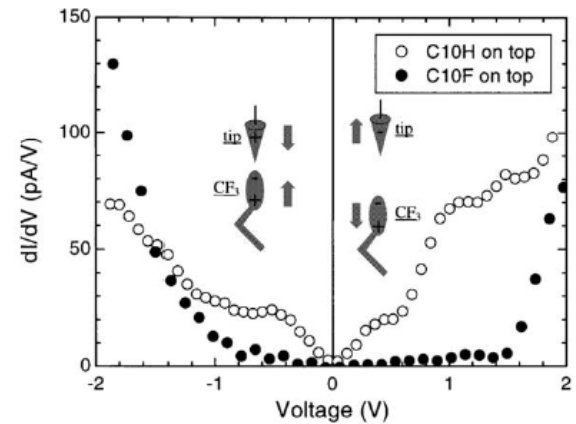
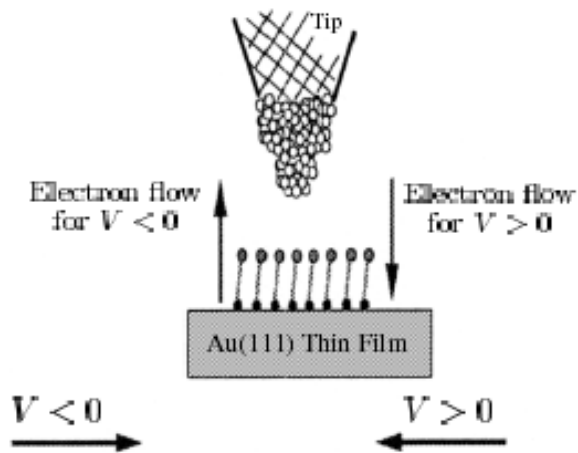
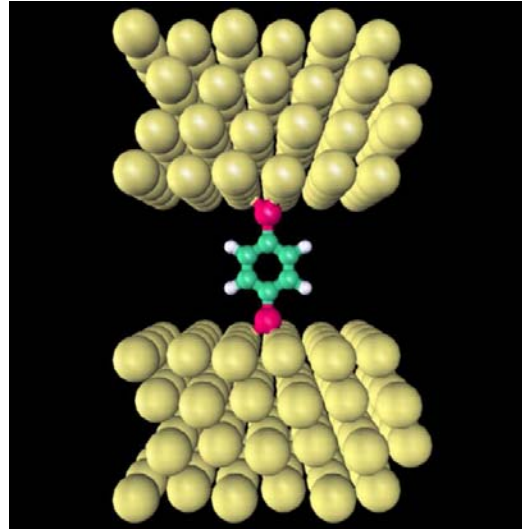


# Electron Transport and Dissipation in Nanoscale Devices

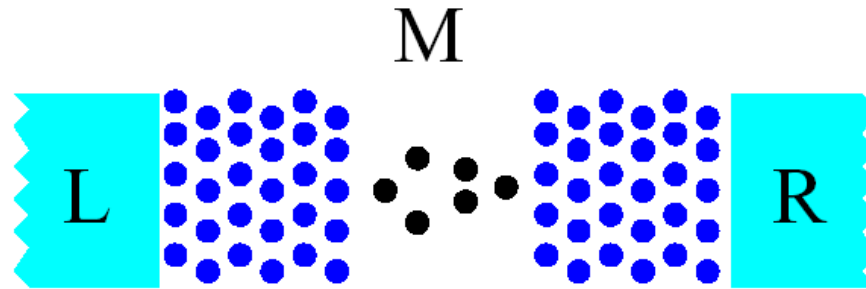
Roberto Car  
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# Nanoscale Electronics



From J. Pflaum et al. *Surface Science* **498**, 89 (2002)

# The standard approach at the meso/nano-scale: transport as a scattering problem

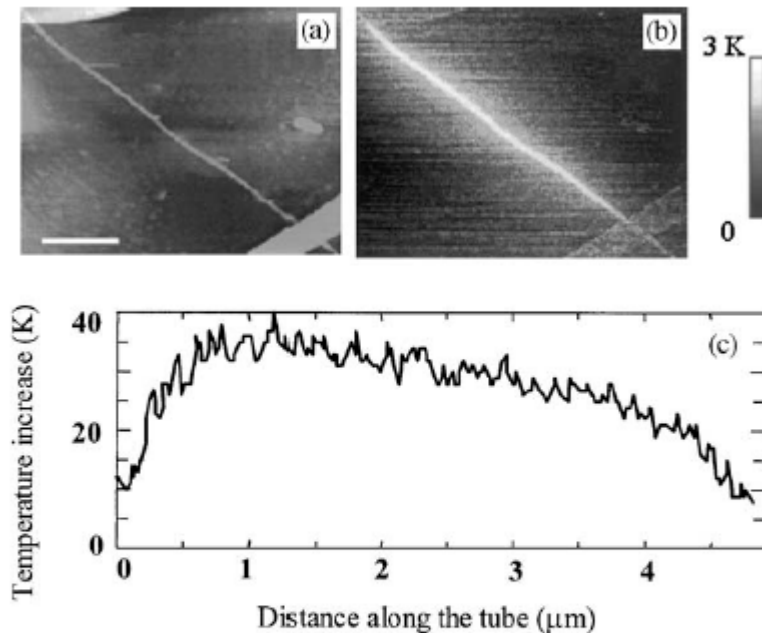


Landauer's formula relates  $I$  to  $V = \frac{\Delta\mu}{e}$

$$I = \frac{2e}{h} \int_{\mu_L}^{\mu_R} dE T(E)$$

**Ballistic transport:** no- inelastic scattering, no- acceleration

# At sufficiently high bias inelastic effects are often observed: e.g. local Joule heating in carbon nanotubes



from P.Kim, L.Shi, A. Majumdar, P.L. McEuen, *Physica B* **323**, 67-70 (2002)

Fig. 3. (a) Topographic image of a MWNT device. Scale bar represent 1  $\mu\text{m}$ . (b) the corresponding thermal signal simultaneously taken with (a). The applied bias voltage on the MWNT was 1 V and the current was 22  $\mu\text{A}$ . (c) Temperature profile along the tube axis.

