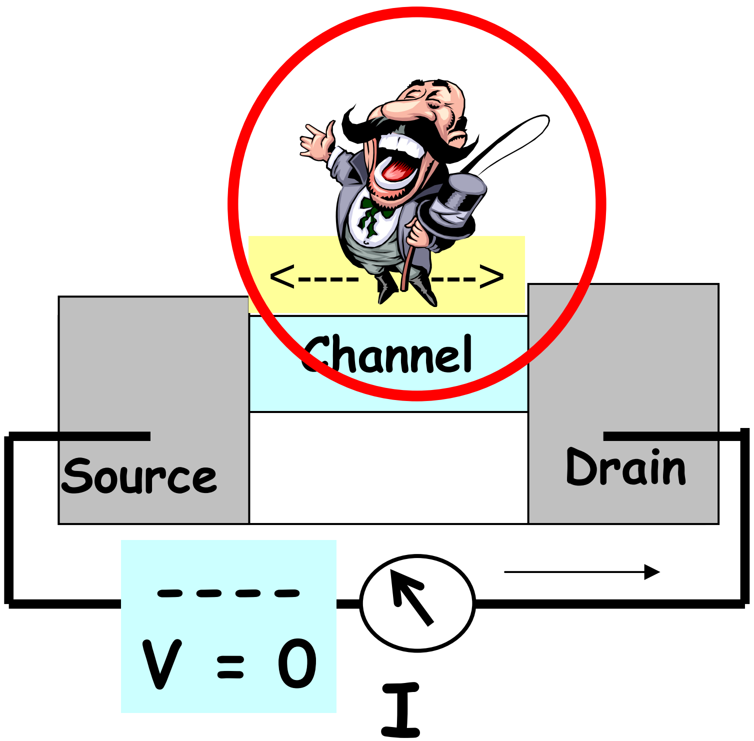
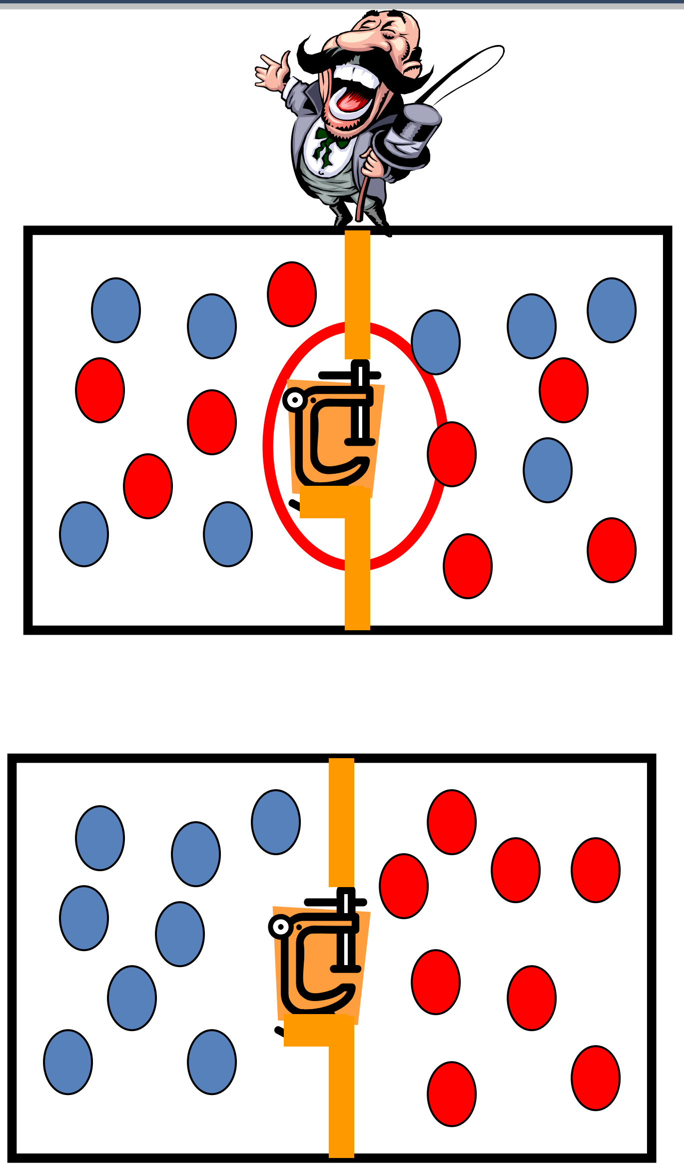
Nanodevices and Maxwell's Demon

Electronic demon

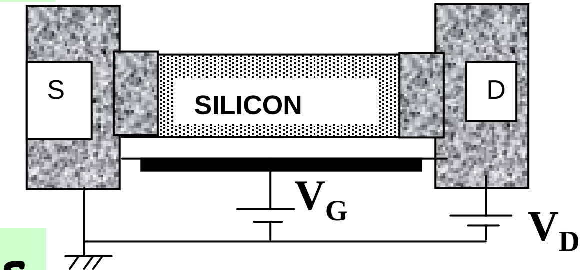




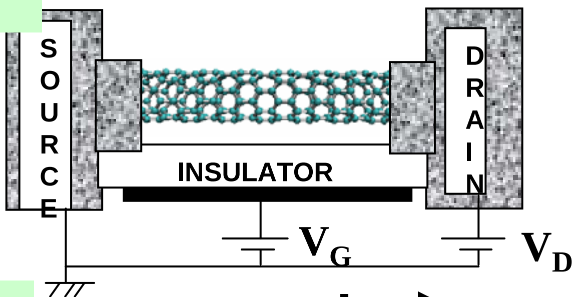
For a detailed write-up of this lecture
See arXiv:condmat/0704.1623

