Correlated quantum systems out of equilibrium: Methods, Applications, Challenges

Martin Nuss, supervised by Wolfgang von der Linden & Enrico Arrigoni

TUG

Materials Day Graz, 24.10.2013

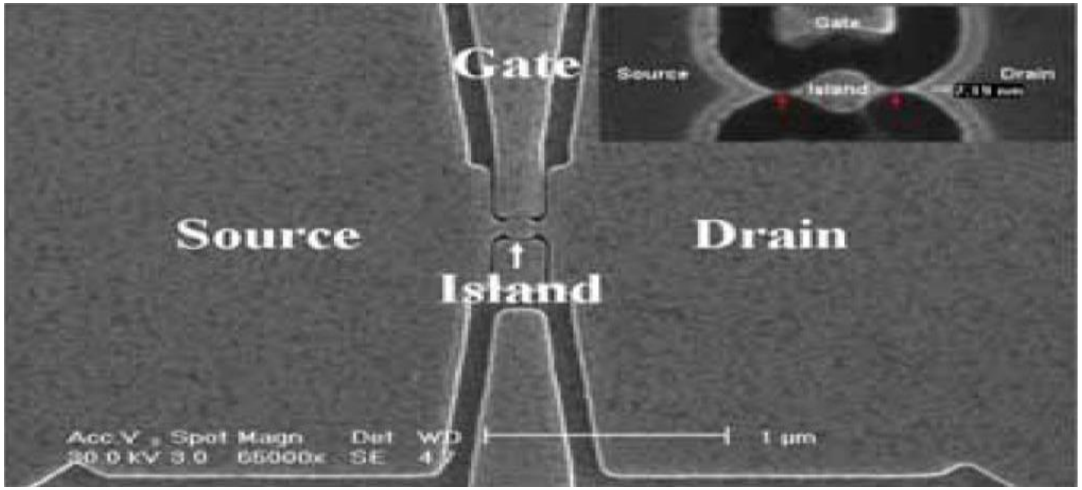
itp^{cp}

Agenda

I — Quantum many body systems out of equilibrium

II — Transport through a quantum dot

single quantum dot



Wu etal (2010)

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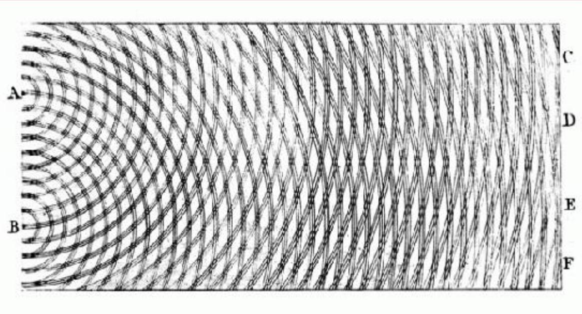
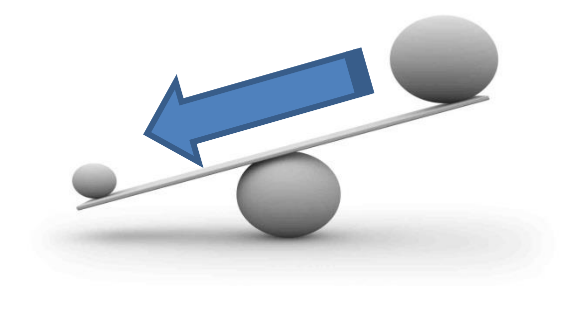
Quantum many body systems out of equilibrium

quantum mechanics



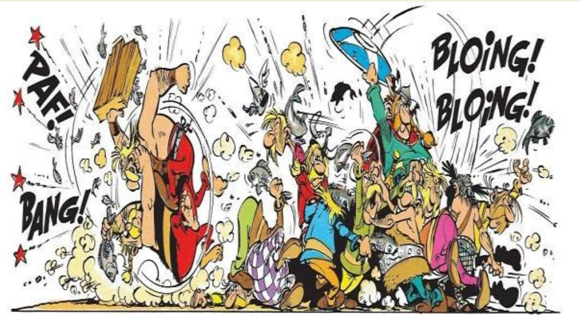
Young Royal Society (1803)

non equilibrium



www.nessnet.eu

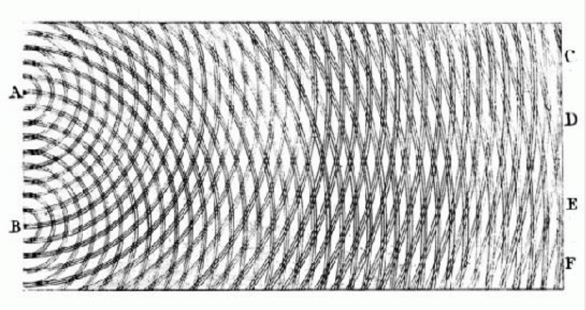
many body interactions



c Goscinny & Uderzo Ehapa

Quantum many body systems out of equilibrium

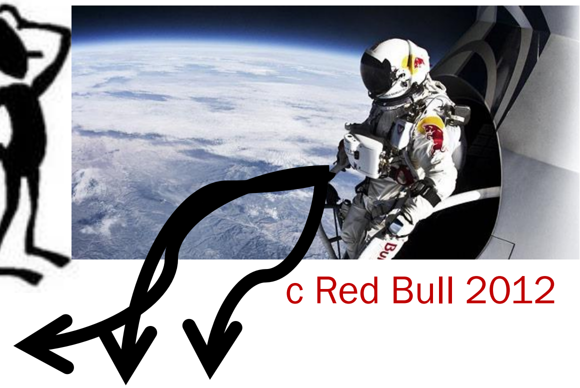
quantum mechanics



Young Royal Society (1803)

- described by Schrödinger wave equation
- probabilities instead of deterministic trajectories

classical



c Red Bull 2012

- „objects“ propagate as waves but interact like particles

de Broglie wavelength $\lambda \approx \dfrac{\text{Planck's constant}}{\text{mass x velocity}}$

F.J. Himpsel Univ. Wisconsin

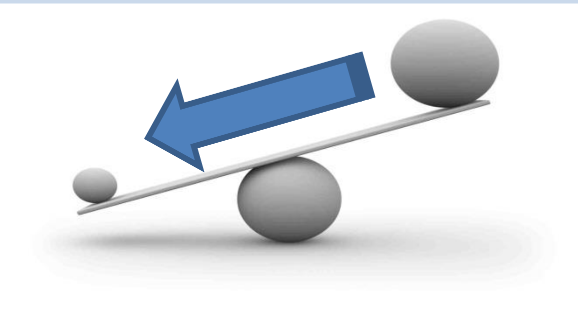
clintonpower.com.au

rantingants.com

Electron:	mass= 10^{-30} kg,	velocity= 1 eV	λ = 1 nm
NFL ball in the hands of Brett Favre:	mass= 0.4 kg,	velocity= 30 m/s	$\lambda = 10^{-34}$ m

