On the Effects of Electron-Phonon interaction on transport through Carbon Nanotubes

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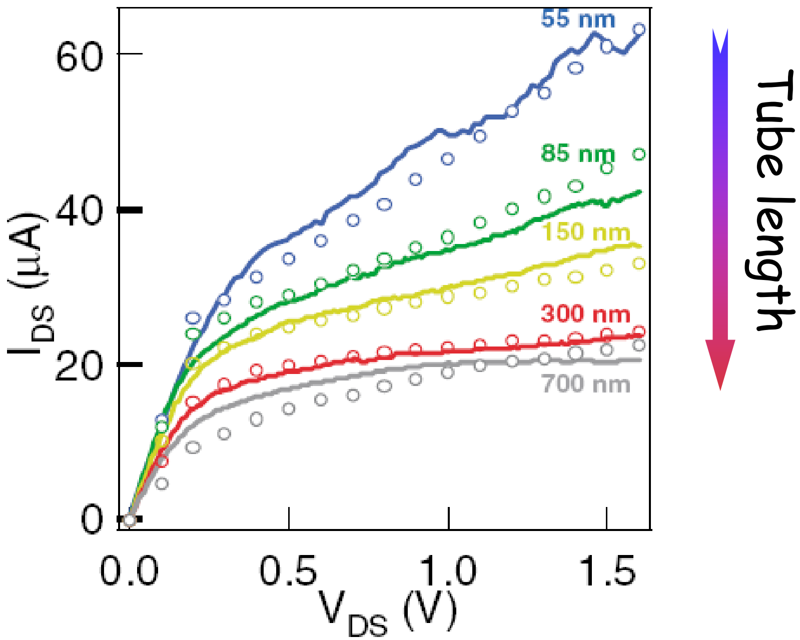
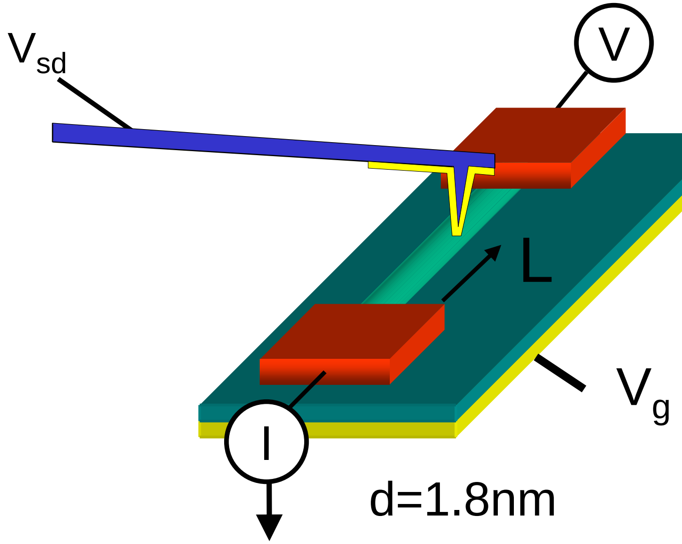
Outline of the talk

- **Motivation: E-ph effects** → Transport; Electronic and Phonon bandstructures
- **Peierls-like mechanism: Model and simple picture**
- **Predictions: experimental consequences on transport**

Conclusions

Motivation 1: E-ph interaction leads to current saturation at high bias voltage

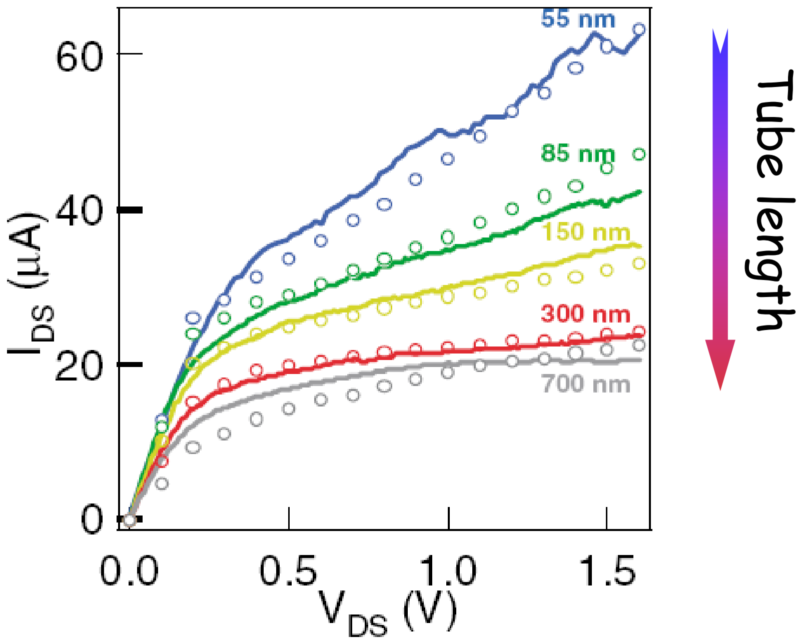




A. Javey et al PRL **92**, 106804 (2004), see also Park et al., Nano Lett. 2004.

- For short metallic tubes there is a change in the slope of the I-V curve.
- The current saturates at high biases for long tubes.

Motivation 1: E-ph interaction leads to current saturation at high bias voltage



A. Javey et al PRL **92**, 106804 (2004), see also Park et al., Nano Lett. 2004.

Most of the studies are based on the use of the Boltzmann equation

↓

Main input: Inelastic scattering rates (FGR)

Quantitative disagreement, hot phonons scenario n~2-5

M. Lazzeri et al, PRL **95**, 236802 (2005).

Are we missing anything beyond the scope of semiclassical approaches?

Applicability?

Short lengths, Low dimensionality…

Motivation 2: E-Ph effects on electronic bandstructure

Efficiency of Peierls Instability in Carbon Nanotubes?

Are Fullerene Tubules Metallic?

J. W. Mintmire, B. I. Dunlap, and C. T. White
Naval Research Laboratory, Washington, DC 20375-5000
(Received 9 October 1991)

Phys. Rev. Lett. **68**, 638 (1992).

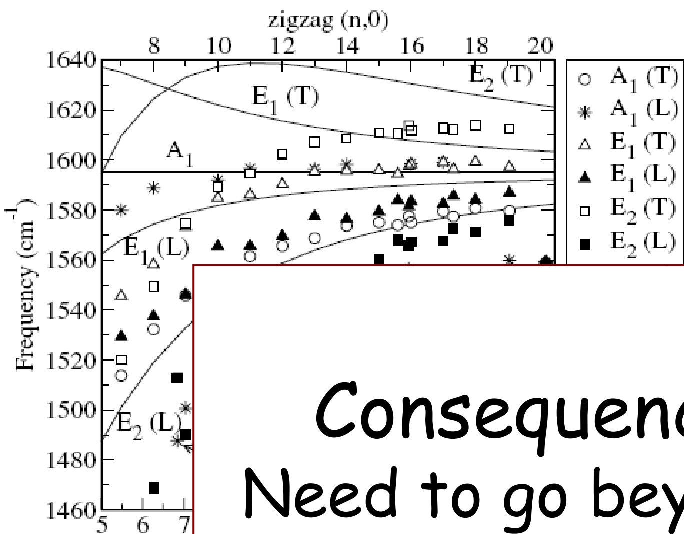
Yes, Carbon Tubules remain metallic at temperatures above 10K and not very short radii.

