

Title: Fundamental Aspects of Transport in Condensed Matter and Atomic Physics

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URL: <http://pirsa.org/12030067>

Abstract: I will discuss some of the most basic questions in fermionic and bosonic transport, such as the conditions for the existence of a steady-state current, its uniqueness, the role of interactions and spin statistics, its entanglement entropy, etc. This will lead me to introduce an alternative viewpoint to conduction - the micro-canonical formalism of transport - which is ideal to study the above issues [1]. I will point out the similarities and differences with the widely used Landauer formalism, and advance a series of predictions that can be verified by loading ultra-cold atoms into artificial optical lattices.

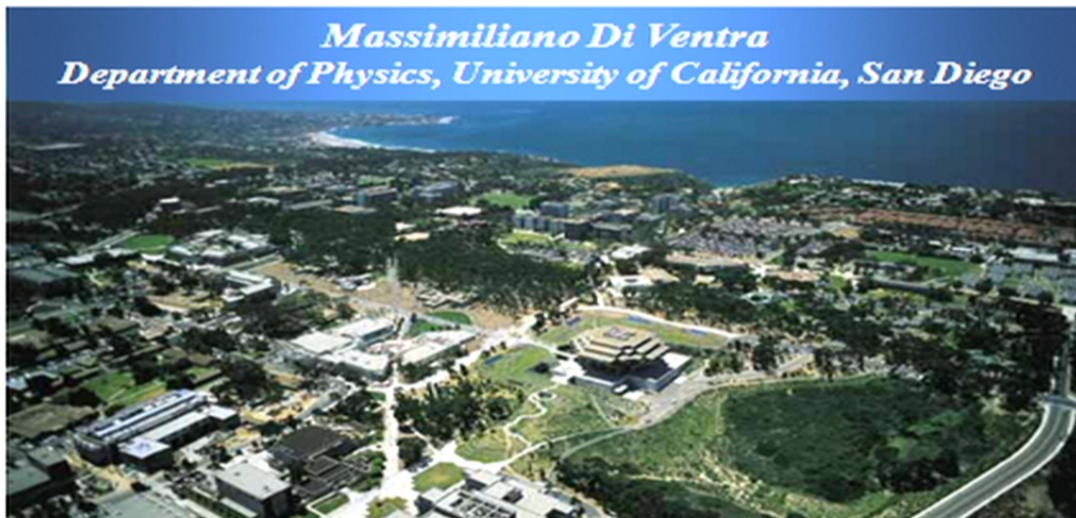
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`<div>[1] M. Di Ventra, Electrical Transport in Nanoscale Systems (Cambridge University Press, 2008). </div></div></div>`

Fundamental aspects of transport in condensed matter and atomic physics

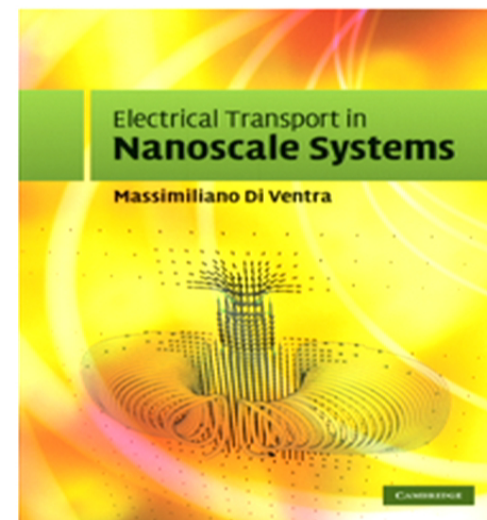


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Collaborators

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Mike Zwolak (OSU)
Roberto D'Agosta (Spain)
Giovanni Vignale (U. Missouri)

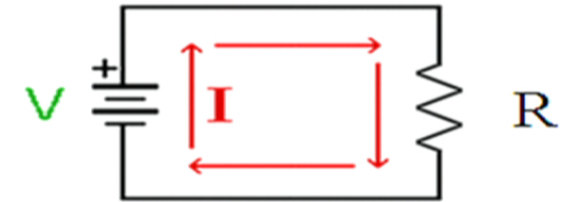
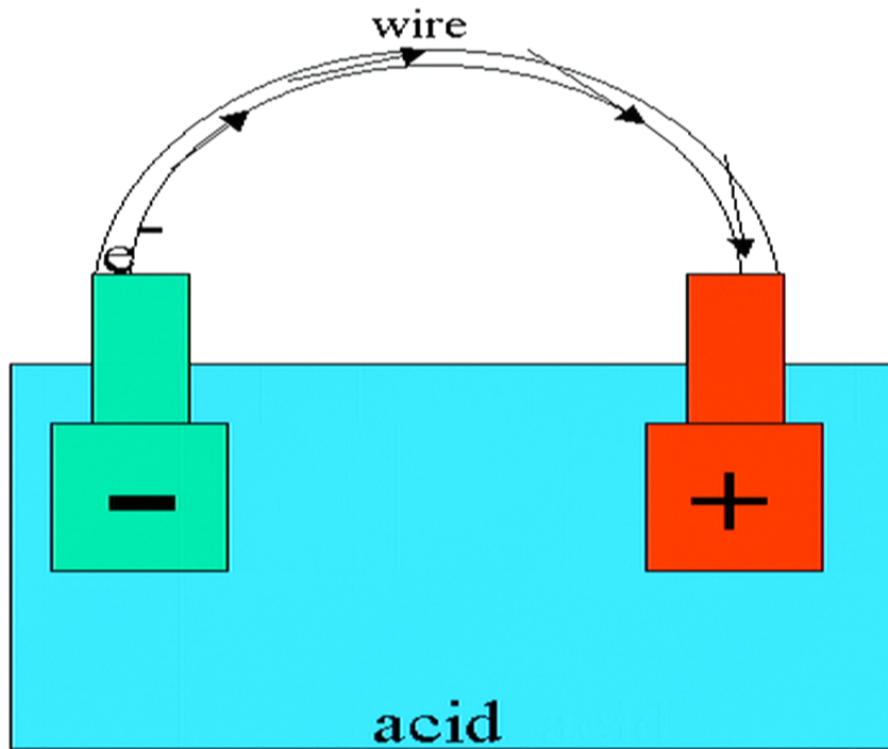


Outline



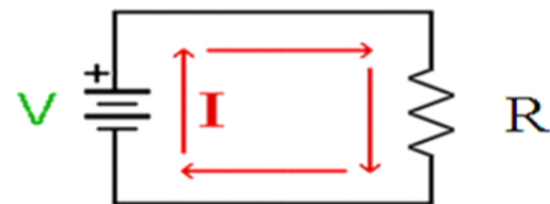
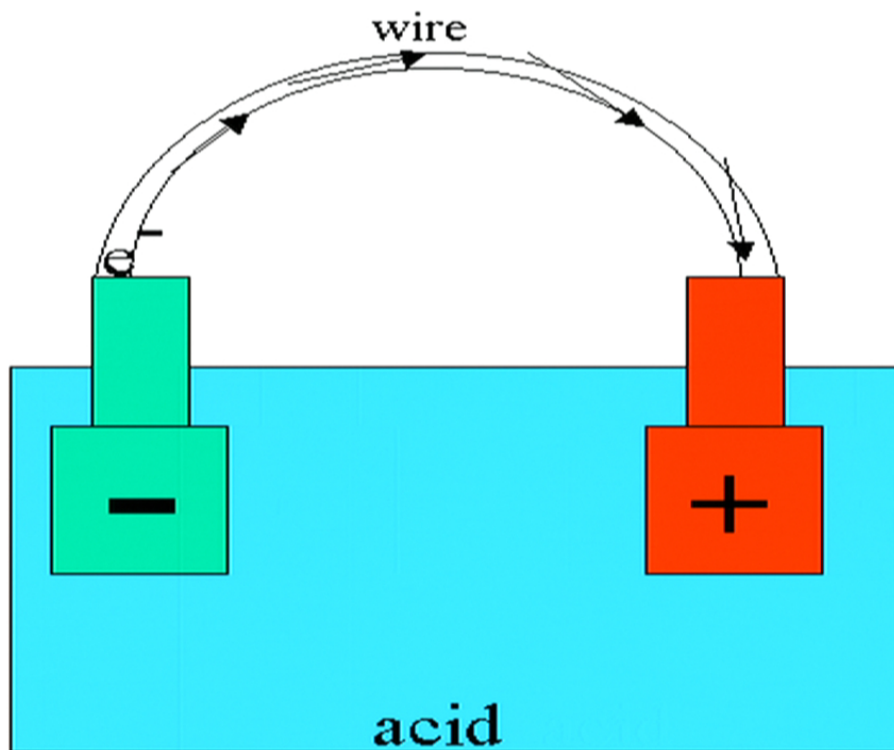
- Introduction to the transport problem
- Many-body effects related to viscosity of the electron liquid (large for structures with smaller transmissions)

What do we want to describe ?



$$R^{-1} = G = \frac{dI}{dV}$$

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$$R^{-1} = G = \frac{dI}{dV}$$

Solved ? Not quite, especially at the atomic level !

Why is the problem difficult (and interesting) ?



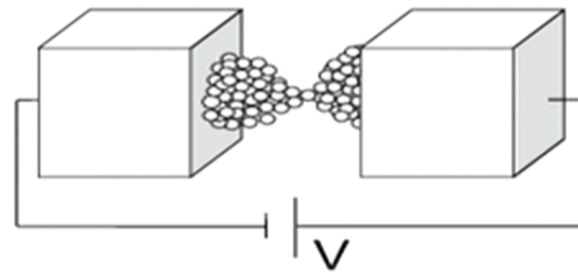
- **The system is out of equilibrium**
(non-equilibrium statistical mechanics is still an open subject; do we need to go beyond Hamiltonian dynamics?)
- **Interactions among electrons**
(Coulomb blockade, correlations, non-Fermi liquid behavior)
- **Interactions among electrons and ions**
(e.g., el-phonon scattering, current-induced forces)
- **Interaction with the environment**
(dissipation and dephasing)
- **Physical properties are quite sensitive to atomic details**

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From experiment to model system

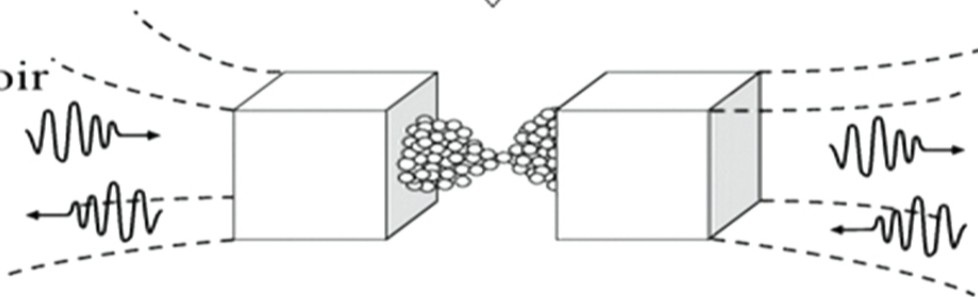
Approximation 1: *open quantum systems*

Closed system



reservoir

μ_L



reservoir

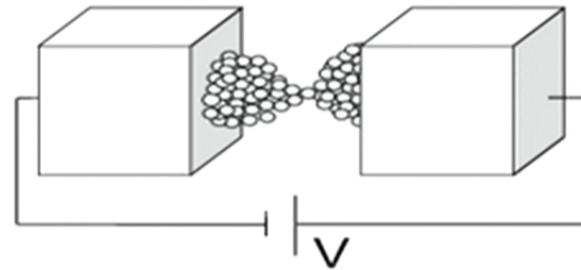
$\mu_R = \mu_L - eV$

Open system: dynamical interaction with reservoirs

From experiment to model system

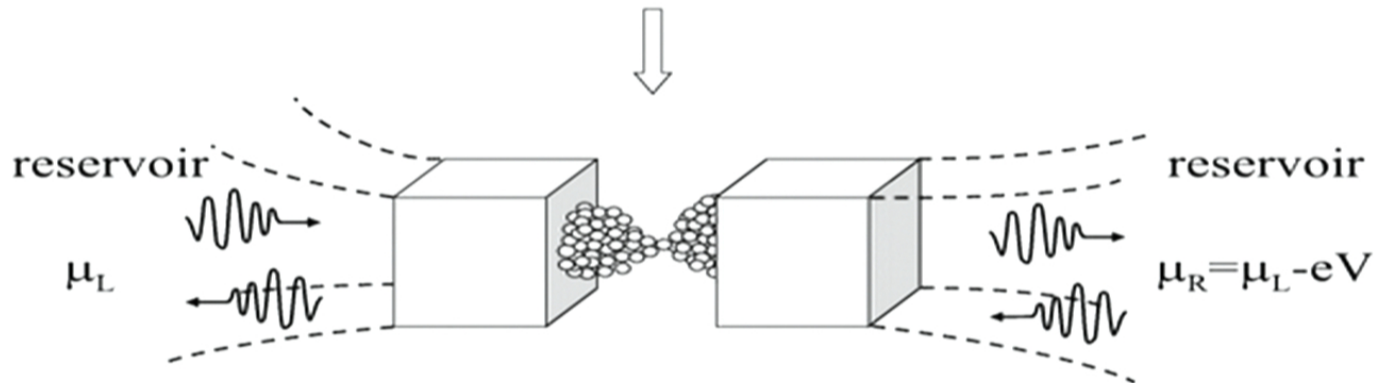
Approximation 1: open quantum systems

Closed system



$$H = H_S + H_{\text{Battery}} + H_{\text{int}}$$

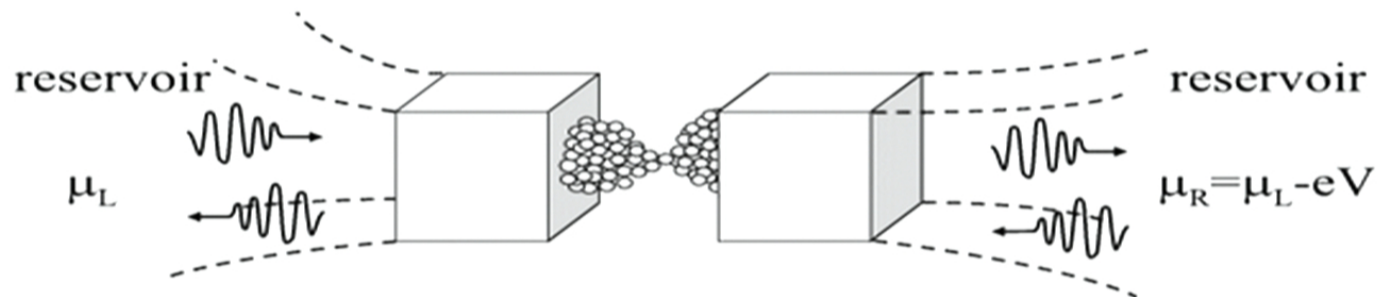
$$\rho_S = \text{Tr}_{\text{Battery}} \rho$$



Open system: dynamical interaction with reservoirs

From experiment to model system

Approximation 1: open quantum systems



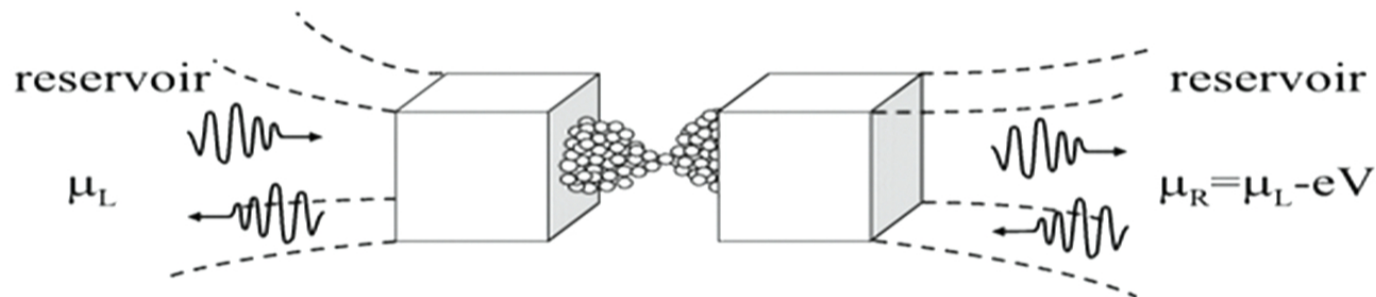
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In general, no closed equation of motion for ρ_S

From experiment to model system

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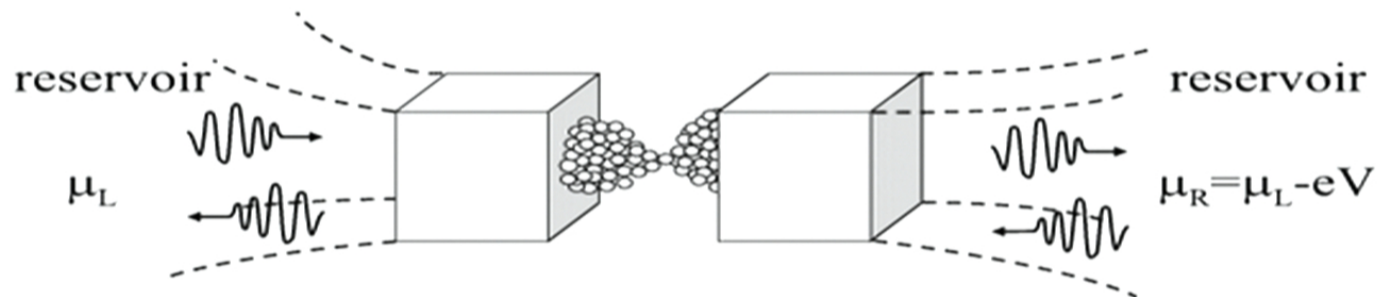
Battery dense spectrum
No initial correlations
Small interaction