Unified viewpoint: Materials

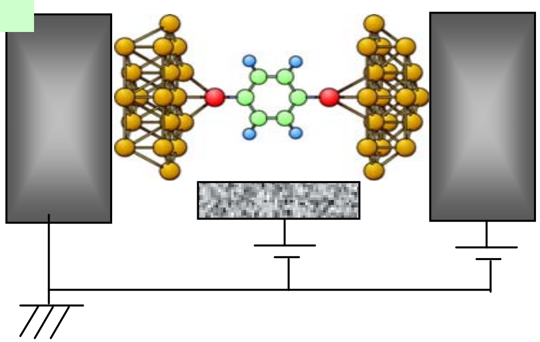
Nanowires



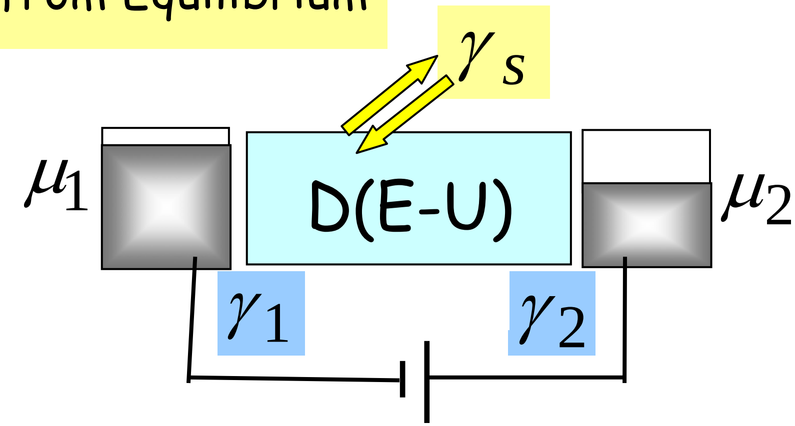
Nanotubes /Graphene

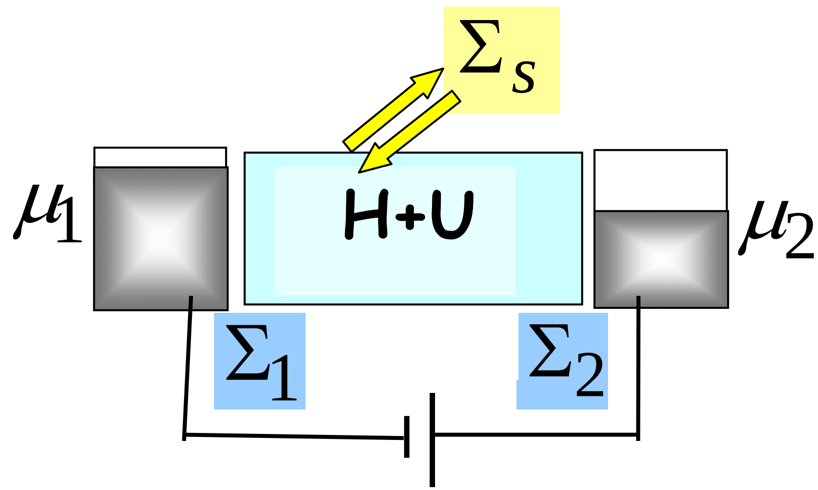


Molecules



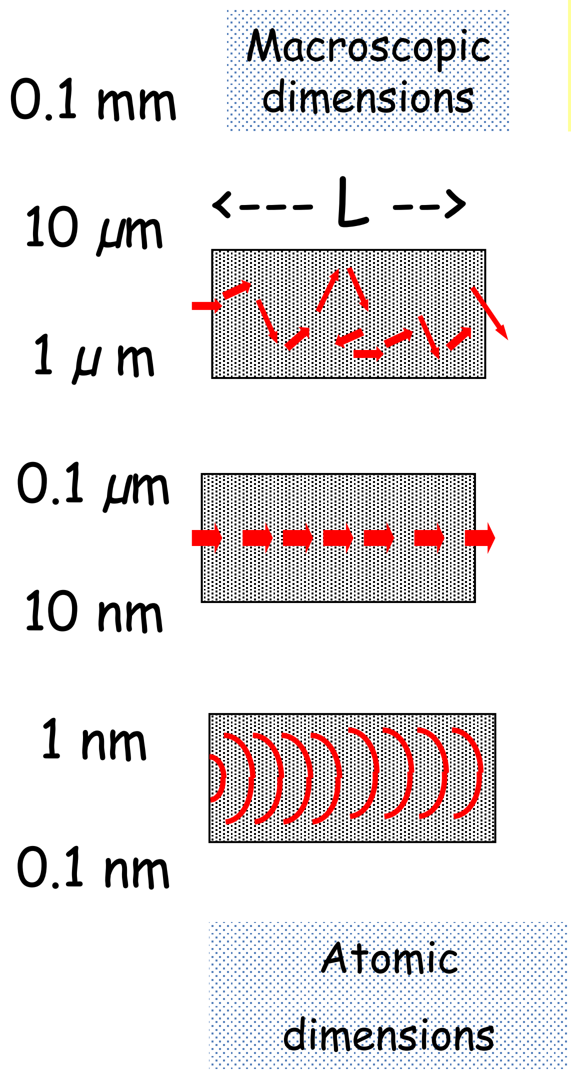
Quantum Transport
Far from Equilibrium



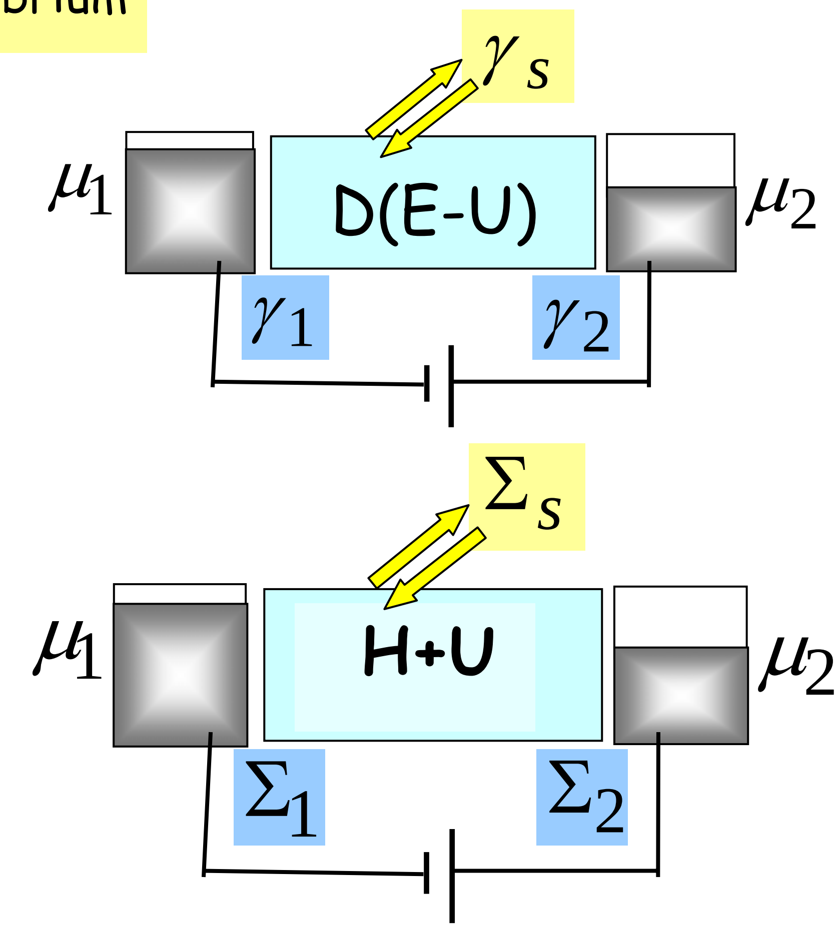


$$\Gamma = i\left[\Sigma - \Sigma^{+}\right]$$

Unified viewpoint: Ballistic to Diffusive



Quantum transport far from equilibrium



$$\Gamma = i\left[\Sigma - \Sigma^{+}\right]$$

Top-down view

Macroscopic dimensions

0.1 mm

10 μm

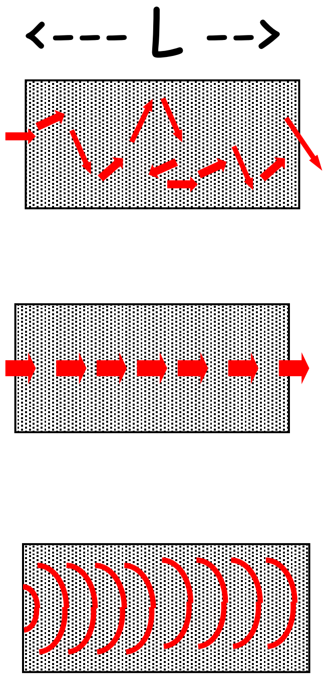
1 μm

0.1 μm

10 nm

1 nm

0.1 nm



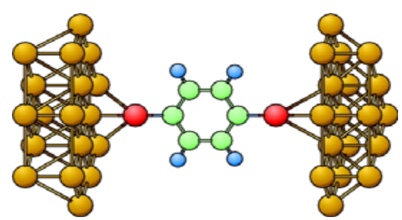
Atomic dimensions

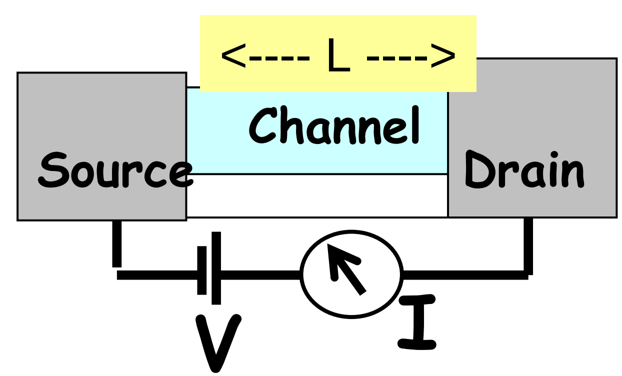
$$G = \sigma A / L$$

$$\sigma = e^2 n \tau / m$$

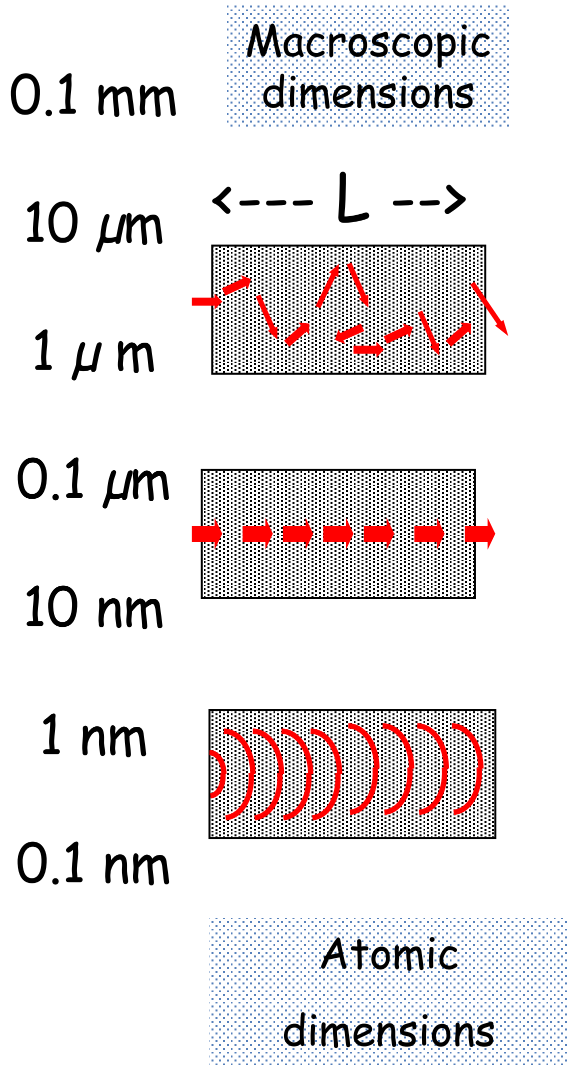
$\tau = ?$ "Very complicated"

m = ? n = ?





Bottom-up view



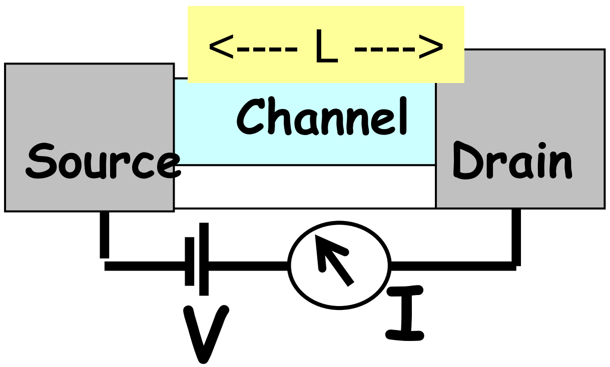
$$G = \sigma A/L$$

$$\gamma \sim \frac{2\hbar D}{L^2} \rightarrow D\gamma \sim A/L$$

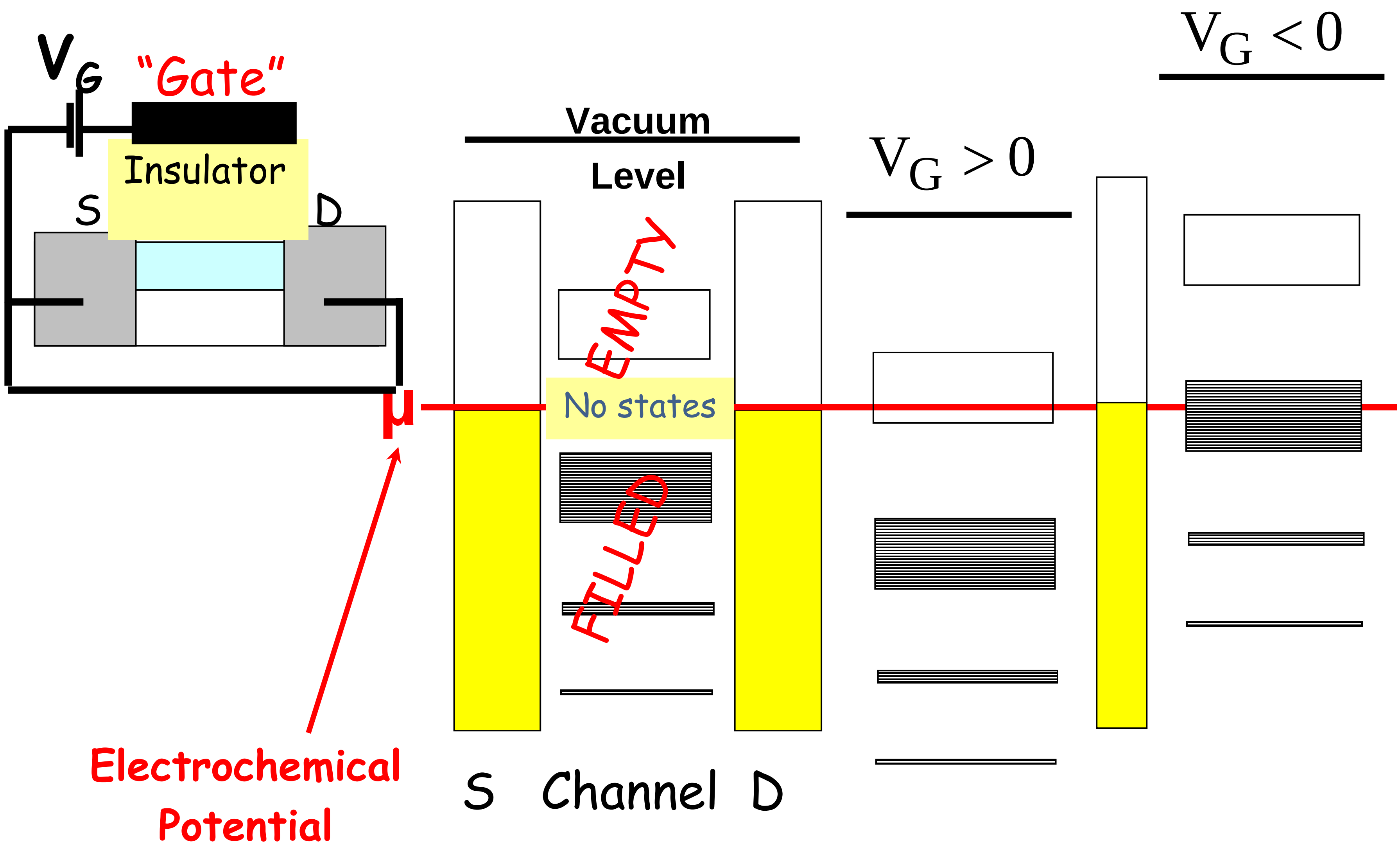
$$G = (e^2/h)(\pi D\gamma), \qquad D \sim AL$$

$$\gamma \sim \frac{\hbar v}{L} \rightarrow D\gamma \sim A$$

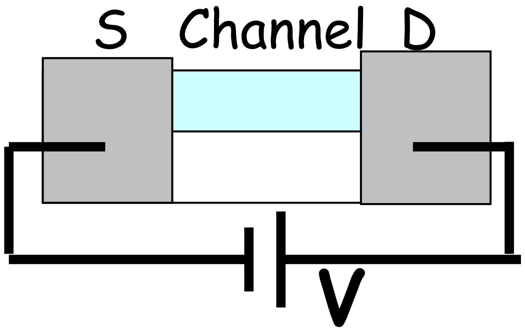
$$G = \underbrace{(e^2/h)}_{1/25.8\ K\Omega}$$

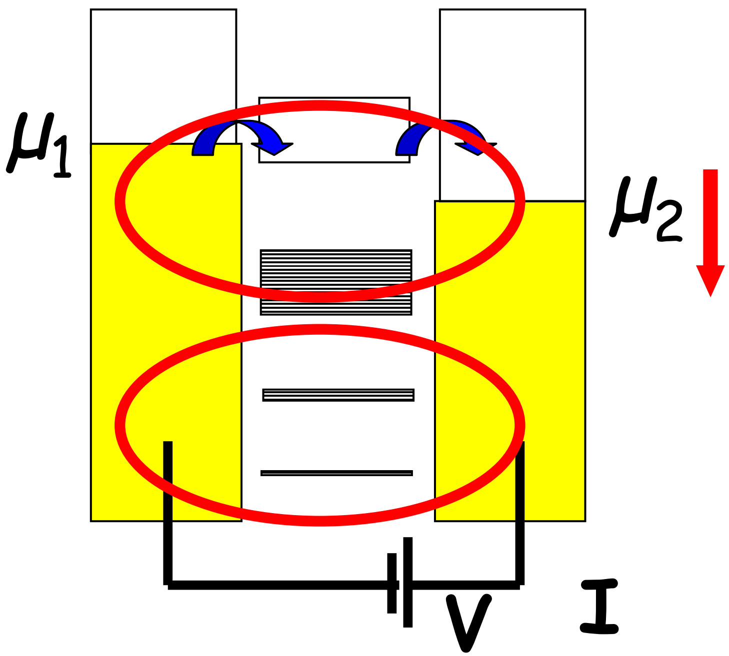


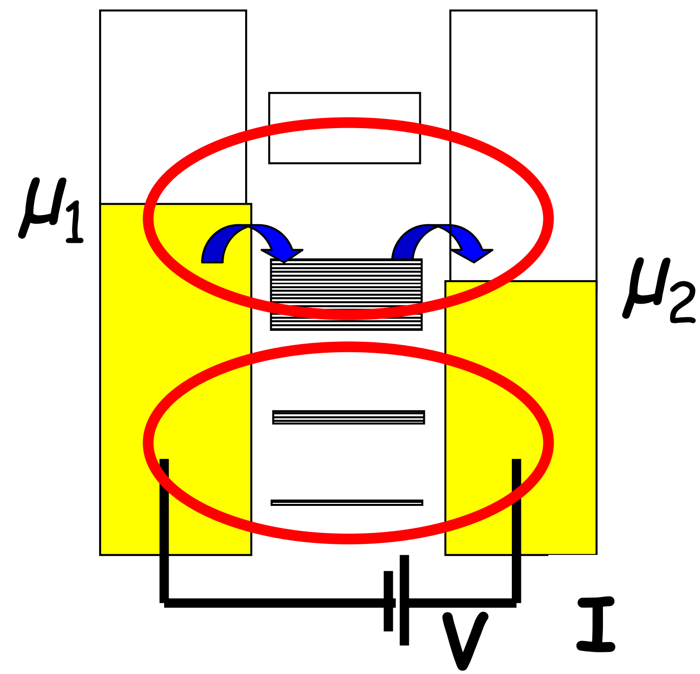
Equilibrium Energy Level Diagram



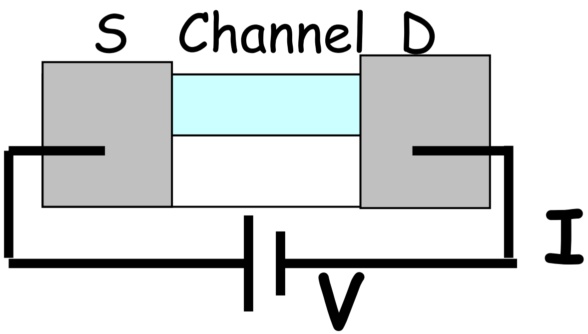
What makes electrons flow?