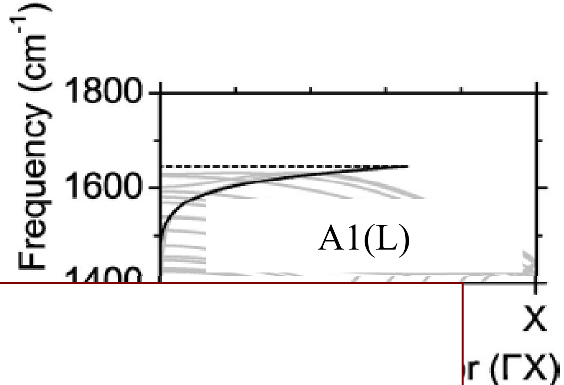
Connetable et al;, PRL **94**, 015503 (2005)
Figge et al., PRL **86** 4572 (2001)

However, there are important effects on the phonon bandstructure that remain even at room temperatures…

Motivation 2: E-Ph effects on phonon bandstructure

E-Ph interaction leads to softening of A1(L) mode at the Gamma point





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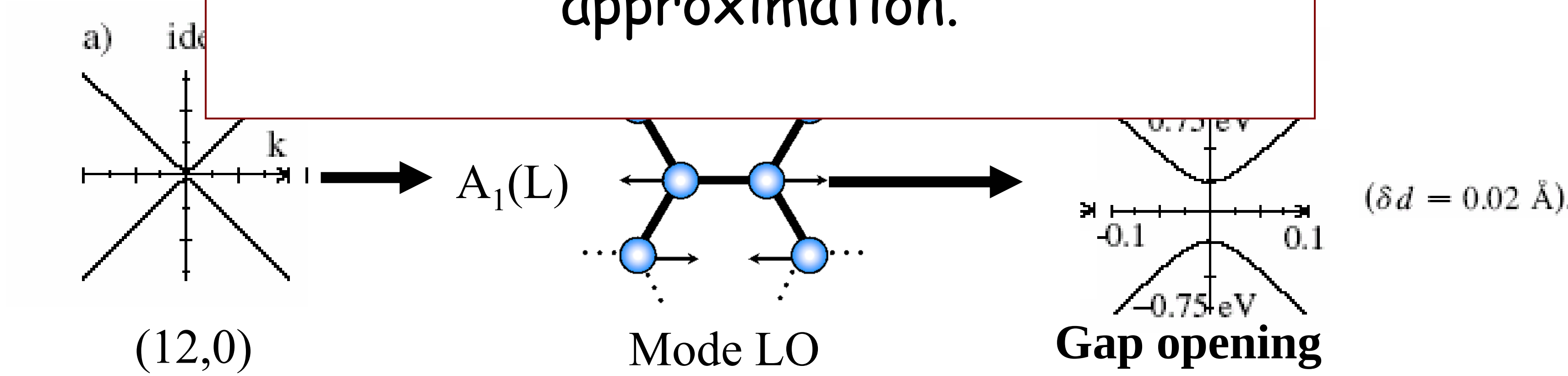
Consequences on transport?
Need to go beyond FGR and adiabatic approximation.



Fock space approach for inelastic transport

mapping of the many-body problem (one electron interacting with phonons) into a one-particle problem in a higher dimensional space.

Variational (non-perturbative) scheme

E. V. Anda et al. Braz. J. Phys. **24**, 330 (1994).

J. Bonča, S. A. Trugman, Phys. Rev. Lett. **75**, 2566 (1995).

n phonons

$$|\, j, n \rangle$$

one electron at site *j*

$$|\, j, n_1, n_2, \ldots \rangle$$

Calculation of the elastic and inelastic transmission coefficients in the e-ph Fock space, plus self-consistent treatment for the electronic distributions to compute the current.

E. Emberly & G. Kirczenow, PRB 61, 5740 (2000)

LFT, H.M. Pastawski & S.S. Makler, PRB **64**, 193304 (2001)

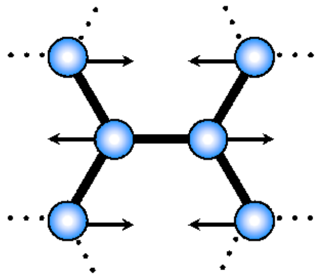
Starting Point: Hamiltonian Description

$$H = H_e + H_{e-ph} + H_{ph}$$

Electronic Hamiltonian:
pi-orbitals model

$$H_e = -\gamma_0 \sum_{\langle i,j \rangle} \left[c_i^+ c_j + h.c. \right],$$

optic $A_1(L)$ phonons



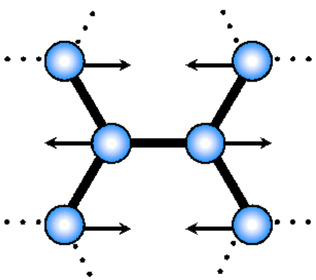
The e-ph Hamiltonian is described via the SSH model

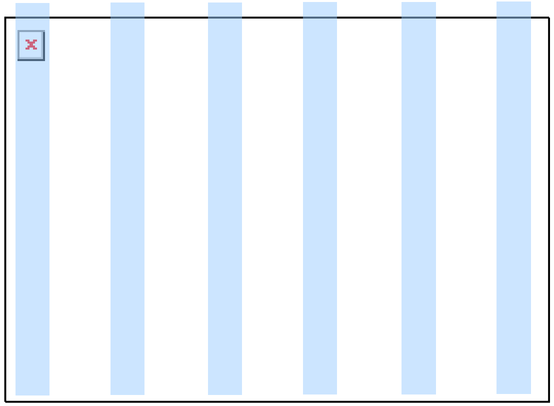
$$H = H_e + H_{e-ph} + H_{ph}$$

SSH model for the e-ph interaction (linear corrections to the atomic displacements) + quantization

$$\gamma_{i,j} = \gamma_{i,j}^{(0)} + \alpha \left(\hat{\delta} \cdot \Delta \overrightarrow{R}_{i,j}\right)$$

$$\sum_{\langle i,j \rangle} \left[\gamma_{i,j}^{e-ph} c_i^{+} c_j (b_{A_1(L)}^{+} + b_{A_1(L)}) + h.c.\right]$$

