Steady-state characteristics of correlated quantum many-body systems out of equilibrium

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

Oberseminar TU Graz, Graz, 24.10.2013

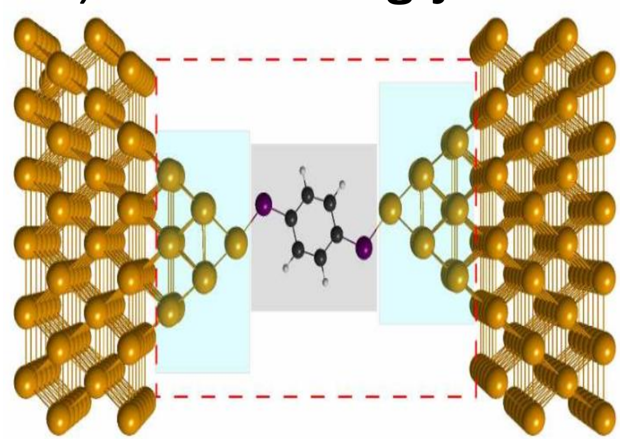
Agenda

I	Transport in a one dimensional material
II	Current-voltage characteristics of a molecular junction
III	Steady state of a correlated quantum dot

1) $Li_{0.9}Mo_6O_{17}$

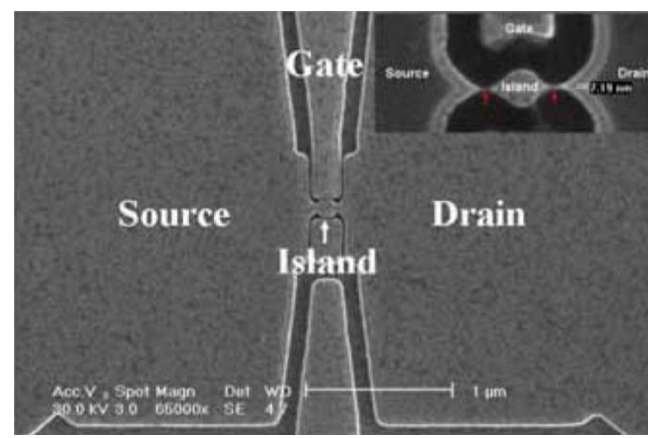
Allen (2013)

2) molecular ring junction



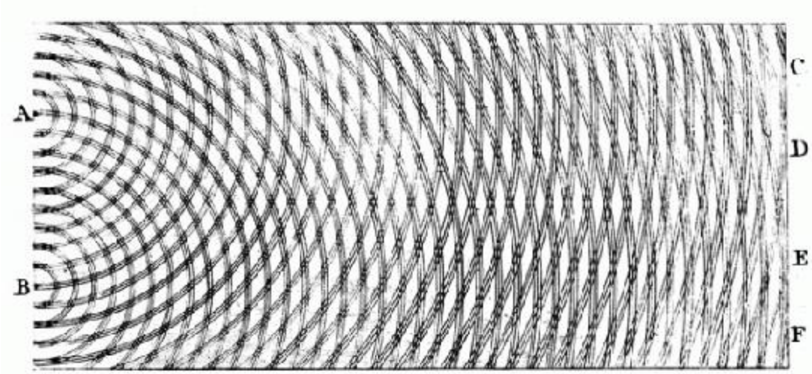
Ryndyk etal (2012)

3) single quantum dot



Wu etal (2010)

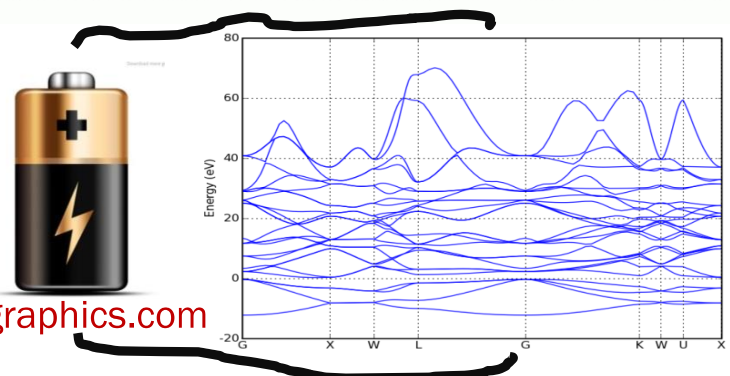
Quantum many body systems out of equilibrium



Young Royal Society (1803)