Quantum many body systems out of equilibrium

non equilibrium



www.nessnet.eu

- thermodynamic equilibrium
  - „energy“ minimization
  - ideal $PV = NkT$
  - no current
- exception ?
  - typical timescales
  - linear response

- non equilibrium
  - time dependent action
  - time dependence
  - transient / dissipation / steady state
  - typical timescales
  - $T_{observe} < T_{relax}$

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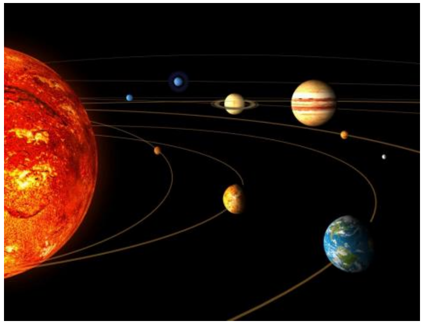
Quantum many body systems out of equilibrium

many body interactions

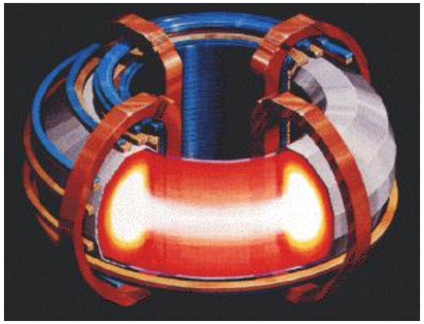
c Goscinny & Uderzo Ehapa

classical: solar system



c ESA

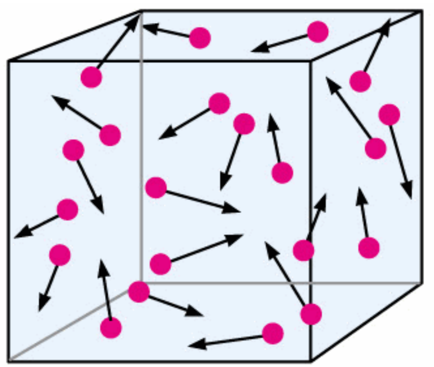
semi classical: fusion plasma



centpeus.blogspot.co.at

quantum: electrons in metals

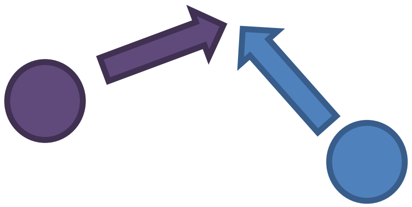
hdwallpapersinn.com



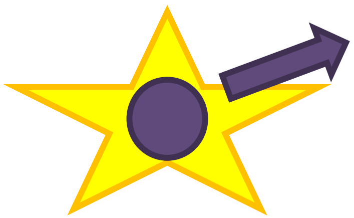
quantumfreak.com

- Many interacting particles: difficult!
- Even more so if quantum particles!

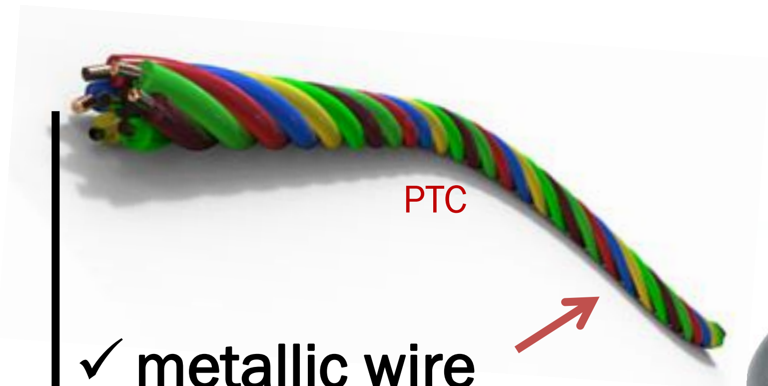
Problem: interactions



Solution: approximations

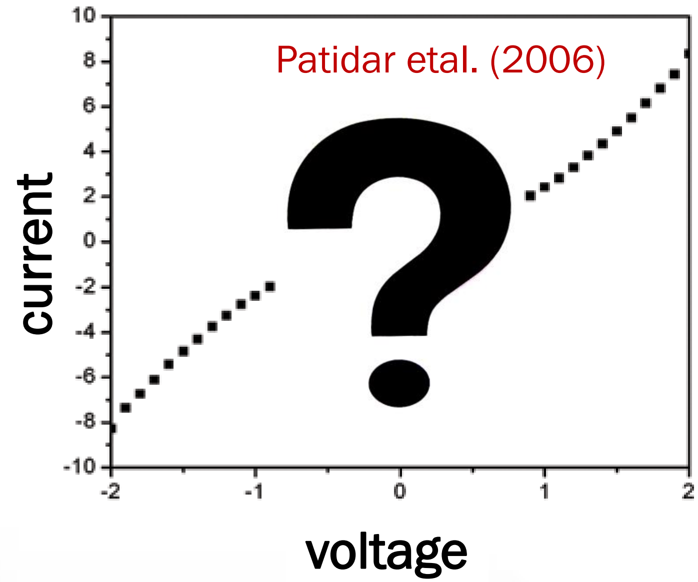


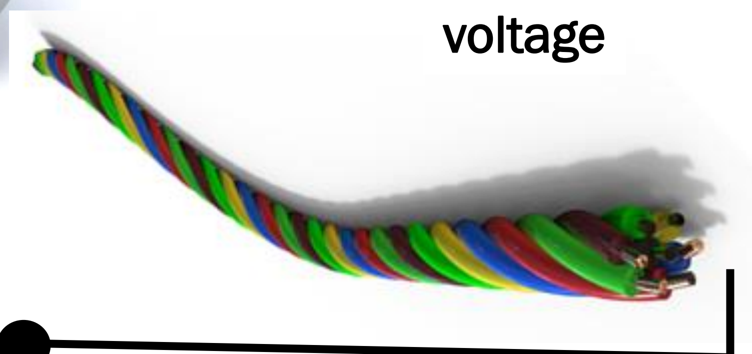
Electrical transport through „some object“