More recent experiments indicate that heating starts at the contacts and is more prominent at the injection contact (private communication)

# **Boltzmann's equation, the standard approach for bulk transport, includes dynamics and dissipation**

$$\frac{df}{dt} = \left( \frac{\partial f}{\partial t} \right)_{field} + \left( \frac{\partial f}{\partial t} \right)_{collisions}$$

**Steady State:**

$$\left( \frac{\partial f}{\partial t} \right)_{field} = - \left( \frac{\partial f}{\partial t} \right)_{collisions}$$

$f \equiv f(x, p; t)$  is a classical probability distribution

# The challenge

When the dimensions of a device are comparable to the electron wavelength, the **semi-classical** Boltzmann equation should be replaced by a **quantum-mechanical** Liouville-Master equation for the reduced density operator describing a quantum system coupled to a heat bath

$$f \rightarrow S$$

$$\frac{dS}{dt} = -i[H, S] + \mathcal{C}[S]$$

**Steady State**  $i[H, S] = \mathcal{C}[S]$

# Master equation is derived from First-Principles

$$H_T = H + R + V$$

$$R = \sum_{\alpha} \omega_{\alpha} a_{\alpha}^{\dagger} a_{\alpha} = \int d\omega g(\omega) \omega a_{\omega}^{\dagger} a_{\omega}$$

$$V = \sum_i L_i F_i = \sum_{n,m,\alpha} \gamma_{n,m}^{\alpha} c_n^{\dagger} c_m a_{\alpha}^{\dagger} + h.c.$$

$$i \frac{\partial Z}{\partial t} = [H_T, Z]$$

Solve for the reduced density operator  $S(t) = \text{Tr}_R Z(t)$

# Important approximations

- treat  $V$  to 2<sup>nd</sup> order in perturbation theory
- assume that the harmonic bath is in thermal equilibrium
- make Markov approximation, i.e. **coarse-graining in time** so that on the time scale of system damping electron-phonon scattering processes are treated as instantaneous processes via Fermi's golden rule

$$\tau_c \ll t \ll T_R$$



# The collision operator

$$\mathcal{C}[S] = - \sum_{n,m} \Gamma_{m,n} \left( L_{n,m} L_{m,n} S + S L_{n,m} L_{m,n} - 2 L_{m,n} S L_{n,m} \right)$$

$$L_{n,m} = c_n^\dagger c_m \quad \Gamma_{n,m} = \begin{cases} |\gamma_{n,m}|^2 (\bar{n}_\omega + 1) g(\omega), & \omega = \varepsilon_m - \varepsilon_n \\ |\gamma_{n,m}|^2 \bar{n}_\omega g(\omega), & \omega = \varepsilon_n - \varepsilon_m \end{cases}$$

The phonon occupation numbers originate from the *fluctuations* of the bath (via the bath spectral functions)  
The difference between emission and absorption processes ensures *detailed balance*:

$$\frac{\Gamma_{n,m}}{\Gamma_{m,n}} = e^{\beta(\varepsilon_m - \varepsilon_n)}$$

Notice:  $S$  is an N-particle density operator

# Making the problem tractable

- **We adopt an effective single-particle formulation (like the time dependent Hartree approximation) that includes self-consistently electron-electron interactions**
- **We adopt periodic boundary conditions to deal with a closed (rather than an open) electronic system**

# Periodic Supercell Approach

*A ring geometry* allows current flow



...But a *static* uniform electric field breaks translational invariance

The difficulty is solved in a *dynamic* approach by adopting a different *gauge* for the electric field

**x-gauge**      $\mathcal{E} = -\nabla \varphi, \quad \varphi = -\mathcal{E} \cdot x$

**v-gauge**      $\mathcal{E} = -\frac{\partial A}{c \partial t}, \quad A = -c \mathcal{E} t$

The  $v$ -gauge corresponds to a *ring geometry* in which an electric current is induced by a magnetic flux

The electrons are subject to a steady electromotive force: coupling to a heat bath prevent them from accelerating indefinitely

## The resulting Liouville-Master equation (in the time-dependent Hartree approximation)

$$\dot{S}_{n,m} = -i \sum_p \left( H_{n,p}^\varepsilon(t) S_{p,m} - S_{n,p} H_{p,m}^\varepsilon(t) \right) + \left( \delta_{n,m} - S_{n,m} \right) \sum_p \left( \Gamma_{n,p} + \Gamma_{m,p} \right) S_{p,p} - S_{n,m} \sum_p \left( \Gamma_{p,n} + \Gamma_{p,m} \right) \left( 1 - S_{p,p} \right)$$

Here: 
$$H^\varepsilon(t) = \frac{(p - \varepsilon t)^2}{2} + U_0(x) + \int dx' \frac{\delta n(x'; t)}{|x - x'|}$$