1) quantum mechanics

Schrödinger equation
quantum statistics



psdgraphics.com

2) non equilibrium

transient / dissipation / steady state

3) many body interactions

in general impossible to solve
-> approximations

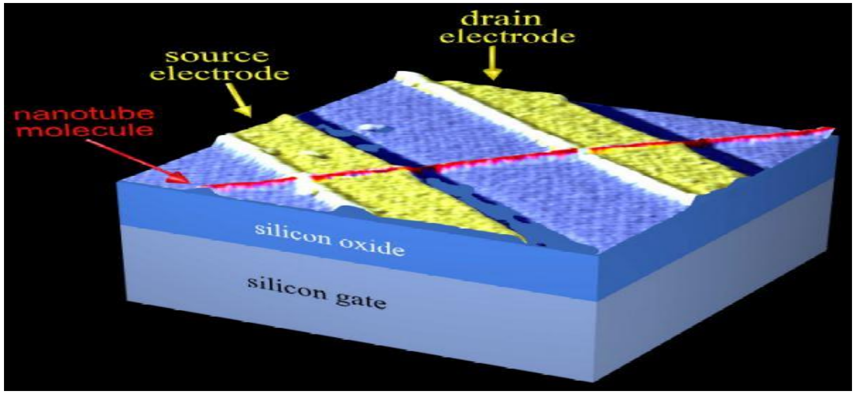
c Goscinny & Uderzo Ehapa

Quantum many body systems out of equilibrium

quantum mechanics	non equilibrium	many body
Emission characteristics of GaN and AlGaInP based Light Emitting Diodes		
SEMICLASSICAL	YES	NO
Interaction effects in Helium Atom Scattering from semimetal Surfaces		
YES	YES	PARTLY
Electrolyte-gated organic field-effect transistor for sensing applications in aqueous media		
SEMICLASSICAL	YES	NO
Enzymatic Cellulose Hydrolysis: New Approaches in the Investigation of Biocatalytic processes via In-situ Liquid Atomic Force Microscopy		
PARTLY	YES	NO
Focused ion beam processing of low melting polymers: new perspectives due to optimized patterning strategies		
NO	YES	NO
A SIMULATION PROCEDURE FOR LIGHT-MATTER INTERACTION AT DIFFERENT LENGTH SCALES		
MULTISCALE	PROBABLY	NO
Simultaneous photoacoustic and laser-ultrasound imaging		
NO	YES	NO

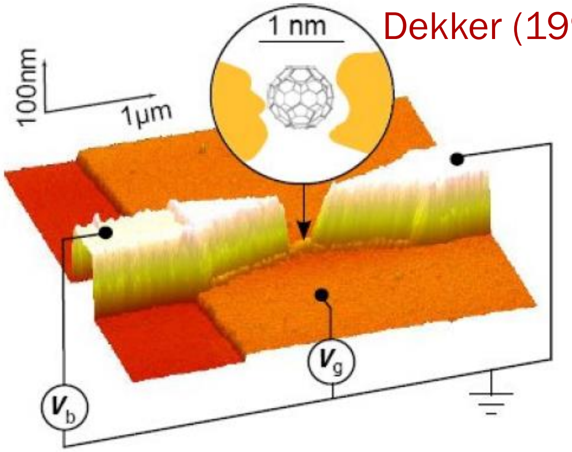
Example systems

- transport in nanoscopic devices
  - temperature gradients
  - voltage bias
  - magnetic fields



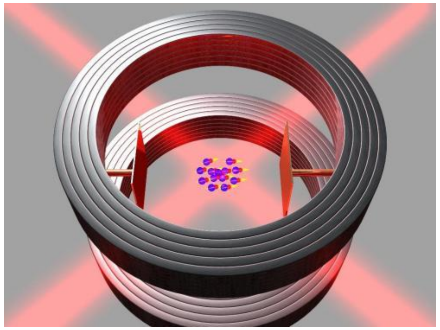
Dekker (1998)

- transport through molecular junctions



Yao (1999)

- ultra cold atomic gases
  - quantum quenches
  - expansion
  - external „fields“



Modugno etal (2009)