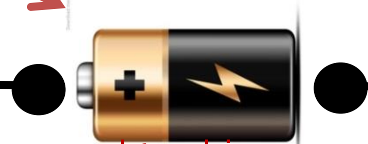

PTC

- ✓ metallic wire
- ✓ „some object“
- ✓ voltage source

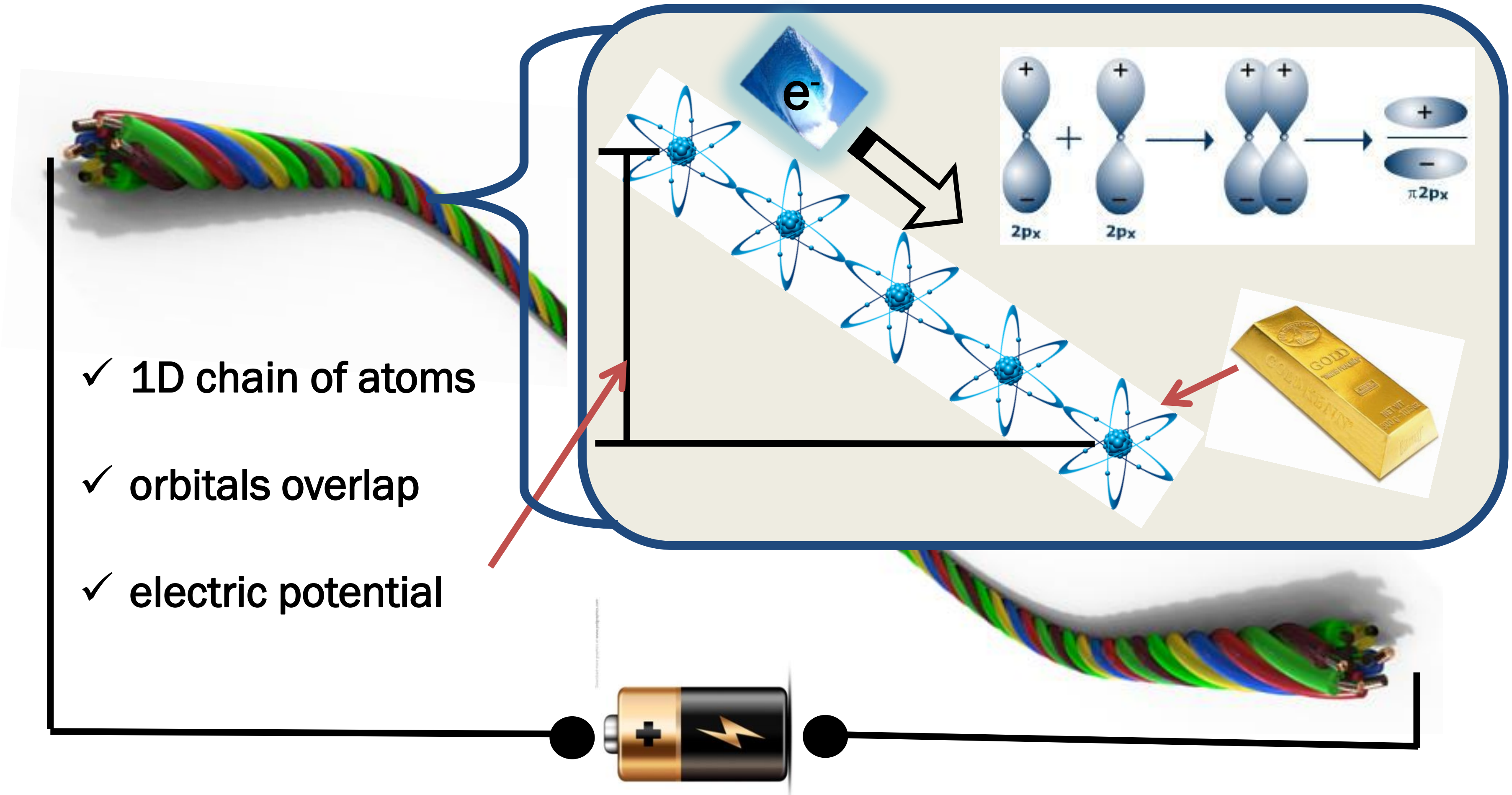

complast





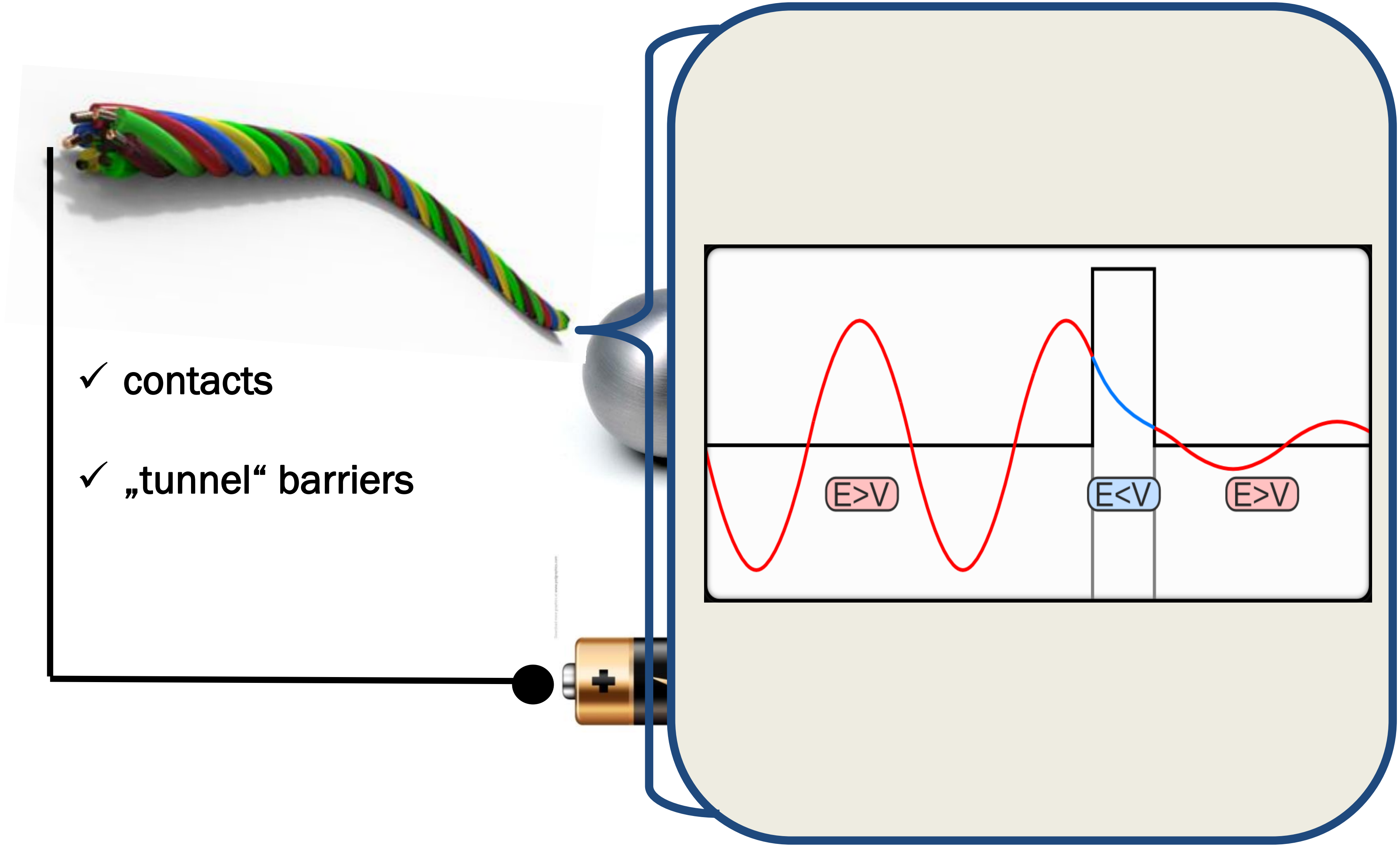

psdgraphics.com

A similar quantum system



- ✓ 1D chain of atoms
- ✓ orbitals overlap
- ✓ electric potential

A similar quantum system