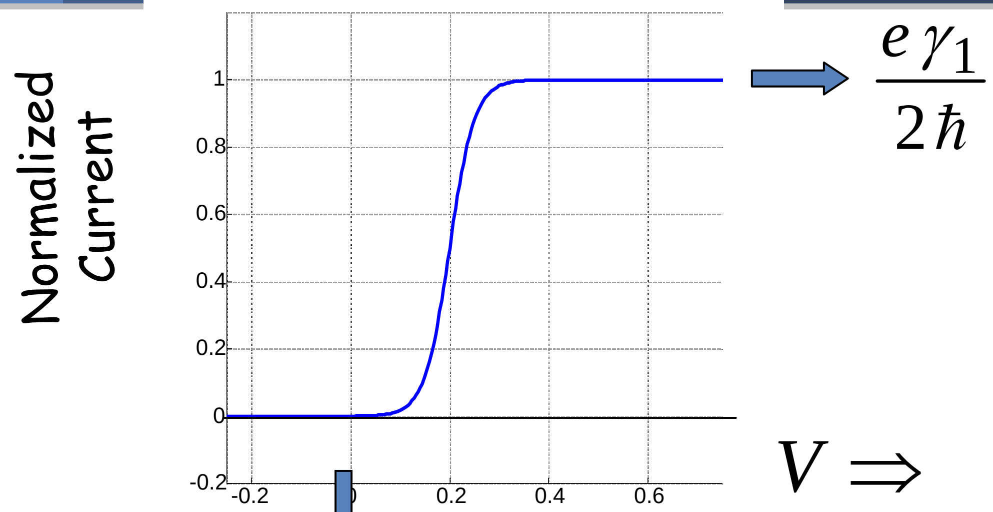


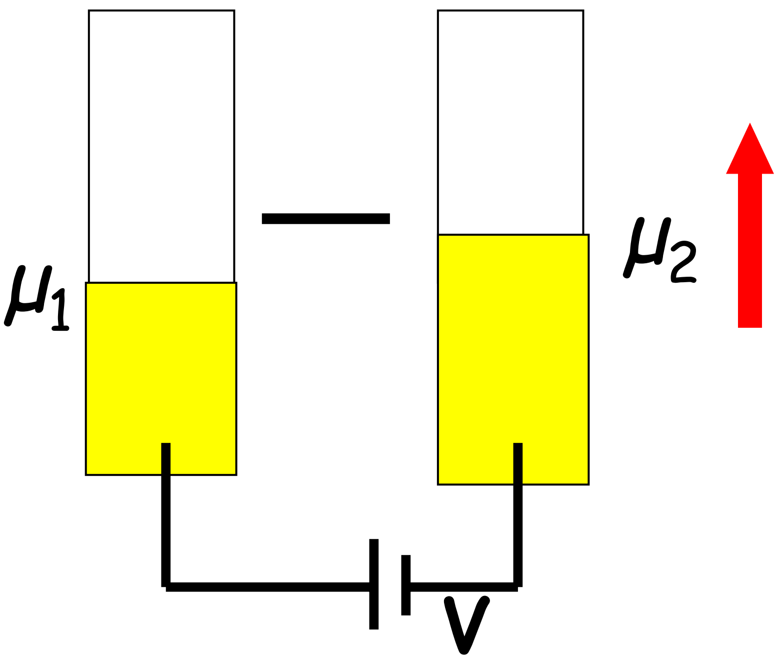


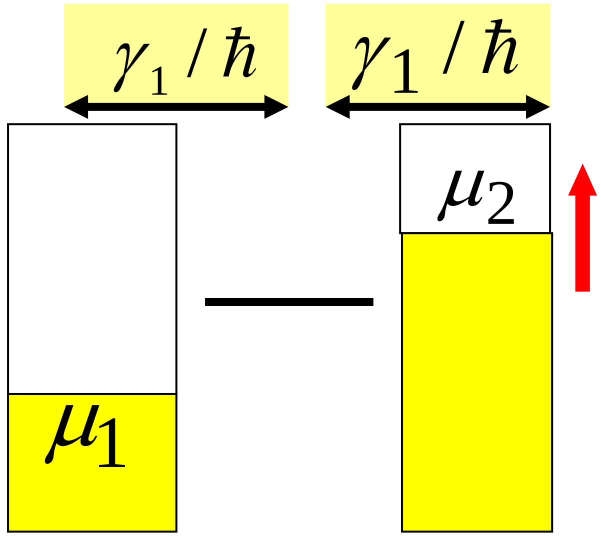


Current through a 1-level conductor

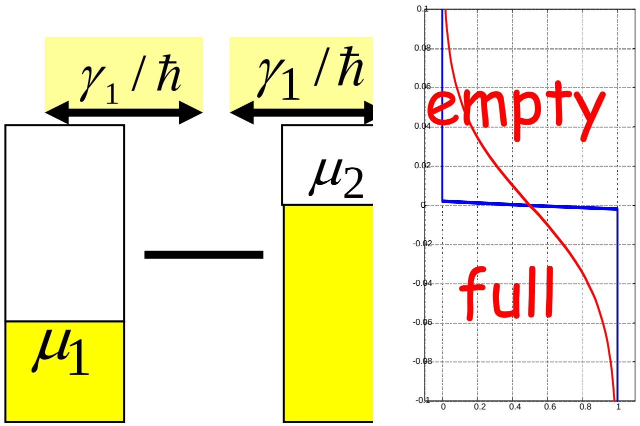


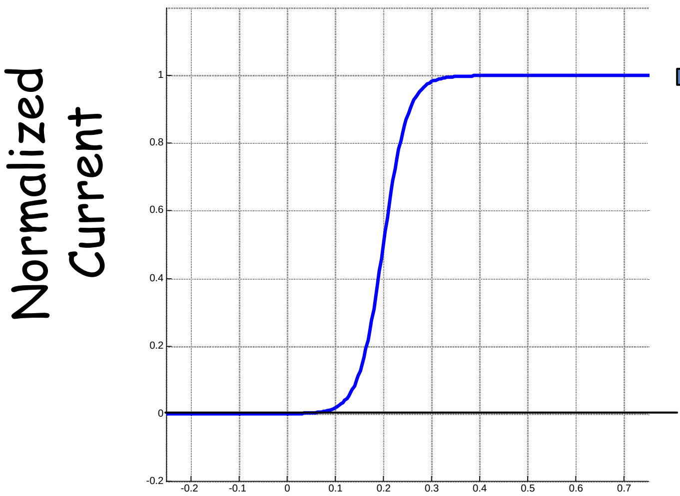






Conductance ?

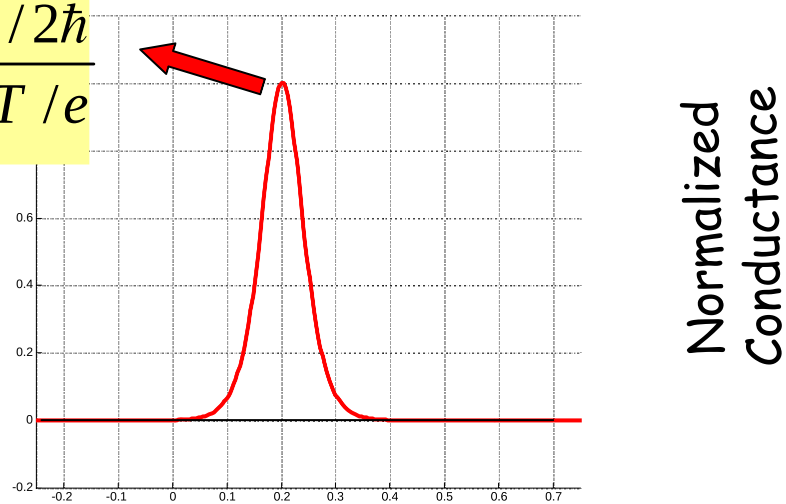




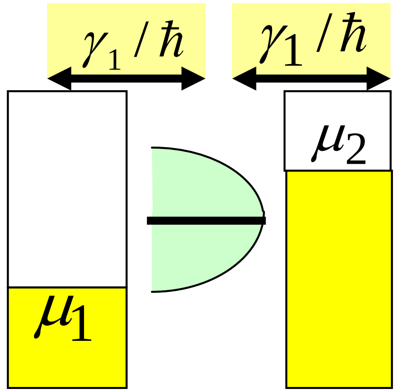
$\Rightarrow \dfrac{e\gamma_1}{2\hbar}$

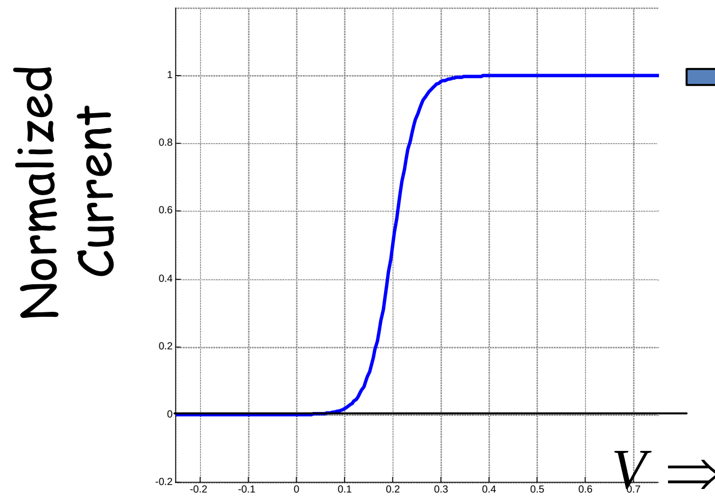
$V \Rightarrow$

$$\frac{dI}{dV} \sim \frac{e\gamma_1/2\hbar}{4kT/e}$$



Conductance quantum

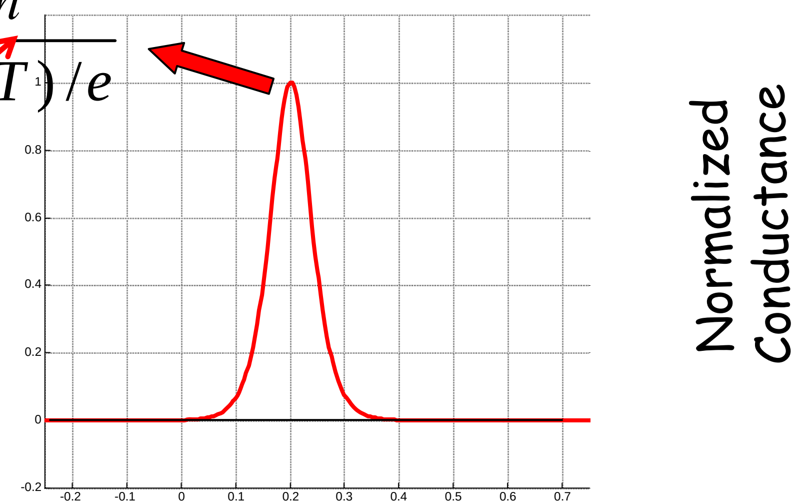




$$\Rightarrow \frac{e\gamma_1}{2\hbar}$$

$$\frac{dI}{dV} \sim \frac{e\gamma_1/2\hbar}{(2\gamma_1 + 4kT)/e}$$

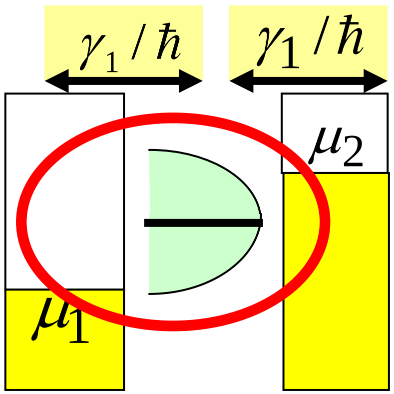
$$\sim \quad e^2/4\hbar \quad if \quad \gamma_1 >> kT$$



Conductance quantum

$$\sim \quad e^2/2\pi\hbar \quad \sim \quad 1/25.8\ K\Omega$$

Conductance quantum



Measurement of the conductance of a hydrogen molecule

R. H. M. Smit*, Y. Noat*†, C. Untiedt*, N. D. Lang‡, M. C. van Hemert§ & J. M. van Ruitenbeek*

* *Kamerlingh Onnes Laboratorium, Universiteit Leiden, PO Box 9504,*

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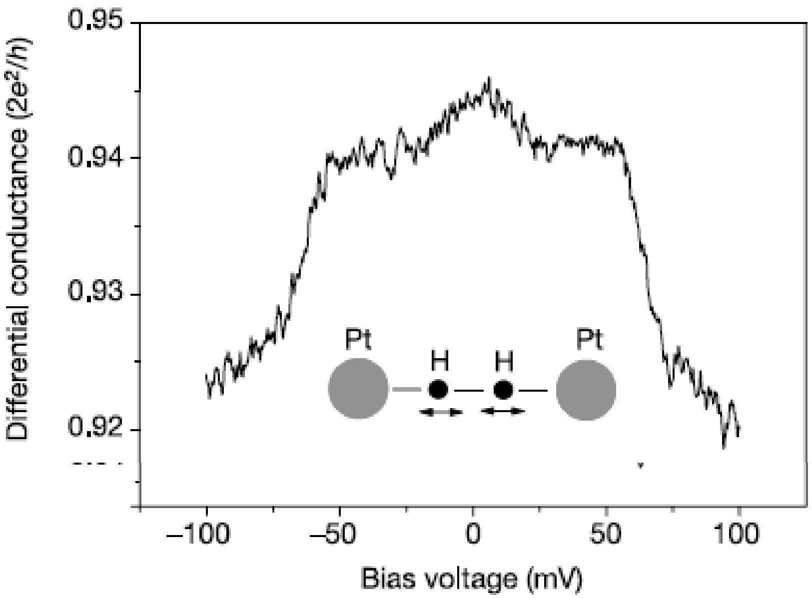
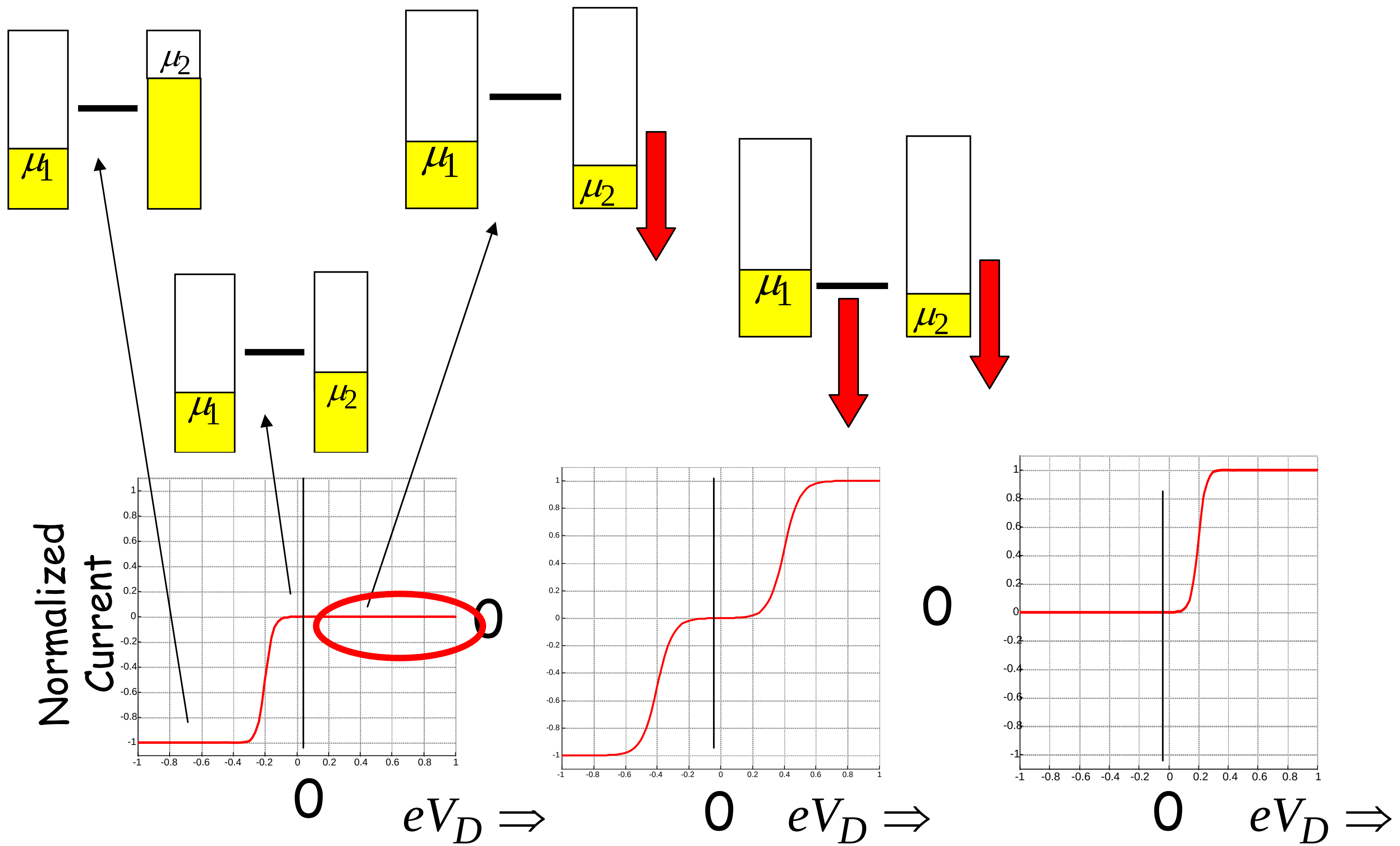