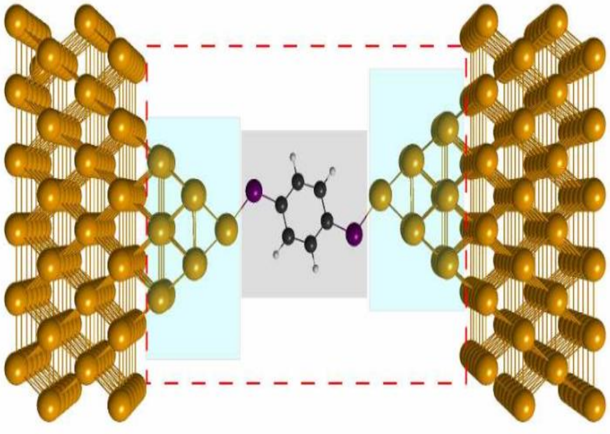
- ultra fast pump probe spectroscopy

Overview

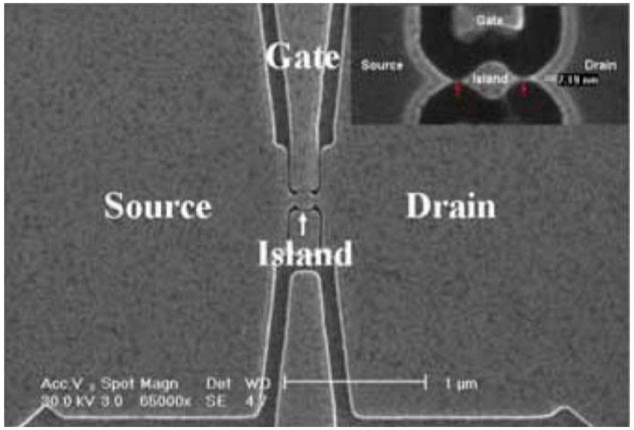
1) $Li_{0.9}Mo_6O_{17}$

- **Density Functional Theory**
- **Dynamical Mean Field Theory**
- **Linear Response Transport**

2) molecular ring junction



3) single quantum dot



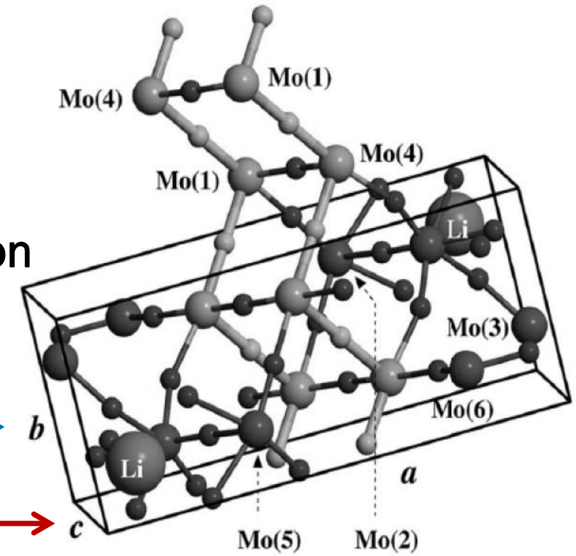
$Li_{0.9}Mo_6O_{17}$

dos Santos etal. *PRB* **74**, 045117 (2006)

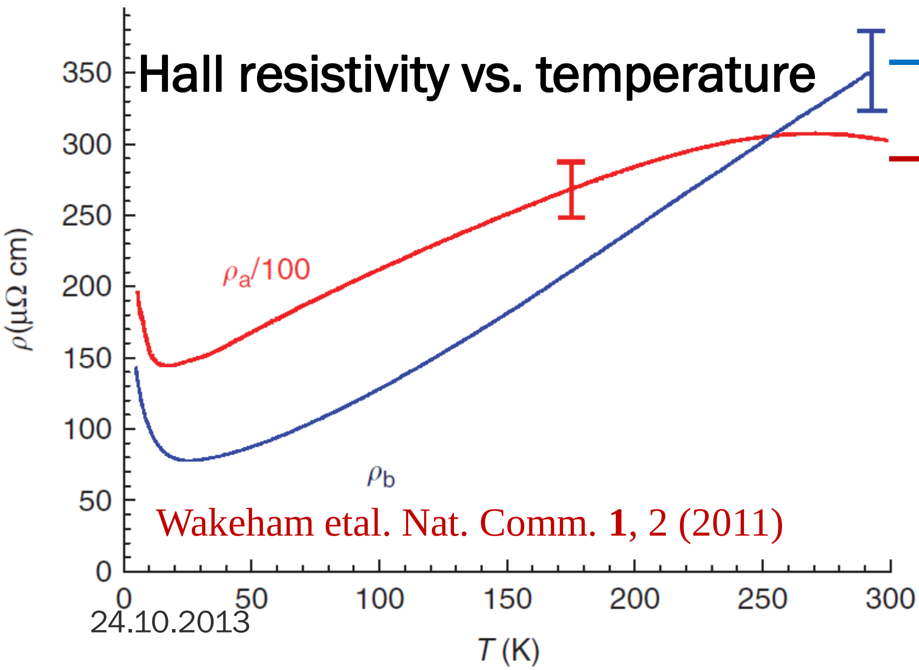
cleaved lithium purple bronze

(J. W. Allen)