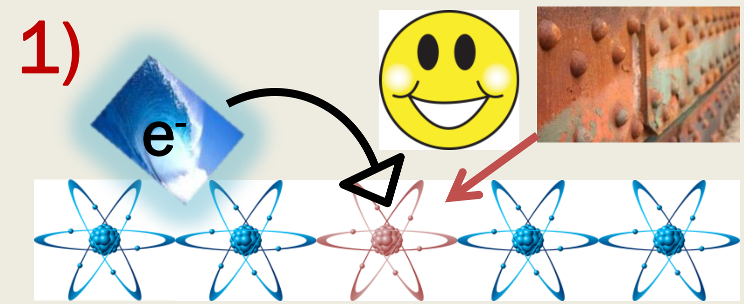
- ✓ contacts
- ✓ „tunnel“ barriers

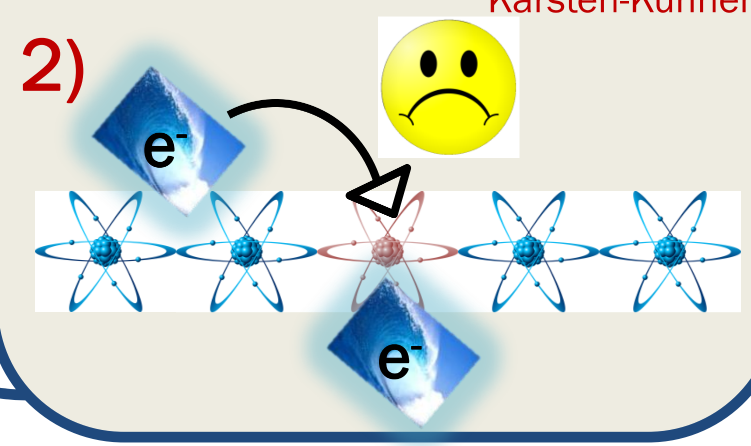
A similar quantum system

- ✓ quantum dot
- ✓ one interacting „atom“

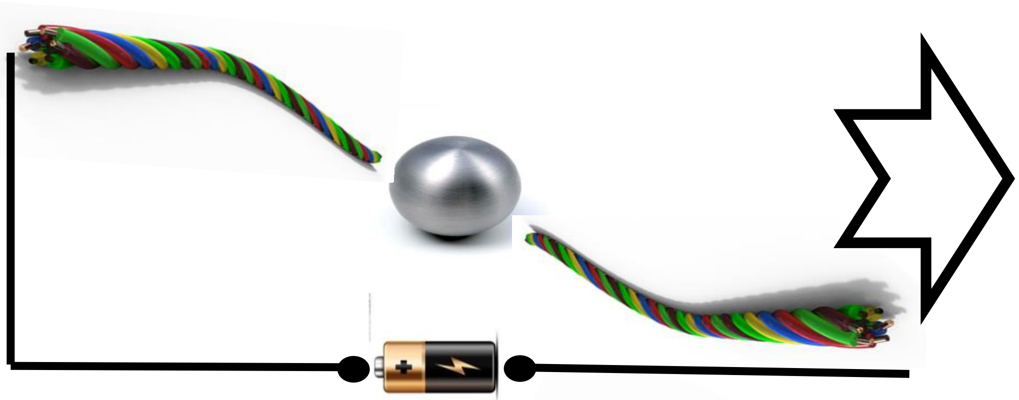
Coulomb repulsion

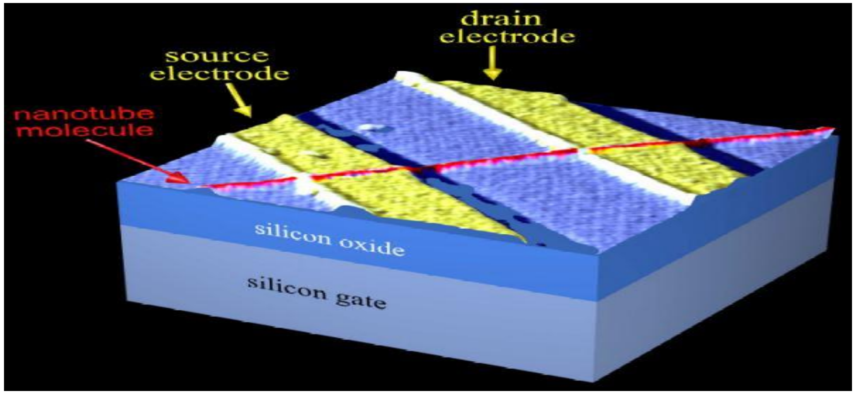
$$\boldsymbol{F}_{12} = k_e \frac{q_1 q_2 \hat{\boldsymbol{r}}_{21}}{r^2}$$