In general, no closed equation of motion for ρ_S

From experiment to model system

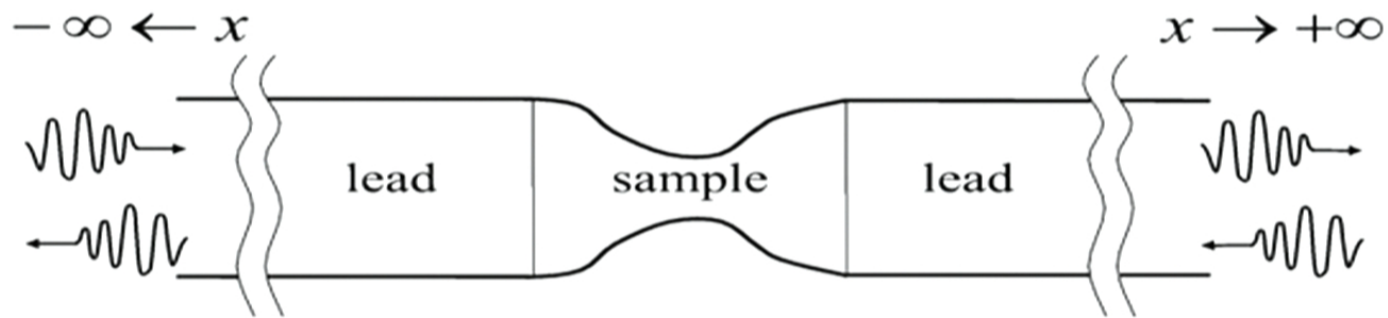
Approximation 2: ideal steady state



Assume existence of at least one steady state solution

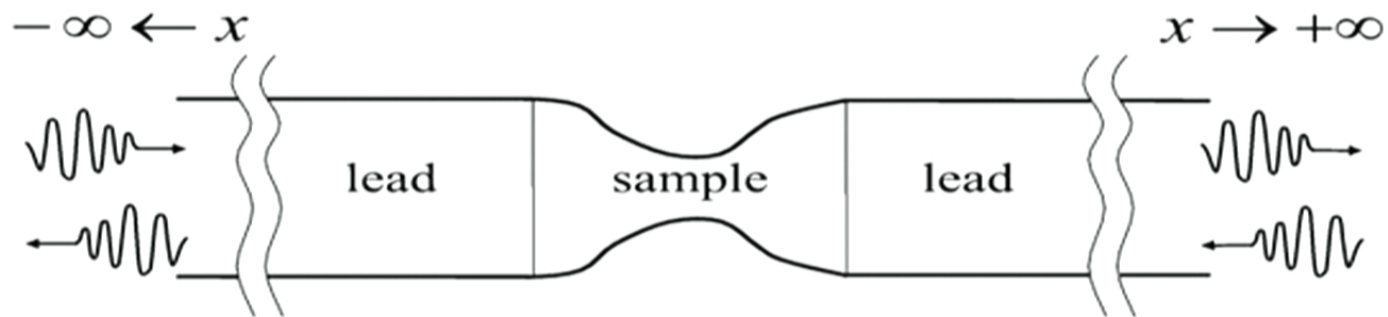
From experiment to model system

Approximation 3: *“openness” vs boundary conditions*



From experiment to model system

Approximation 3: “openness” vs boundary conditions

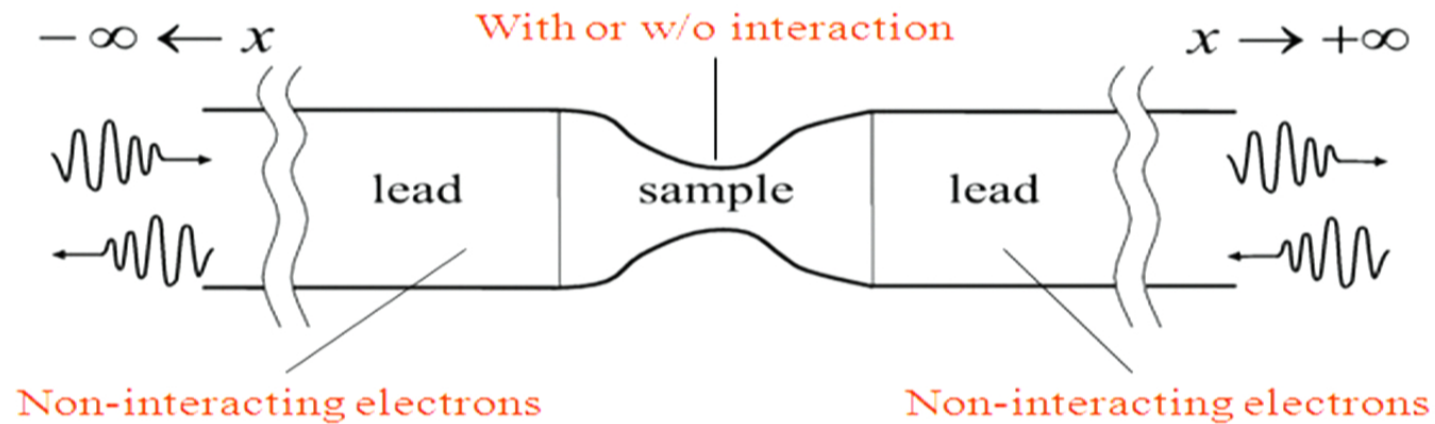


Loss of information

closed system (with battery) \rightarrow open system \rightarrow closed and infinite *different* system

From experiment to model system

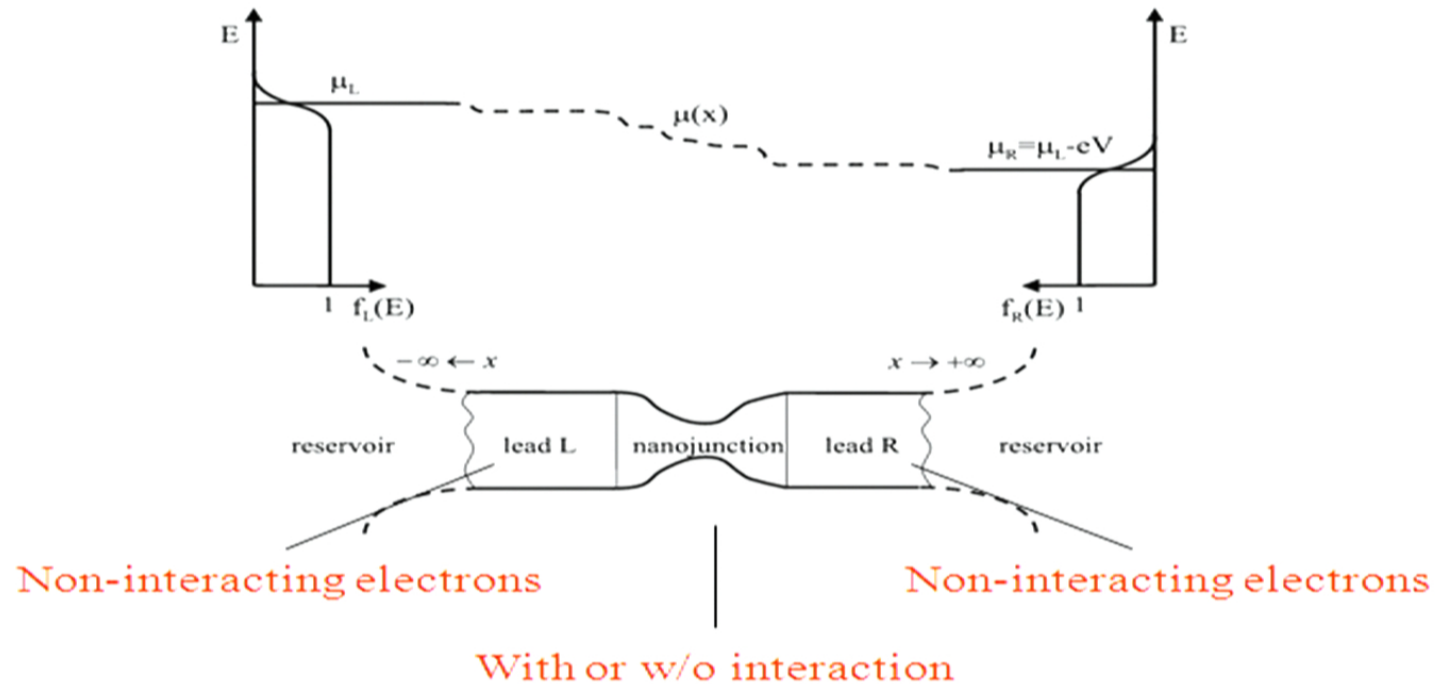
Approximation 4: *mean-field approximation*



If leads are interacting NO closed equation of motion for the current !

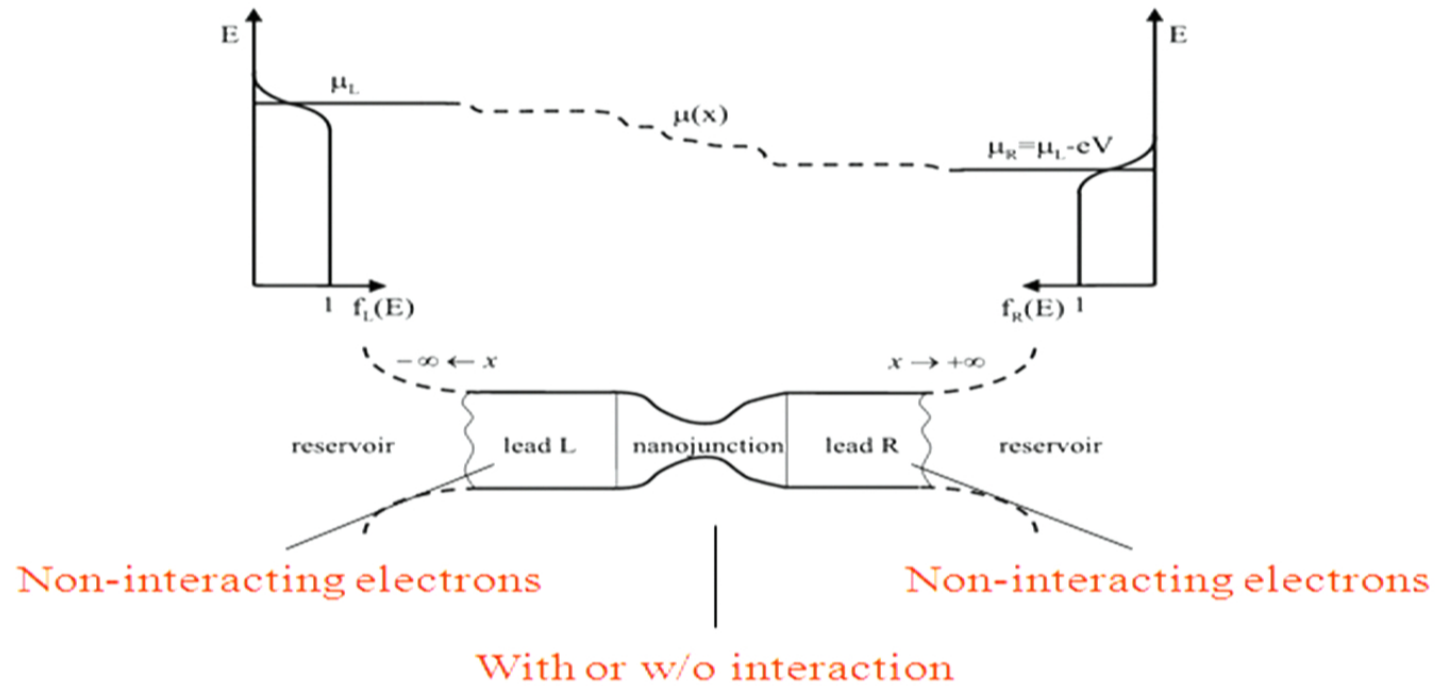
From experiment to model system

Approximation 5: *independent channels and energy filling*

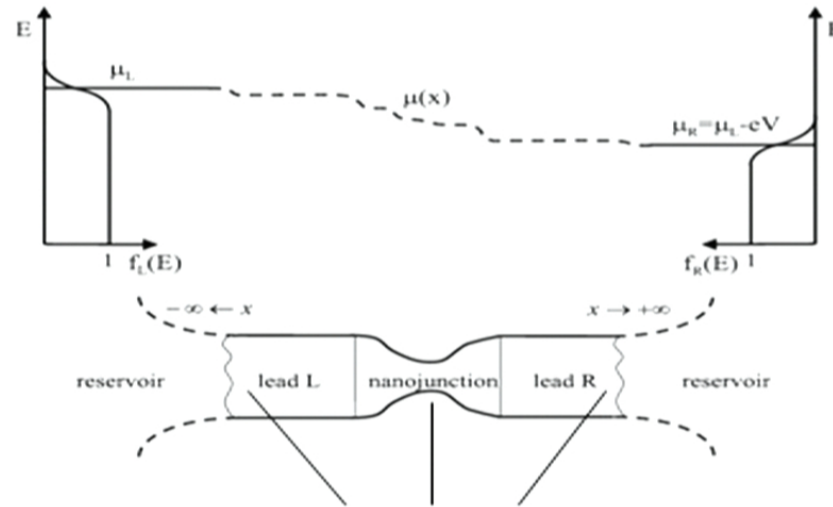


From experiment to model system

Approximation 5: *independent channels and energy filling*



The Landauer current

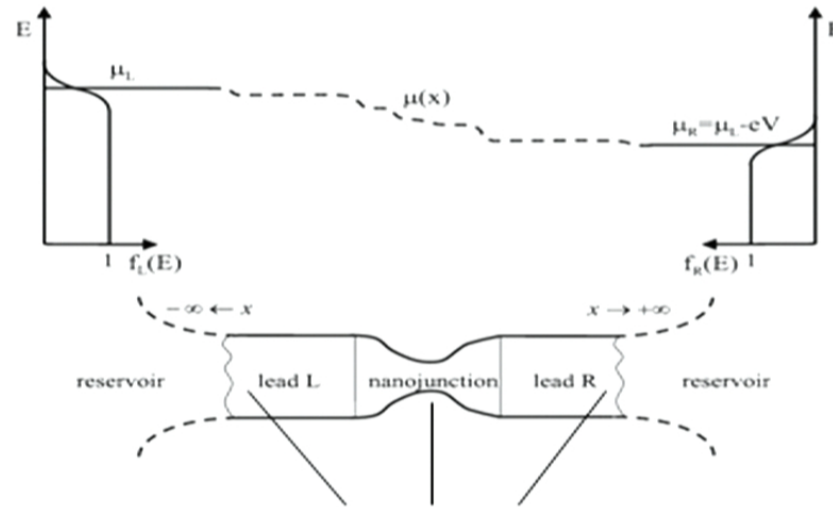


Non-interacting electrons

From scattering theory

$$I = \frac{e}{\pi\hbar} \int dE [f_L(E) - f_R(E)] T(E) \equiv \frac{e}{\pi\hbar} \int dE [f_L(E) - f_R(E)] \text{Tr} \{ \Gamma_R G^+ \Gamma_L G^- \}$$

The Landauer current



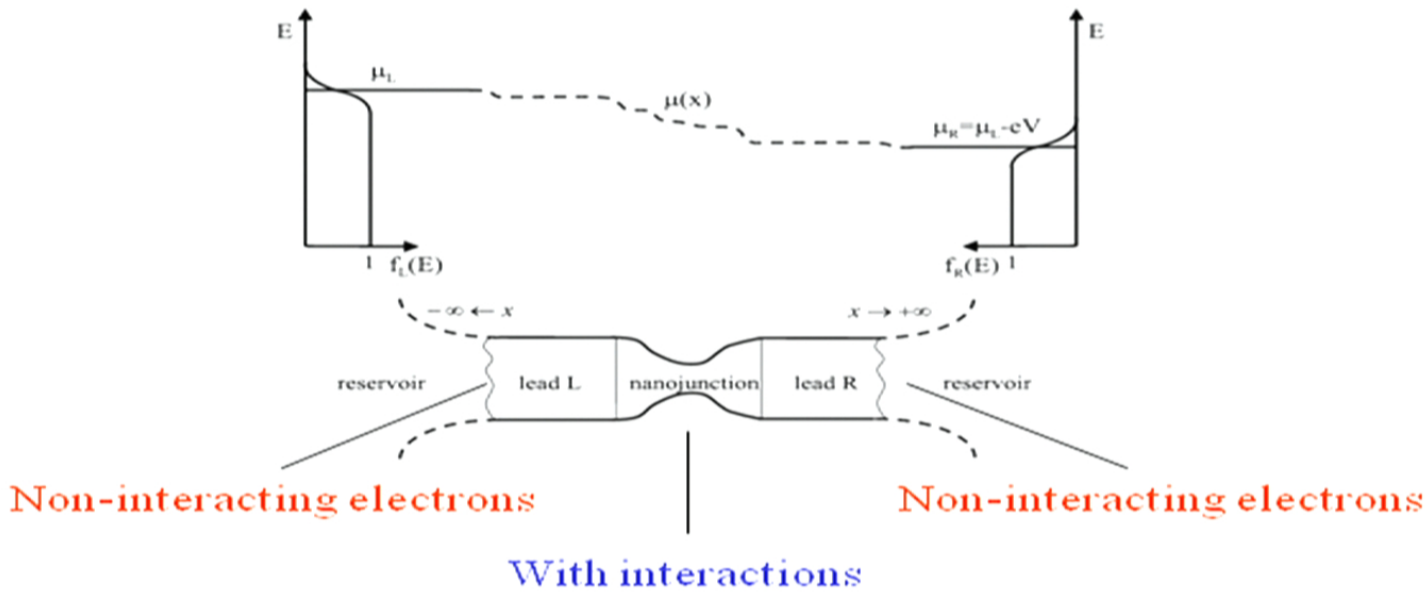
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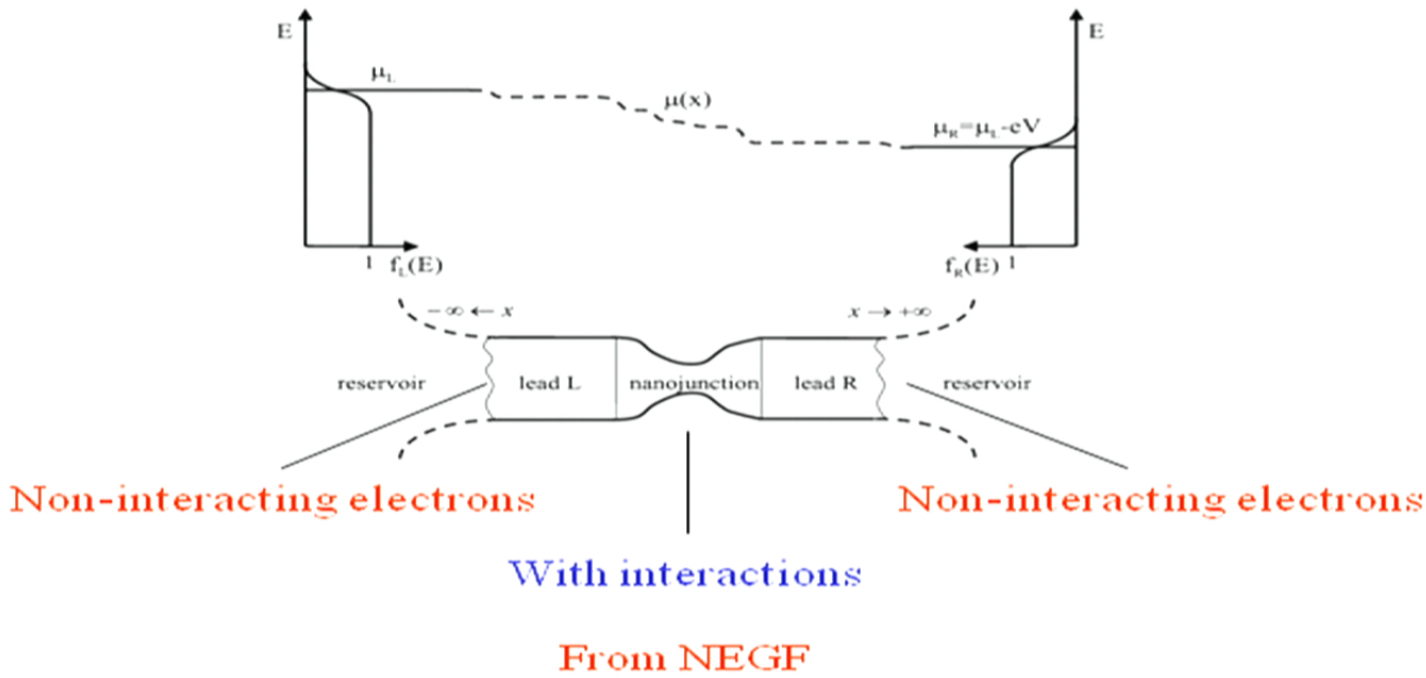
This formula has nothing to do with NEGF !!!