A form that includes exchange-correlation effects can be derived within Time-Dependent Current Density Functional Theory

The electric field is systematically “gauged” away to avoid indefinite “growth” of the Hamiltonian

The transition probabilities are given by:

$$\Gamma_{n,m} = \begin{cases} |\gamma_{n,m}|^2 (\bar{n}_\omega + 1) g(\omega), & \omega = \varepsilon_m - \varepsilon_n \\ |\gamma_{n,m}|^2 \bar{n}_\omega g(\omega), & \omega = \varepsilon_n - \varepsilon_m \end{cases}$$

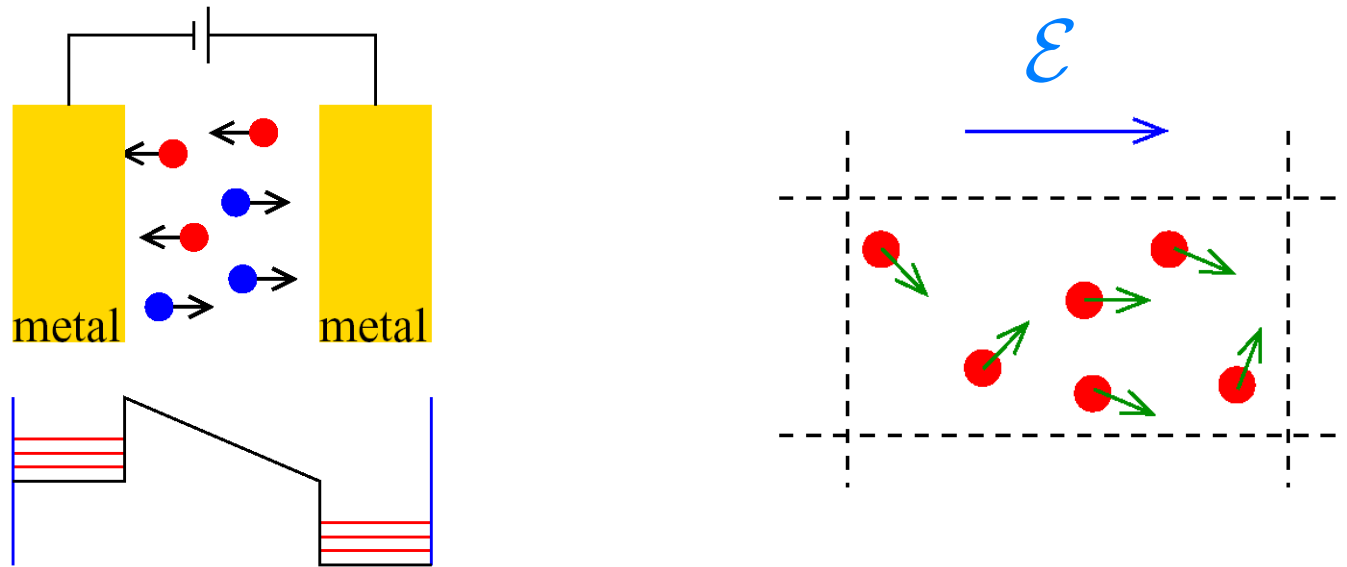
The difference between emission and absorption processes ensures *detailed balance*:

$$\frac{\Gamma_{n,m}}{\Gamma_{m,n}} = e^{\beta(\varepsilon_m - \varepsilon_n)}$$

This guarantees that in absence of external electromotive force the equilibrium electron distribution is the Fermi Dirac distribution

$$\dot{S}_{n,n} = (1 - S_{n,n}) \sum_p \Gamma_{n,p} S_{p,p} - S_{n,n} \sum_p \Gamma_{p,n} (1 - S_{p,p}) = 0$$

# This is analog to **Non Equilibrium Molecular Dynamics (NEMD)** in a classical context



System can be modeled with **periodic boundary conditions** plus coupling to a thermostat

# A simple application: a 1D DBRTS

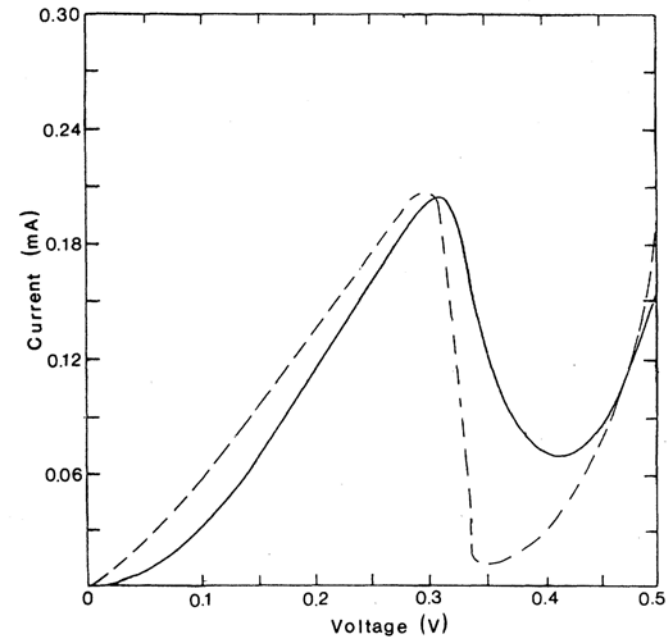
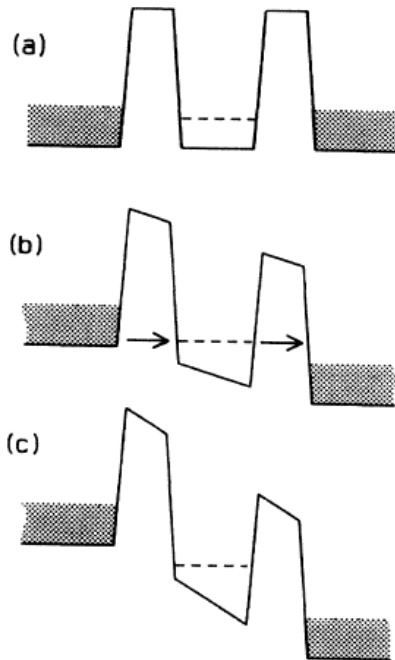