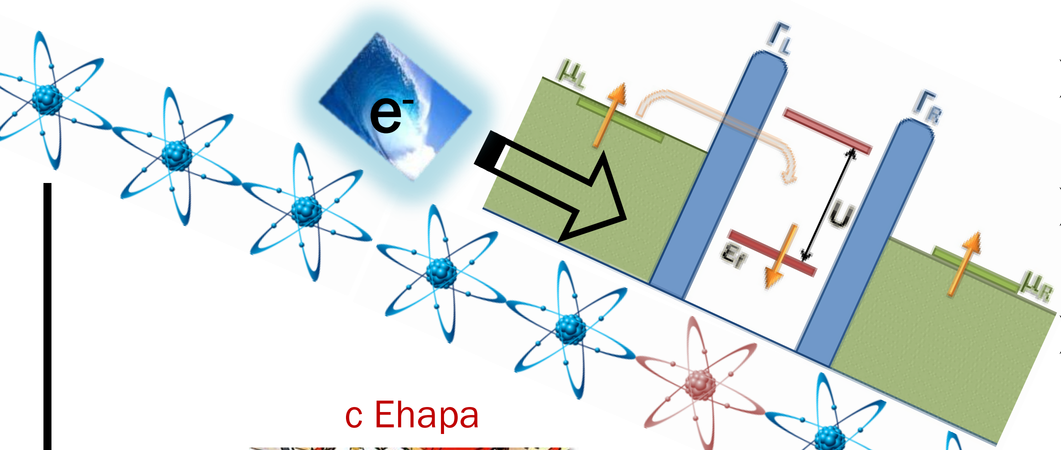
A similar quantum system



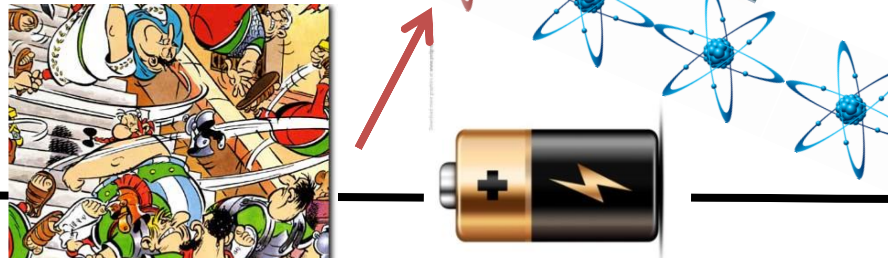


Dekker (1998)

- electrons in a 1D quantum wire
- electrons interact
- electric potential makes them „go“



c Ehapa



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How to obtain answers?

in general unsolvable → strategy?

A) <u>steady state</u>: non equilibrium Variational Cluster Approach:

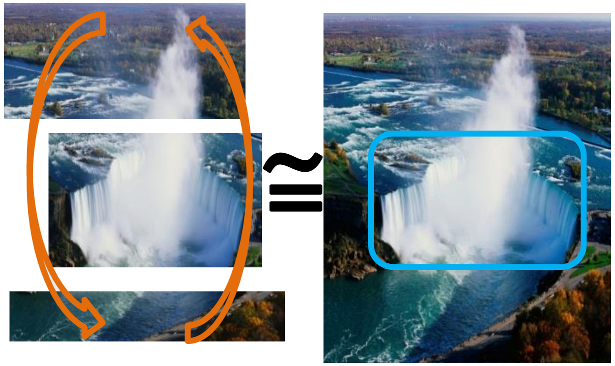
1)

2)

3)

4)

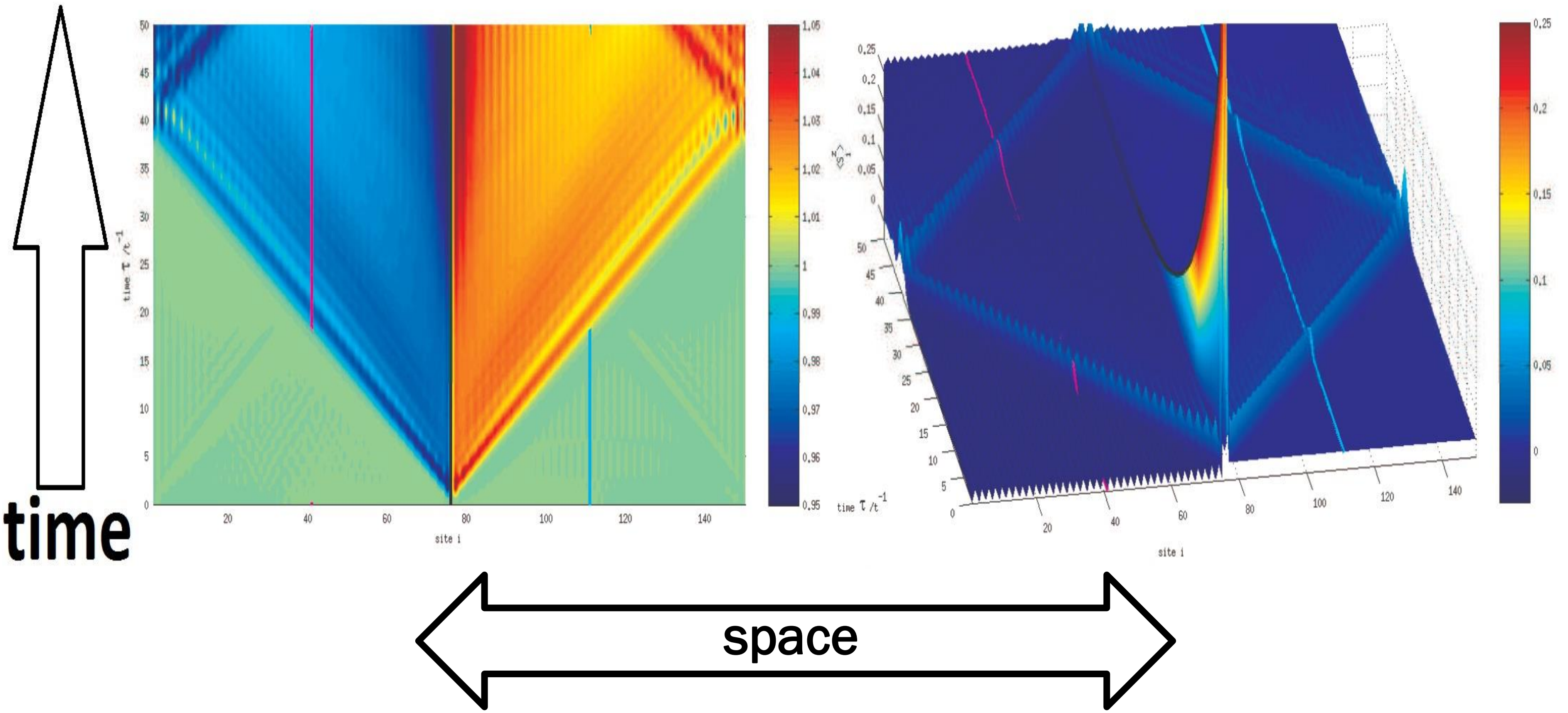
5)