Interacting sample



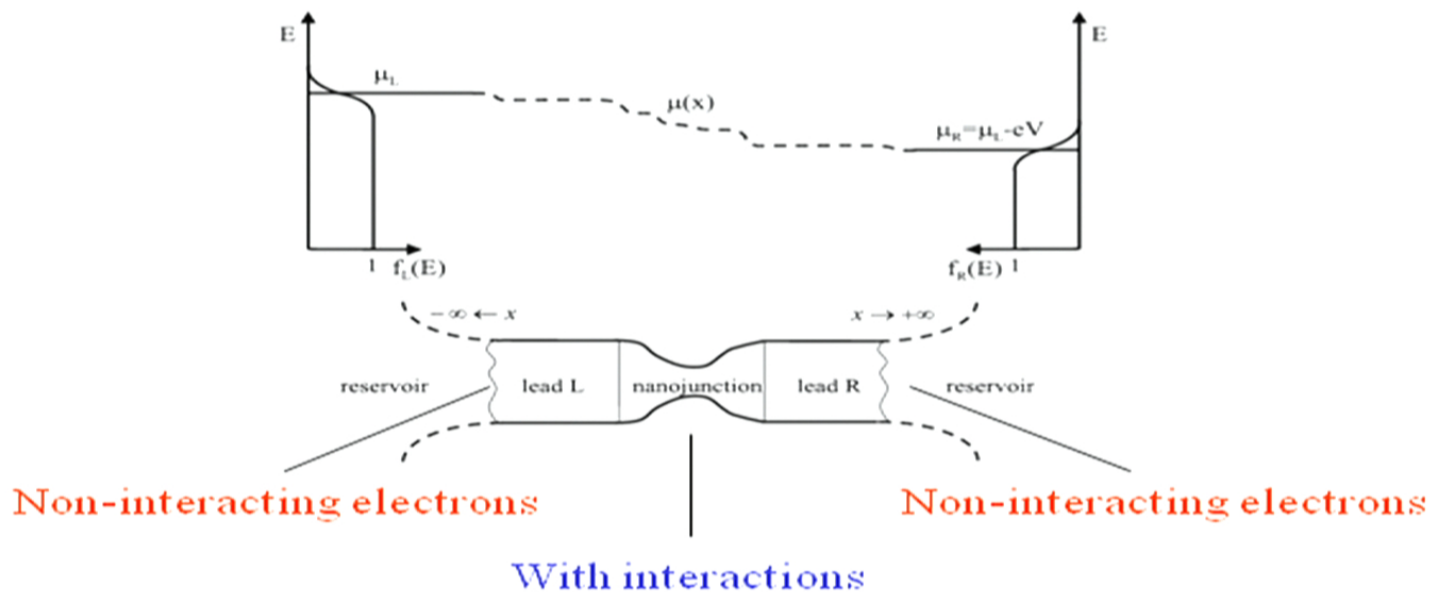
Meir and Wingreen, 1992

Interacting sample



Meir and Wingreen, 1992

Interacting sample



From NEGF

$$I = \frac{ie}{\hbar} \int \frac{dE}{2\pi} \text{Tr} \left\{ [\Gamma_L(E) - \Gamma_R(E)] G^< + [f_L(E)\Gamma_L(E) - f_R\Gamma_R(E)] [G^+(E) - G^-(E)] \right\}$$

Meir and Wingreen, 1992

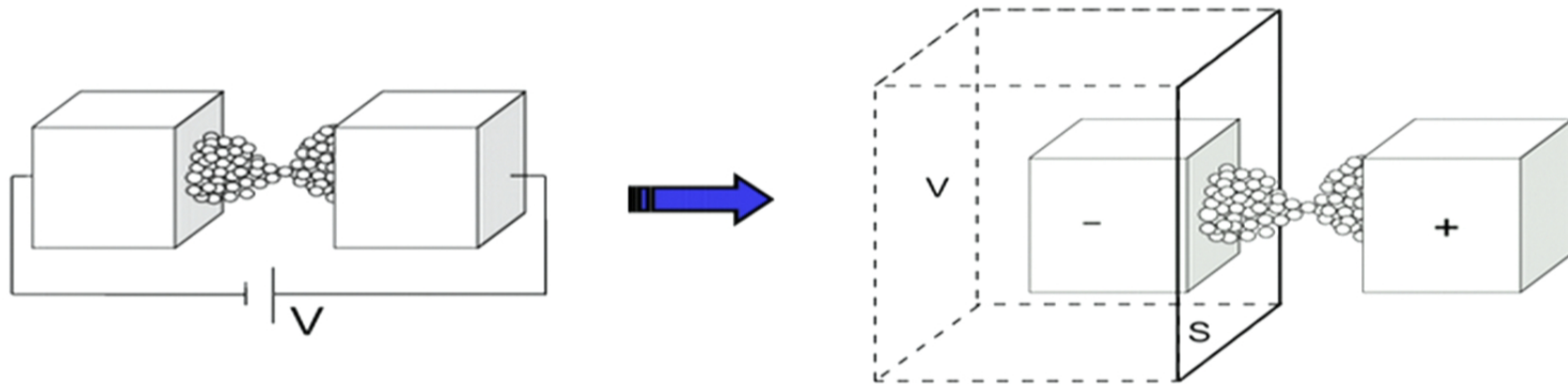
Outline



- Introduction to the transport problem
- Many-body effects related to viscosity of the electron liquid (large for structures with smaller transmissions)
- Properties of steady states and predictions

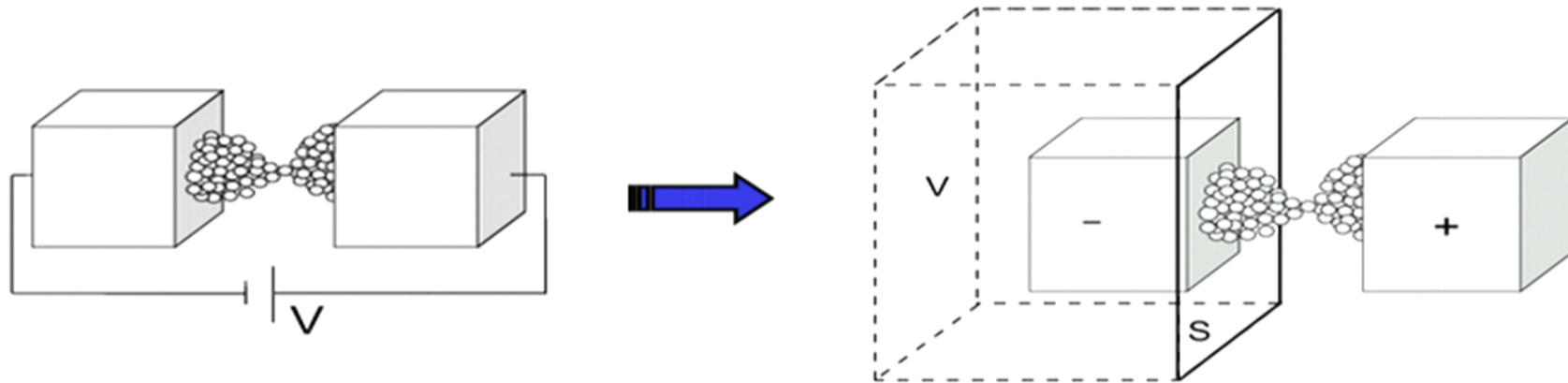
Theory: Microcanonical picture of transport
Experiments: Atomic gases in optical lattices

Interactions in the whole system: the microcanonical picture of transport



M. Di Ventra, T.N. Todorov, (J. Phys. Cond. Matt. 2004)

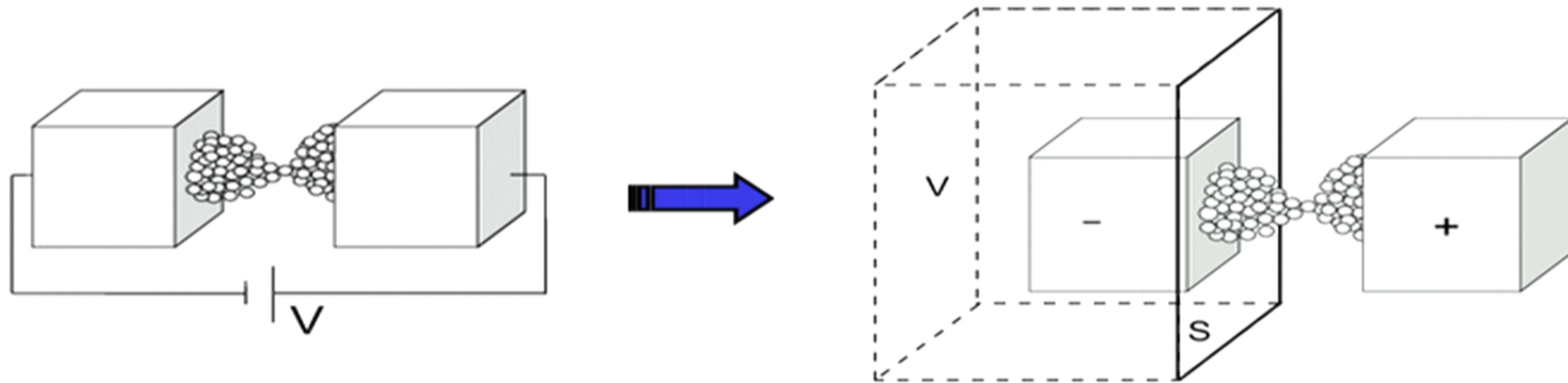
Interactions in the whole system: the microcanonical picture of transport



$$I_{exact} = \int_S \mathbf{j}_{exact} ds = \int_V \nabla \cdot \mathbf{j}_{exact} dv \stackrel{\nabla \cdot \mathbf{j} = -\frac{\partial n}{\partial t}}{=} \int_V \nabla \cdot \mathbf{j}_{KS} dv = \int_S \mathbf{j}_{KS} ds = I_{KS}$$

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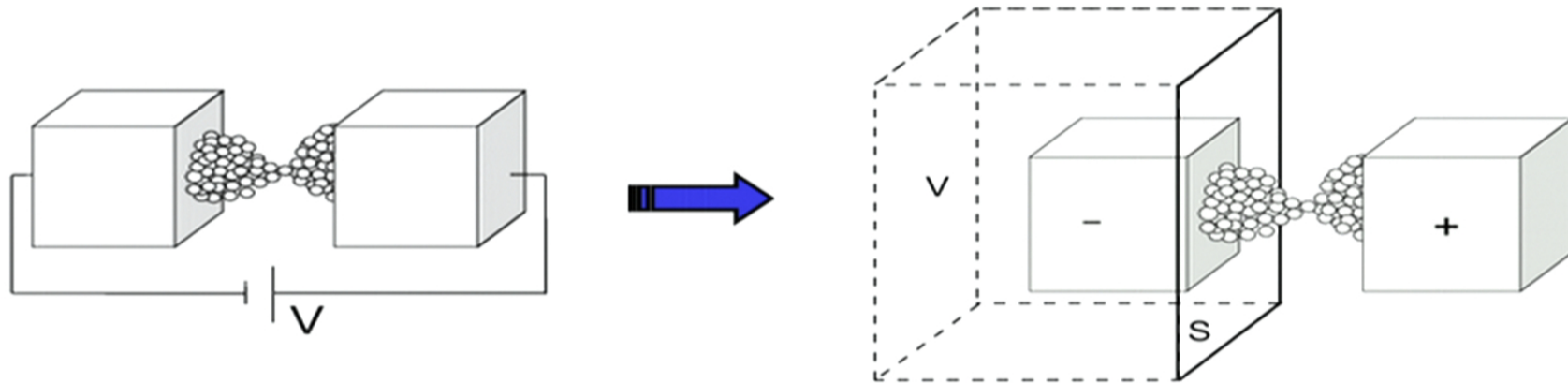
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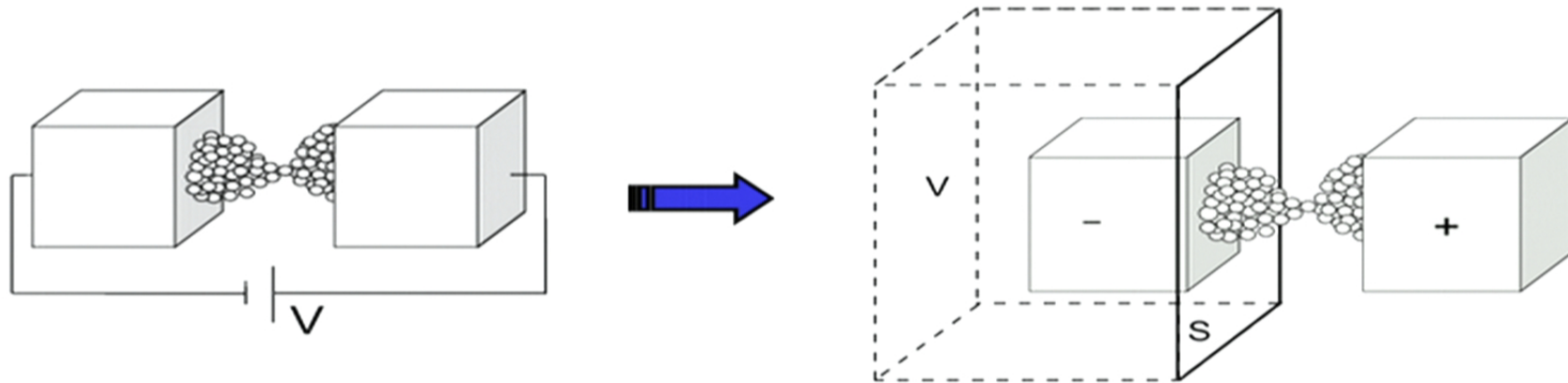
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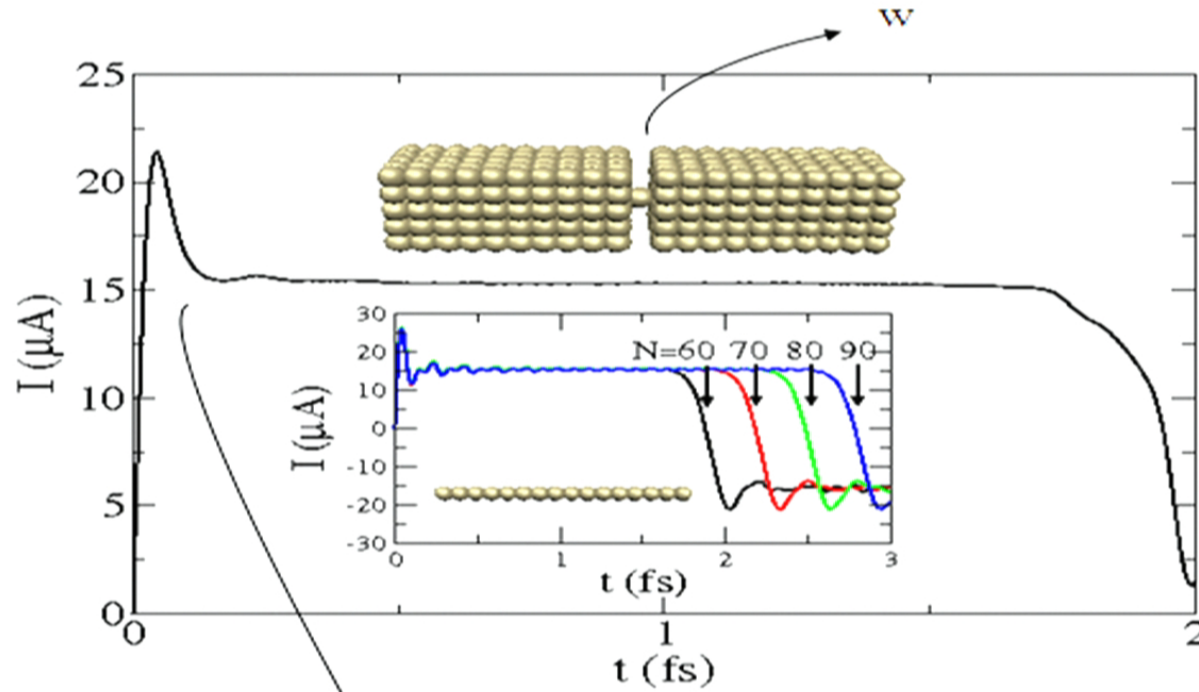
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Fast relaxation of momentum