Importance of electrostatics



Importance of electrostatics

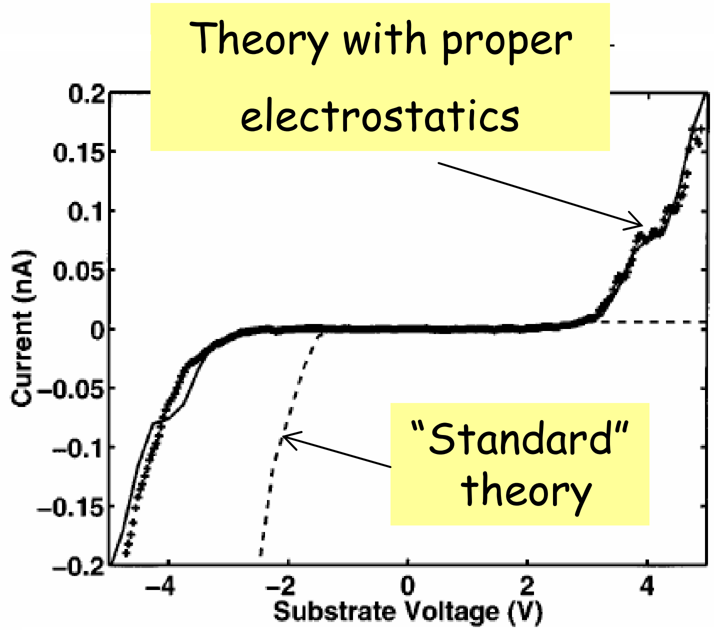
JMBER 13 PHYSICAL REVIEW LETTERS 29 SEPTEMBER 1997

Current-Voltage Characteristics of Self-Assembled Monolayers by Scanning Tunneling Microscopy

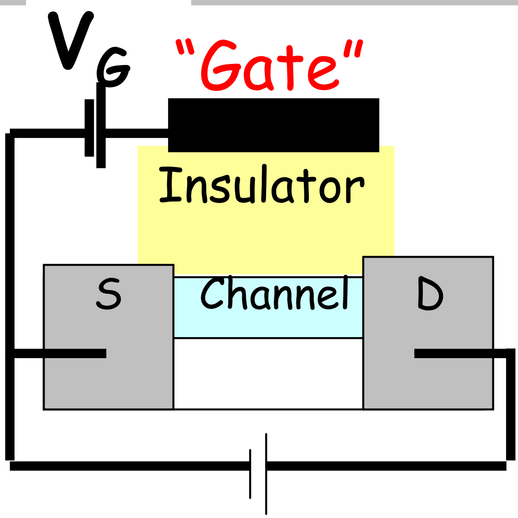
Supriyo Datta and Weidong Tian
ool of Electrical and Computer Engineering, Purdue University, West Lafayette, Indiana 47907-1285

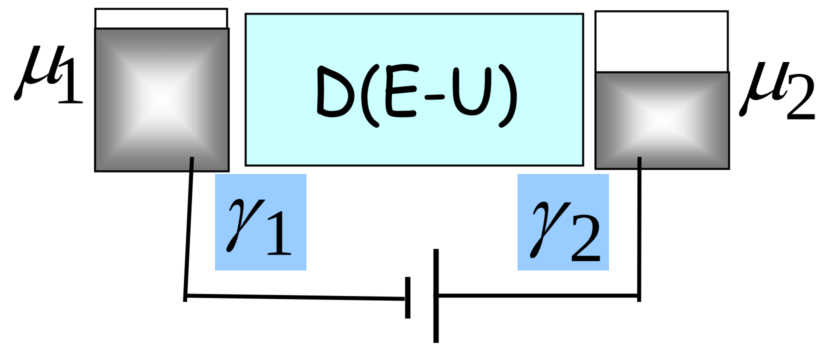
Seunghun Hong and R. Reifen
Department of Physics, Purdue University, West Lafa

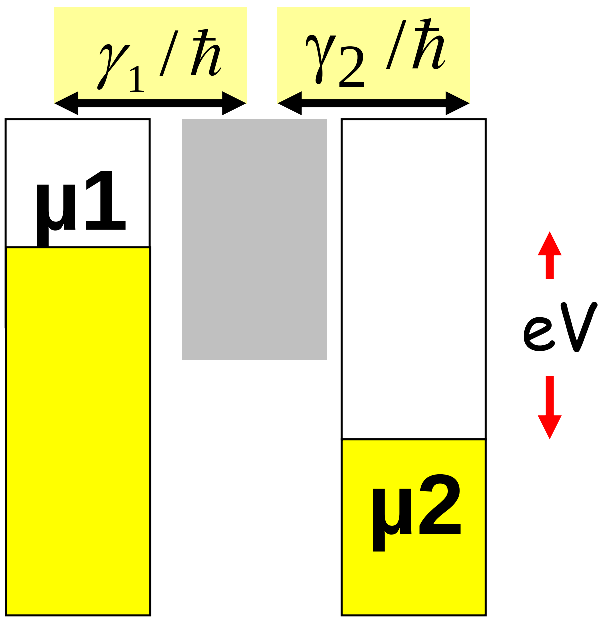
Jason I. Henderson and Clifford P
Department of Chemistry, Purdue University, West La
(Received 9 June 1997)

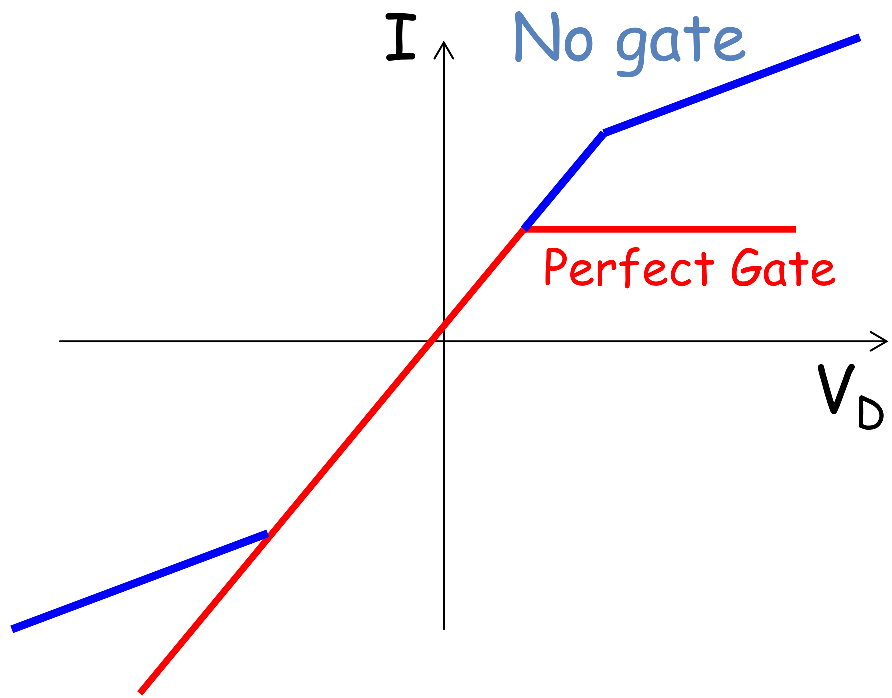


Electrostatics of a Nanotransistor

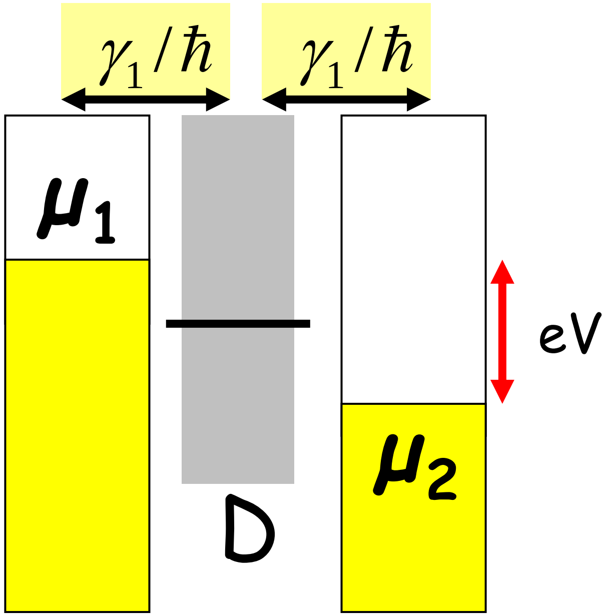








Conductance: for any DOS, D



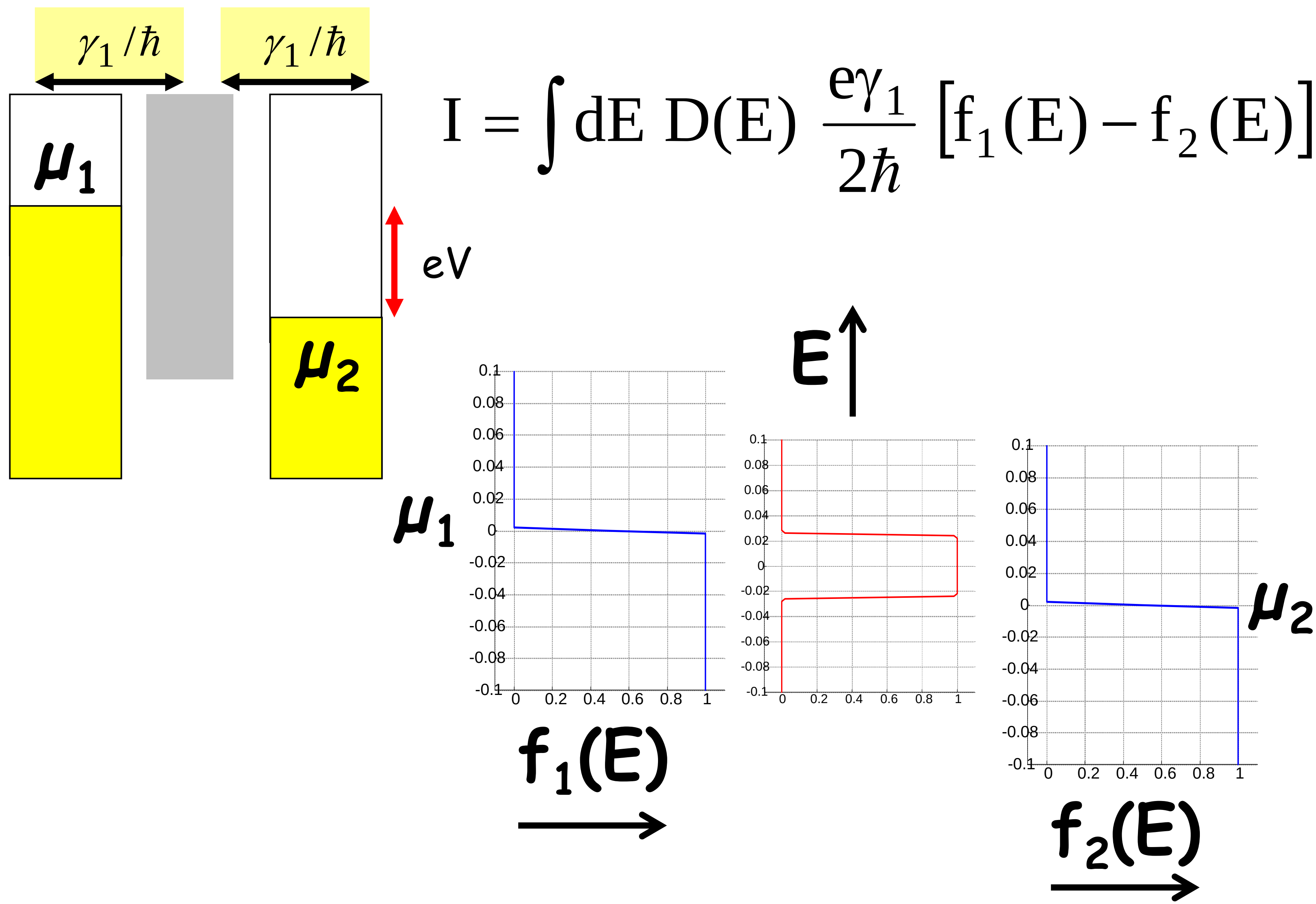
$$I \sim \underbrace{\frac{e\gamma_1}{2\hbar}}_{\text{Current per state}} \underbrace{D\,eV}_{\text{Number of states}}$$

D: Density of states

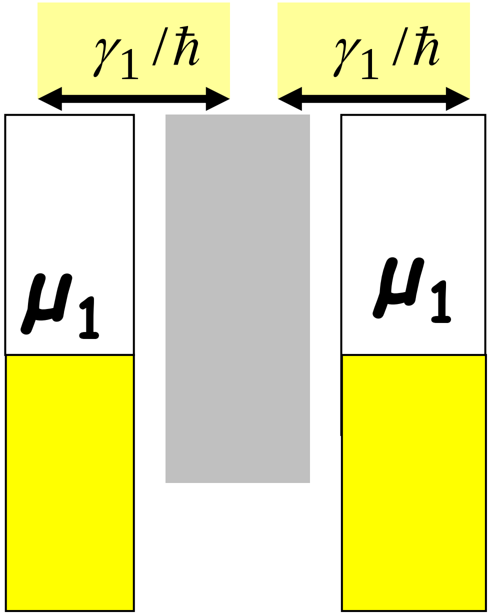
$$I/V = \underbrace{\frac{e^2}{2\pi\hbar}}_{\text{Conductance Quantum}} \underbrace{\pi D \gamma_1}_{\text{Transmission}}$$

Current versus voltage

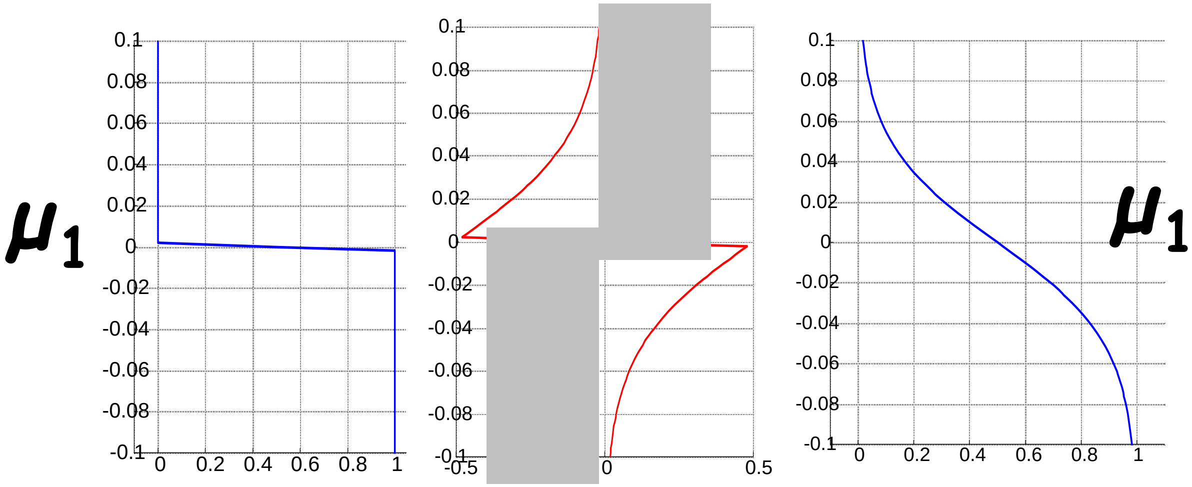
$$I = \int dE\ D(E)\ \frac{e\gamma_1}{2\hbar}\left[f_1(E) - f_2(E)\right]$$