„chains“ in b direction



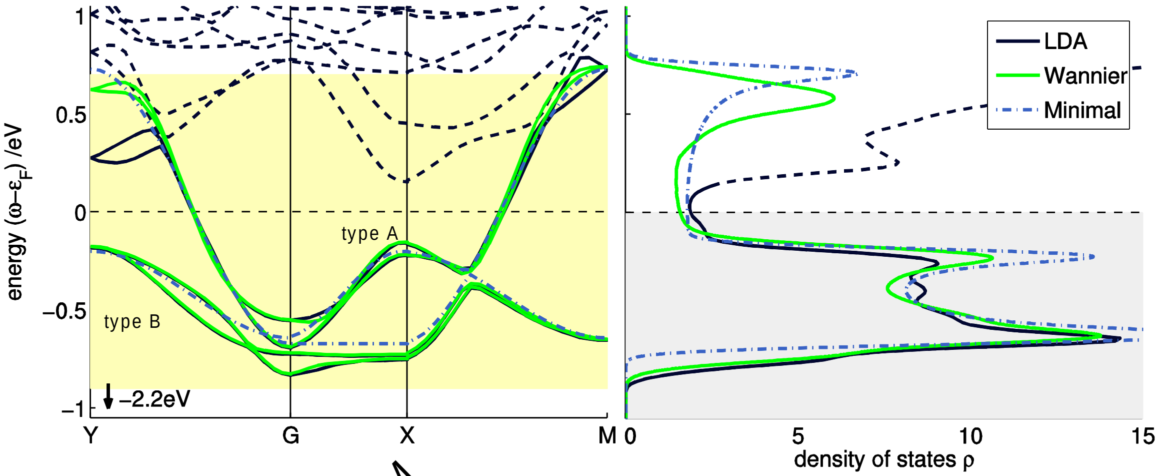
Hall resistivity vs. temperature



Wakeham etal. Nat. Comm. **1**, 2 (2011)

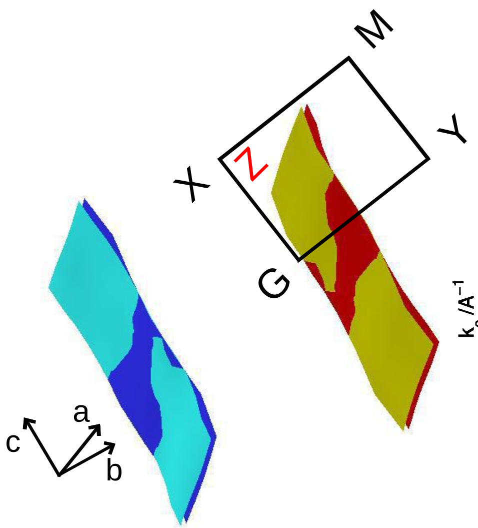
- metal-insulator-trans. @ 24 K
- superconductivity @ < 2 K
- possibly charge density wave
- highly anisotropic

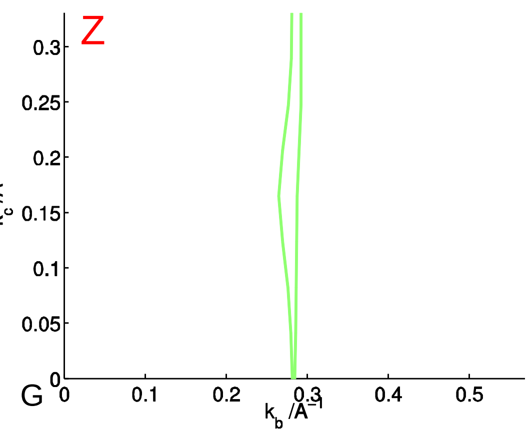
Ab-initio electronic structure

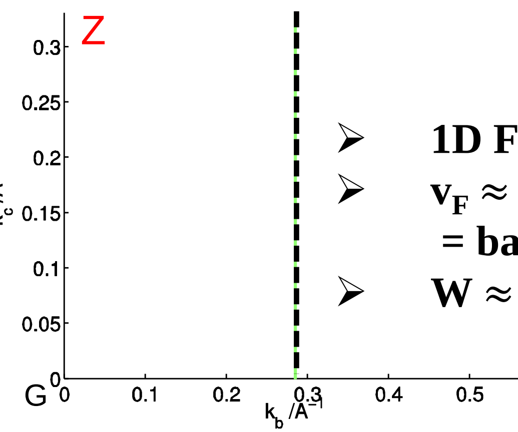


- **Density Functional Theory**
- **Local Density Approximation**
- **all electron, Wien2k, FP-LAPW**

- **4 bands close to Fermi energy**
- ***Mo 4d* character**
- **originate from 4 *Mo* atoms / unit cell**