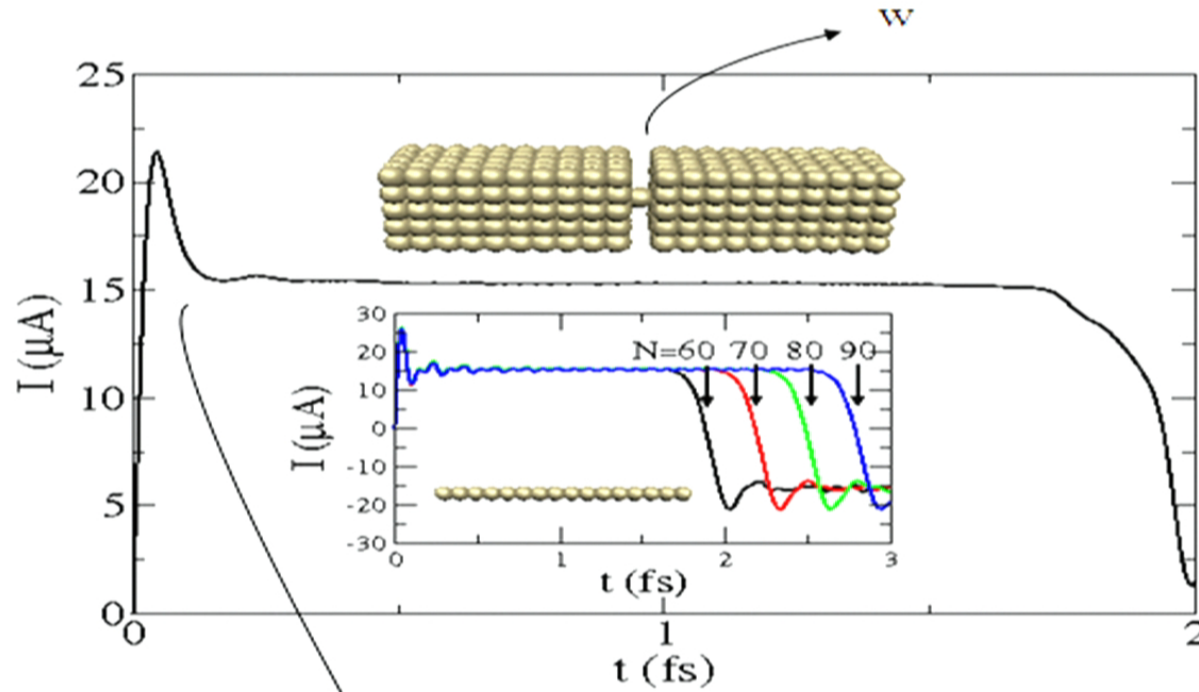


momentum relaxation time

$$1/v_c \sim t_c \sim \hbar/\Delta E \sim m w^2/\pi^2 \hbar^2 \sim 1 \text{ fs}$$

Bushong, Sai and M. Di Ventra (Nano Letters 2005)

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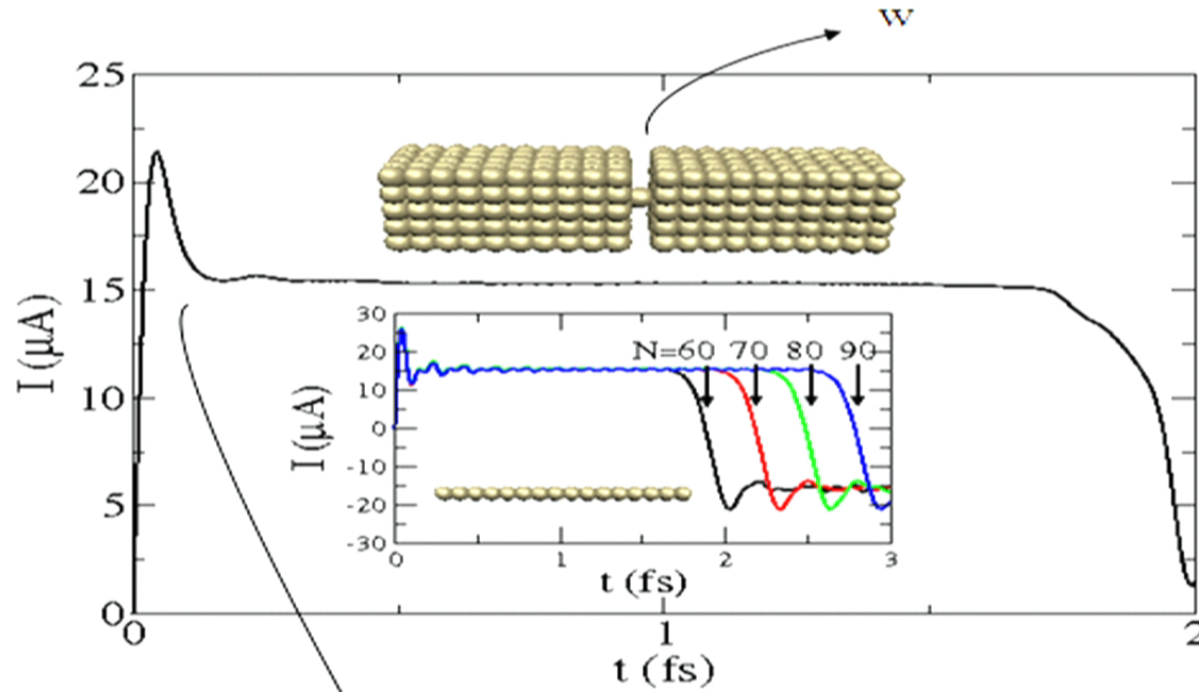


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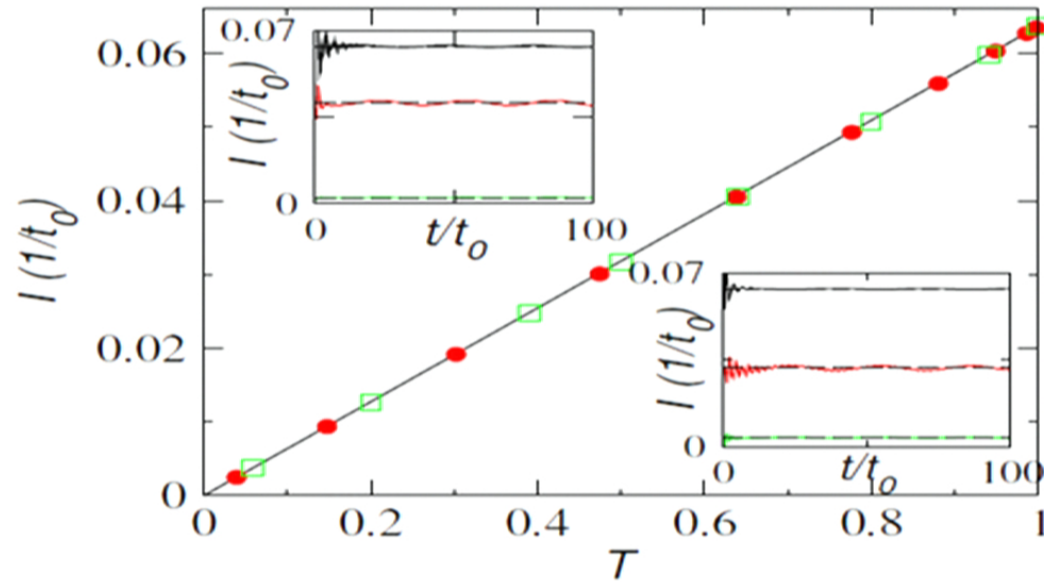
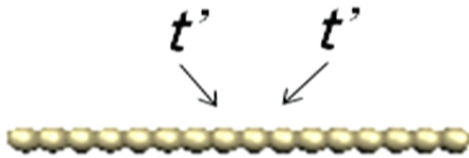


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Comparison with Landauer formula



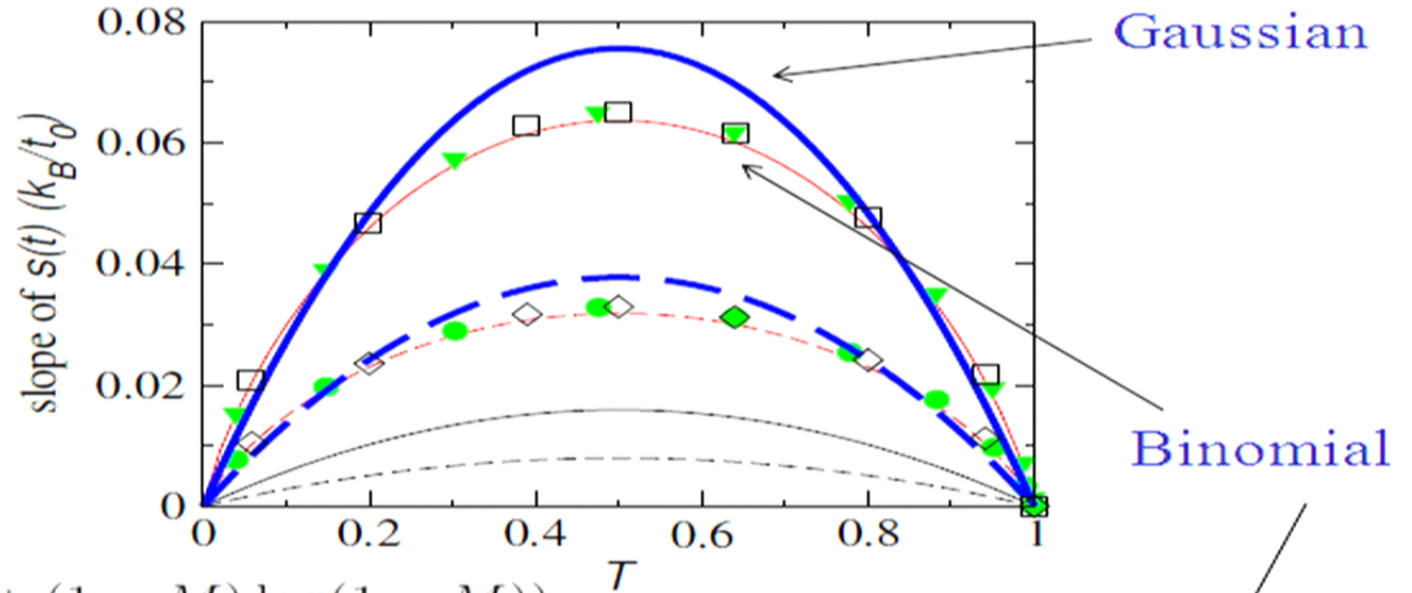
$$H = H_L + H_R + H_C$$

$$H_{L/R} = -\tilde{t} \sum_{\langle ij \rangle, L/R} c_i^\dagger c_j + E_{L/R} \sum_{i \in L/R} c_i^\dagger c_i$$

$$H_C = -\tilde{t}' (c_{N/2}^\dagger c_{N/2+1} + c_{N/2+1}^\dagger c_{N/2})$$

Chen, Zwolak and Di Ventra, in preparation

Entanglement entropy



Exact

$$s = -\text{Tr}(M \log M + (1 - M) \log(1 - M))$$

$$M = P_L C(t) P_L$$

$C(t)$ = correlation matrix

P_L = projection operator

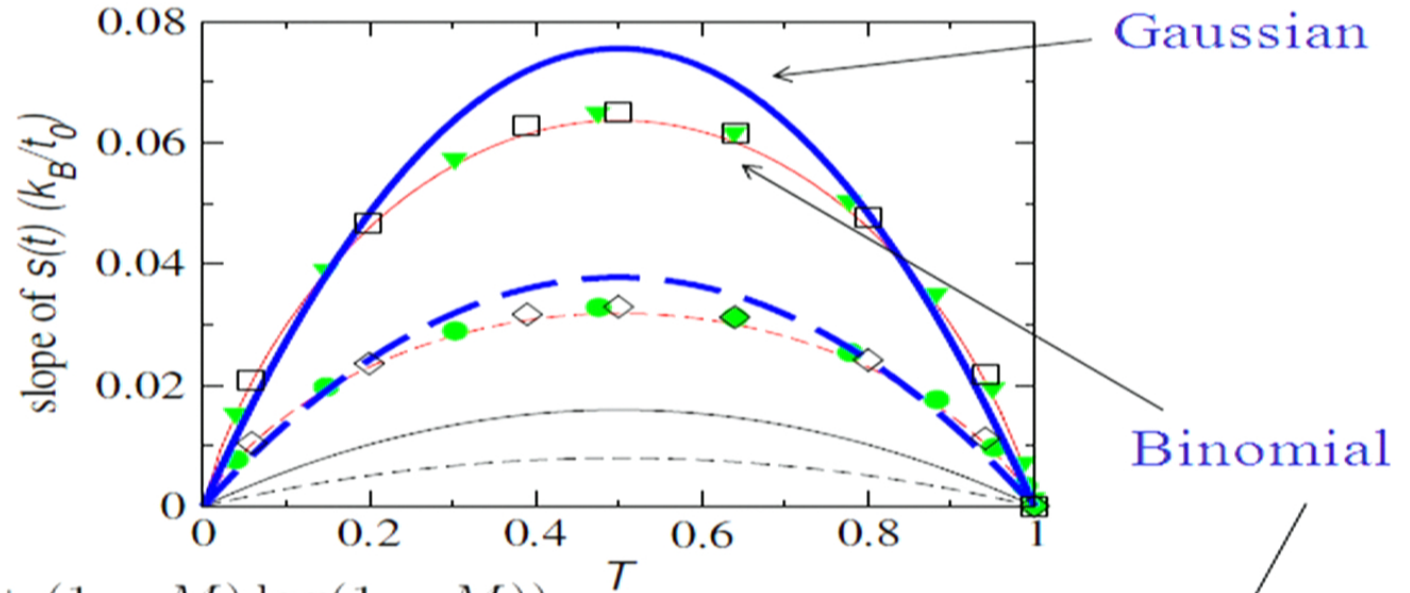
Approximate

$$s(t)/t = -2 \frac{\mu_B}{h} [T \log T + (1 - T) \log(1 - T)].$$

Chen, Zwolak and Di Ventura, in preparation

Klich and Levitov, PRL 2009

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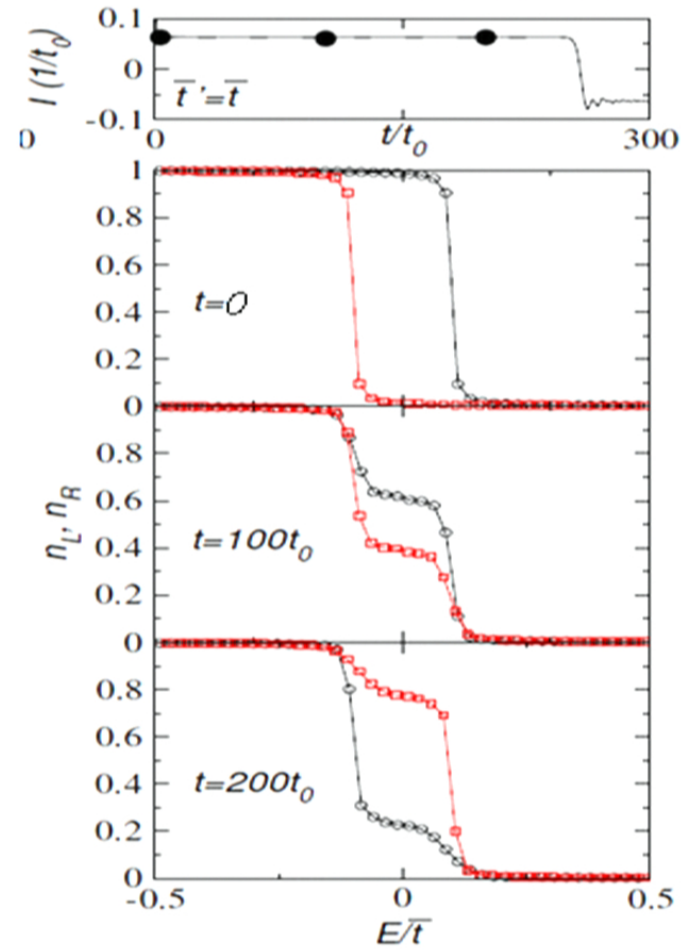
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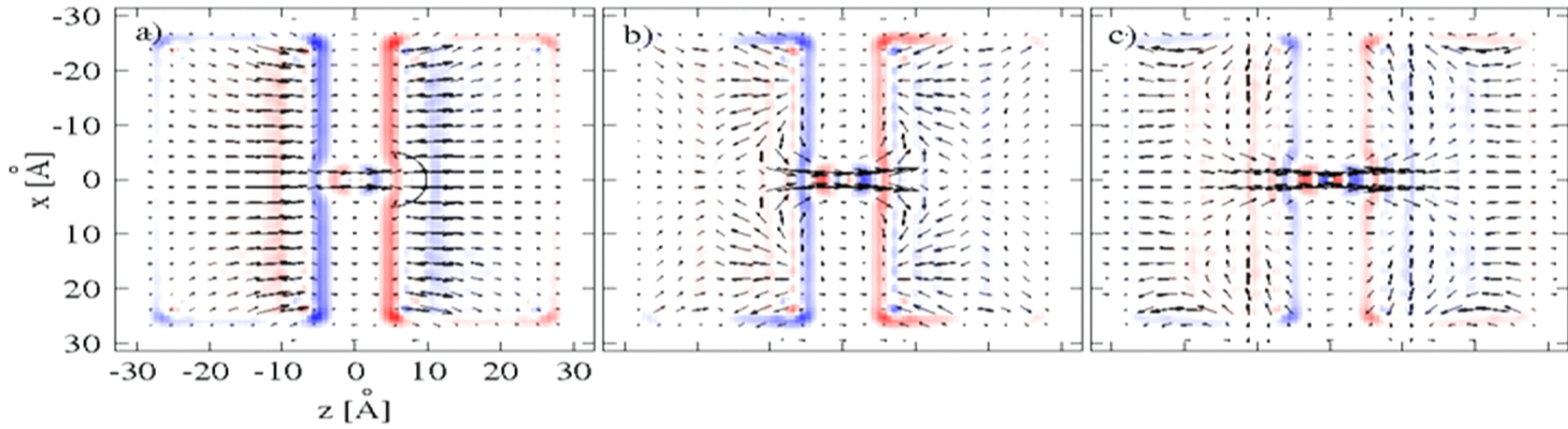
Klich and Levitov, PRL 2009

The existence of a steady state is unrelated to the existence or not of Fermi distributions



Chen, Zwolak and Di Ventra, in preparation

Electron flow



Quasi-2D electron liquid,
 TDDFT
 $V=0.2V$

$$\left[i\hbar \frac{\partial}{\partial t} - \frac{1}{2m} \left(-i\hbar \nabla - \frac{e}{c} A_{xc}(r,t) \right)^2 - V_{ext}(r,t) \right] \phi_x^{KS}(r,t) = 0$$

Sai, Bushong, Hatcher, and Di Ventra, PRB 2007

$$i\hbar \frac{d|\Psi(t)\rangle}{dt} = H|\Psi(t)\rangle$$

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⇔ Exact!

$$\begin{array}{l}
 n = \text{density} \\
 v = j/n
 \end{array}
 \left\{
 \begin{array}{l}
 D_t n + n \nabla \cdot v = 0 \quad \longrightarrow \text{continuity} \\
 mn D_t v_j + \nabla_i P_{ij} + n \nabla_j V_{ext} = 0 \quad \longrightarrow \mathbf{F=ma}
 \end{array}
 \right.$$

|
 Information on all e-e interactions (generally unknown)

A hydrodynamic formulation is more natural in QM than in classical physics

Martin and Schwinger, Phys. Rev. (1959)

Anticipates TDDFT by many years !