FIG. 2. Experimental (solid) and theoretical (dashed)  $I$ - $V$  curves for a resonant-tunneling diode. The theoretical curve is calculated by the simple tunneling model.



Our model: a 1D wire (flat potential) in contact with a double barrier resonant tunneling structure in a ring geometry

We adopt a simple model for the e-ph coupling:

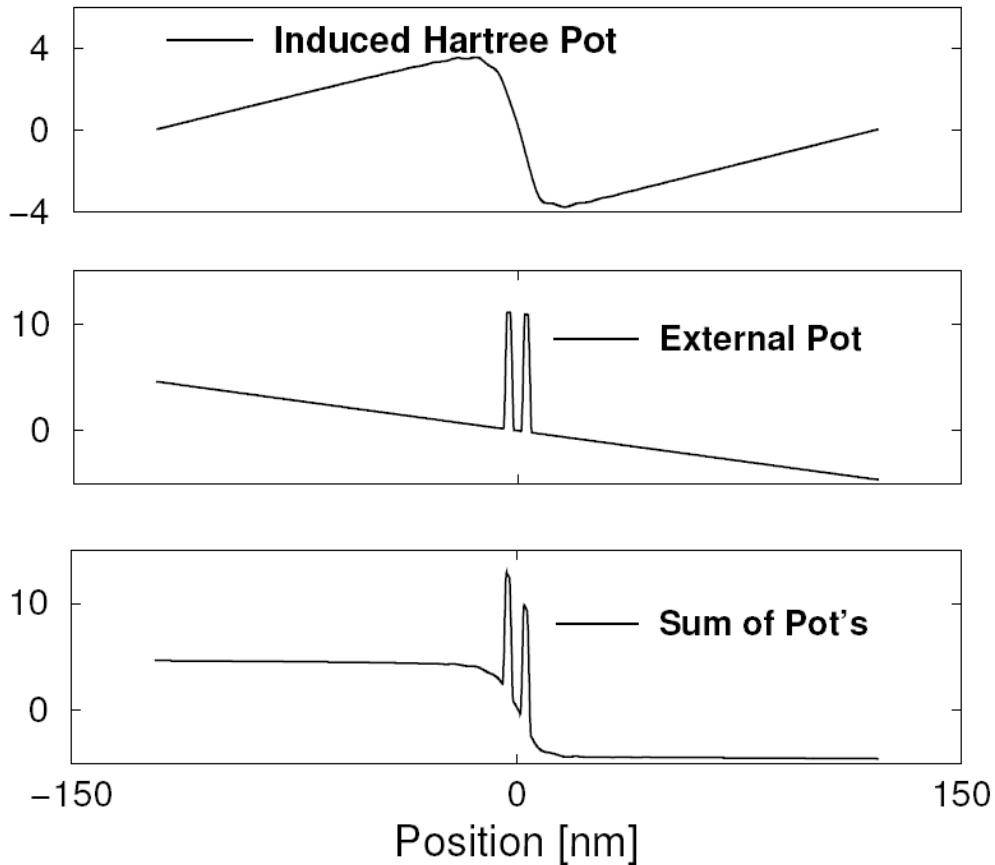
$$\Gamma_{n,m} = \begin{cases} |\gamma|^2 (\bar{n}_\omega + 1) \omega^2, & \omega = \varepsilon_m - \varepsilon_n \\ |\gamma|^2 \bar{n}_\omega \omega^2, & \omega = \varepsilon_n - \varepsilon_m \end{cases}$$

We study the steady state behavior:

$$\frac{dS_{n,m}}{dt} = 0$$

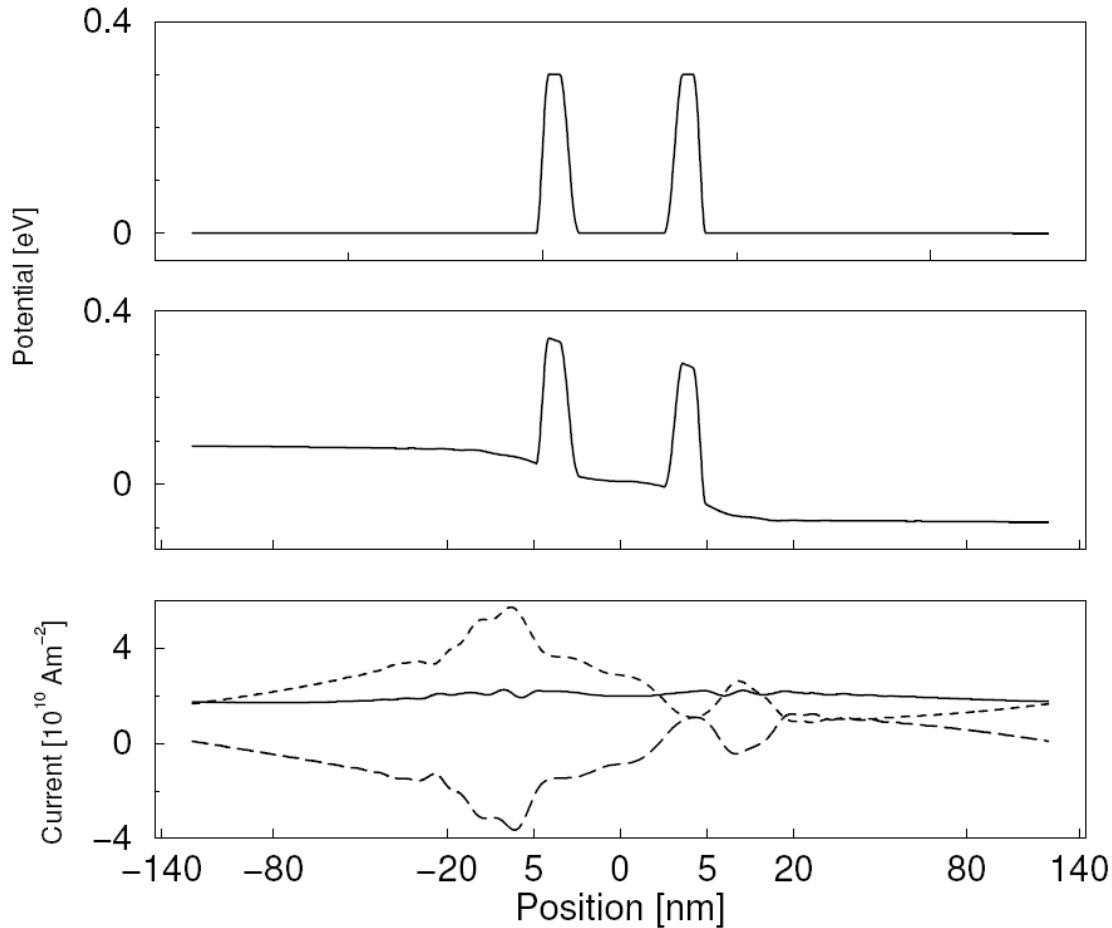


## Tunneling Barrier Potentials



The external field is represented here by a scalar potential varying linearly along the wire.

This is the position gauge, but the calculations are performed in the velocity gauge in which the field is represented by a vector potential varying linearly in time.



On the coarse grained time scale of Markovian dynamics the

physical current is  $j(x;t) \equiv j_H(x;t) + j_C(x;t)$

$$j_H(x) = Tr\{S\hat{J}(x)\}, \quad j_C(x) = Tr\{\mathcal{D}(S)\hat{J}(x)\}, \quad \hat{J}(x) = \frac{1}{2}[\hat{p}\delta(x - \hat{x}) + \delta(x - \hat{x})\hat{p}]$$

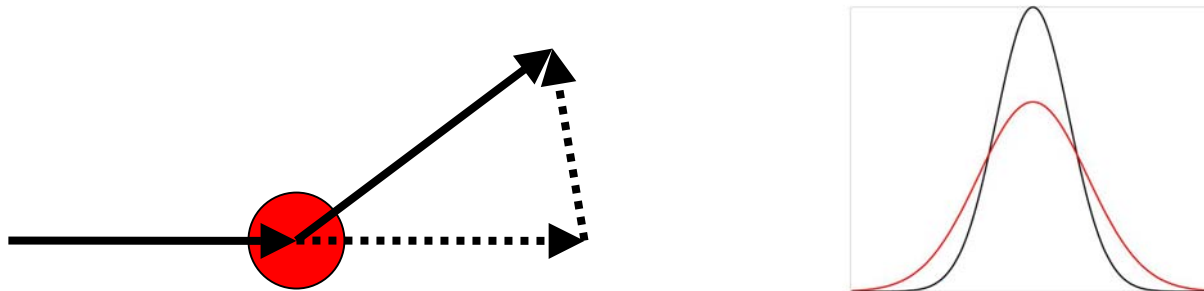
# The current due to collisions with the bath

$$\bar{j}_c(\mathbf{x}, t) = \lim_{t_0 \rightarrow t} \frac{1}{\Delta t} \int_{t_0}^t dt' \text{Tr} \{ (S(t') - S_H(t')) \mathbf{J}(\mathbf{x}) \}$$

- It is a coarse grained current
- The difference between  $S(t')$  and  $S_H(t')$  is calculated to leading order of perturbation theory
- Any dependence on  $t_0$  disappears (Markov approximation)