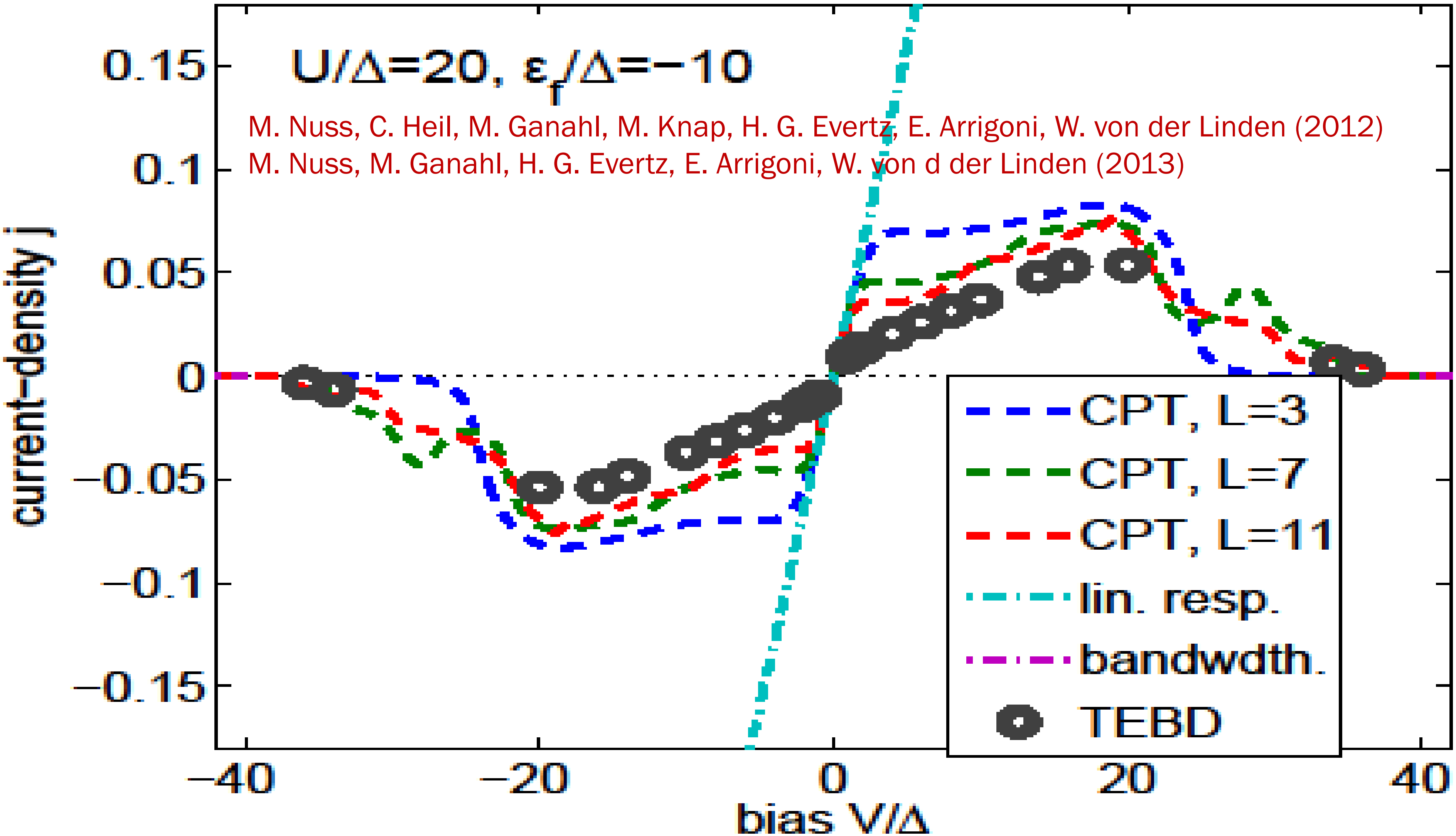
B) <u>time evolution</u>: Density Matrix Renormalization Group

- time dependent Schrödinger equation: partial differential equation
- special Ansatz: represent many body wavefunction in optimal basis