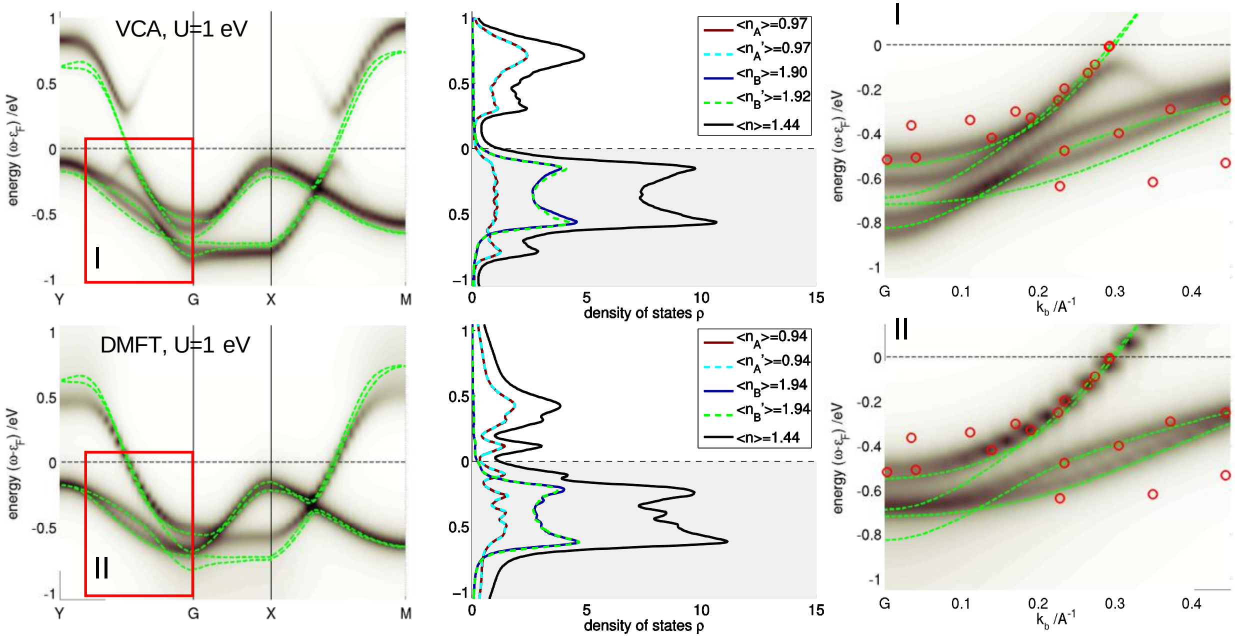


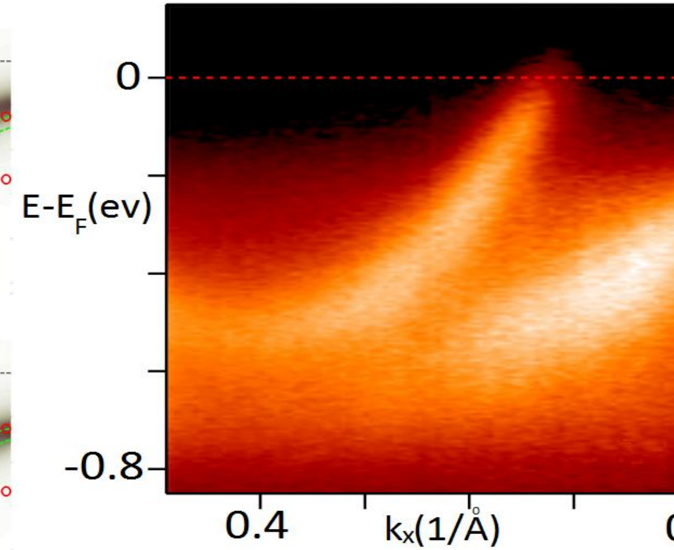


- **1D Fermi surface**
- **$v_F \approx 10^5$ m/s = bad metal**
- **$W \approx 1.5$ eV**

Nuss & Aichhorn (2013)

Interacting electronic spectra





Angle Resolved Photo EmiSsion

Wang etal. PRL **96**, 196403 (2006)

- **Dynamical Mean Field Theory for Wannier model + local U=1eV**
- **(extended) Variational Cluster Aproach for U=1eV**
- **Agreement with experimental ARPES data**

For details see our poster (14) in the afternoon!

Linear response transport

- **low temperature, small scattering γ ≈ 0.05eV**
- **anisotropy via numeric solution of full Wannier model**

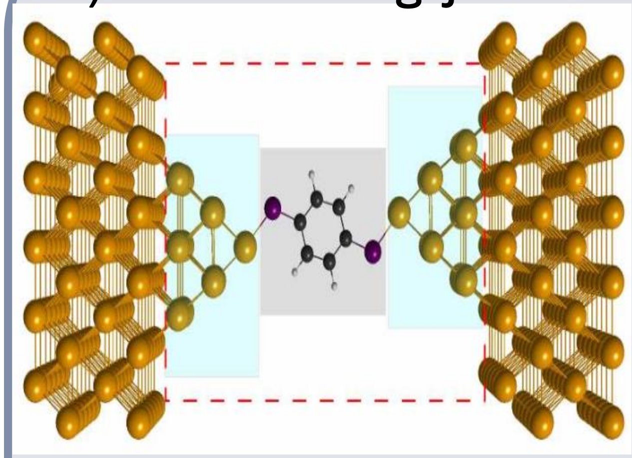
$$\sigma_{bb} = \frac{4e^2}{h\gamma}\frac{b}{ac}\sqrt{(2t_{AA})^2 - \mu^2} \overset{\mu\approx 0}{\approx} N_{\text{spin}}N_{\text{band}}\frac{D}{R_K\gamma}\frac{b}{ac}$$