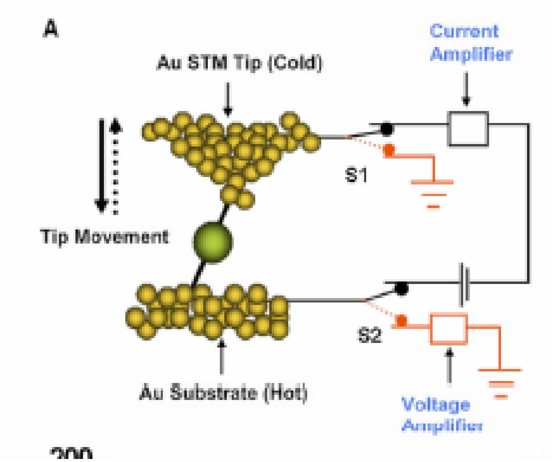
Current versus temperature



$$I = \int dE \; D(E) \; \frac{e\gamma_1}{2\hbar} \left[f_1(E) - f_2(E) \right]$$



Molecular Thermoelectricity

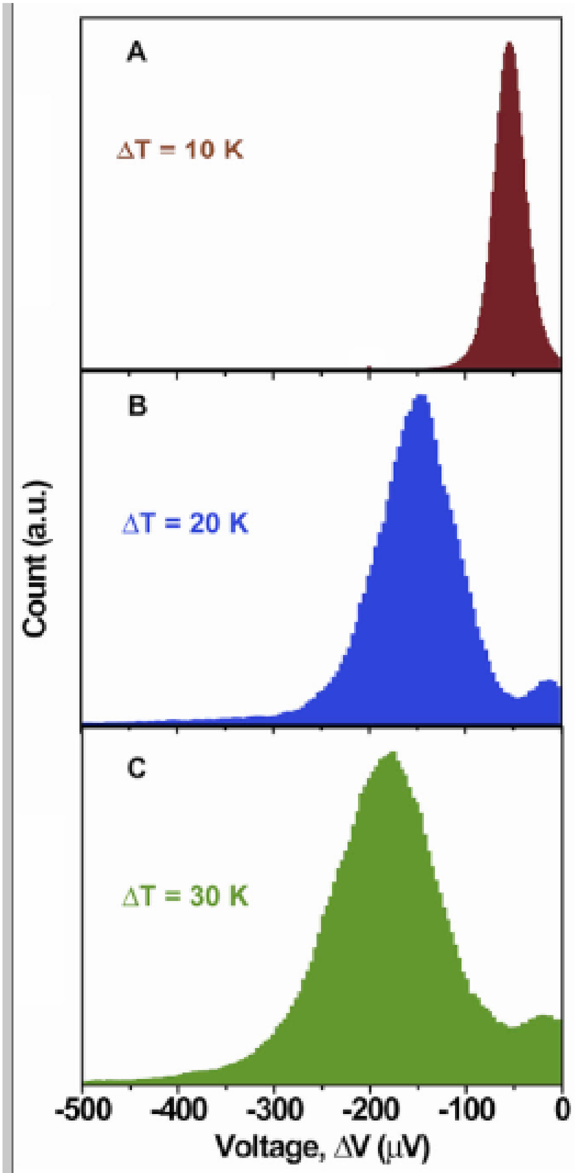


Thermoelectricity in Molecular Junctions

Pramod Reddy,[1*] Sung-Yeon Jang,[2,3*†] Rachel A. Segalman,[1,2,3‡] Arun Majumdar[1,3,4‡]

By trapping molecules between two gold electrodes with a temperature difference across them, the junction Seebeck coefficients of 1,4-benzenedithiol (BDT), 4,4′-dibenzenedithiol, and 4,4′′-tribenzenedithiol in contact with gold were measured at room temperature to be +8.7 ± 2.1 microvolts per kelvin (μV/K), +12.9 ± 2.2 μV/K, and +14.2 ± 3.2 μV/K, respectively (where the error is the full width half maximum of the statistical distributions). The positive sign unambiguously indicates p-type (hole) conduction in these heterojunctions, whereas the Au Fermi level position for Au-BDT-Au junctions was identified to be 1.2 eV above the highest occupied molecular orbital level of BDT. The ability to study thermoelectricity in molecular junctions provides the opportunity to address these fundamental unanswered questions about their electronic structure and to begin exploring molecular thermoelectric energy conversion.

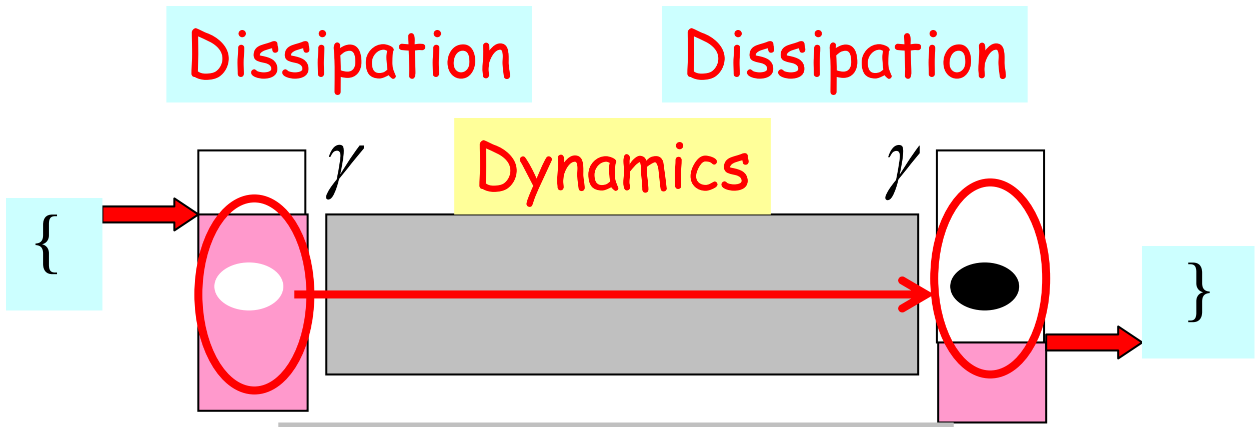
Experiment:
Reddy, et al., Science, 315 16 March, 2007.
Theory:
Paulsson and Datta, PRB 67, 241403 (2003),



From ballistic to diffusive transport

Separate dynamics
+ dissipation

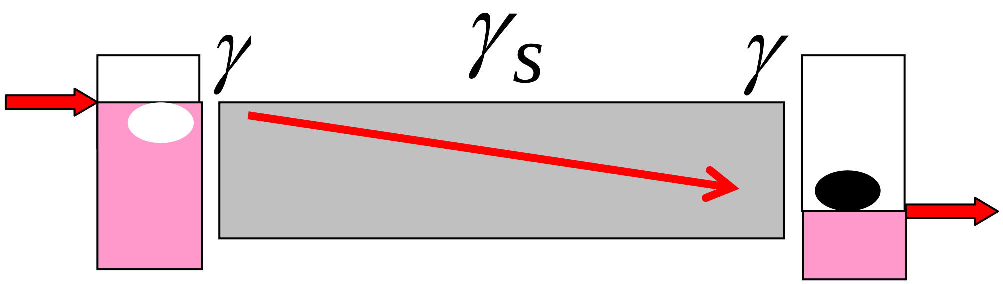
Landauer
model



Newton's law
Schrodinger equation

Mixed dynamics
+ dissipation

Boltzmann
NEGF



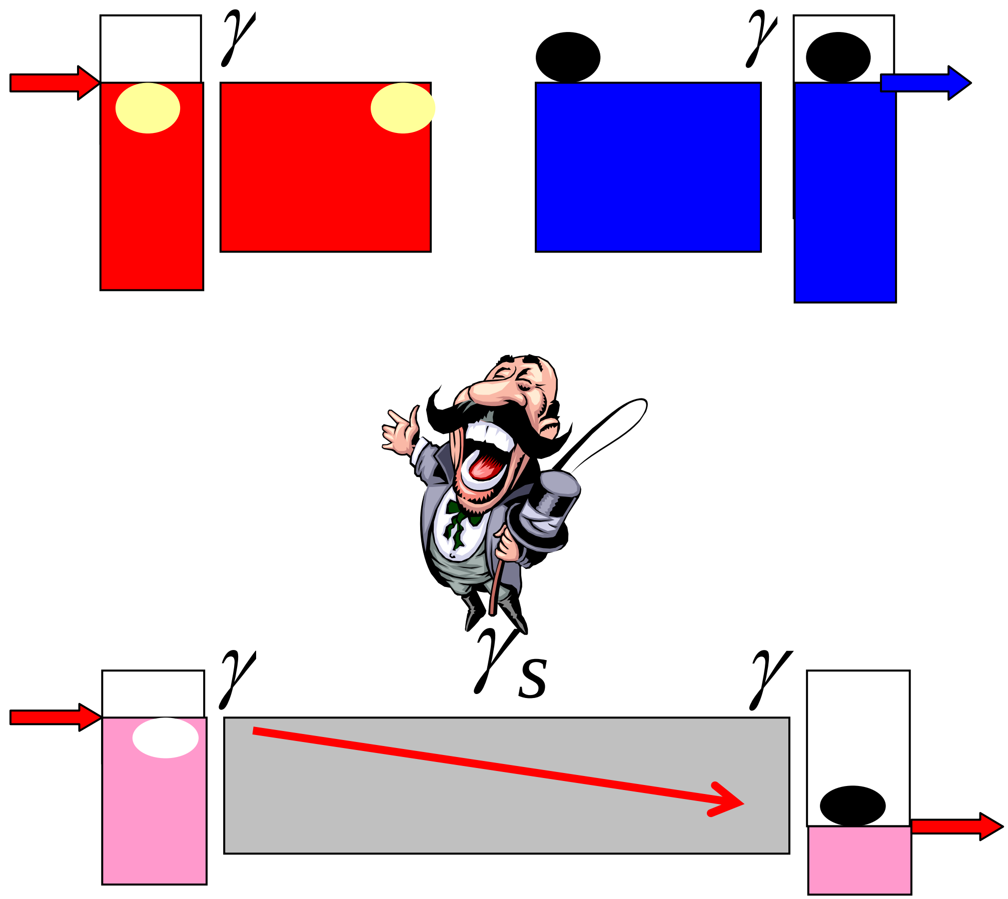
Maxwell's demon as an energy conversion device

Need two groups of states:

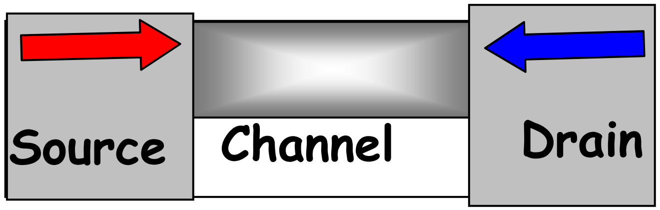
"Red"

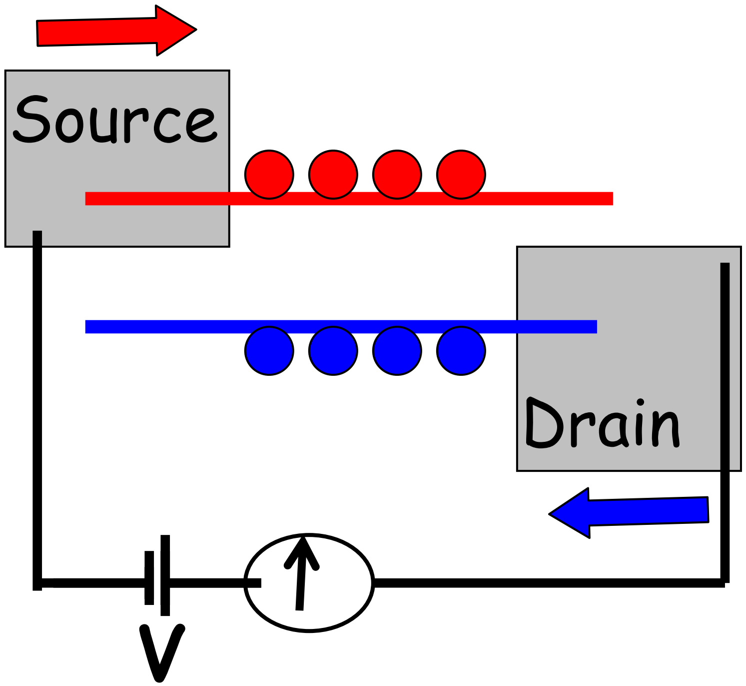
&

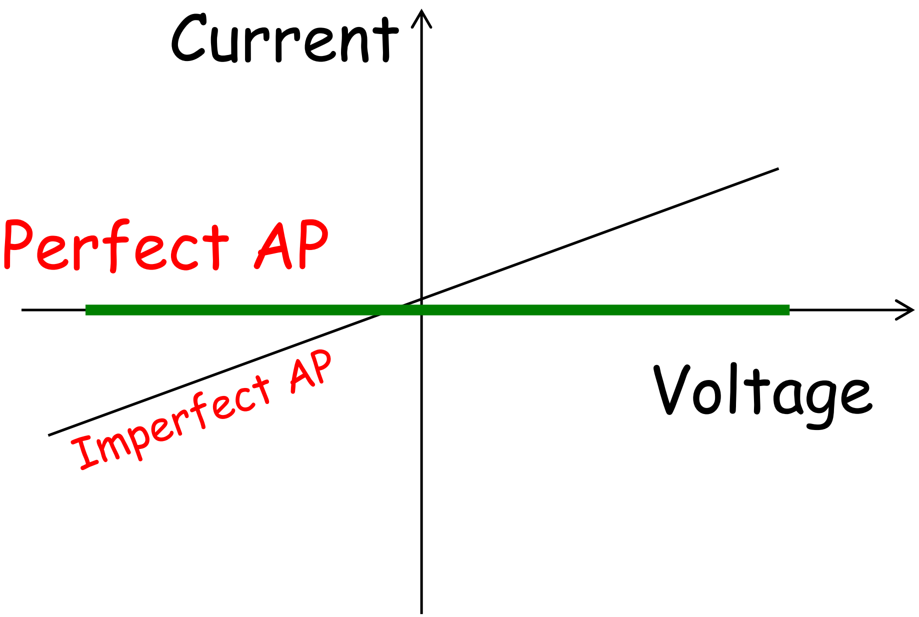
"Blue"