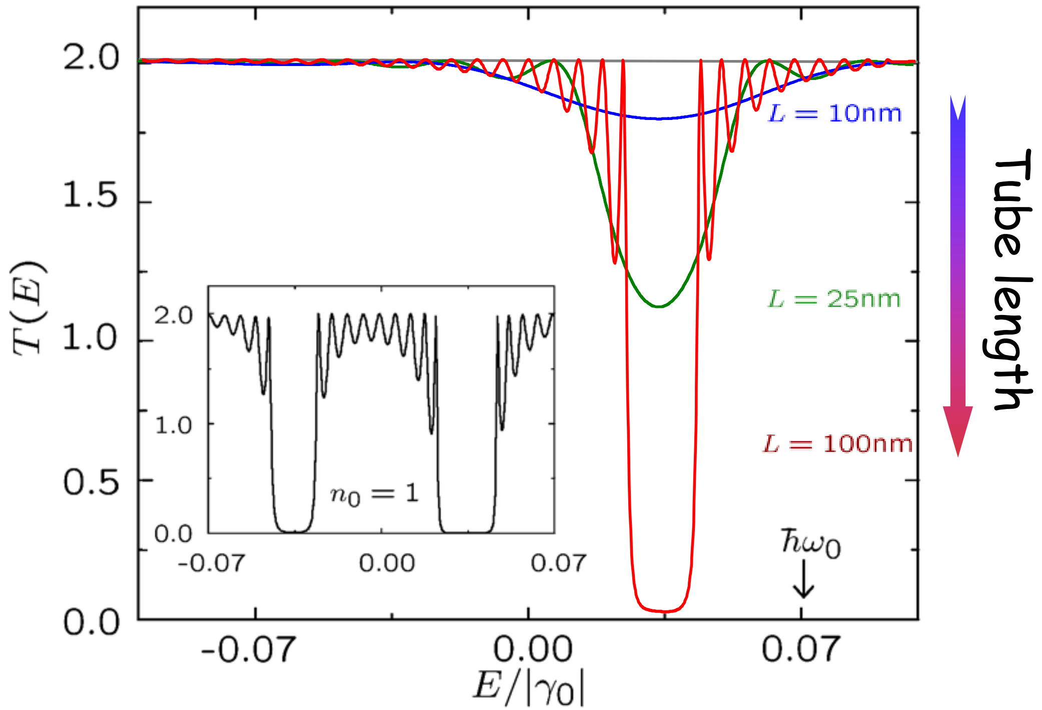




Numerical results for the transmission through a clean tube

kT=0, n_0=0

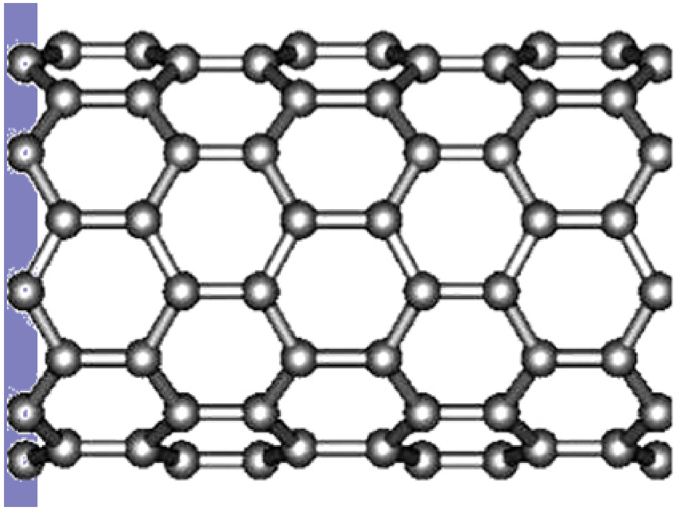
As the tube length increases a dip develops at half the phonon energy above the CNP. (below)



(Perfect) Inelastic backscattering with phonon emission. (absorption)

Divide and Conquer Strategy

Mode decomposition in the direction perpendicular to the tube axis



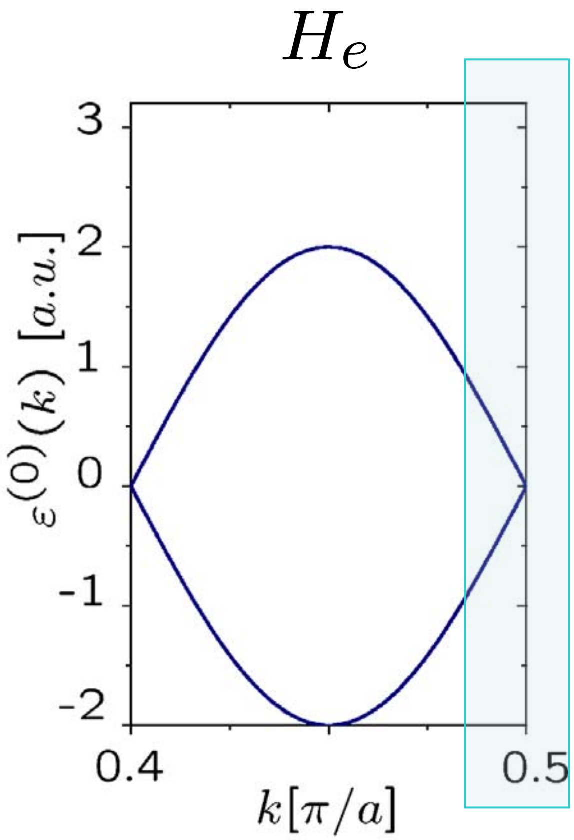
(N,0)

N independent circumferential modes

Linear chain with hoppings γ_0 and γ_q.

The e-ph interaction with A_1(L) phonon modes does not couple different spatial circumferential modes.

For metallic tubes, only 2 circumferential modes contribute close to the CNP.


H_e
3
2
1
0
-1
-2
$\varepsilon^{(0)}(k)$ $[a.u.]$
0.4
0.5
$k[\pi/a]$

The e-ph interaction lifts the degeneracy between Fock states thus leading to the opening of energy gaps

$$H = H_e + H_{e-ph} + H_{ph}$$

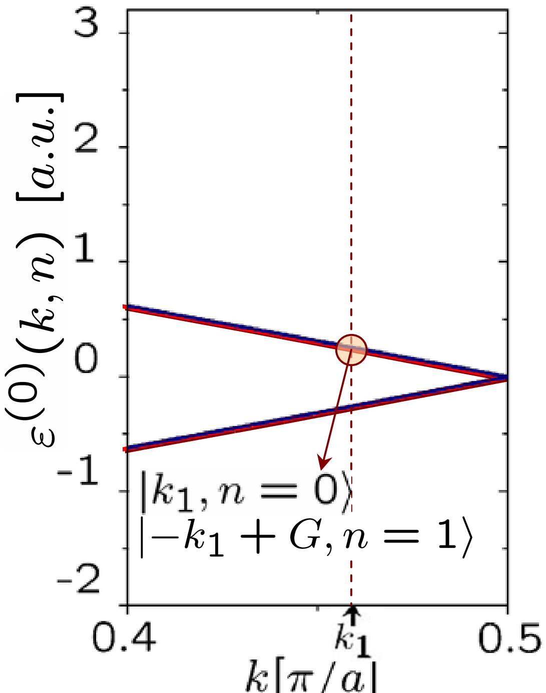
$$\langle -k_1 + G, n \pm 1 | H_{e-ph} | k_1, n \rangle \neq 0$$