Ref.	ρ_a	ρ_b	ρ_c	ratio
	mΩcm	mΩcm	mΩcm	
Greenblatt etal. SSC 51, 681 (1984)	2470	9.5	-	260:1:-
Chen etal. EPL 89, 67010 (2010)	64.5	16	854	4.5:1:50
Choi etal. PRB 69, 085120 (2004)	-	1.7	-	-:1:-
Luz etal. PRB 76, 233105 (2007)	110(40)	19(1)	47(5)	6(2):1:2.5(4)
Mercure etal. PRL 108, 187003 (2007)	30	0.4	600	80:1:1600
Xu etal. PRL 102, 206602 (2009)	-	0.4	-	100:1:>100
Wakeham etal. NatComm. 1, 2 (2011)	-	-	-	100:1:-
Wannier model	$\approx 430\gamma$	$\approx 1.8\gamma$	$\approx 600\gamma$	240:1:330
minimal model	-	$\approx 2\gamma$	-	-:1:-

Overview

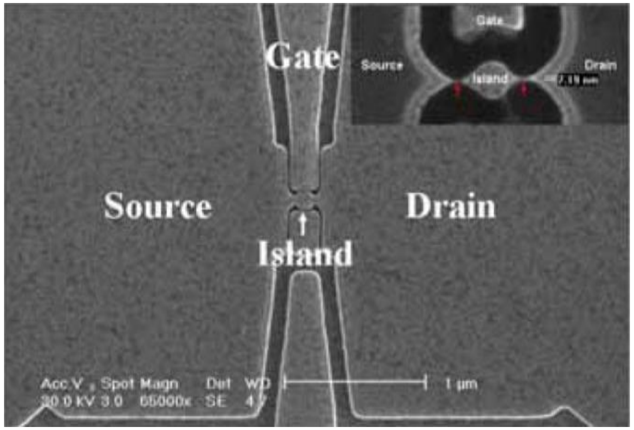
1) $Li_{0.9}Mo_6O_{17}$

2) molecular ring junction

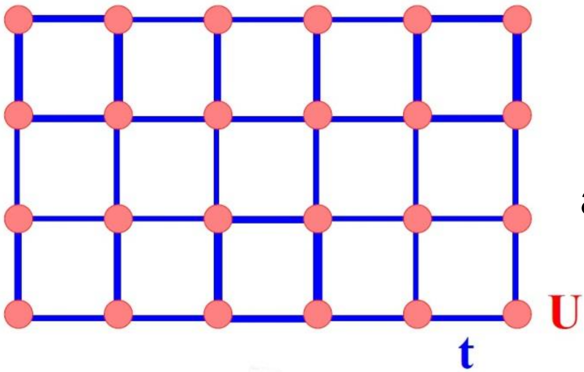


- non equilibrium
  Cluster
  Perturbation
  Theory

3) single quantum dot



Many body cluster methods



given $\hat{\mathcal{H}}$

ask for G

in general unsolvable

strategy ?

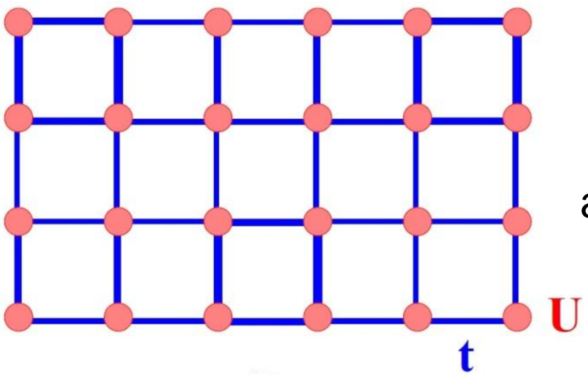
1)

2)

3)

4)

Many body cluster methods



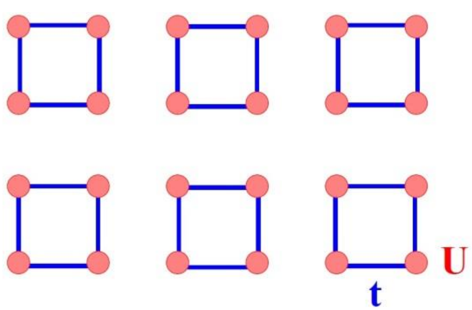
given $\hat{\mathcal{H}}$

ask for G

in general unsolvable

strategy ?