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R. D'Agosta and M. Di Ventra, JPCM (2006)

$$D_t n + n \nabla \cdot \mathbf{v} = 0$$

$$mn D_t \mathbf{v}_j + \nabla_i P_{ij} + n \nabla_j V_{ext} = 0$$

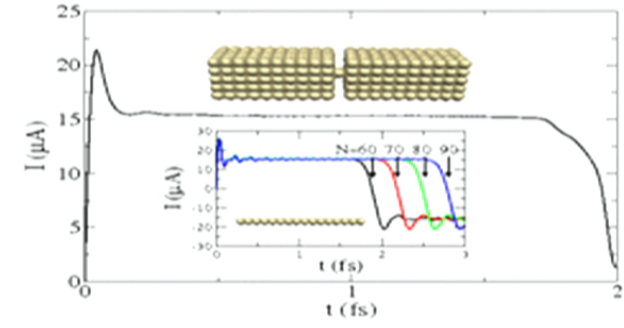
$$P_{ij} \stackrel{|}{=} F[P_{ijk} = F[P_{ijkl} = \dots]]$$

$$1) \frac{1}{m} \sum I[f] P_i P_j = D_t P_{ij} + P_{ij} \nabla \cdot \mathbf{v} + P_{ik} \nabla_k \mathbf{v}_j + P_{kj} \nabla_k \mathbf{v}_i + \nabla_k P_{ijk}^{(3)}$$

R. D'Agosta and M. Di Ventra, JPCM (2006)

Quantum Navier-Stokes equations

$$\left\{ \begin{aligned} D_t n + n \nabla \cdot \mathbf{v} &= 0 \\ mn D_t v_j + \nabla_i P_{ij} + n \nabla_j V_{ext} &= 0 \\ P_{ij} &= F[P_{ijk} = F[P_{ijkl} = \dots]] \end{aligned} \right.$$



$$1) \frac{1}{m} \sum I[f] P_i P_j = D_t P_{ij} + P_{ij} \nabla \cdot \mathbf{v} + P_{ik} \nabla_k v_j + P_{kj} \nabla_k v_i + \nabla_k P_{ijk}^{(3)}$$

$$2) \quad \Delta E \Delta t \simeq \hbar \rightarrow v_c = \Delta E / \hbar$$

$$\downarrow v / (L \max(\omega, v_c)) \ll 1$$

$$3) P_{i,j} = P \delta_{ij} - \eta \left(\nabla_i v_j + \nabla_j v_i - \frac{2}{3} \delta_{i,j} \vec{\nabla} \cdot \vec{v} \right) \quad \boxed{\eta \propto \hbar n}$$

R. D'Agosta and M. Di Ventra, JPCM (2006)

Conductance quantization from hydrodynamics

$$\begin{cases} D_t n + n \nabla \cdot \mathbf{v} = 0 \\ mn D_t v_j + \nabla_j P - \eta \tilde{\pi}_{ij} + n \nabla_j V_{ext} = 0 \end{cases}$$



1D, stationary, non-viscous fluid

$$\frac{v^2}{2} + \frac{P}{n} + V_{ext} = \text{const} \quad \longleftrightarrow \quad \text{Bernoulli}$$

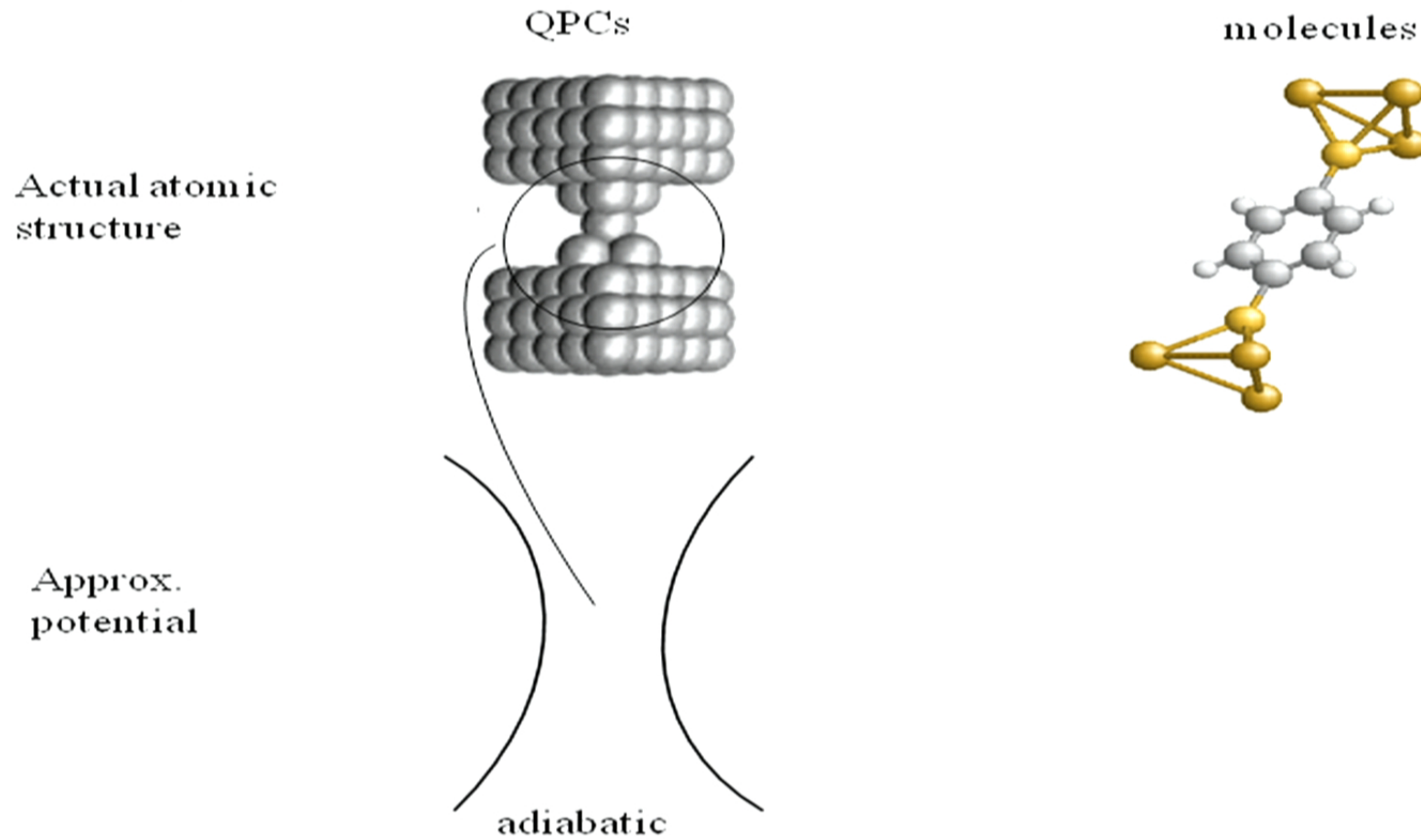
$$\frac{P}{n} = \frac{(\pi \hbar m)^2}{2m^2}$$



$$I = \frac{e^2}{h} V$$

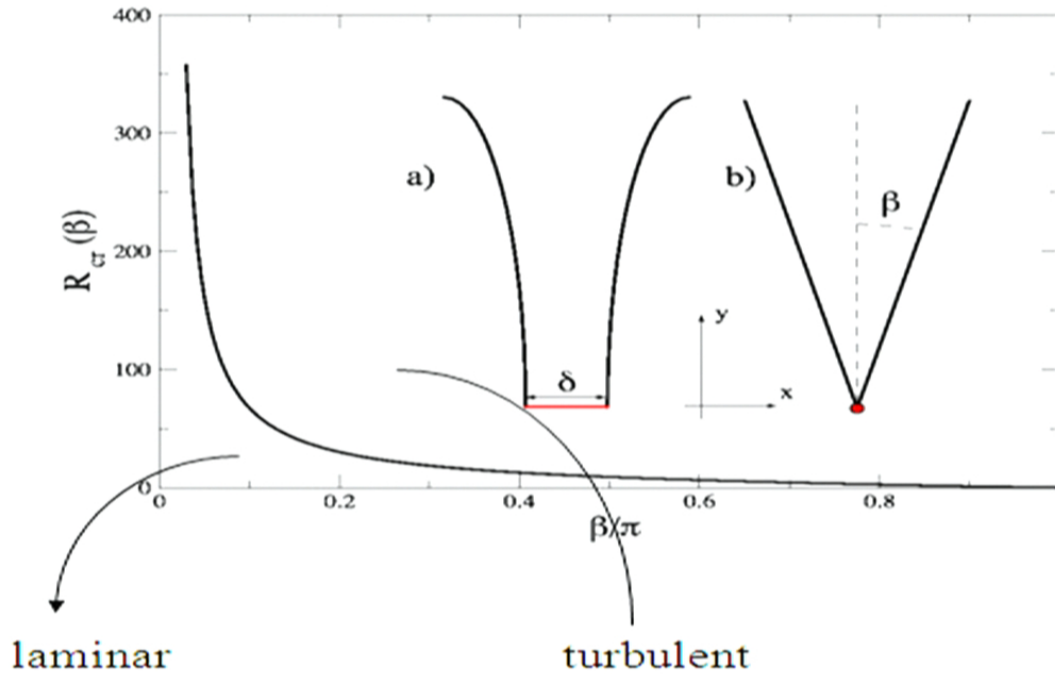
Quantized conductance is the one of a 1D ideal, non-viscous charged fluid

Turbulence in nanoscale systems



D'Agosta and M. Di Ventra, JPCM (2006)

Turbulence in nanoscale systems



$$Re = \frac{mI}{e\eta}$$

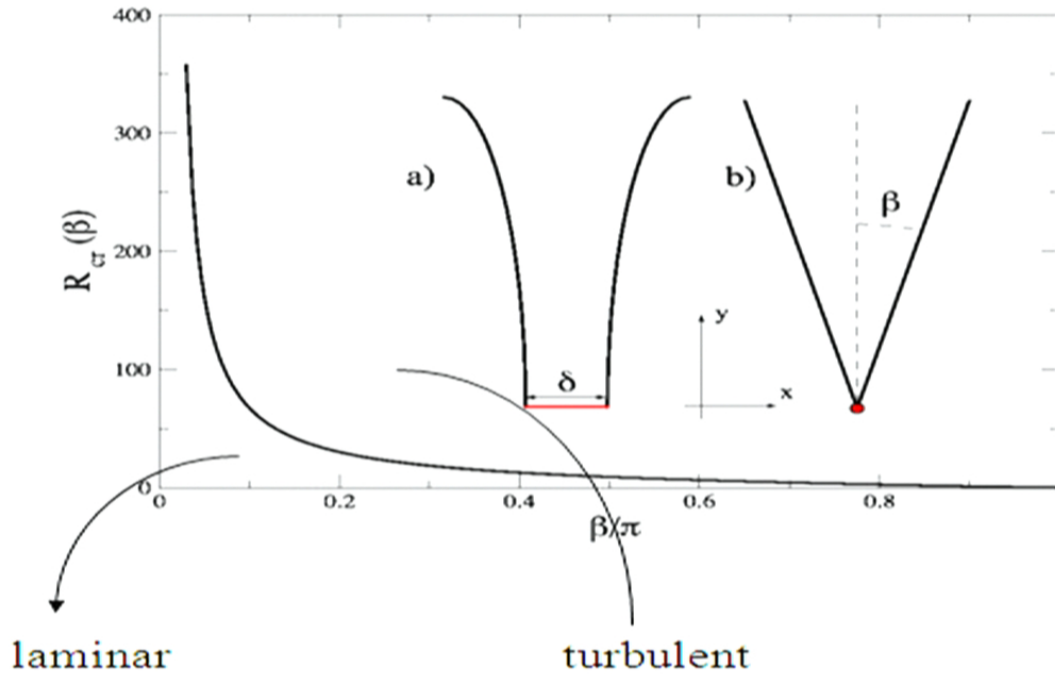
Adiabatic constrictions
(e.g., QPC),
laminar flow

Nonadiabatic constrictions
(e.g., molecules),
turbulent flow

$$\eta_e \approx 10^{-2} \eta_{air}$$

D'Agosta and M. Di Ventra, JPCM (2006)

Turbulence in nanoscale systems



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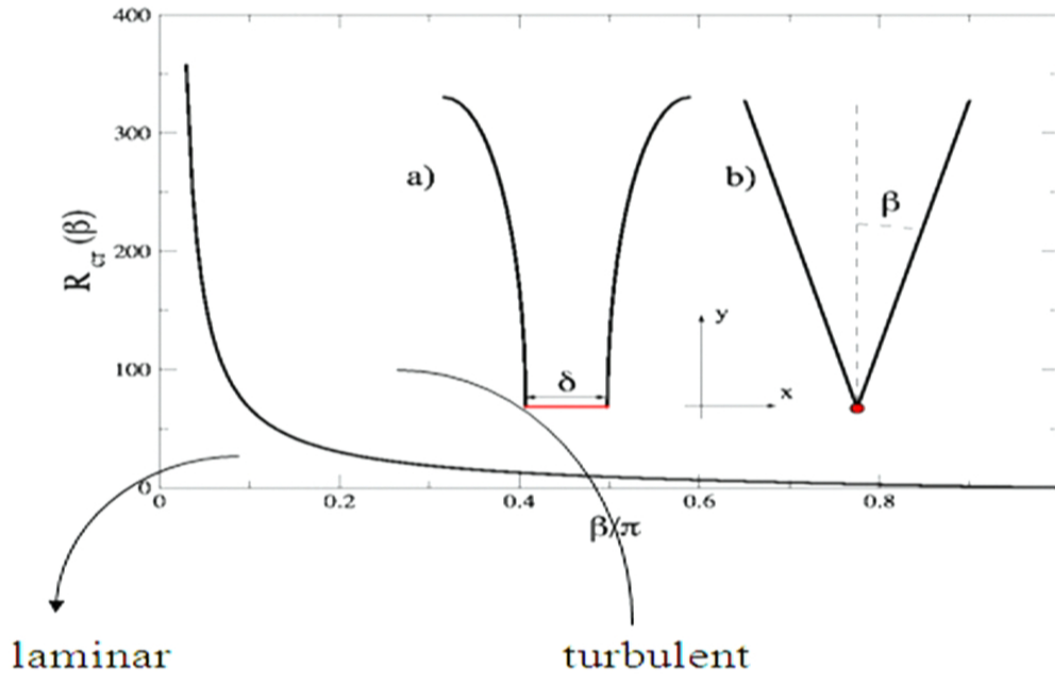
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$$Re = \frac{mI}{e\eta}$$

Adiabatic constrictions
(e.g., QPC),
laminar flow

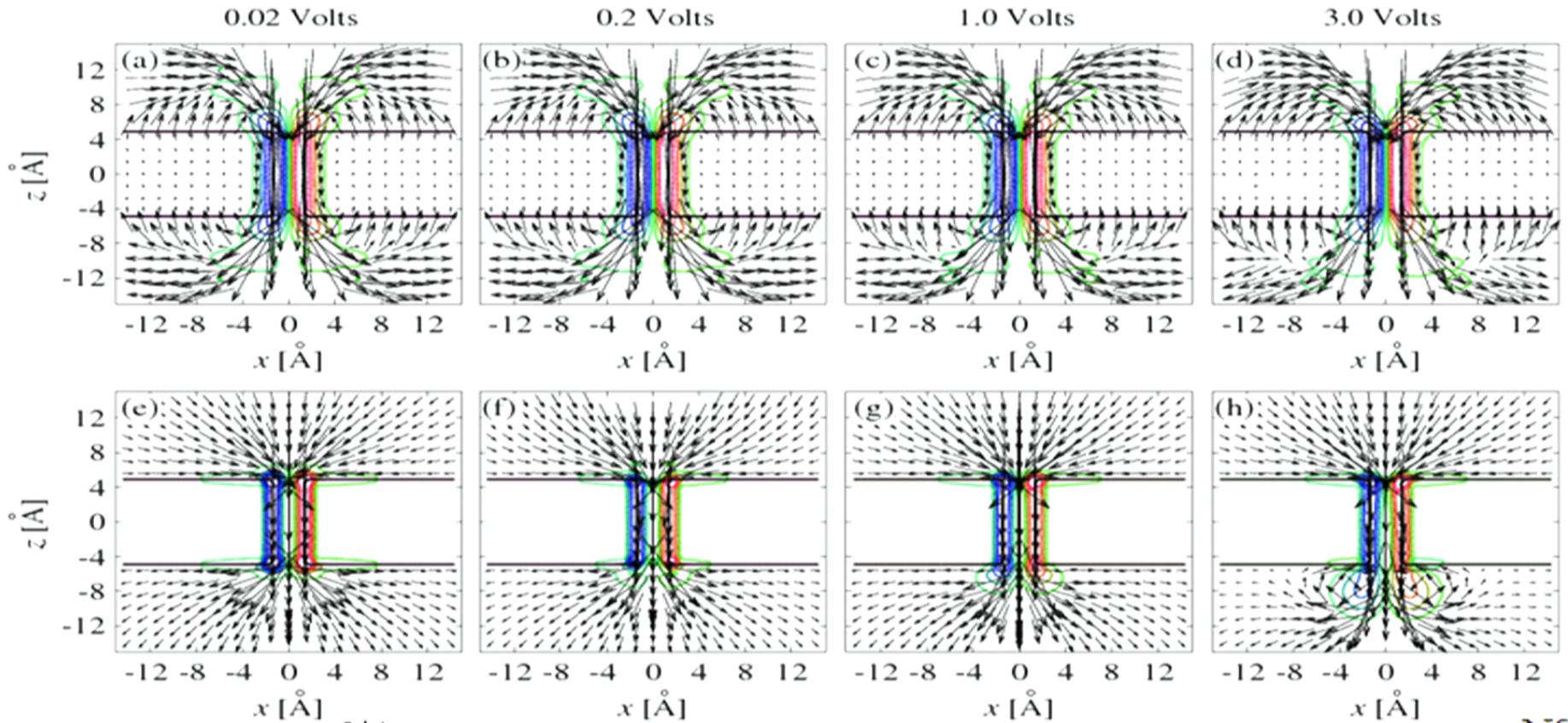
Nonadiabatic constrictions
(e.g., molecules),
turbulent flow

$$\eta_e \approx 10^{-2} \eta_{air}$$

D'Agosta and M. Di Ventra, JPCM (2006)