Lifting of degeneracy in Fock space driven by phonon emission or absorption

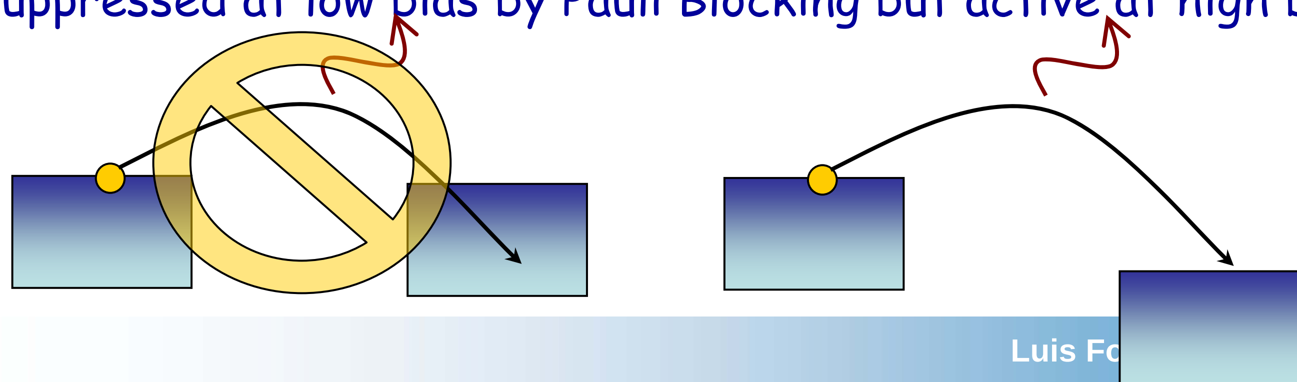
↓

$$\text{Energy gaps} \quad 2 \times \Delta\gamma^{e-ph}$$

$H_e H_{ph}$



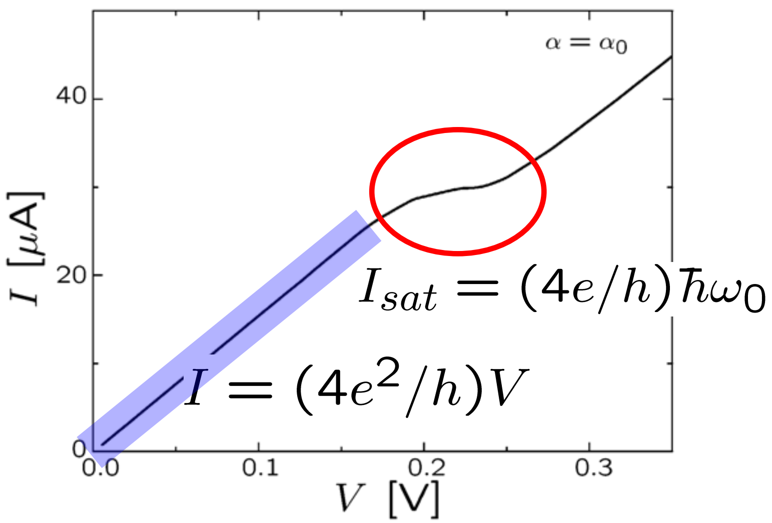
Suppressed at low bias by Pauli Blocking but active at high bias



Consequences on the I-V characteristics?

At low bias voltage the opening of the transmission gap is prevented by Pauli blocking.

But is activated for bias voltages in the order of the phonon energy leading to an onset of current saturation (of about 30μA).

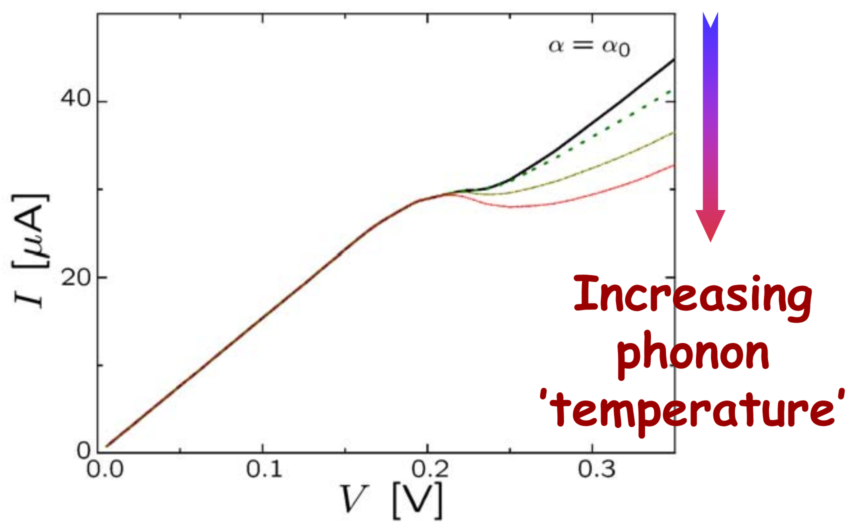


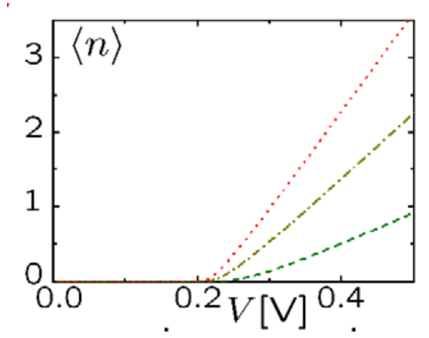
Consequences on the I-V characteristics

At low bias voltage the opening of the transmission gap is prevented by Pauli blocking.

But is activated for bias voltages in the order of the phonon energy leading to an onset of current saturation (of about 30μA).

$$I_{sat} = (4e/h)\hbar\omega_0$$





LFT and S. Roche, Phys. Rev. Lett. **97**, 076804 (2006).

Conclusions

We have shown a mechanism involving optical phonon emission (absorption) which leads to nonequilibrium energy gaps at half the optic $A_1(L)$ phonon energy, $\hbar\omega_0/2$, above (below) the CNP.

This mechanism develops when the system is driven out of equilibrium.

Quantum charge pumping in an open ring with a single-parameter

Luis Foà Torres

Outline

Introduction

Driven systems, Quantum Charge Pumping

Adiabatic parametric scattering theory.

Beyond the adiabatic theory

Floquet Theory: some basics

Transmittances and time-averaged currents in a single particle picture

Pumping in an open ring with a single parameter

Conclusions and Perspectives

Driven systems

What is the influence of excitations by electromagnetic fields and time-dependent gate voltages on the electron transport?

Photon assisted tunneling

Driven systems

Present theoretical and experimental interests

Adiabatic and non adiabatic pumping of electrons

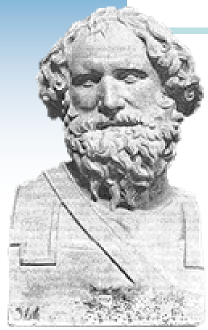
Also used in the context of the tunneling time problem

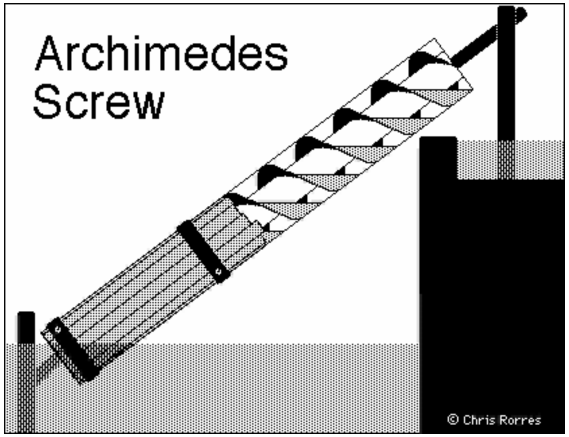
...