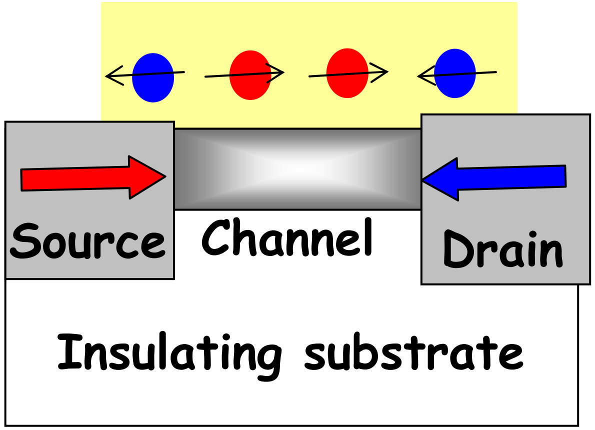
Anti-parallel (AP) Spin Valve

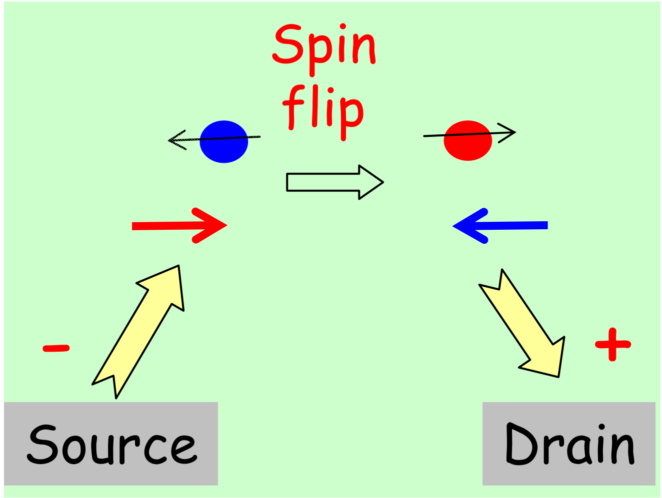


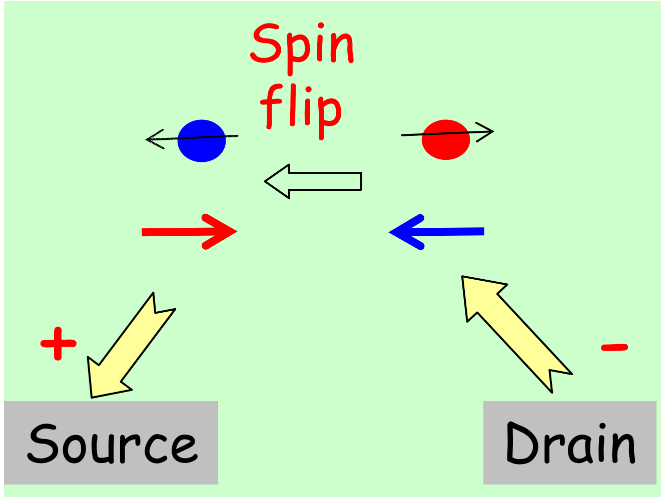


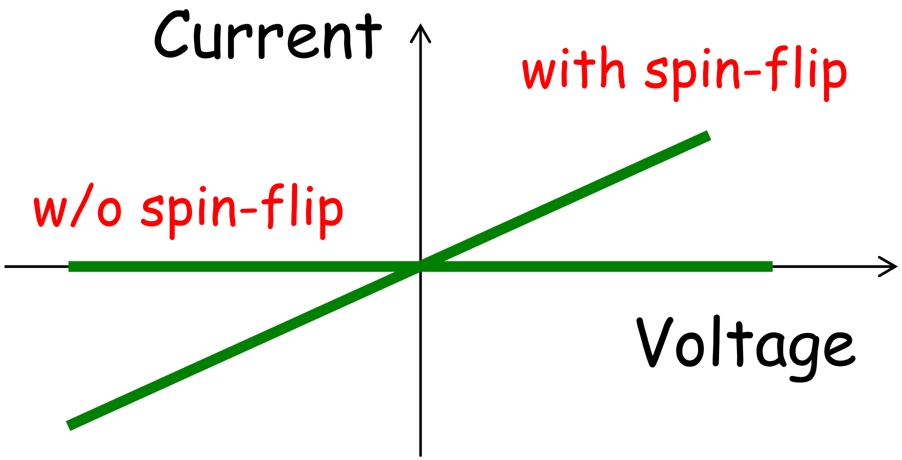


Perfect AP with Spin-flip Impurities

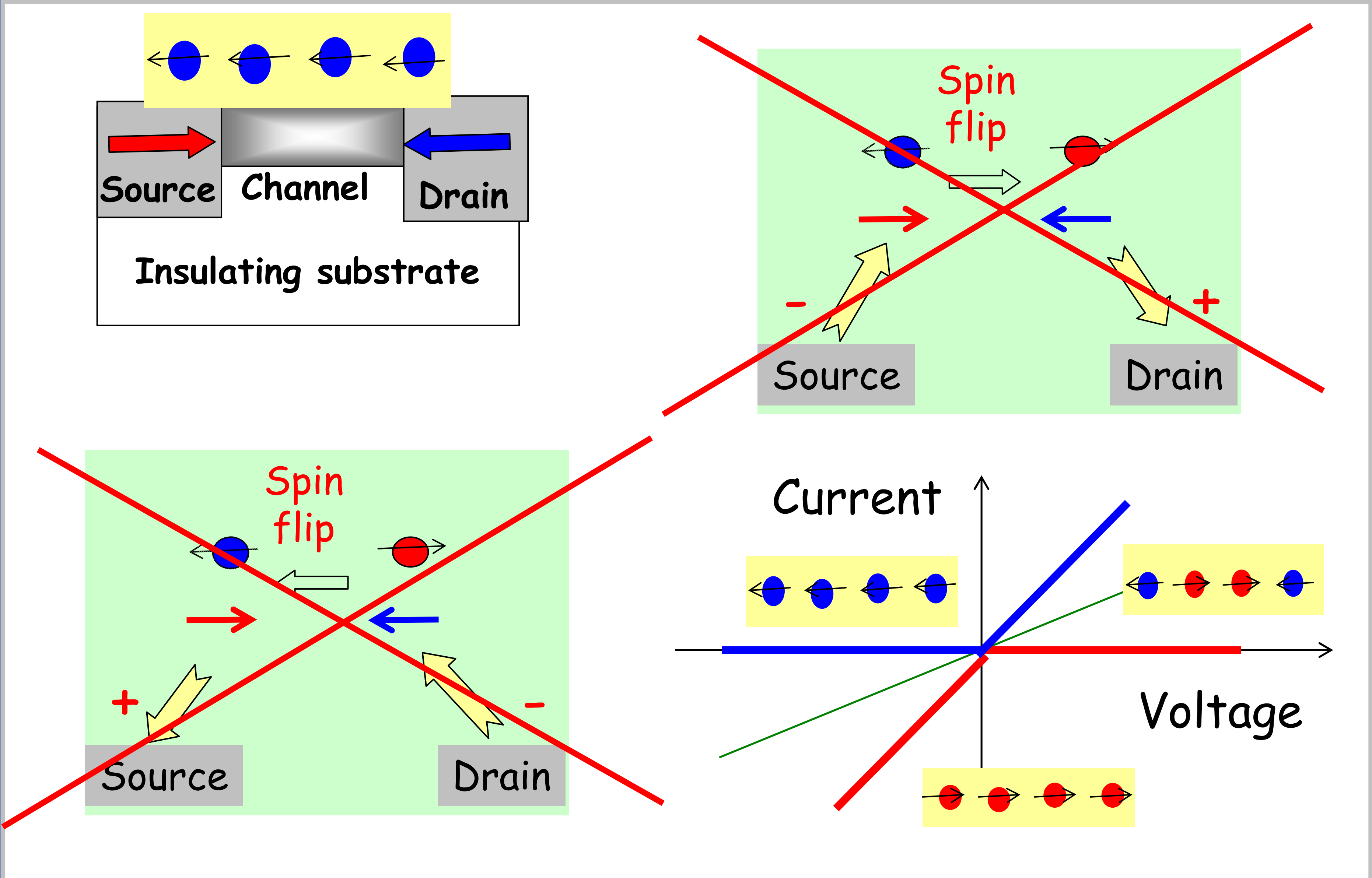




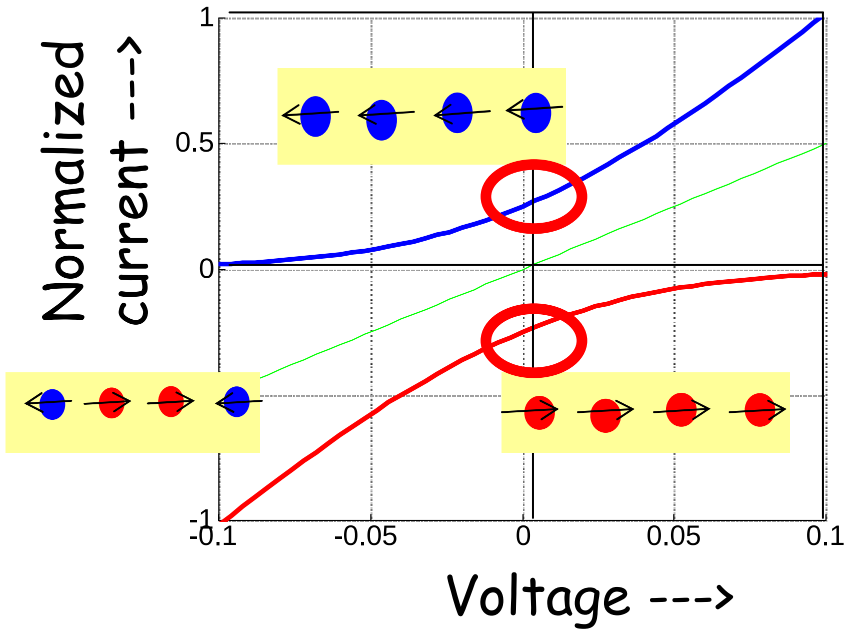


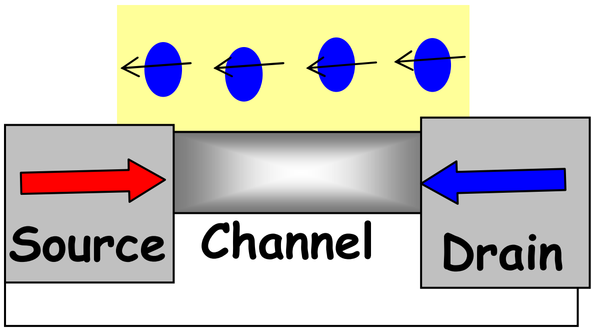


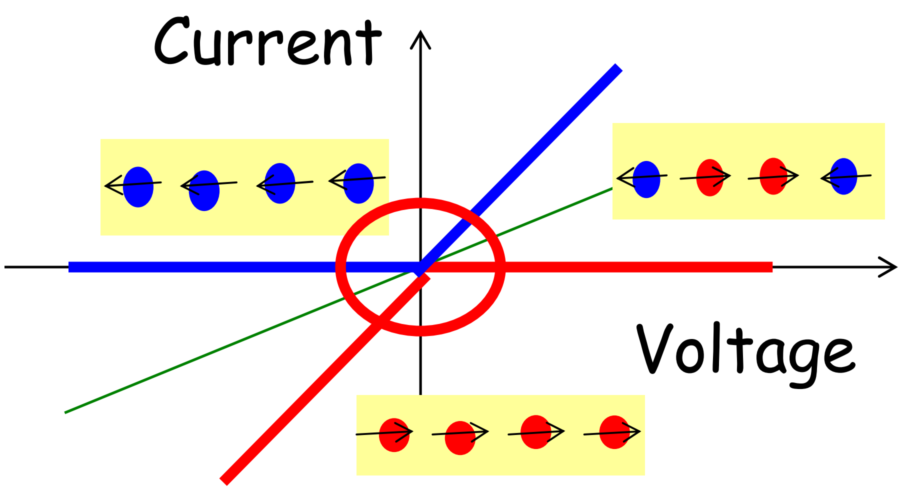
Perfect AP with Spin-polarized gate



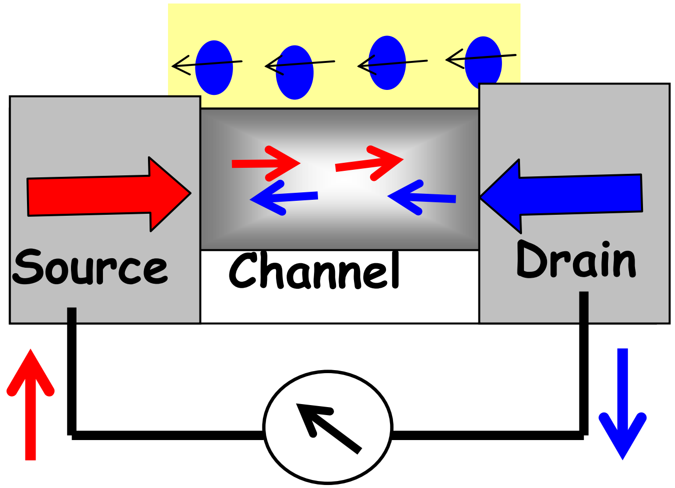
Current at zero voltage ! !