1) CUT



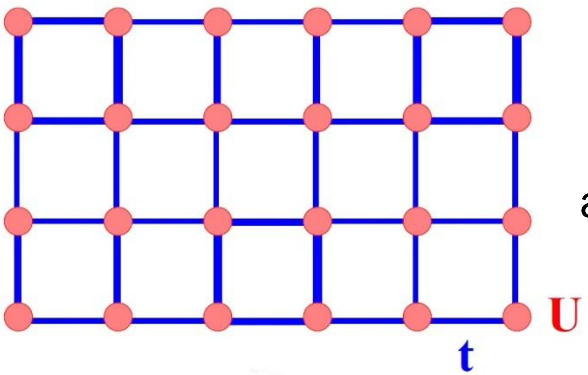
2)

3)

4)

Martin Nuss

Many body cluster methods



given $\hat{\mathcal{H}}$

ask for G

in general unsolvable

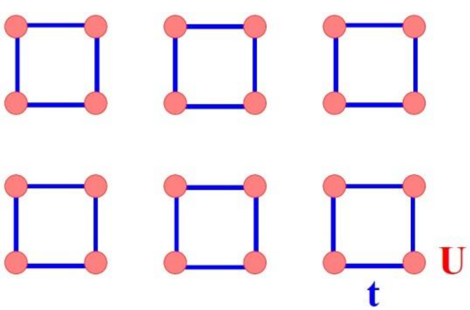
strategy ?

1) CUT

2) SOLVE

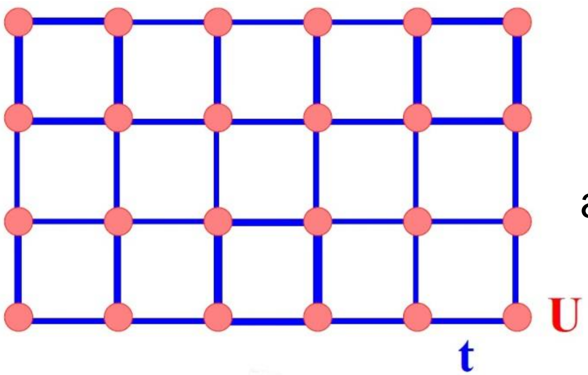
3)

4)



$G_{cluster}$ = exactly solvable

Many body cluster methods



given $\hat{\mathcal{H}}$

ask for G

- **Cluster Perturbation Theory (CPT)**

C. Gros, R. Valenti (1993)
D. Sénéchal, D. Perez, M. Pioro-Ladriére (2000)

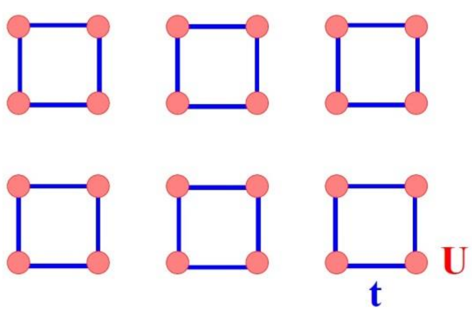
first order strong coupling perturbation theory

1) CUT

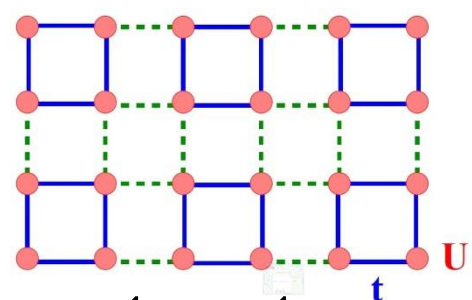
2) SOLVE

3) GLUE

4) $\sum = \sum_{cluster}$

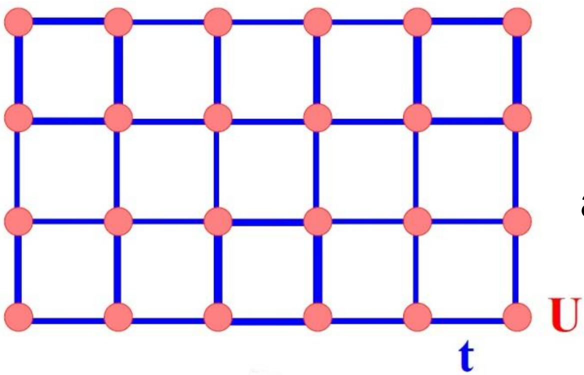


$G_{cluster}$ = exactly solvable



$$G^{-1} = G^{-1}_{cluster} - T$$

Many body cluster methods

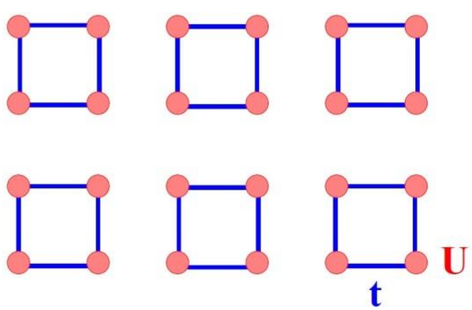


given $\hat{\mathcal{H}}$

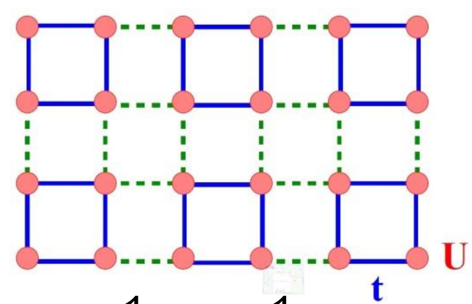
ask for G

- **Cluster Perturbation Theory (CPT)**
  C. Gros, R. Valenti (1993)
  D. Sénéchal, D. Perez, M. Pioro-Ladriére (2000)
- **Variational Cluster Approach (VCA)**
  M. Potthoff, M. Aichhorn, C. Dahnken (2003)
- Cellular Dynamical Mean-Field Theory (CDMFT)
- Dynamical Cluster Approximation (DCA)