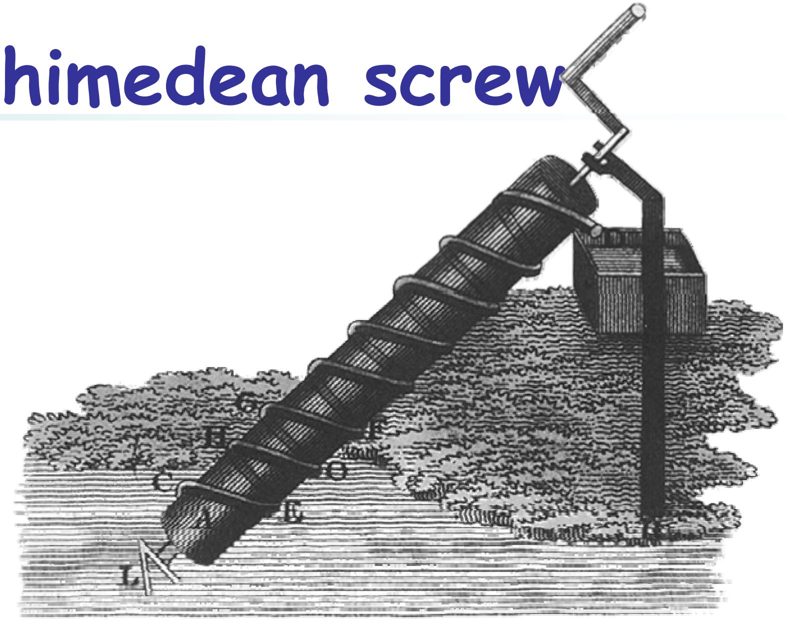
Theory for driven quantum transport is less developed as compared with the time-independent case.

Calculations are usually restricted to the lowest order in the amplitude of the driving field.

Classical Pumps: the Archimedean screw







Archimedes, 3rd century BC.

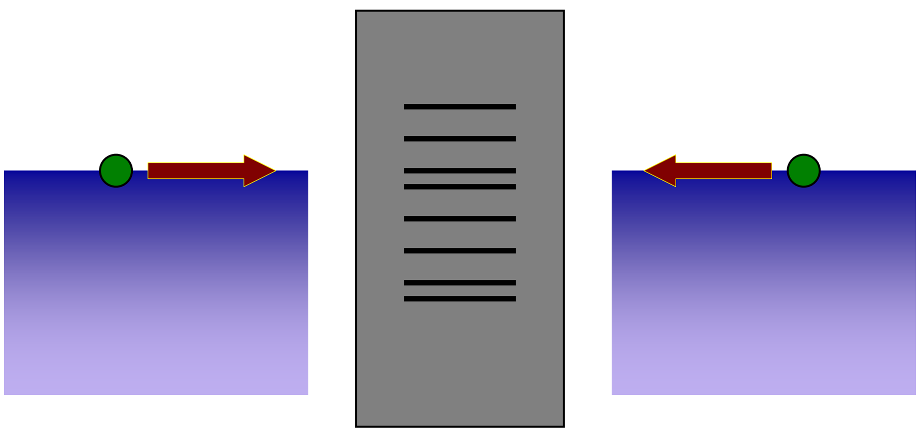
Pumping in the Quantum domain

Quantum Pumping

Generation of a directed current (dc) at ***zero*** bias potential.

Necessary condition for pumping.

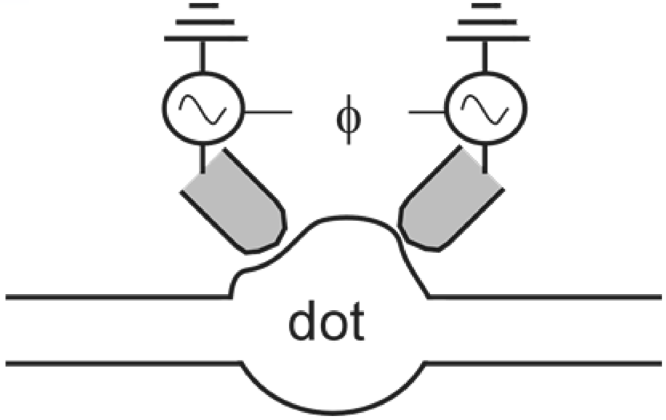
$$T_{\rightarrow} \neq T_{\leftarrow}$$



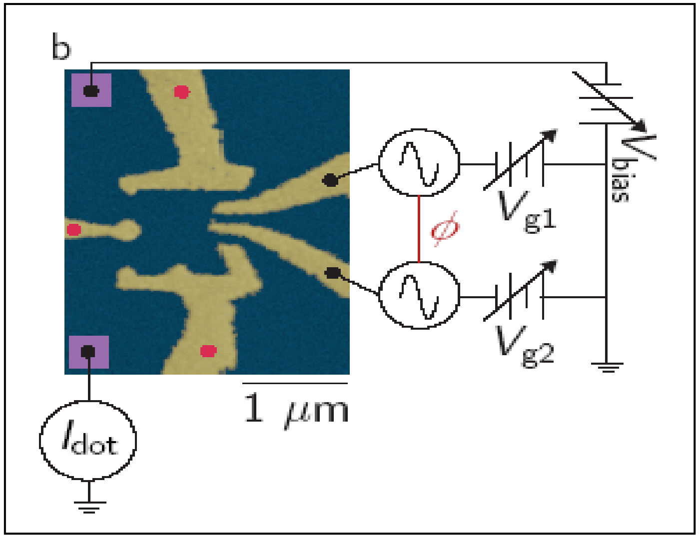
Left-right symmetry breaking.

Pumping in the Quantum domain

Typical Setup

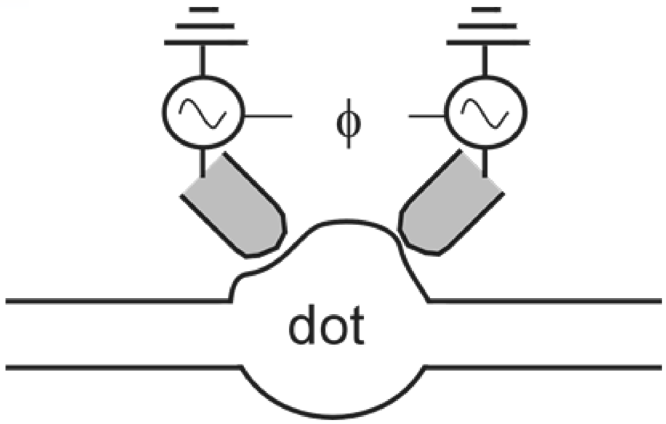


M. Switkes et al Science **283**, 1905 (1999).



Pumping in the Quantum domain

Typical Setup



M. Switkes et al Science **283**, 1905 (1999).

- Ballistic quantum dot.
- Cyclic two-parameter deformation of the dot.

ω_0 Modulation frequency.

ϕ Phase difference.