Electron turbulence

TDCDFT



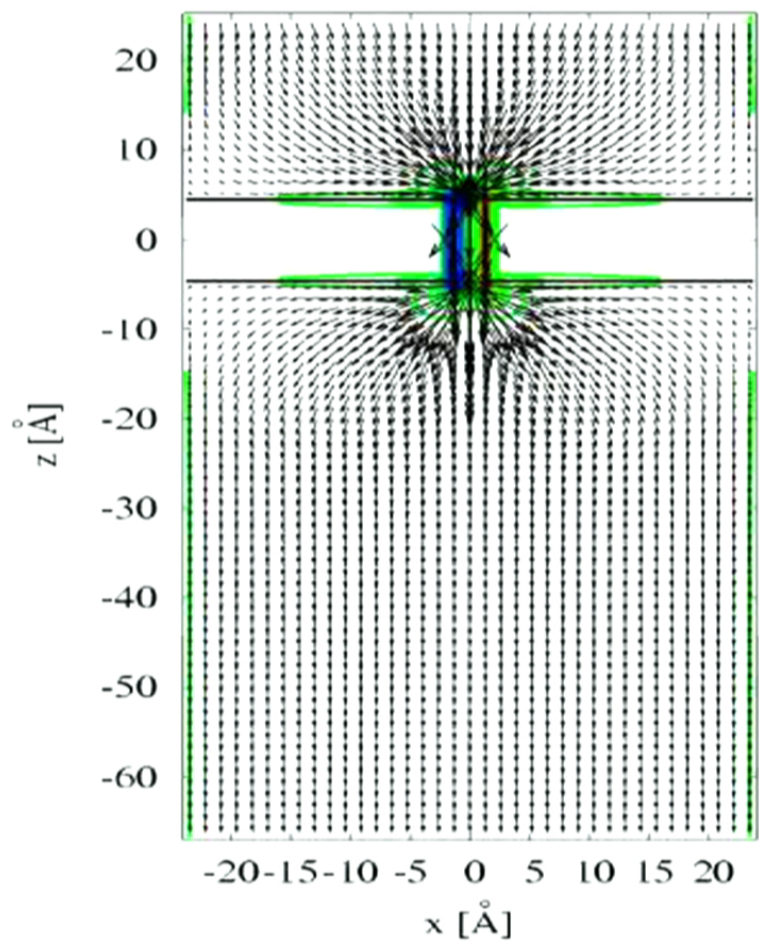
$$\lambda_0 \sim l \left(\frac{R_{cr}}{Re} \right)^{3/4}$$

nanoscale, for fully developed turbulence

NS

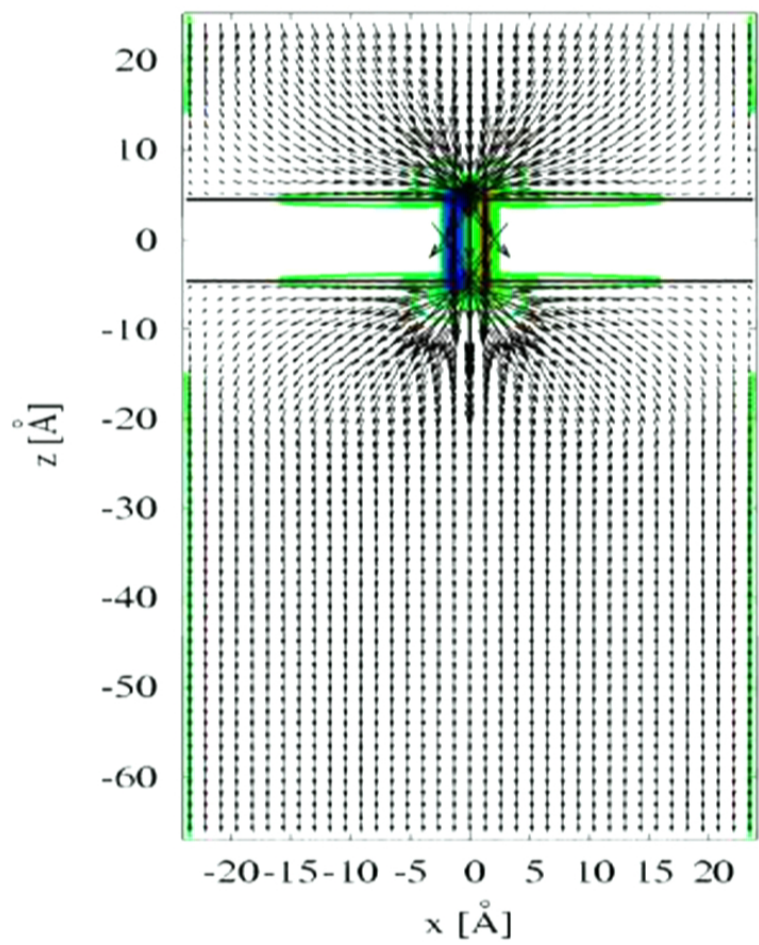
Bushong, Gamble, and M. Di Ventra (Nano Lett. 2007); D'Agosta and Di Ventra JPCM (2006)

23.80 fs



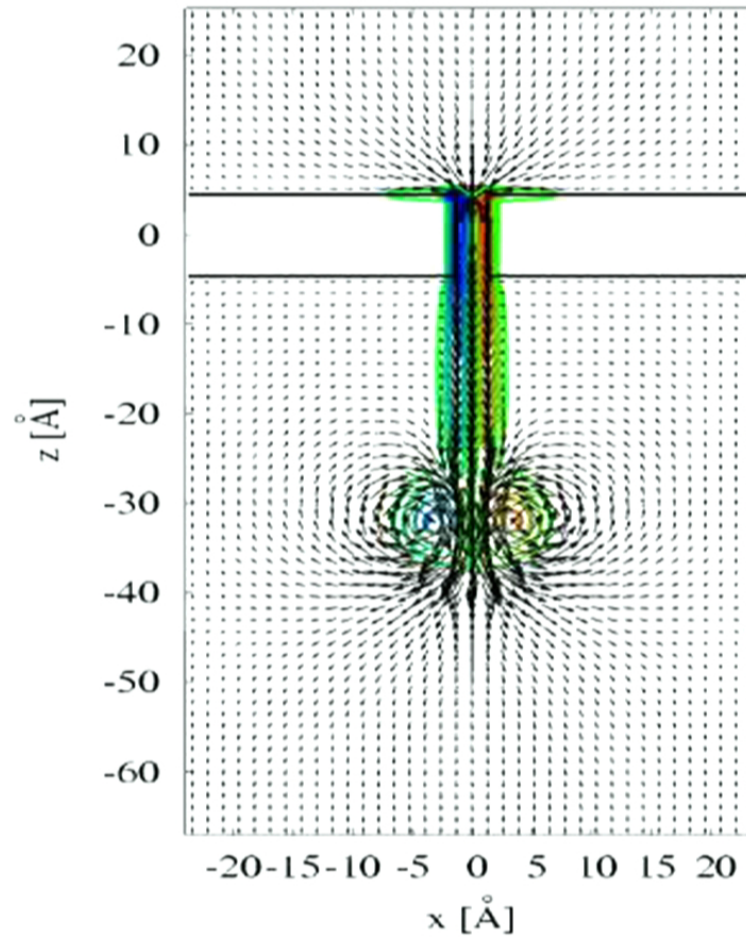
Bushong, *Journal of Applied Physics* 101, 043105 (2007)

26.30 fs

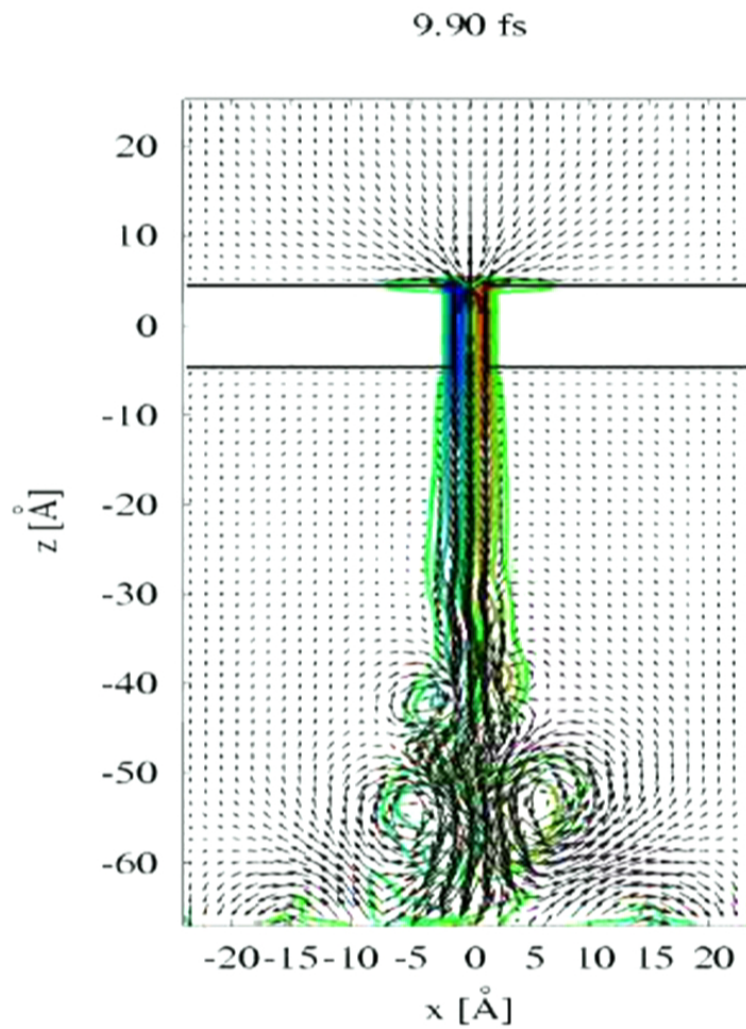


Bushong, *Journal of Applied Physics* 101, 043105 (2007)

3.70 fs



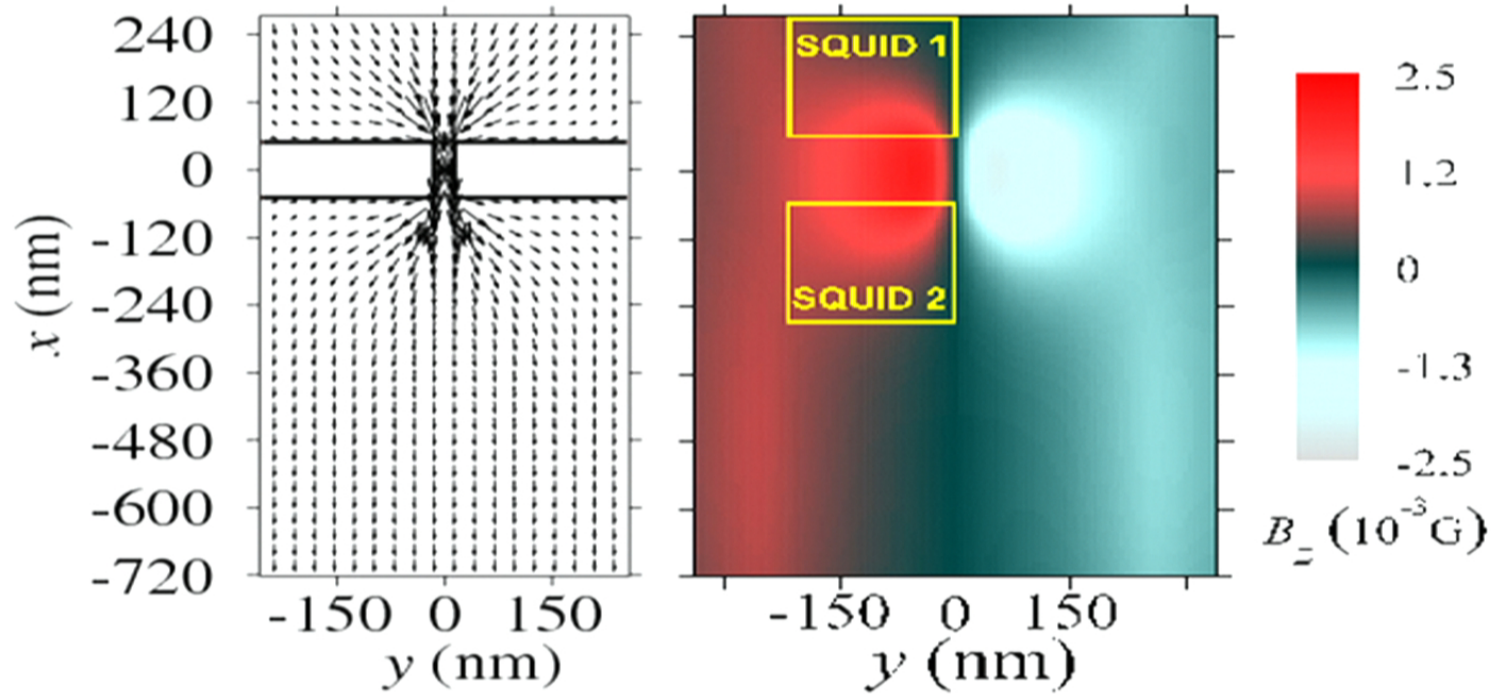
Bushong, *Journal of Applied Physics*, 101, 043105 (2007)



Bushong, *Journal of Applied Physics*, 101, 043105 (2007)

Possible exp. verification

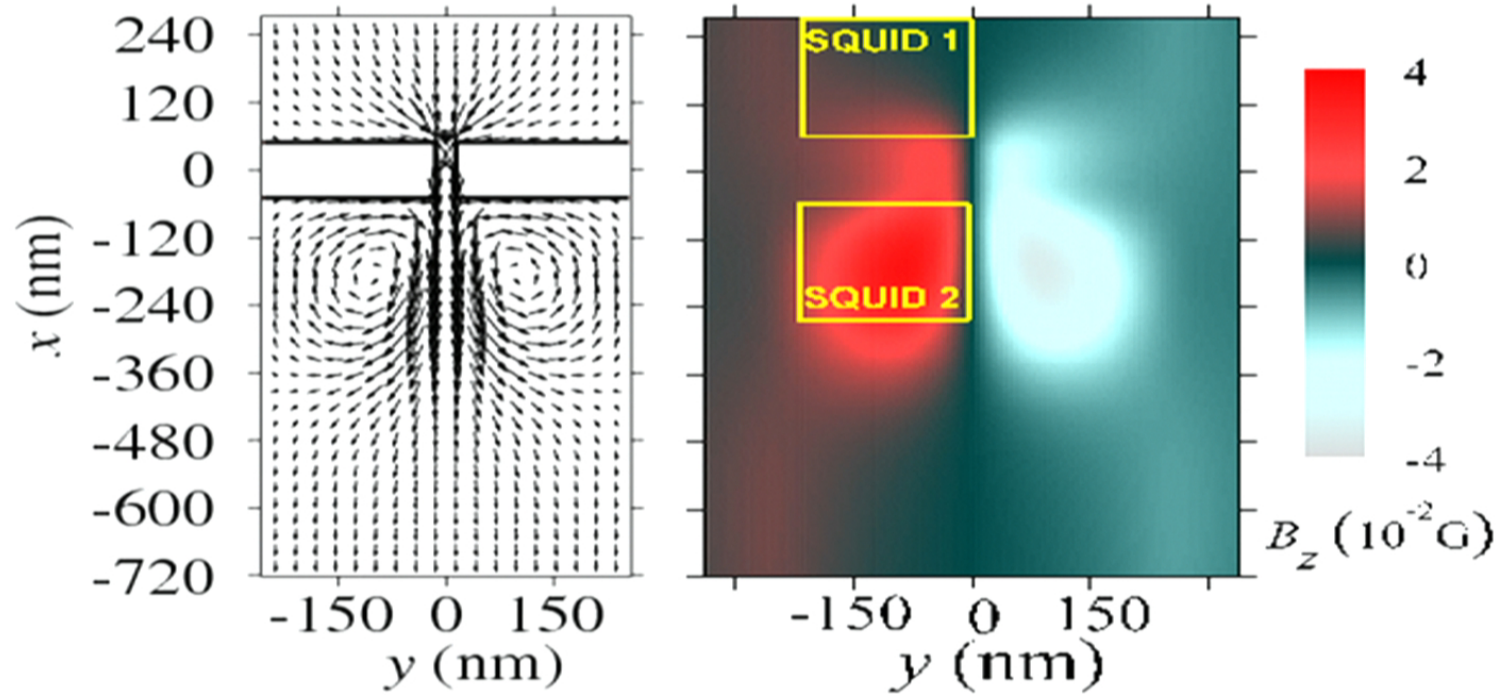
Laminar



Bushong, Pershin and M. Di Ventra (Phys. Rev. Lett. 2007)

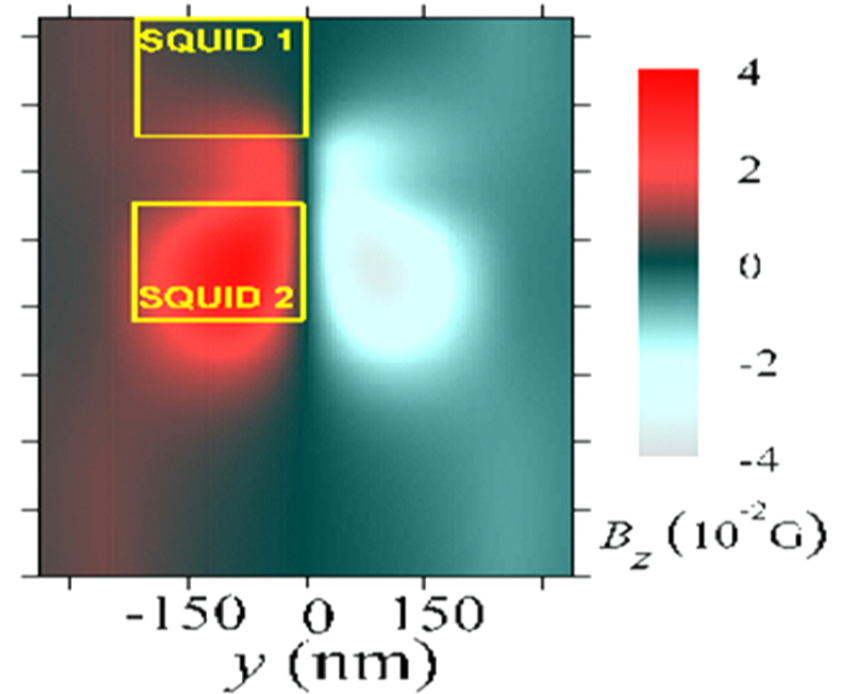
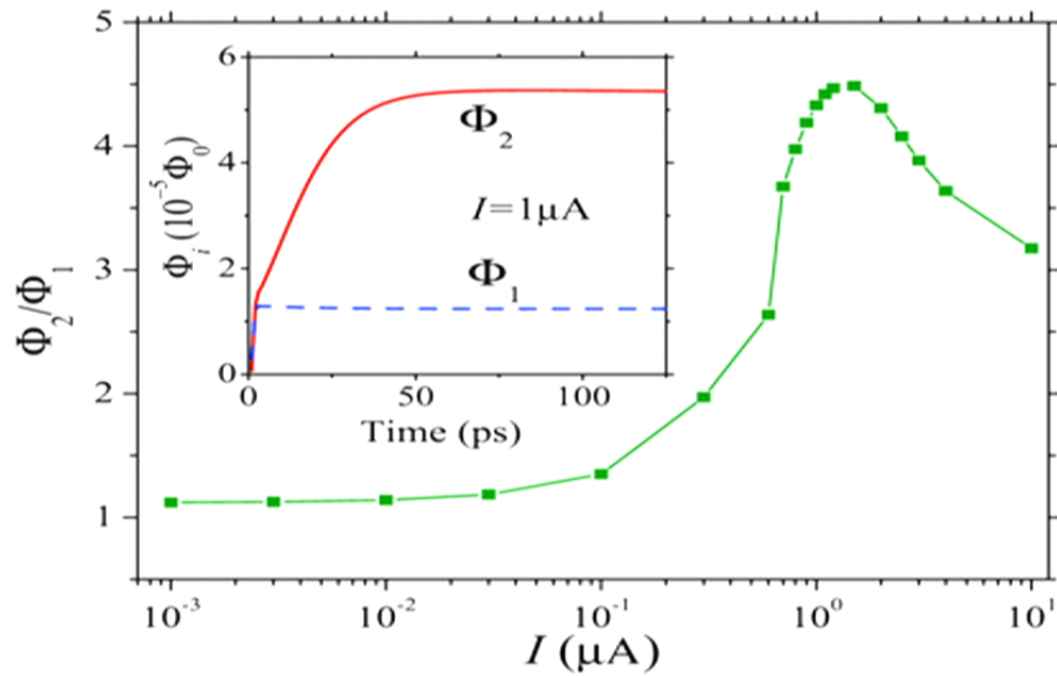
Possible exp. verification