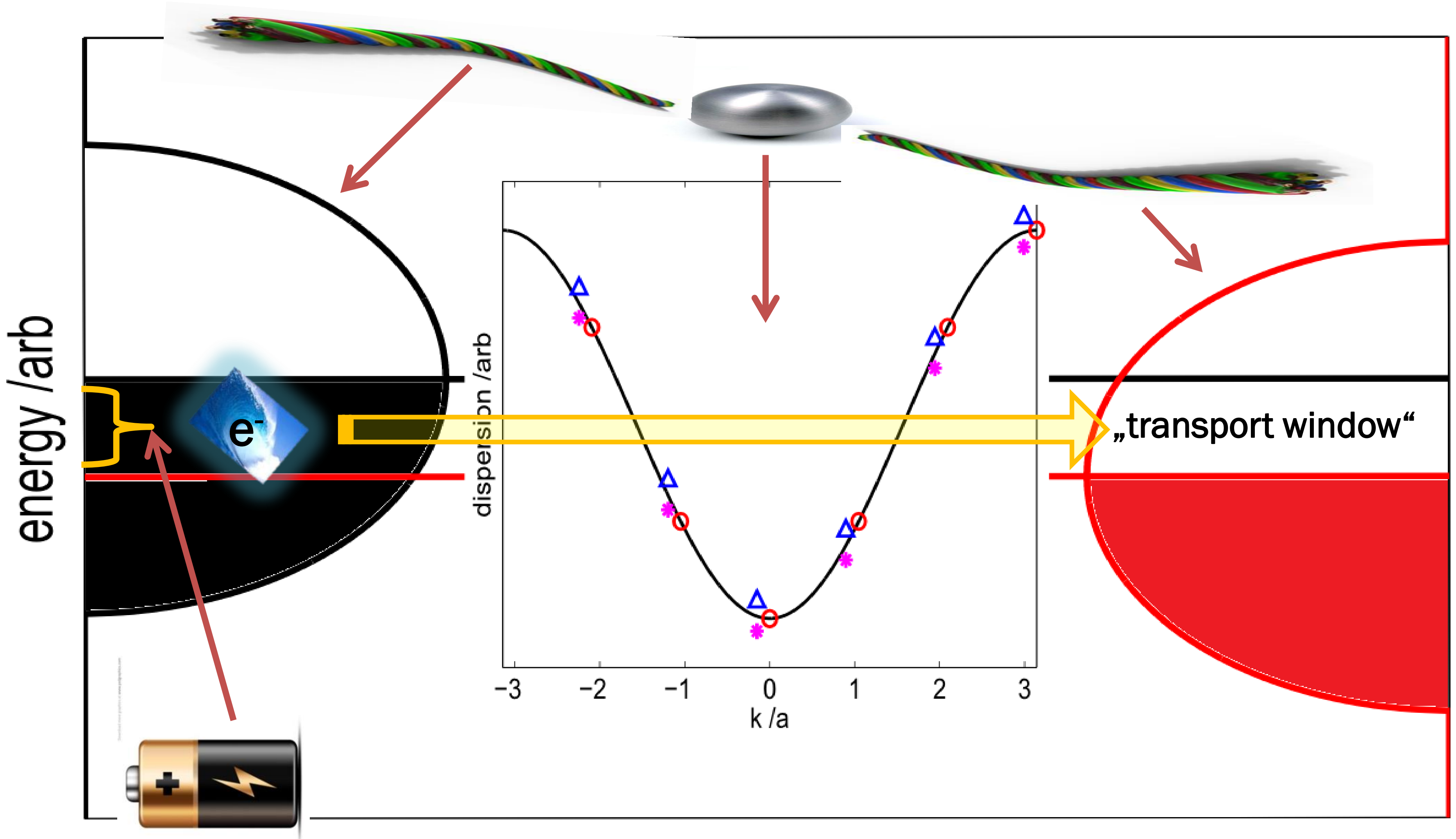
Electronic density + magnetization



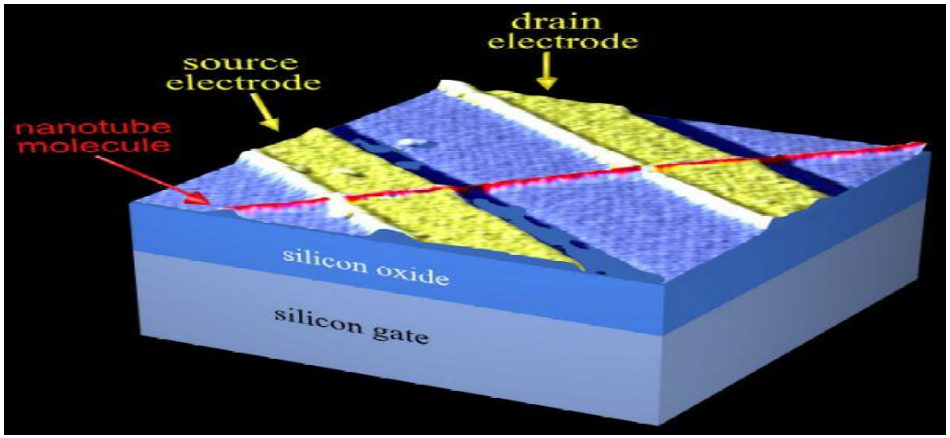
Current-voltage characteristics



Current-voltage characteristics



Conclusions + outlook



- steady state of a single quantum dot

- quantum dots and impurity systems
- molecular junctions and electronics
- correlated materials + layered heterostructures
- ultracold atomic gases + quantum simulators
- composite systems, phonons, light matter interaction, …

For different application see our poster (14) in the afternoon!


Non equilibrium group at
TUG
Prof. Wolfgang von der Linden
Prof. Enrico Arrigoni
Prof. Hans Gerd Evertz
Martin Nuss
Antonius Dorda
Delia Fugger
Max Sorantin
Markus Aichhorn
Martin Ganahl
Anna Fulterer
Michael Knap
Christoph Heil
Benjamin Kollmitzer

Thank you!

maybe some day:

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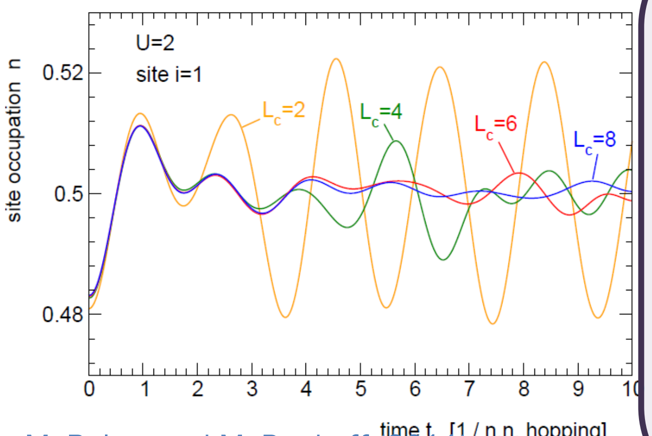
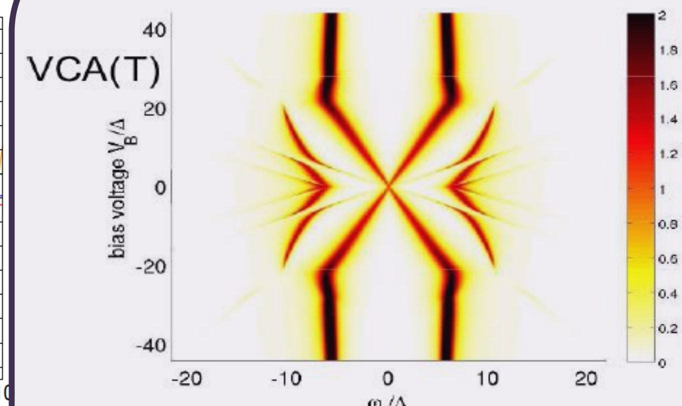
Non equilibrium Variational Cluster Approach

time evolution by CPT



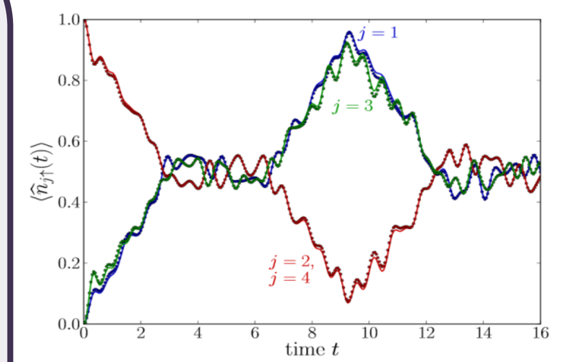
M. Balzer and M. Potthoff (2011)

steady state of quantum dots



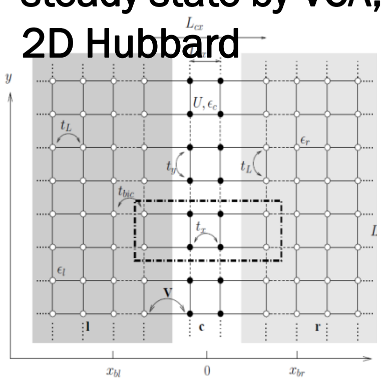
M. Nuss, C. Heil, M. Ganahl, M. Knap, H. G Evertz, E. Arrigoni, W. vd Linden (2012)