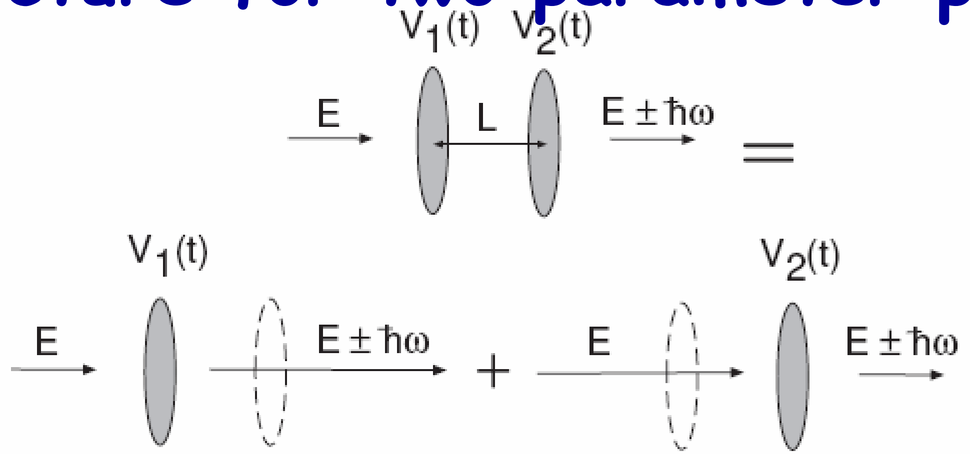
Different operational regimes according to the magnitude of

$$\frac{\omega_0}{\tau_T^{-1}} \begin{cases} << 1, \text{"}\, adiabatic \text{"}\; QP \\ >> 1, \text{"}\, non-adiabatic \text{"}\; QP \end{cases}$$

Dwell time in the dot.

A simple picture for two parameter pumping

M. Buettiker



Two different alternatives for inelastic processes.

$$T = T^{(0)}(E;E) + T^{(+)}(E+\hbar\omega;E) + T^{(-)}(E-\hbar\omega;E).$$

$$T^{(+)} = \left|\mathcal{A}^{(1,+)} + \mathcal{A}^{(2,+)}\right|^2.$$

$\longrightarrow$ $\mathcal{A}_{\rightarrow}^{(1,+)} \approx \alpha V \mathrm{e}^{-\mathrm{i}\varphi_1} \mathrm{e}^{\mathrm{i}\left(k+\frac{\omega}{v}\right)L},$ $\mathcal{A}_{\rightarrow}^{(2,+)} = \mathrm{e}^{\mathrm{i}kL} \alpha V \mathrm{e}^{-\mathrm{i}\varphi_2}.$

$\longleftarrow$ $\mathcal{A}_{\leftarrow}^{(1,+)} = \mathrm{e}^{\mathrm{i}kL} \alpha V \mathrm{e}^{-\mathrm{i}\varphi_1}.,$ $\mathcal{A}_{\leftarrow}^{(2,+)} \approx \alpha V \mathrm{e}^{-\mathrm{i}\varphi_2} \mathrm{e}^{\mathrm{i}\left(k+\frac{\omega}{v}\right)L}$

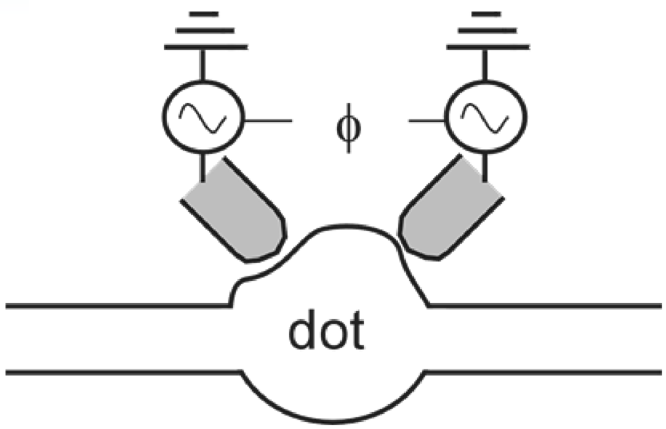
The interference terms are different!

$$T_{\rightarrow}^{(+)} \neq T_{\leftarrow}^{(+)}.$$

M. Buettiker and M. Moskalets, cond-mat/0502229.

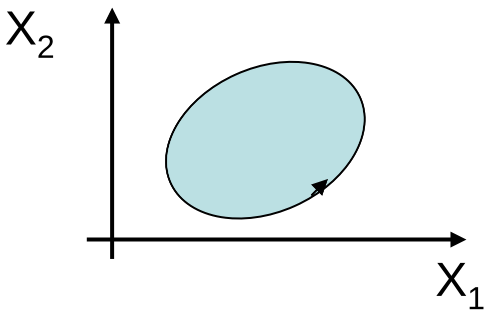
Parametrical theory for adiabatic pumping

P. W. Brouwer, PRB **44**, 10135R (1998).



Parametric pumping theory: *S-matrix* approach at low-frequency (first order in Omega).

$$S(X_1(t), X_2(t))$$



Main outcome of this theory:
The average pumped **current is proportional to the area in parameter space**.

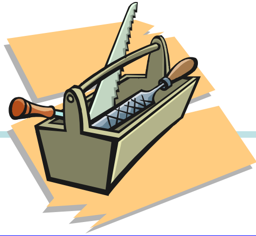
Hence, at least two out of phase time-dependent parameters are needed to achieve pumping.

Why does the parametric scattering theory require at least two parameters? What is the difference with a situation with only one parameter?

Is it possible to operate a pump with a single parameter?

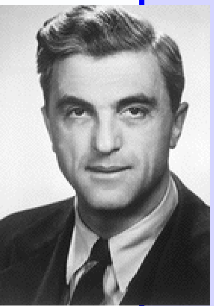
What is the minimal number of parameters needed to obtain QP? what symmetries should they break?

Let us think beyond the adiabatic parametric scattering matrix theory... this means using either strong driving amplitudes or high frequencies...



Floquet Theory

(a brief summary)



Spatially periodic systems	*periodically time-dependent* systems
Bloch theorem	**Floquet theorem**
assures the existence of *quasi-momenta* associated with the Bloch functions.	assures the existence of *quasi-energies* and Bloch-type states (Floquet's states).

$$\left(\hat{H}(x,t) - i\hbar\frac{\partial}{\partial t}\right)\psi(x,t) = 0.$$

$$\hat{H}(t) = \hat{H}(t+T)$$

There is a complete set of solutions of the form:

$$\boxed{\psi_\alpha(x,t) = \exp(-i\varepsilon_\alpha t/\hbar)\phi_\alpha(x,t),}$$

SepDynScales.

quasi-energies

Floquet's states or modes

$$\phi_\alpha(x,t+T) = \phi_\alpha(x,t)$$

J. Shirley, PR **138**, B979 (1965); Ya B. Zel'dovich, Sov.Phys. JETP **24**, 1006 (1967).

H. Sambe, PRA **7**, 2203 (1973).

Floquet Theory

$$\hat{H}(t) = \hat{H}(t+T)$$

(a brief summary)