Turbulent



Bushong, Pershin and M. Di Ventra (Phys. Rev. Lett. 2007)

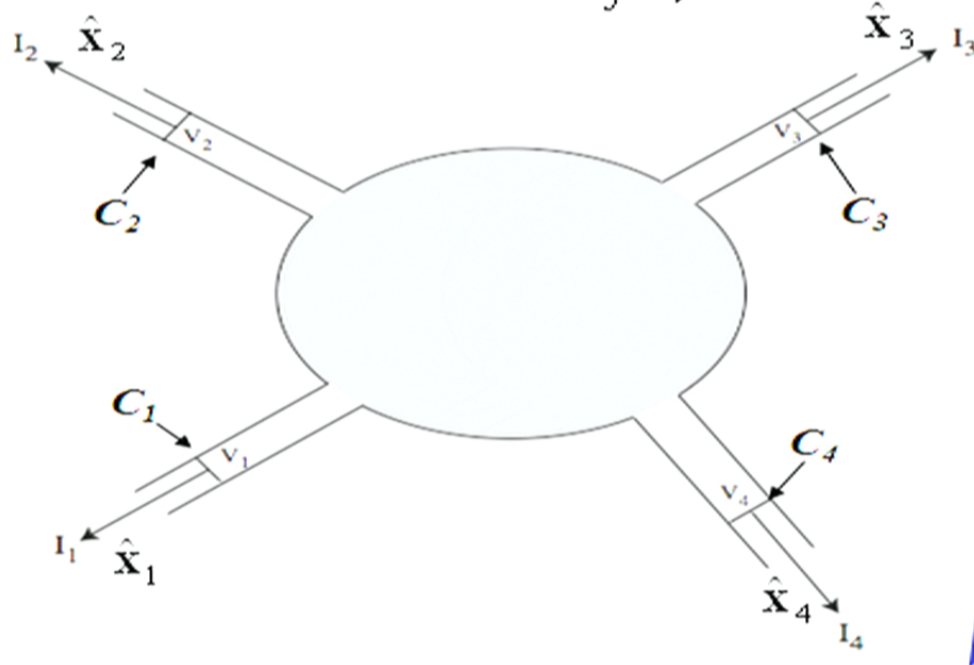
Possible exp. verification



Bushong, Pershin and M. Di Ventra (Phys. Rev. Lett. 2007)

Physical origin of many-body corrections: linear-response theory

$$\mathbf{j}_i(\mathbf{r}) = \sum_j \int_V \sigma_{ij}(\mathbf{r}, \mathbf{r}') \mathbf{E}_j(\mathbf{r}') d\mathbf{r}'$$



Current conservation

$$\partial_i \sigma_{ij}(\mathbf{r}, \mathbf{r}') = 0$$

Gauge invariance

$$\partial_j \sigma_{ij}(\mathbf{r}, \mathbf{r}') = 0$$



$$G_{mn} = - \int_{C_m} d\mathbf{r} \int_{C_n} d\mathbf{r}' \hat{x}_{mi} \sigma_{ij}(\mathbf{r}, \mathbf{r}') \hat{x}_{nj}$$

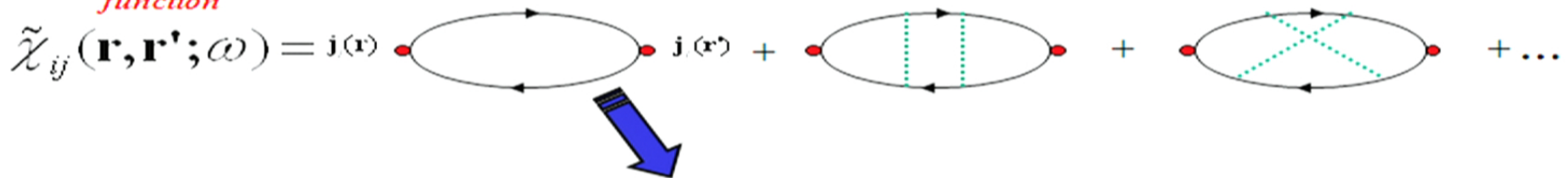
$$m \neq n$$

Physical origin of many-body corrections: linear-response theory



$$\sigma_{ij}(\mathbf{r}, \mathbf{r}') = e^2 \lim_{\omega \rightarrow 0} \frac{\text{Im} \tilde{\chi}_{ij}(\mathbf{r}, \mathbf{r}'; \omega)}{\omega}$$

“Proper” current-current response function



For a non-interacting system

$$\sigma_{ij}(\mathbf{r}, \mathbf{r}') = e^2 \sum_{\alpha, \beta} \frac{\partial f(\epsilon_{\alpha})}{\partial \epsilon_{\alpha}} \delta(\epsilon_{\alpha} - \epsilon_{\beta}) W_{\alpha, \beta}^{i*}(\mathbf{r}) W_{\alpha, \beta}^j(\mathbf{r}')$$



Physical origin of many-body corrections: linear-response theory



$$\begin{aligned}\mathbf{j}_i(\mathbf{r}) &= \sum_j \int_V \sigma_{ij}(\mathbf{r}, \mathbf{r}') \mathbf{E}_j(\mathbf{r}') d\mathbf{r}' \\ &= \sum_j \int_V \underbrace{\sigma_{ij}^{KS}(\mathbf{r}, \mathbf{r}')}_{\text{Kohn-Sham conductivity}} \left[\mathbf{E}_j(\mathbf{r}') + \underbrace{\mathbf{E}_{xc,j}(\mathbf{r}')}_{\text{Exchange-correlation field}} \right] d\mathbf{r}'\end{aligned}$$

In the linear approximation one has

$$\mathbf{E}_{xc,i}(\mathbf{r}) = \sum_j \int_V \underbrace{\rho_{ij}^{xc}(\mathbf{r}, \mathbf{r}')}_{\text{Exchange-correlation resistivity}} \mathbf{j}_j(\mathbf{r}') d\mathbf{r}'$$

$$\rho_{ij}(\mathbf{r}, \mathbf{r}') = \rho_{ij}^S(\mathbf{r}, \mathbf{r}') + \rho_{ij}^{xc}(\mathbf{r}, \mathbf{r}')$$

Sai *et al.* Phys. Rev. Lett. (2005)

Physical origin of many-body corrections: viscosity effects



The visco-elastic xc field in time-dependent current-DFT

$$\mathbf{E}_{xc,i}(\mathbf{r}, \omega) = \underbrace{-\nabla_i V_{xc,0}(\mathbf{r}, \omega)}_{\text{Adiabatic LDA}} - \underbrace{n_0^{-1}(\mathbf{r})}_{\text{equilibrium density}} \underbrace{\partial_j P_{xc,ij}(\mathbf{r}, \omega)}_{\text{exchange correlation stress tensor}}$$

The xc stress tensor

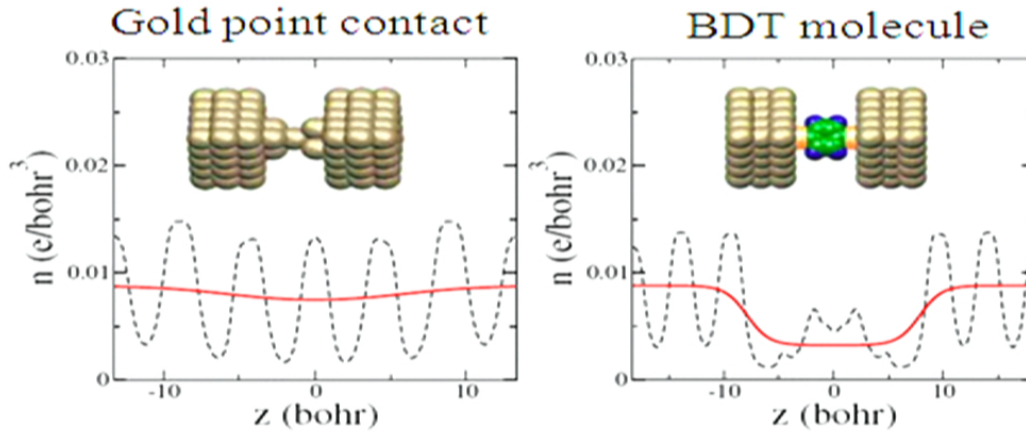
$$P_{xc,ij}(\mathbf{r}, \omega) = \underbrace{\eta(n_0, \omega)}_{\text{Shear viscosity of uniform electron gas}} \left[\frac{\partial_i \delta_j}{\partial_j} + \frac{\partial_j \delta_i}{\partial_i} - \frac{2}{3} \nabla \cdot \mathbf{v} \delta_{ij} \right] + \underbrace{\zeta(n_0, \omega)}_{\text{Bulk viscosity of uniform electron gas } (\sim 0)} \nabla \cdot \mathbf{v} \delta_{ij}$$

The velocity field

$$\mathbf{v}(\mathbf{r}) = \frac{\mathbf{j}(\mathbf{r})}{n_0(\mathbf{r})}$$

[GV, Ullrich, and Conti, PRL 79, 4878 (1997)]

Physical origin of many-body corrections: viscosity effects

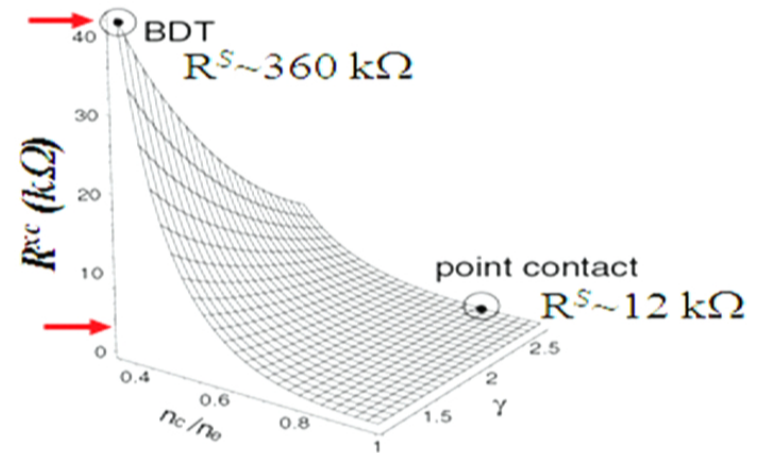


$$R = R^S + R^{xc}$$

Assuming that the system is homogeneous in the transverse direction we obtain

$$R^{xc} \propto \frac{4 \hbar^2}{3e^2 A} \int_a^b \eta[n(z)] \frac{(\nabla_z n)^2}{n^4} dz$$

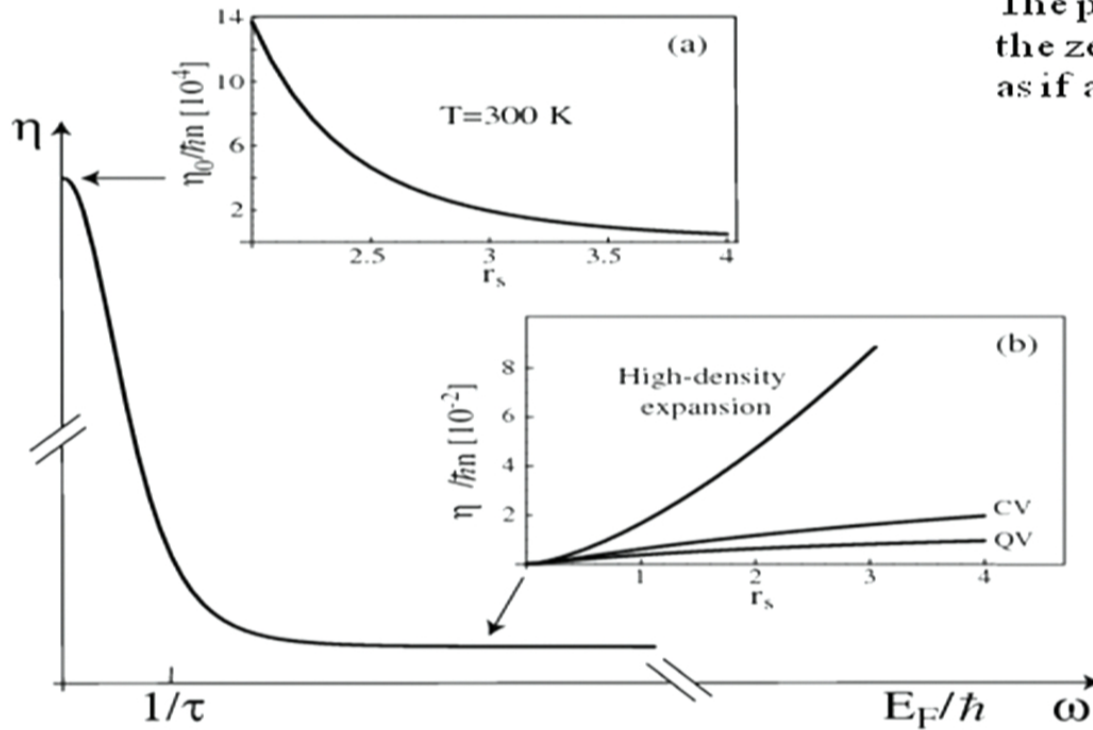
Sai *et al.* Phys. Rev. Lett. (2005)



Physical origin of many-body corrections: viscosity effects



η_0 calculated by Abrikosov&Khalatnikov for the homogeneous Fermi liquid



The presence of a nanostructure cuts off the zero frequency divergence of the viscosity as if an effective temperature is present

$$\eta(\omega \rightarrow 0) = \mu_{\infty} \tau_c$$

Shear modulus Elastic lifetime

$$\tau_c \propto \Delta E / \hbar$$

Vignale and Di Ventra, PRB 2009

Outline



- Introduction to the transport problem
- Many-body effects related to viscosity of the electron liquid (large for structures with smaller transmissions)
- **Properties of steady states and predictions**

Theory: Microcanonical picture of transport

Experiments: Atomic gases in optical lattices

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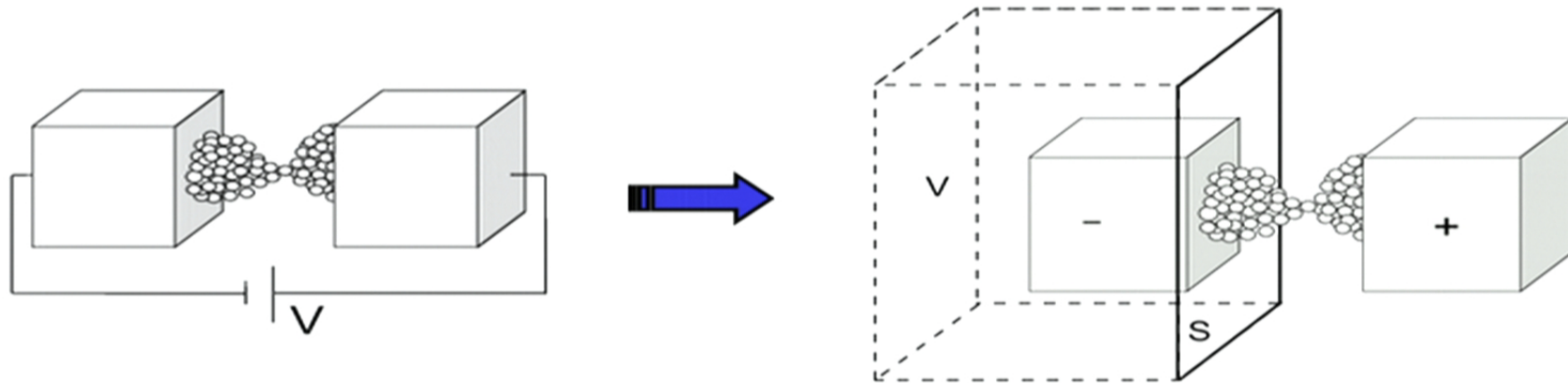


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Theory: Microcanonical picture of transport

Experiments: Atomic gases in optical lattices

Interactions in the whole system: the microcanonical picture of transport



$$I_{exact} = \int_S \mathbf{j}_{exact} ds = \int_V \nabla \cdot \mathbf{j}_{exact} dv \stackrel{\nabla \cdot \mathbf{j} = -\frac{\partial n}{\partial t}}{=} \int_V \nabla \cdot \mathbf{j}_{KS} dv = \int_S \mathbf{j}_{KS} ds = I_{KS}$$

M. Di Ventra, T.N. Todorov, (J. Phys. Cond. Matt. 2004)

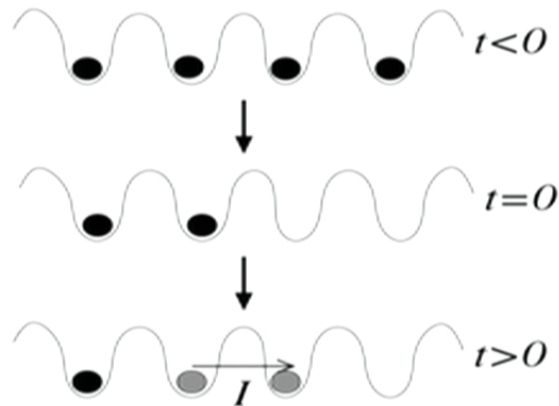
Cold atoms are ideal systems for studying transport phenomena