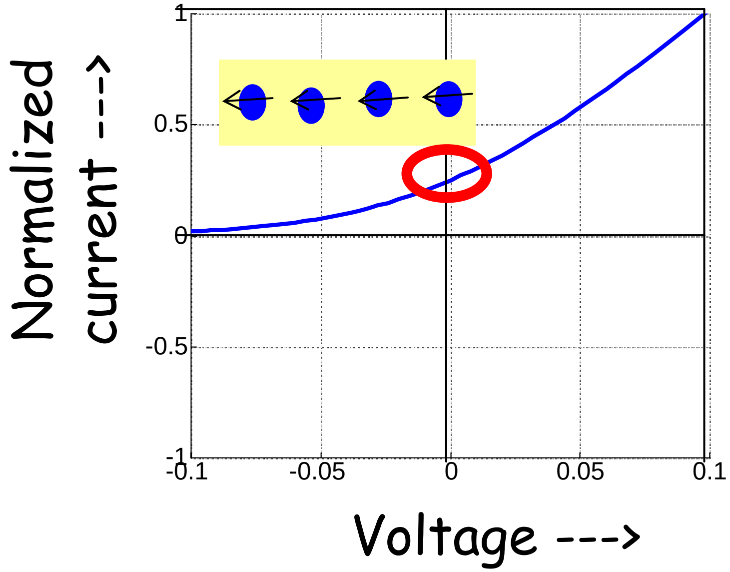


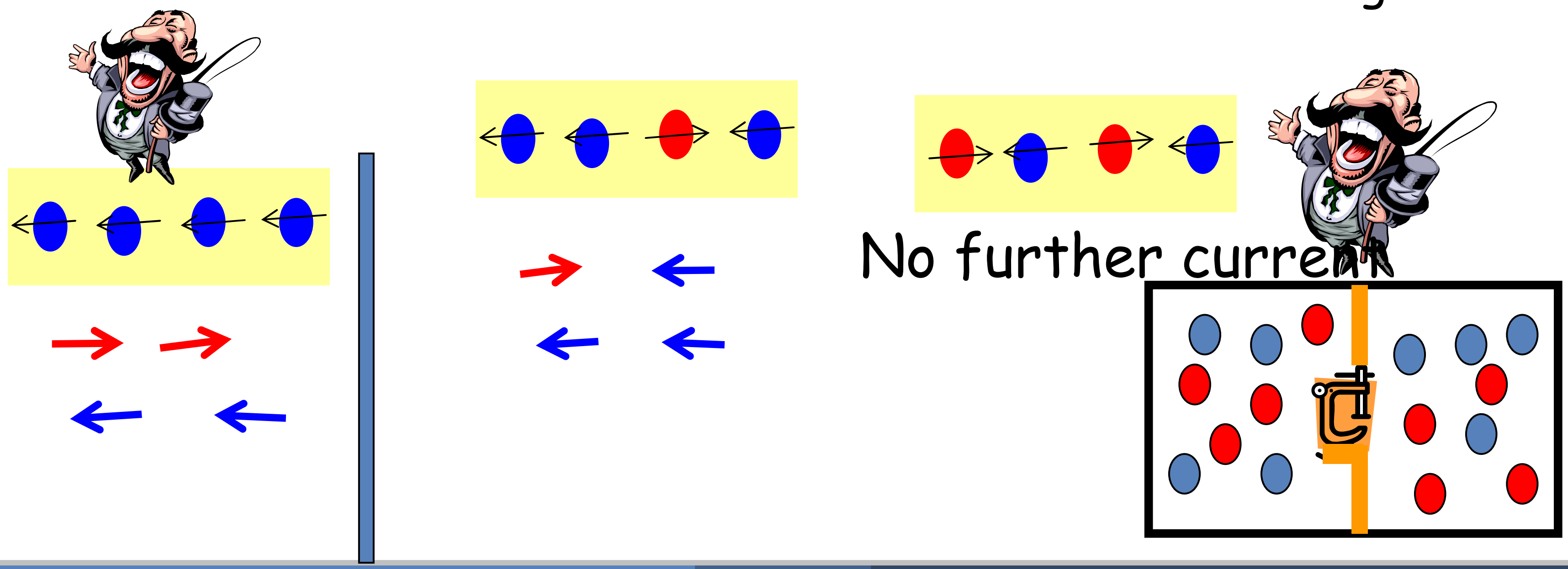




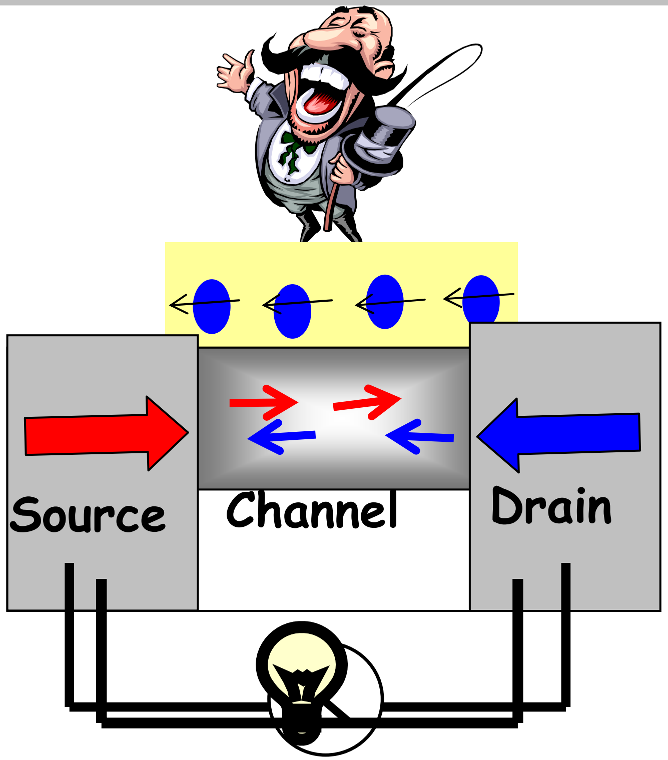
Device as a "demon"

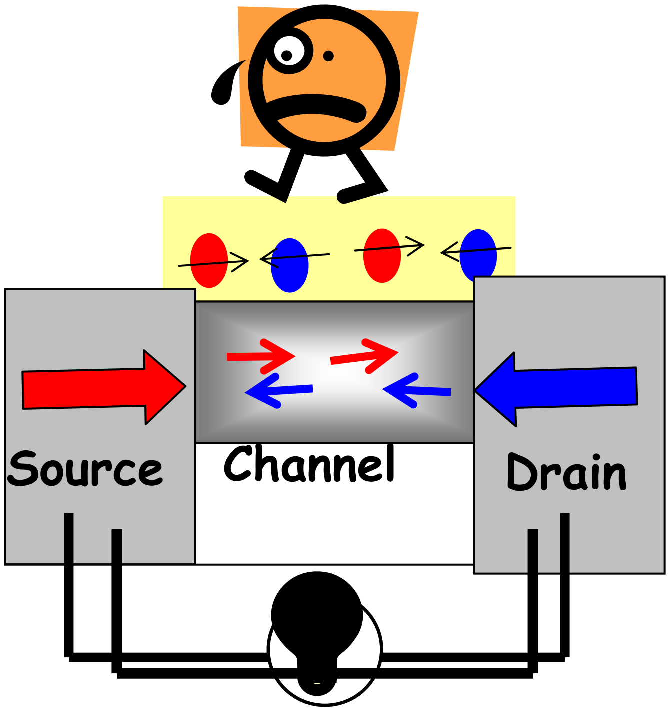




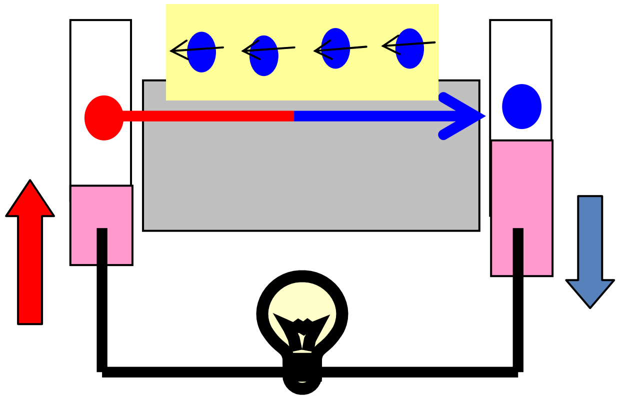


Where did the energy come from?

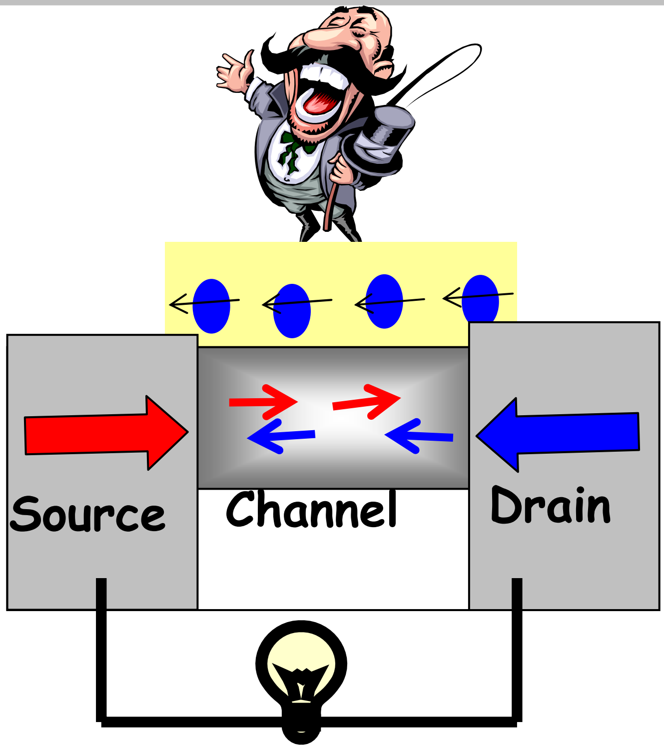


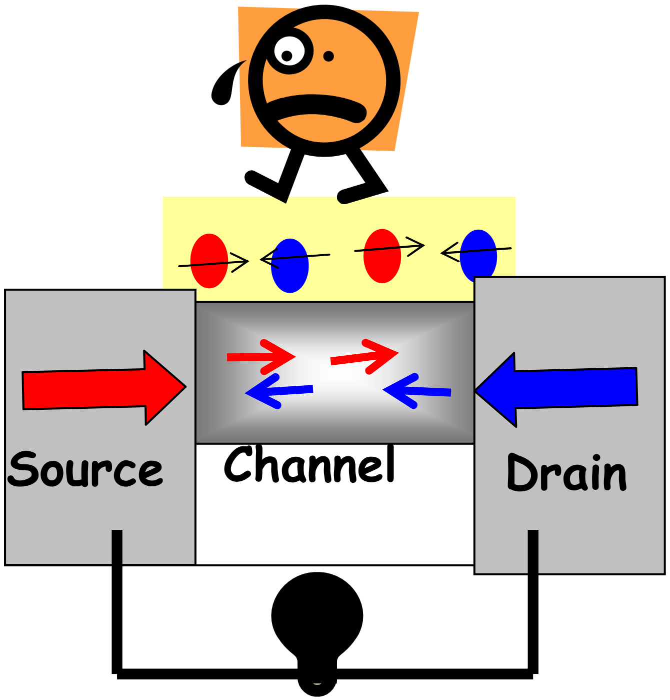


Answer: From the contacts



Second law ?





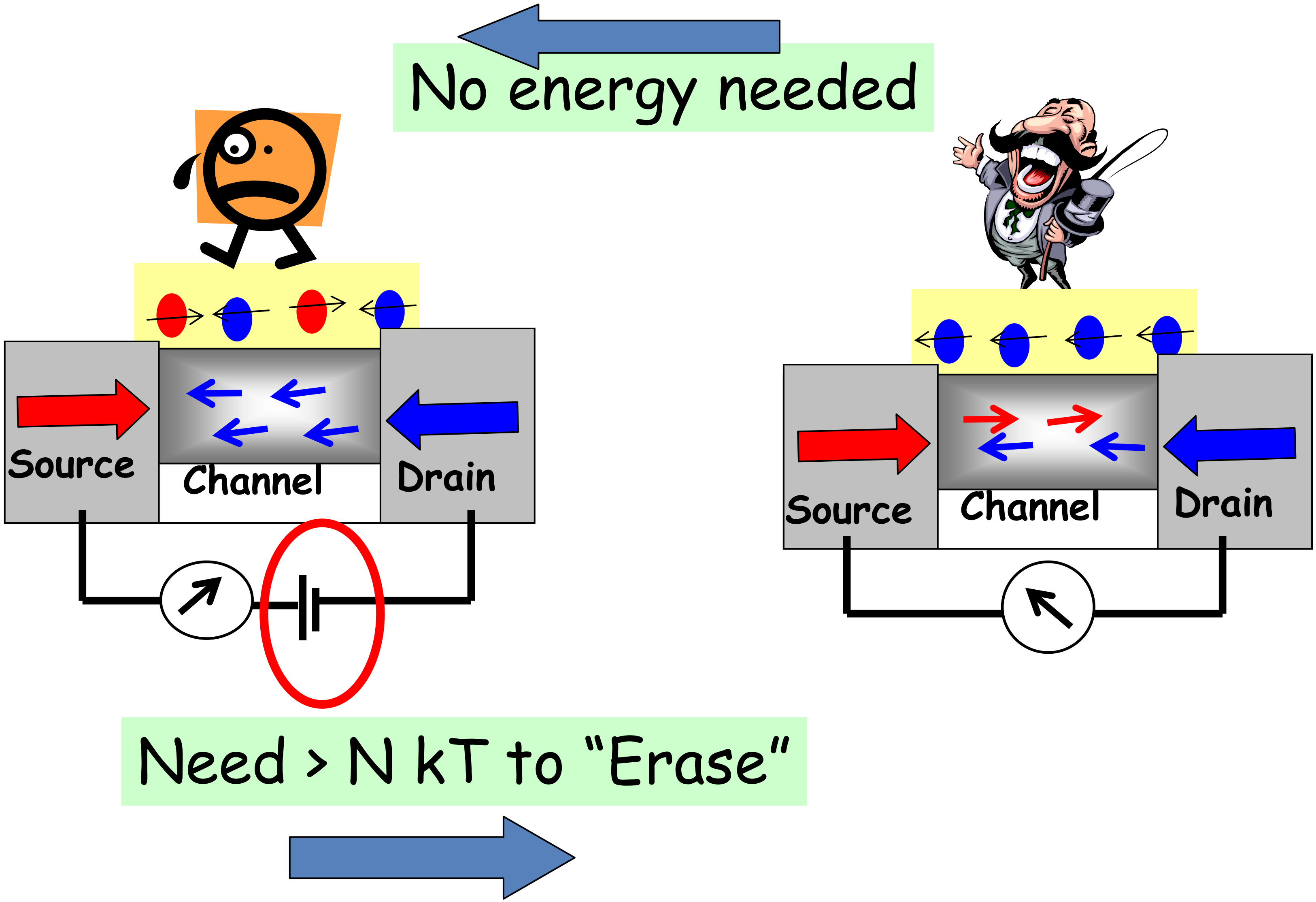
$S = 0$

$S = k \ln W$

$S = Nk \ln 2$

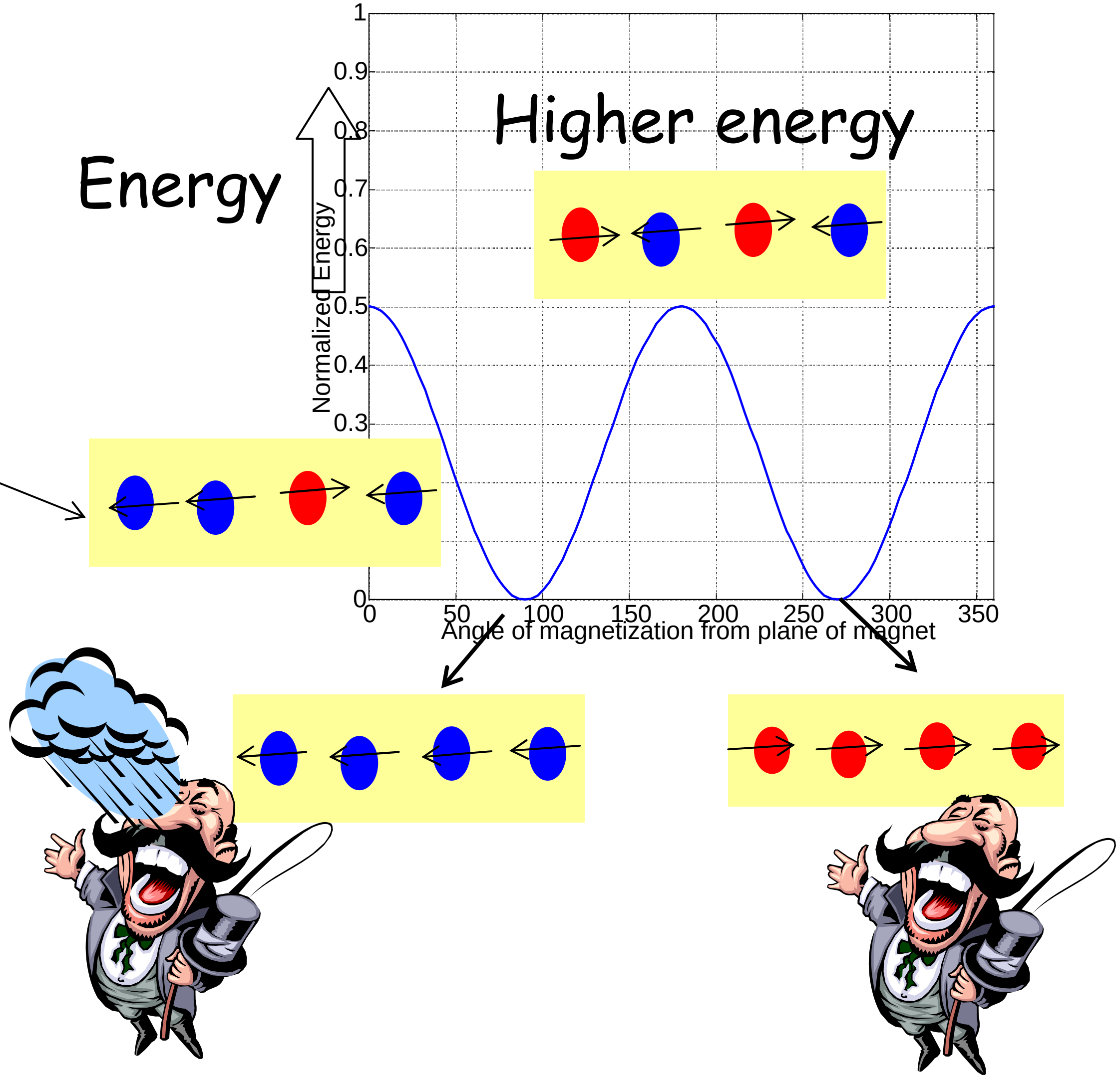
Energy upto $T \Delta S$ may be extracted