dynamical symmetry in 2D



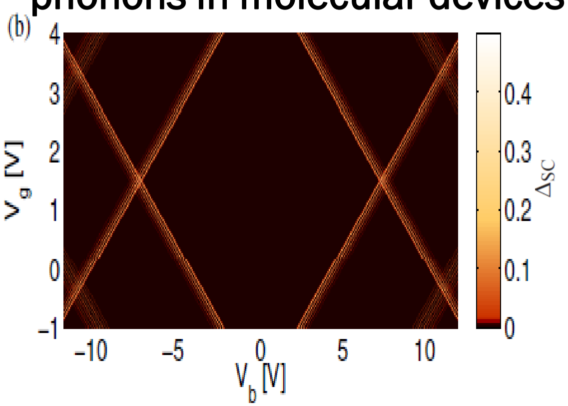
P. Jurgenowski and M. Potthoff (2013)

steady state by VCA, 2D Hubbard



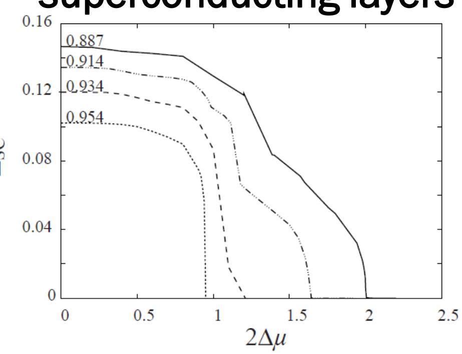
M. Knap, W. vd Linden, E. Arrigoni (2011)

phonons in molecular devices



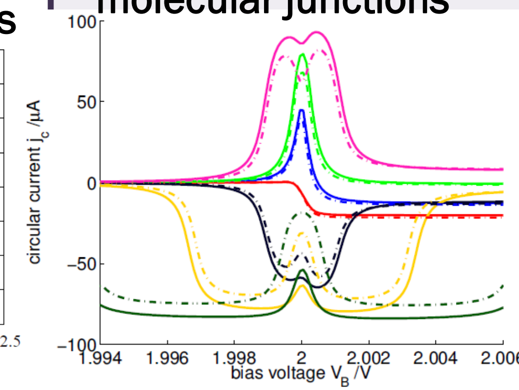
M. Knap, E. Arrigoni, W. von der Linden (2012)

superconducting layers



A. Fulterer, E. Arrigoni (2012)

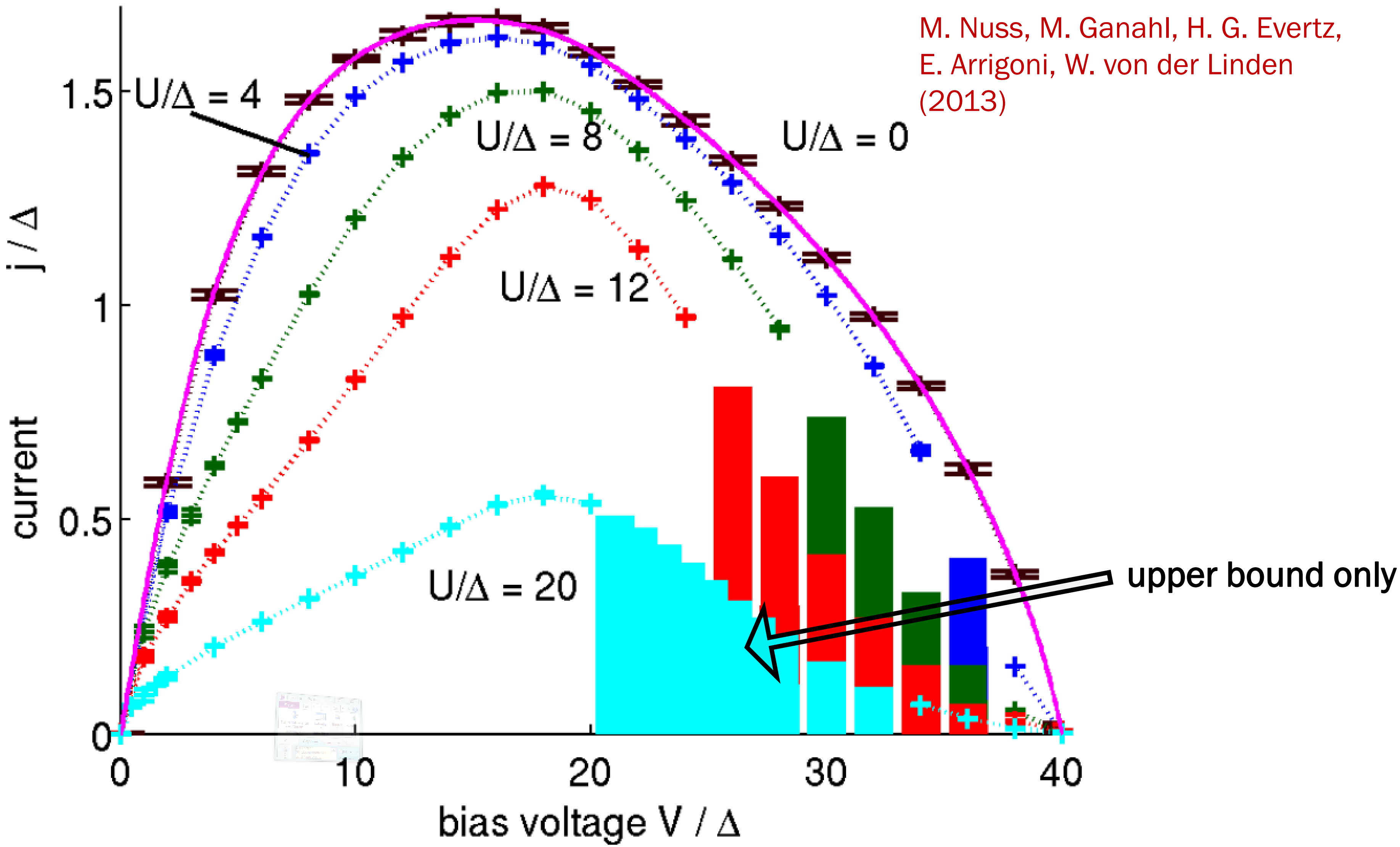
magnetic effects in molecular junctions



M. Nuss, E. Arrigoni, W. vd Linden (2012)

DMRG+TEBD current-voltage characteristics

M. Nuss, M. Ganahl, H. G. Evertz, E. Arrigoni, W. von der Linden (2013)



Time evolution of current