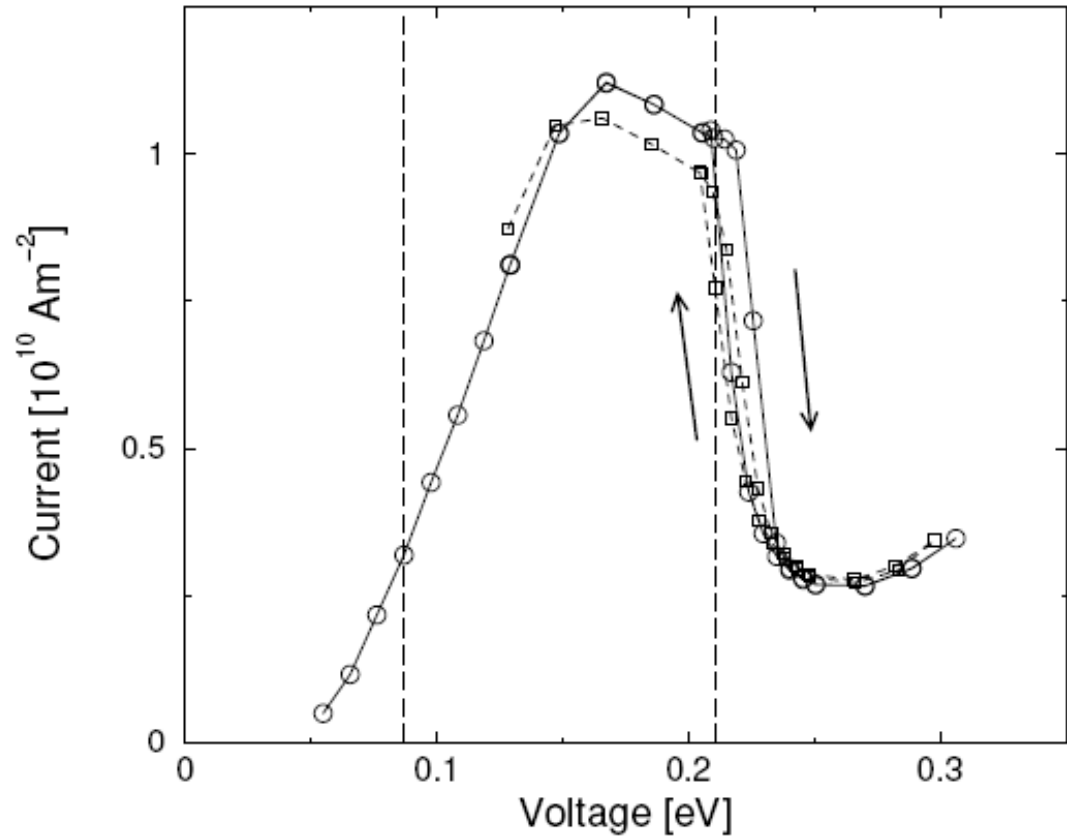
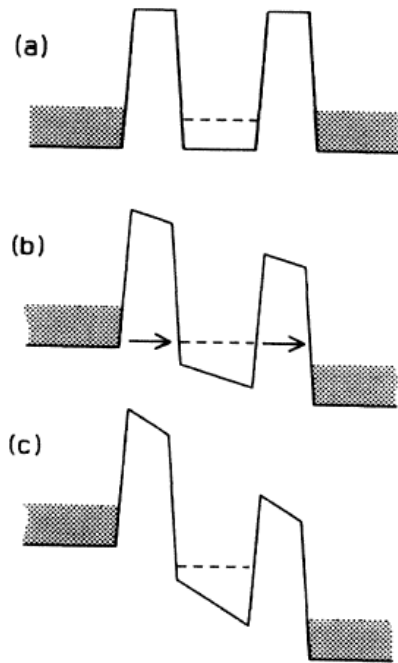
The bath contribution to the current is a *quantum effect* absent from classical master equations (e.g. Fokker-Planck, Boltzmann)

In classical physics momentum and position commute. In quantum mechanics collisions that change the momentum also change the position.

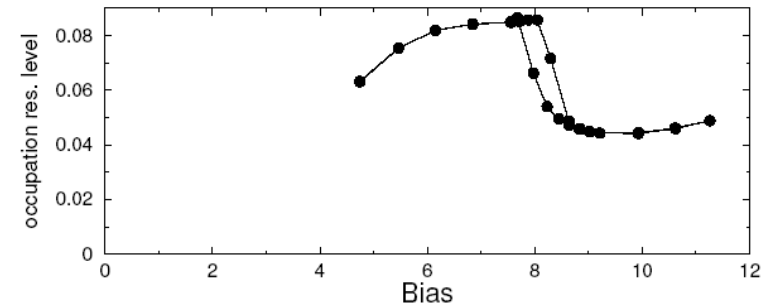
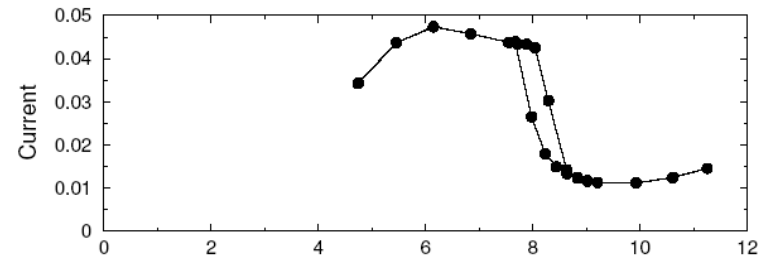
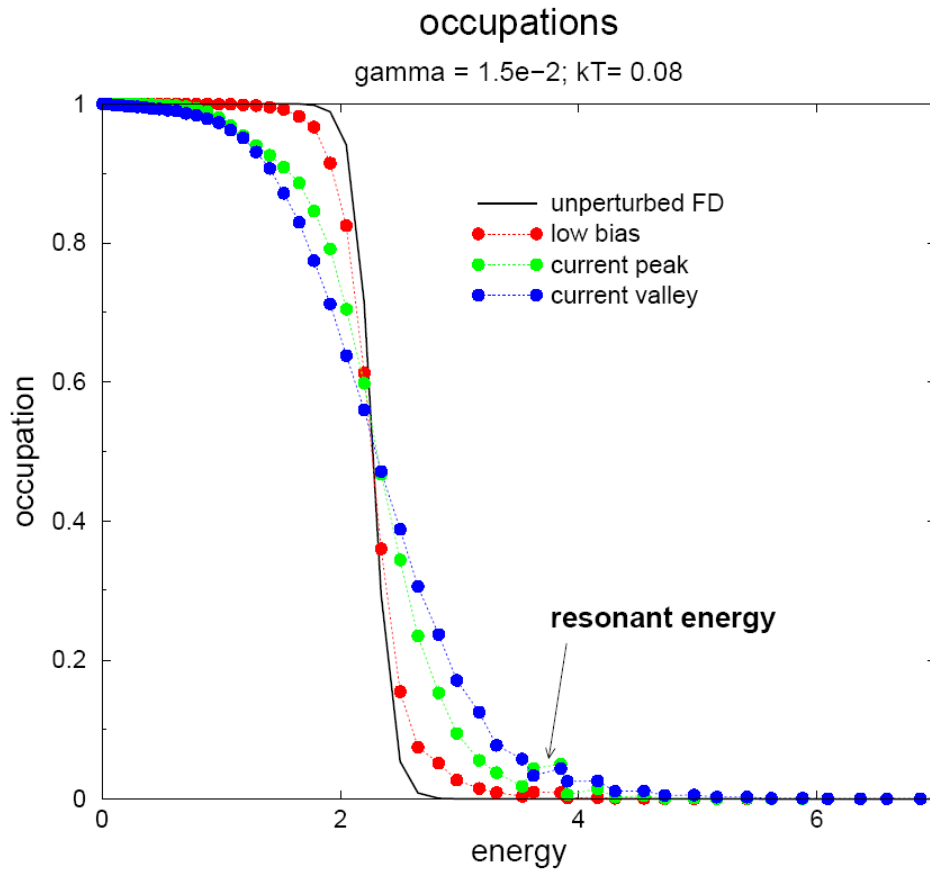