- You can choose:
 1. fermions or bosons
 2. harmonic trap, optical lattice, or both (Box-potential is coming soon!)
 3. single or multi components or species
 4. dimensions (3D, 2D, 1D, or mixed)
- You can tune:
 1. interactions among atoms (via Feshbach resonance)
 2. trap depth or lattice constant
 3. temperature
 4. density / filling factor

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Density-induced transport



1. Loading non-interacting single-species atoms into the ground state.
2. Remove particles on the right half using photons.

$$\langle b_k^\dagger b_{k'} \rangle = n_k \delta_{kk'} \quad c_{ij}(t=0) = \begin{pmatrix} c_{ij} & 0 \\ 0 & 0 \end{pmatrix}$$

$T=0$, N particles:

fermions:

$$\langle b_k^\dagger b_{k'} \rangle = \delta_{kk'}$$

bosons:

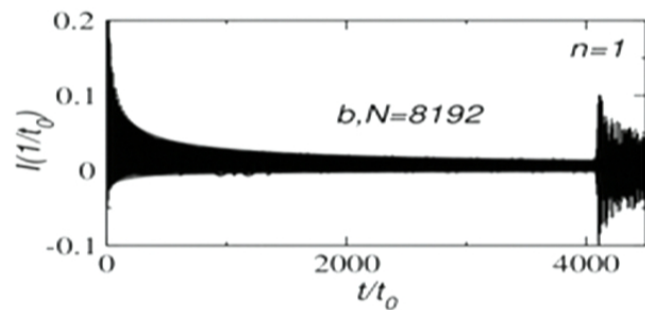
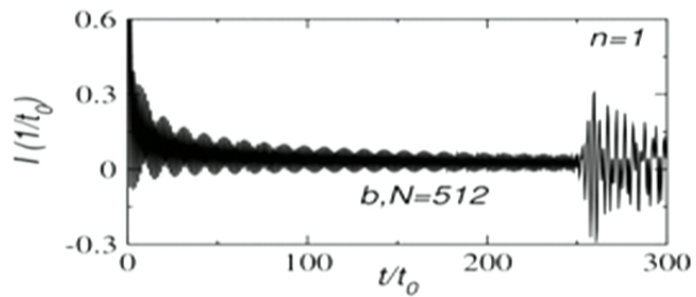
$$\langle b_k^\dagger b_{k'} \rangle = N \delta_{kk'} \delta_{k1}$$

$$D_{kk'}(0) = \sum_{i,j=1}^{N/2} (U^\dagger)_{k'j'} U_{ik} c_{ij}(t=0)$$

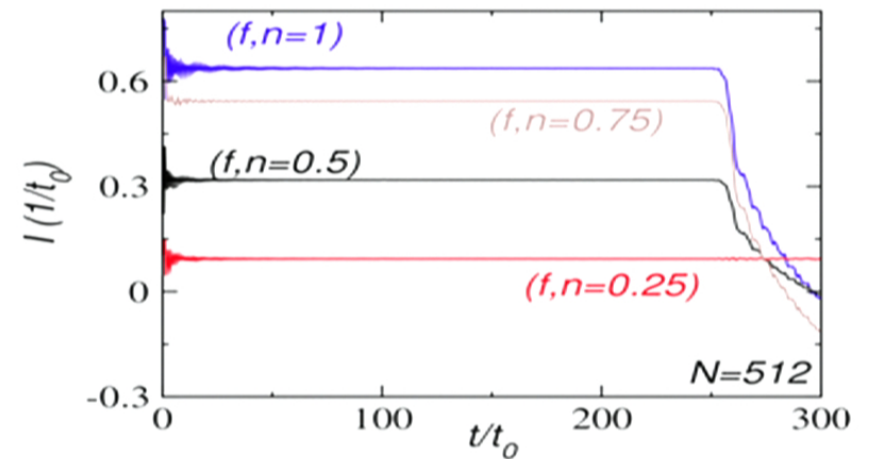
$$c_{ij}(t) = \sum_{k,k'=1}^N (U^\dagger)_{ki} (U)_{jk'} D_{kk'}(0) e^{i(\epsilon_k - \epsilon_{k'})t}$$

Bosonic vs fermionic currents

bosons (quasi-condensate)

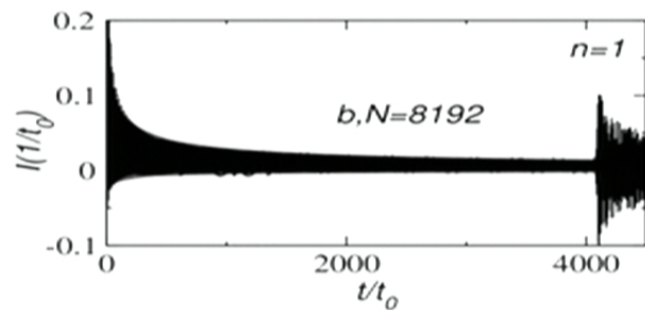
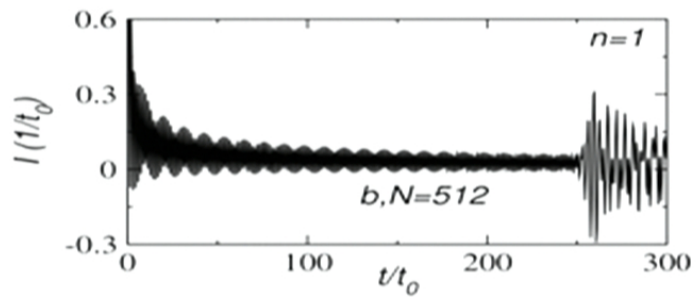


fermions (Fermi sea)

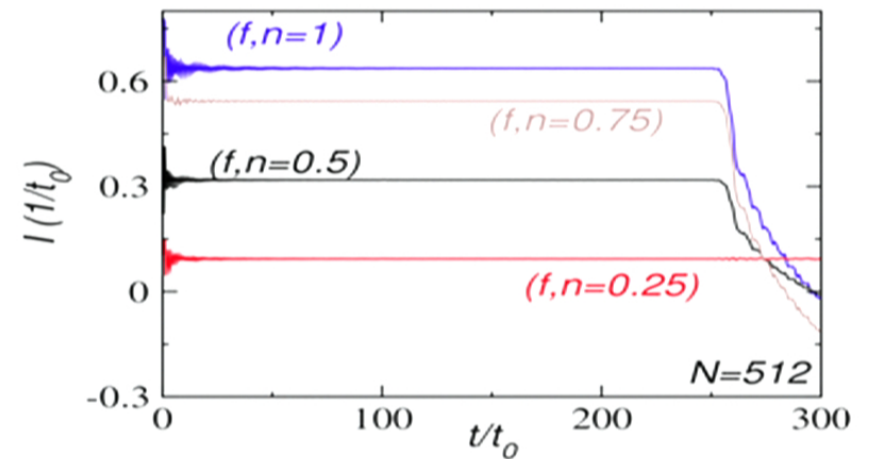


Bosonic vs fermionic currents

bosons (quasi-condensate)

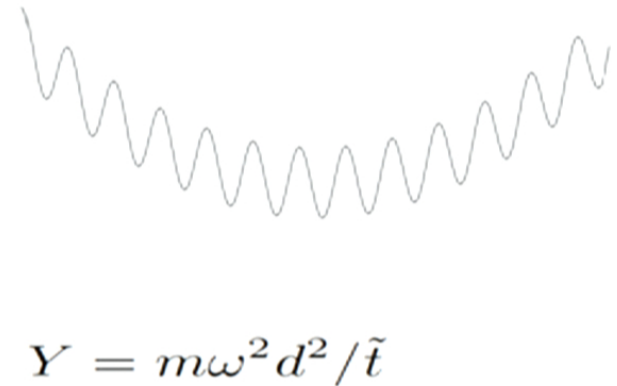
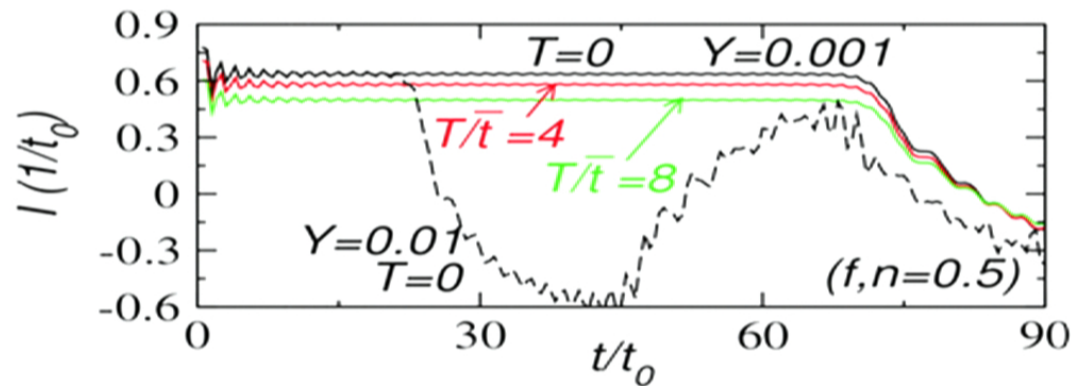


fermions (Fermi sea)



More on the current

- Fermionic QSSC: Robust against trap and T

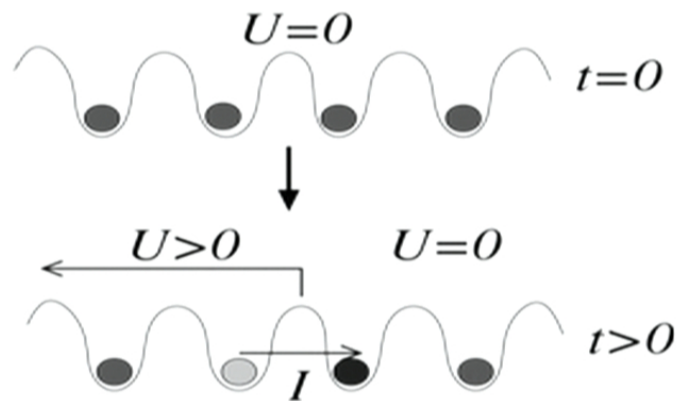


$$Y = m\omega^2 d^2 / \tilde{t}$$

- Bosonic current: Never reaches a finite QSSC even in the thermodynamic limit at $T=0$

$$I \propto N^{-1/2}$$

Interaction-induced transport



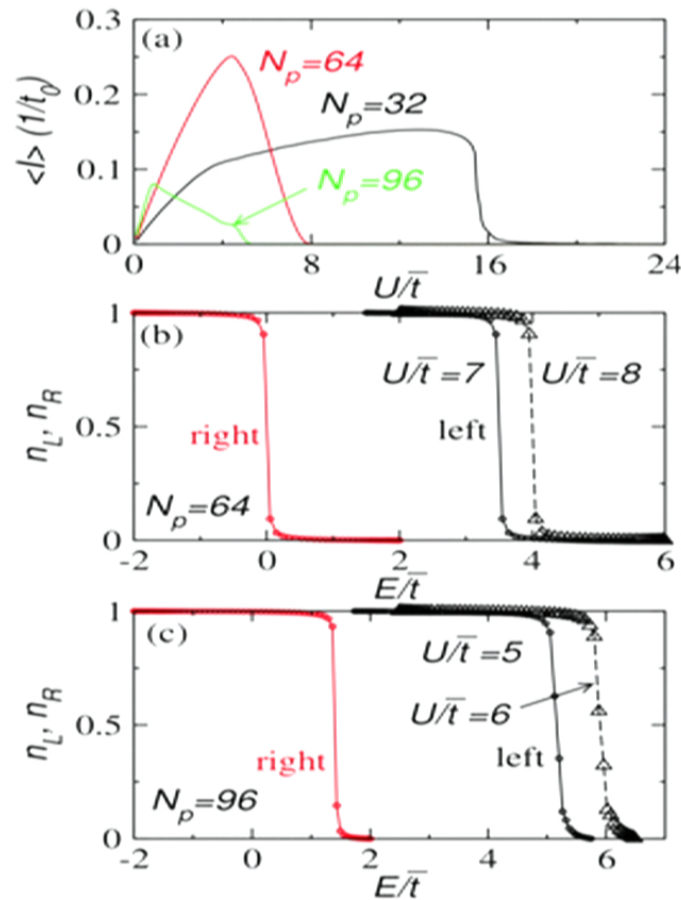
1. Loading non-interacting two-component fermions into the ground state.
2. Turning on interactions on half of the lattice.

$$H_e = H_0 + \sum_{i \in L} U \hat{n}_{i\sigma} \hat{n}_{i\bar{\sigma}}$$

Optically controlled collisions:

Optical Feshbach resonance (coupling to auxiliary channels by photons. Realized in Yb and Sr, proposed for Li.): PRL 105, 050405; PRA 79, 021601; PRL 107, 073202; PRL 108, 010401.

Mismatch of energy spectra



1. The switch-on of U changes the energy dispersion of the left-half lattice.
2. Moving a high-energy particle to a low-energy state or vice versa is forbidden by the underlying quantum dynamics.
3. The blockade is dynamical. (unlike Mott insulator in equilibrium which is due to energy minimization.)

Conclusions



- Landauer approach is an incomplete description of transport

Conclusions



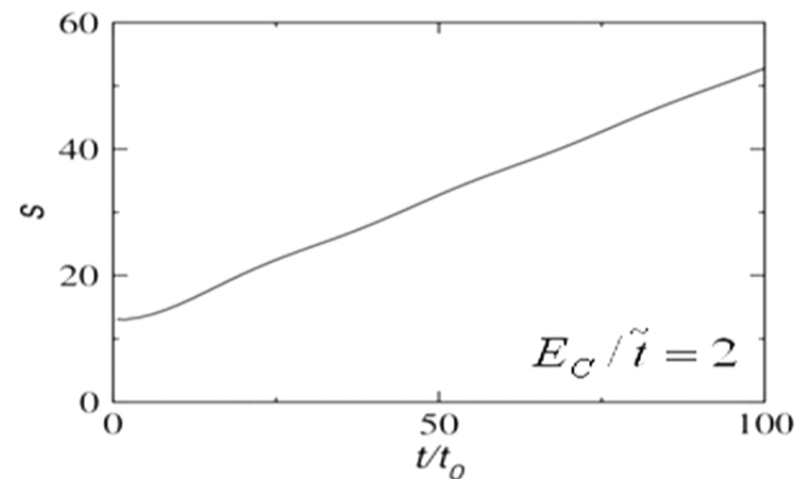
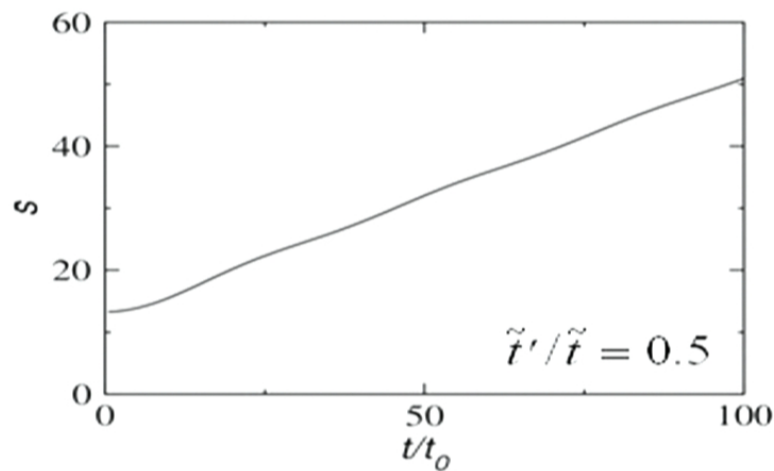
- Landauer approach is an incomplete description of transport
- Many-body effects related to viscosity of the electron liquid (large for structures with smaller transmissions)
- Predictions (some verifiable in atomic lattices):
 - Turbulence of the electron liquid
 - Quasi-steady state formation also in finite systems
 - Fermi distributions not necessary for the existence of a QSS
 - Conducting-nonconducting transition due to interactions

S from MCF Simulations

$$H = \sum_{ij} \tilde{H}_{ij} c_i^+ c_j \Rightarrow \rho_L = \frac{1}{Z_L} \exp(-H_L)$$

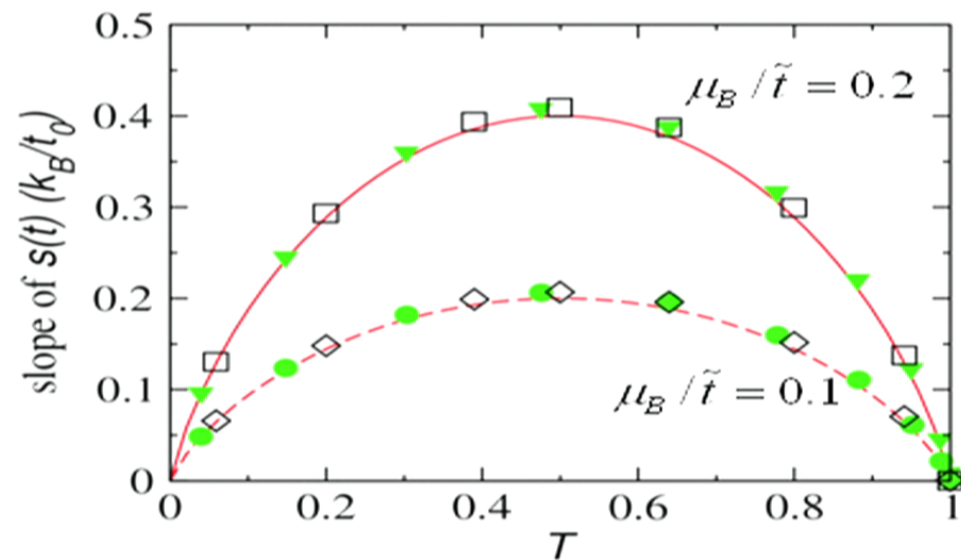
$$M = P_L c_{ij} P_L = \text{Tr}(\rho_L c_i^+ c_j) \quad \Rightarrow \quad M = (1 + e^{\tilde{H}_L})^{-1}$$

$$S_L = -\text{Tr}[\rho_L \log(\rho_L)] = -\text{Tr}[M \log M + (1 - M) \log(1 - M)]$$



Linear-in-time quasi steady state

Comparison of ds/dt



The assumption of a binomial distribution mimics the quantum evolution very well.