There are solutions of the TDSE of the form:

$$\boxed{\psi_\alpha(x,t) = \exp(-i\varepsilon_\alpha t/\hbar)\phi_\alpha(x,t),} \qquad \phi_\alpha(x,t+T) = \phi_\alpha(x,t)$$

Floquet space (Sambe space)

$$\mathbf{R} \otimes \mathbf{T} \qquad |\nu, n\rangle = |\nu\rangle \otimes |n\rangle$$

$$\boxed{\hat{H}_F(x,t)\phi_\alpha(x,t) = \varepsilon_\alpha \phi_\alpha(x,t),}$$

$$\hat{H}_F(x,t) = \hat{H}(x,t) - i\hbar\frac{\partial}{\partial t} \qquad \langle \gamma, m|\hat{H}_F|\nu, n\rangle = \hat{H}_{\gamma,\nu}^{(m-n)} + n\hbar\omega_0\delta_{\gamma,\nu}\delta_{n,m}$$

Time- evolution operator

``Well, in our country,'' said Alice, still panting a little, ``you'd generally get to somewhere else if you ran very fast for a long time as we've been doing.''
Lewis Carroll, "Through the Looking Glass".

$$\boxed{U_{\gamma,\nu}(t,0) = \sum_n \langle \gamma, n|e^{-iH_F t/\hbar}|\nu, 0\rangle e^{in\omega_0 t}.}$$

Beyond the adiabatic scattering theory

Average Current

Single electron picture

$$I_L(t) = \mathrm{i}\frac{e}{\hbar}\left[H(t), N_L\right], \qquad N_L = \sum_{j\in L} c_j^+ c_j$$

$$\bar{I} = \frac{1}{T}\int_0^T dt \langle I_L(t)\rangle$$

$$\boxed{\bar{I} = \frac{e}{2\pi\hbar}\sum_{n=-\infty}^{\infty}\int d\varepsilon \left[T_{RL}^{(n)}(\varepsilon) - T_{LR}^{(n)}(\varepsilon)\right] f(\varepsilon)}$$

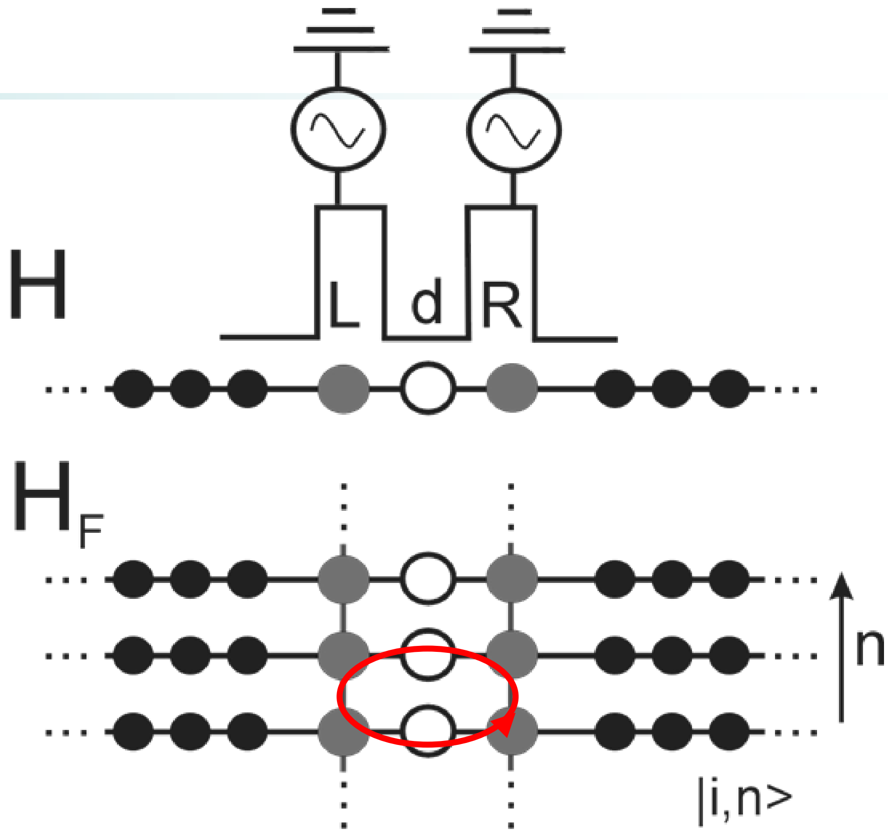
S. Camalet et al, PRB **70**, 155326 (2004).

S. Kohler, J. Lehmann & P. Hänggi, Phys. Reports 2005.

Transmission probability

$$T_{RL}^{(n)}(\varepsilon) = 4\Gamma_R^{(n)}\left|\left\{G_F^R\right\}_{(R,n);(L,0)}\right|^2 \Gamma_L^{(0)} \qquad \hat{G}_F^R = (\varepsilon\hat{I} - \hat{H}_F)^{-1}$$

Example: simple two-parameter pump



Main difference between a situation with one and two driving parameters:

Possibility of having the analog of a magnetic flux in Floquet space.

Words on symmetry breaking and QP, phase rigidity and reciprocity, dynamical symm-breaking.

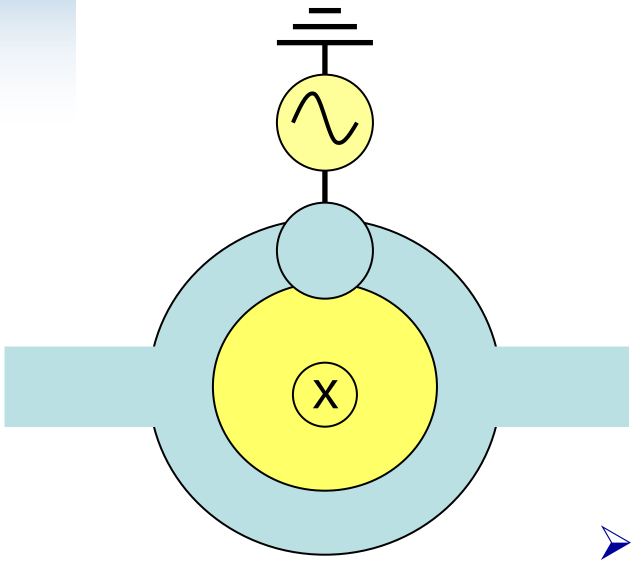
This provides the directional asymmetry needed for quantum pumping.

Directional asymmetry between emission and absorption -> linear effect.

Dynamical LR symmetry breaking.

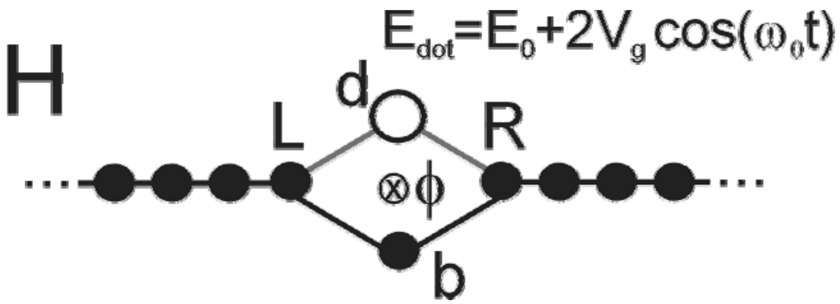
LFT, Phys. Rev. B 72, 235339 (2005).