The effect is present when the system is inhomogeneous on the scale of the electron wavelength (*nano effect*)

# *I-V* characteristics

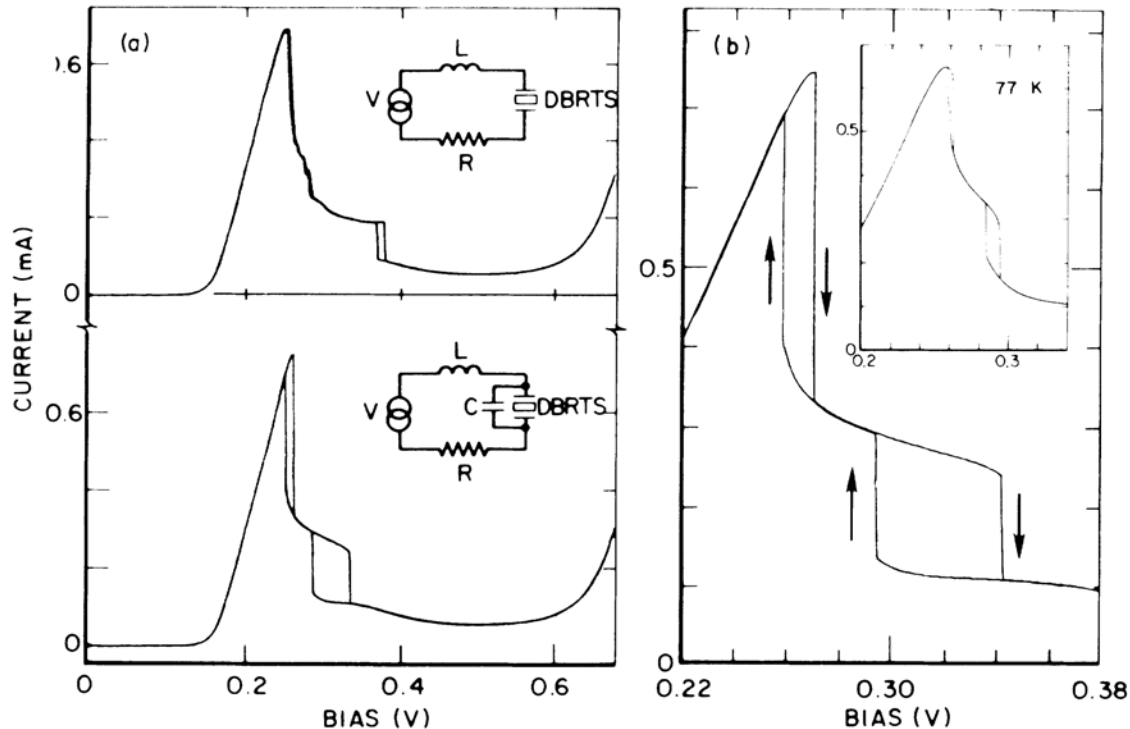


# Deviation from equilibrium



# Intrinsic bistability is observed experimentally

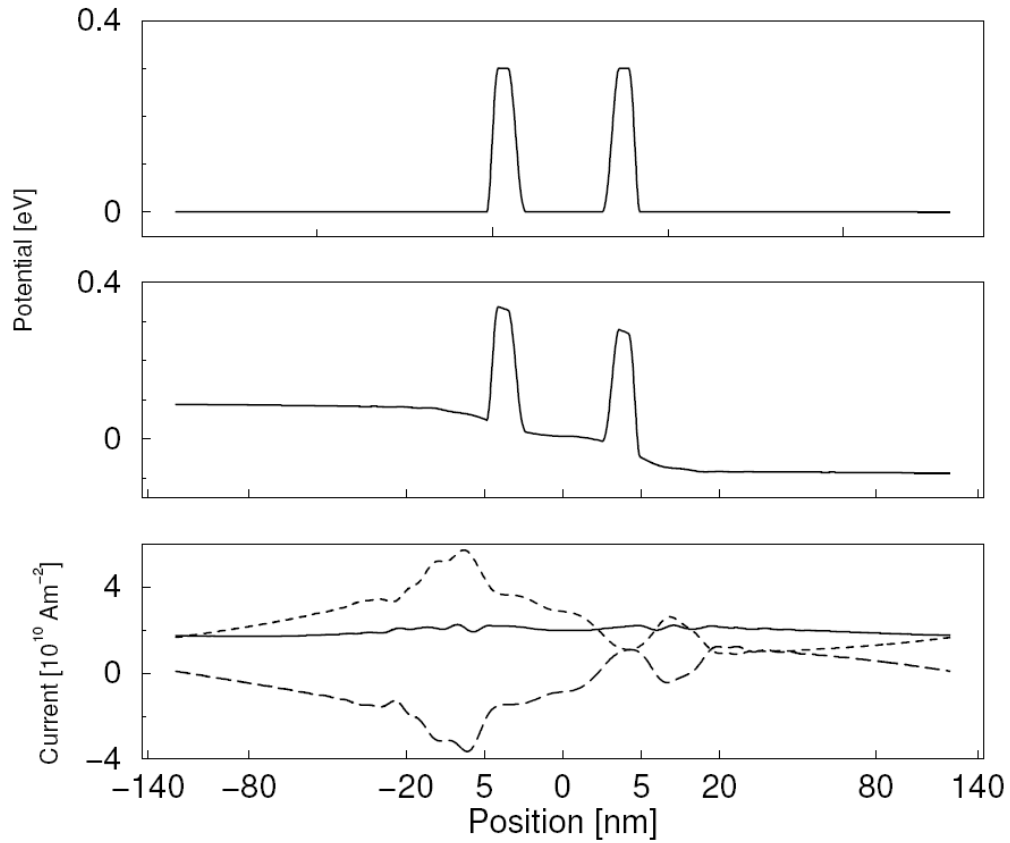
A Double Barrier Resonant Tunneling Structure can be realized with GaAs-AlAs heterostructures



(from Goldman, Tsui, Cunningham, *PRL* 58, 1256 (1987))



# Local Joule Heating

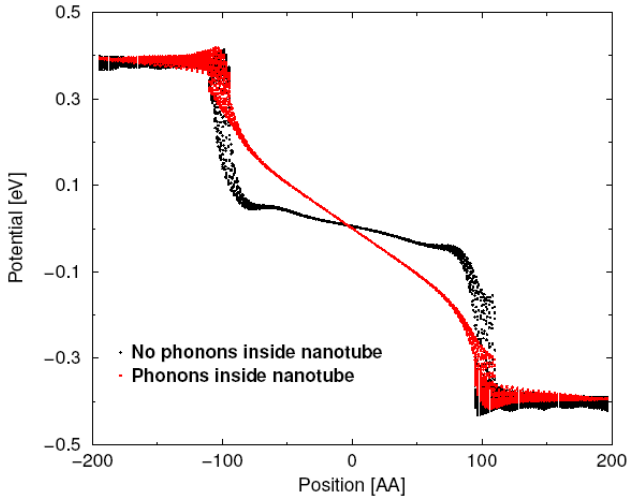
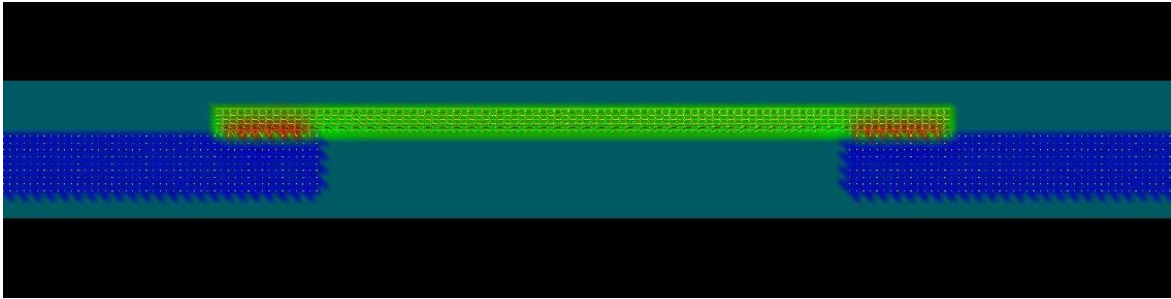


At steady state the injected power is  $W = \int dx \mathcal{E} \cdot j_H(x) = \int dx \mathcal{E} \cdot (j - j_c(x))$

# Perspectives

- Calculations on realistic models (real atoms, molecules and contacts) are possible by exploiting the flexibility of supercell geometries and of electronic structure codes based on DFT
- It will be feasible to use realistic phonon models and electron-phonon couplings
- The approach can be used to study dynamic phenomena within the limits of: (1) average density matrix dynamics, (2) Markov approximation.

# Tight-binding model: an intermediate level of approximation



# Acknowledgements

- Work in collaboration with Ralph Gebauer (ICTP, Trieste)
- Realistic electronic structure implementation under way (S. Piccinin and R. Gebauer)
- Work on Time Dependent Current Density Functional Theory and Master equations in collaboration with K. Burke (Rutgers)
- Funding by DOE, ONR, and NSF.