Resetting the demon takes energy

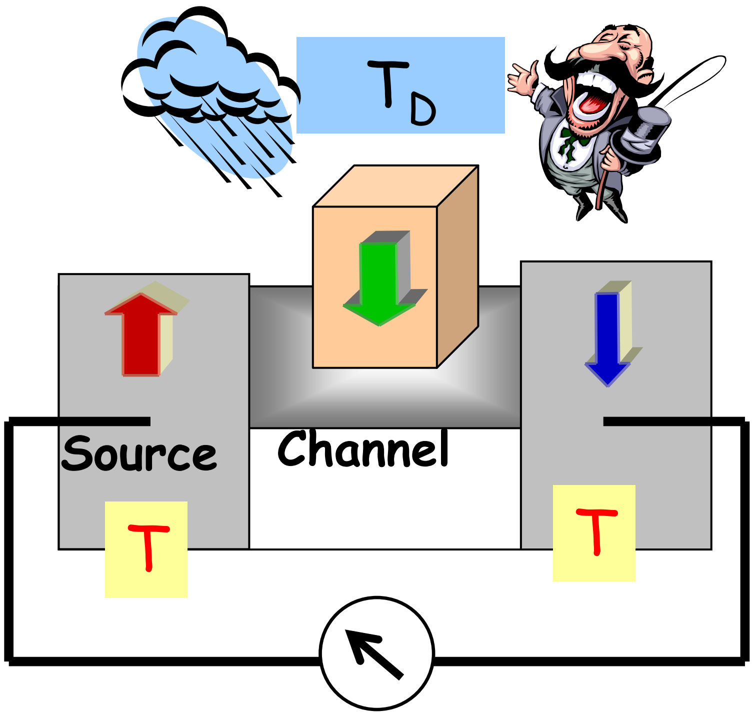


Nanomagnets : Bistable demons

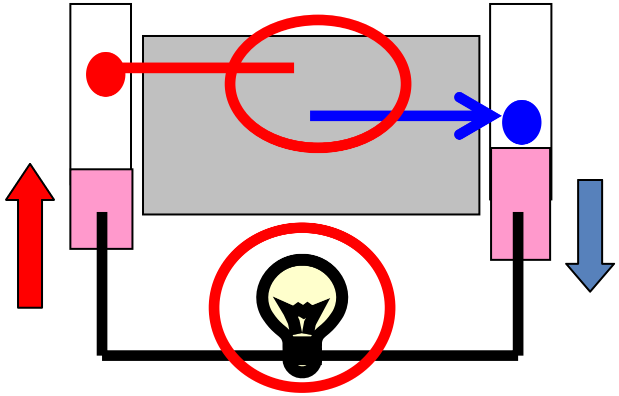
Flipping a spin costs energy



Nanoscale heat engine



Q_1: heat from contacts
Q_2: heat to "magnet"
$Q_1 - Q_2$: useful work

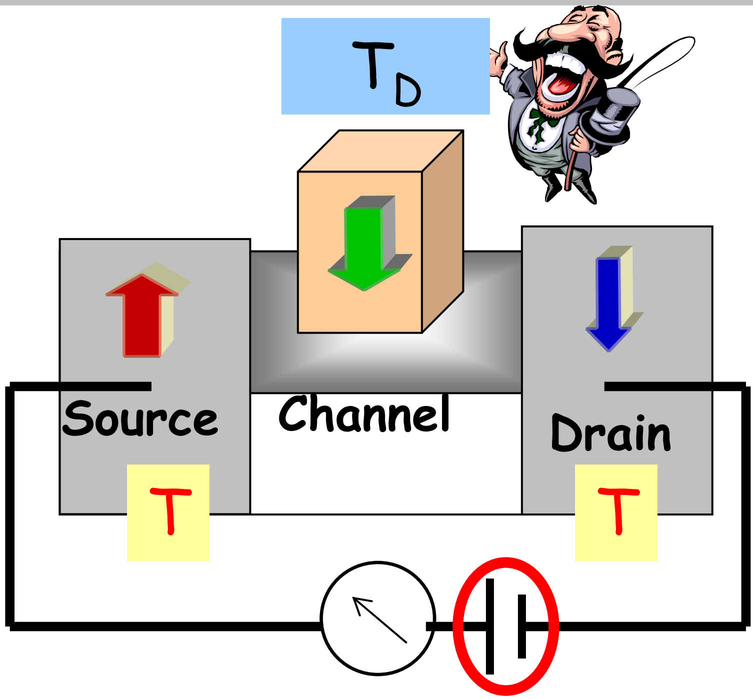


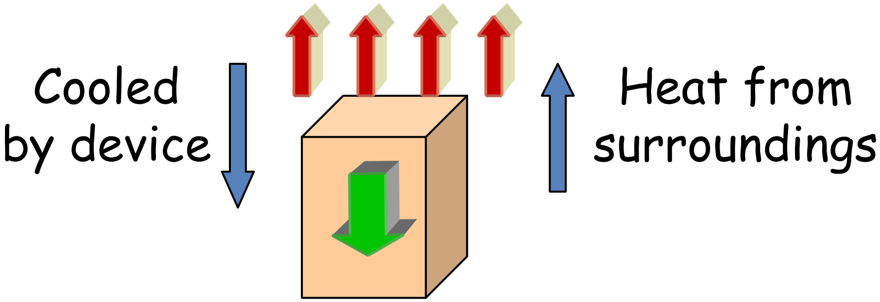
Carnot's principle

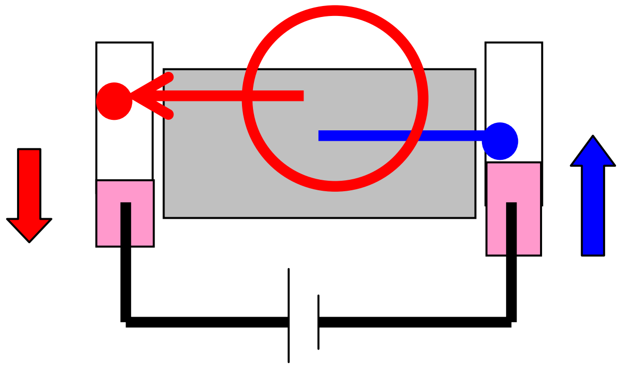
$$\frac{Q_1}{kT} < \frac{Q_2}{kT_D}$$

nanoHUB.org
online simulations and more

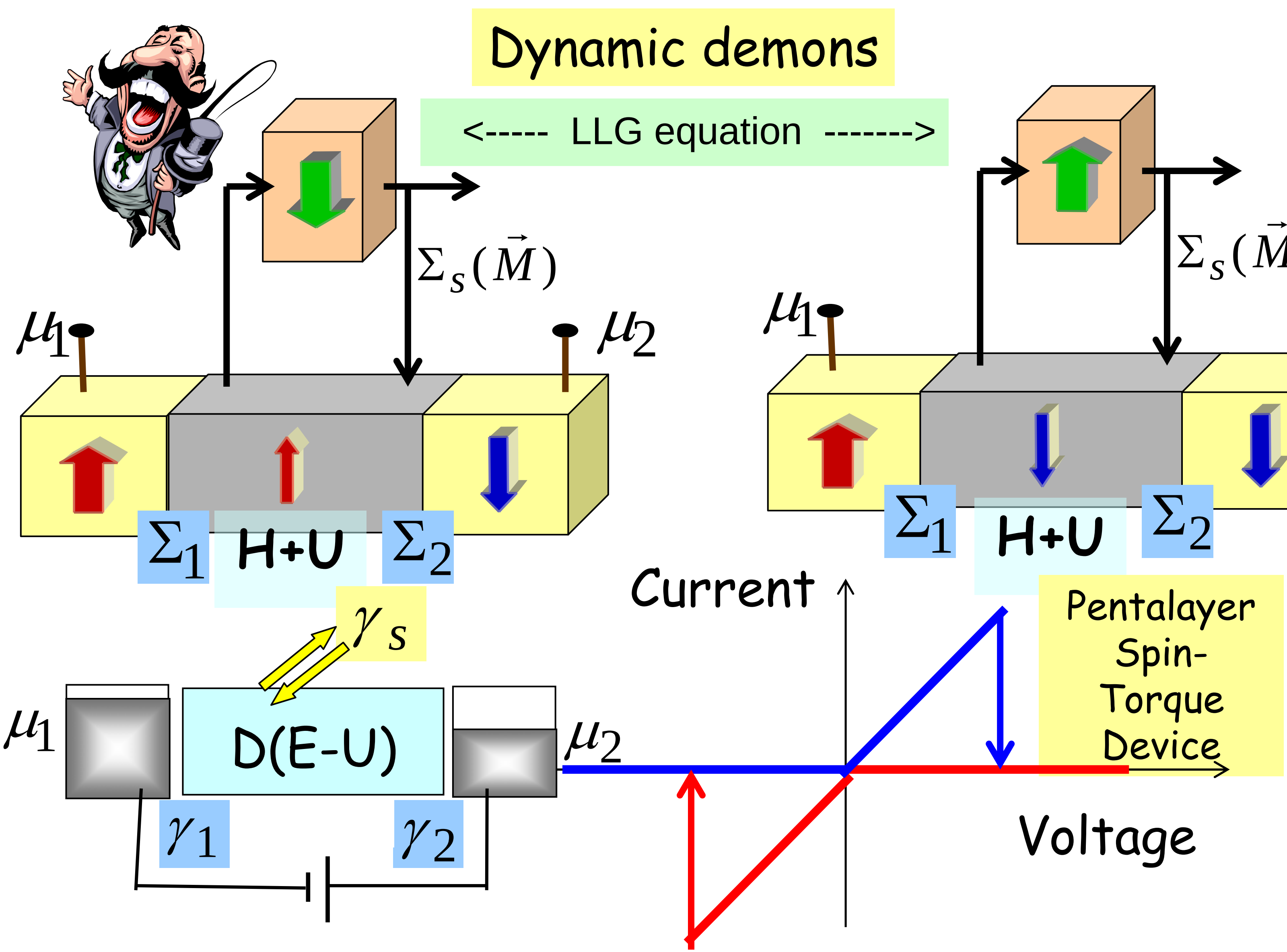
Nanoscale Refrigerator





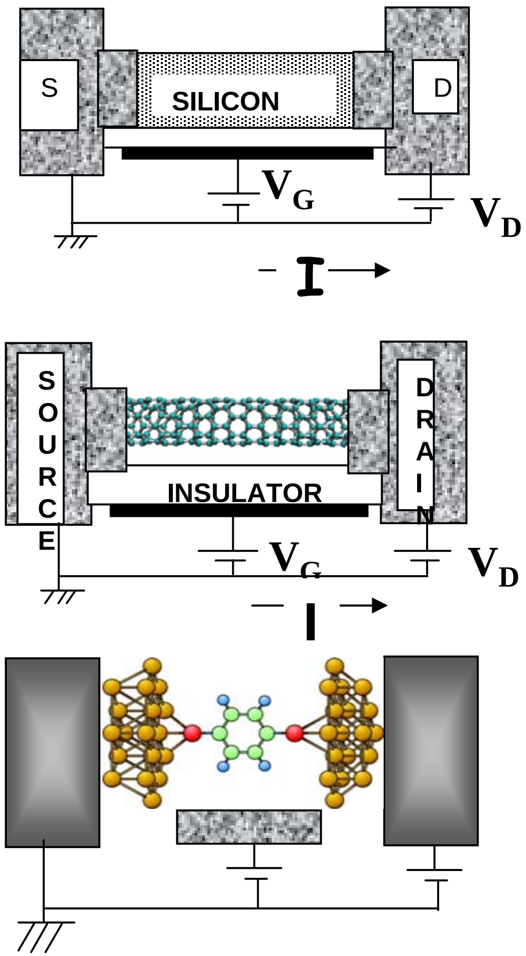


Back to the unified viewpoint



Quantum Transport far from Equilibrium

Materials



Transport Regimes

0.1 mm — Macroscopic dimensions

10 μm

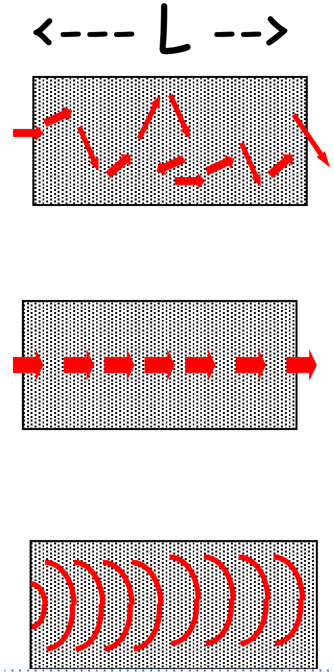
1 μm

0.1 μm

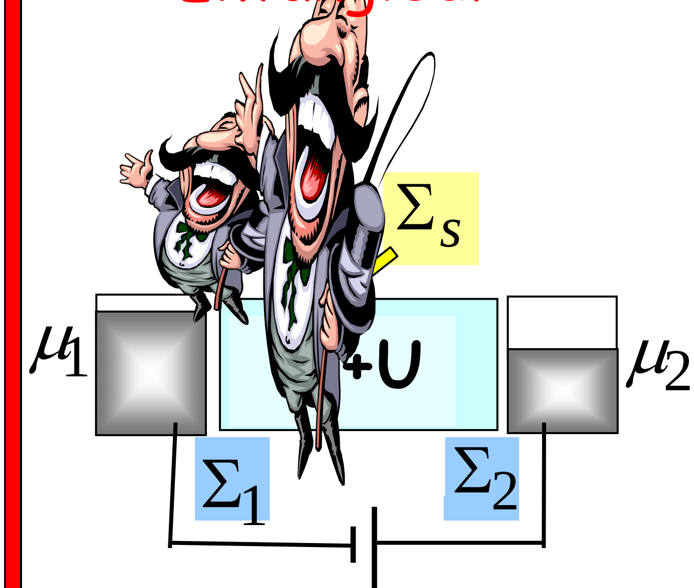
10 nm

1 nm

0.1 nm — Atomic dimensions



Correlated/ Entangled!



Reference:
For a detailed write-up see
arXiv:condmat/0704.1623

Correlated/Entangled "demon"