Pumping in an AB ring using a single parameter



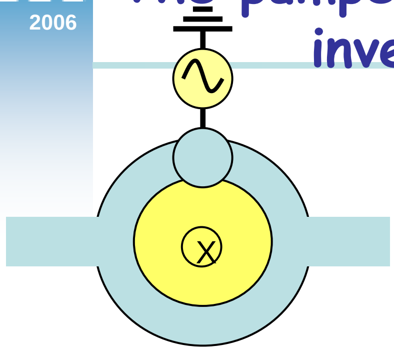
<u>Ingredients</u>

- Static magnetic field — Provides symmetry breaking, directional asymmetry.
- Time-dependent potential — Provides additional inelastic processes removing phase-rigidity.

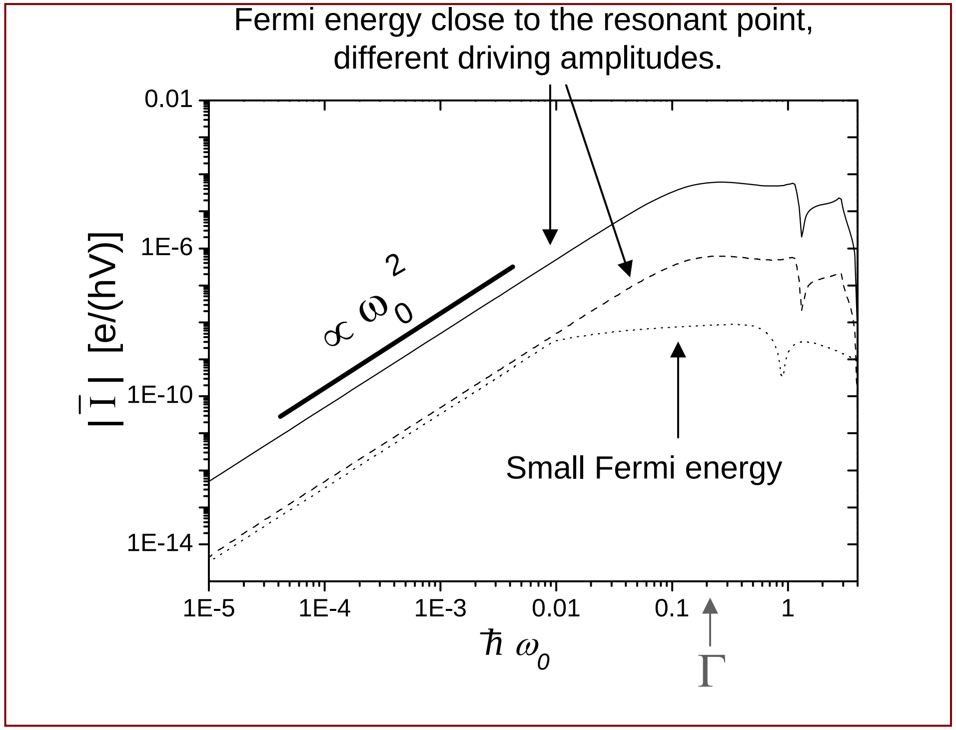


LFT, Phys. Rev. B 72, 235339 (2005).

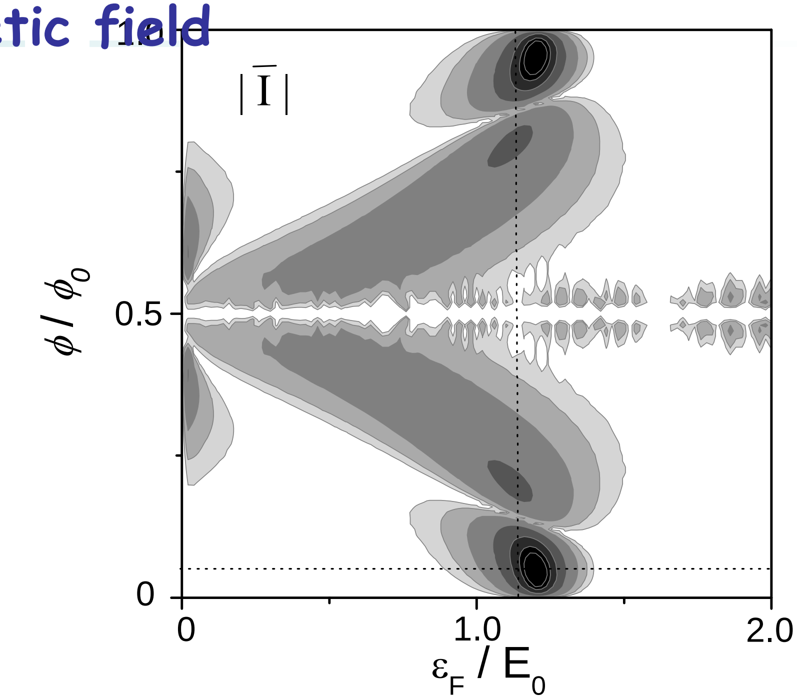
The pumped current is quadratic in Omega and can be inverted by using the magnetic field

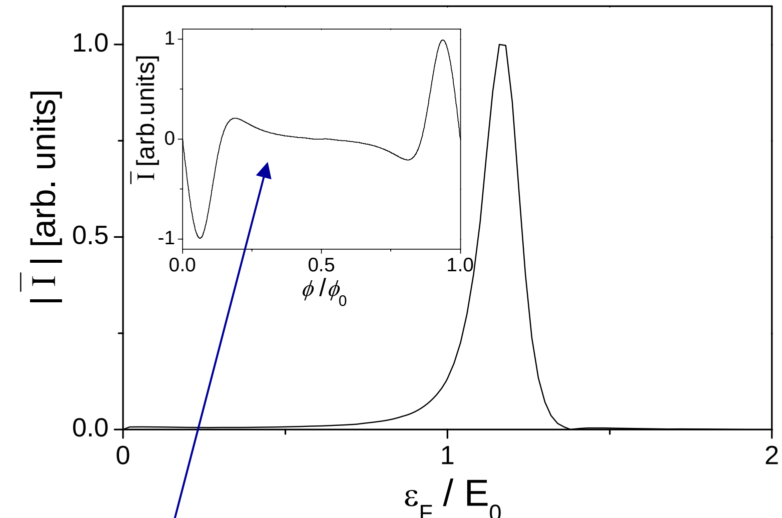


Interplay between spatial interference and PAT,



A similar behavior is observed as a function of the driving amplitude.





The current can be reversed by changing the magnetic flux.

LFT, to appear in Phys. Rev. B; cond-mat/0511223.

Conclusions and Perspectives

- Time independent scheme for time-dependent transport in the presence of cyclic potentials.

⬇

- Quantum pumping in a ring with a single parameter, interplay of PAT and spatial interference.

⬇

These ingredients have the same footing when the problem is formulated in Floquet space.

⇨

- Possibility of reversing the current by changing the magnetic flux.
- Possibility of separating pumping from rectification effects.
- Quantum pumping as an interference effect in Floquet space.