M. Smit, C. Untiedt, G. Rubio Bollinger, R.C. Segers, J.M. van Ruitenbeek,
Phys. Rev. Lett. ***91****, 076805 (2003)*

Observation of parity oscillations in the conductance of atomic chains of Au, Pt, and Ir.



Length histograms and averaged conductance.