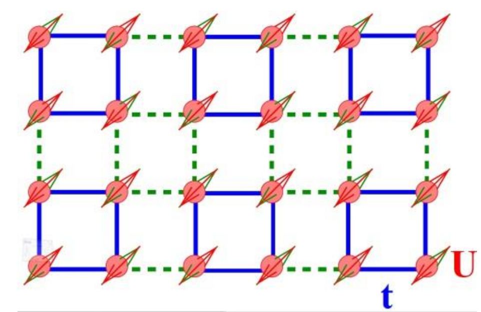
1) CUT 2) SOLVE 3) GLUE 4) ADD FIELDS



$G_{cluster}$ = exactly solvable



$$G^{-1} = G_{cluster}^{-1} - T$$



$$\Sigma = \Sigma_{cluster}(x)$$

M. Potthoff (2003)

+ Variational principle to fix x : Self-energy Functional Approach

Non equilibrium Variational Cluster Approach

$$\tau < \tau_0 : \ \hat{h} \mapsto \hat{h} + \sum_i x_i \hat{\Delta}_i$$

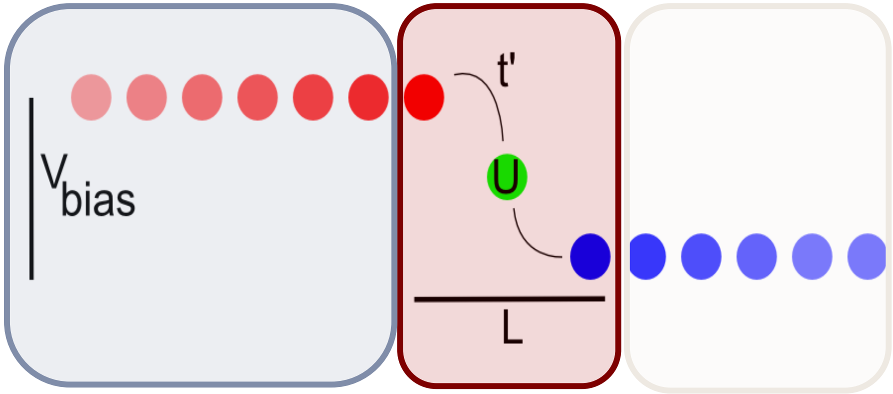
$$\tau > \tau_0 : \ T \mapsto T - \sum_i x_i \hat{\Delta}_i$$

$$\langle \hat{\Delta}_i \rangle_{\text{initial-state}} \stackrel{!}{=} \langle \hat{\Delta}_i \rangle_{\text{steady-state}}$$ = self-consistent feedback

$\cong$

initial reference system *as similar as possible to* the steady-state system

Non equilibrium Variational Cluster Approach

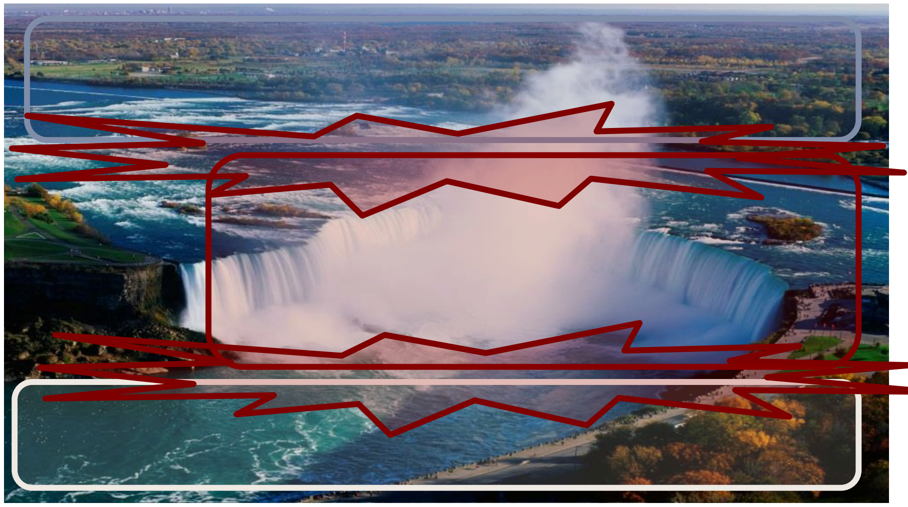


full Dyson

$$G = g + (T + \Delta\Sigma)\,G$$

nCPT („Hubbard I type“)

$$G = g + (T + \Delta\Sigma)\,G$$

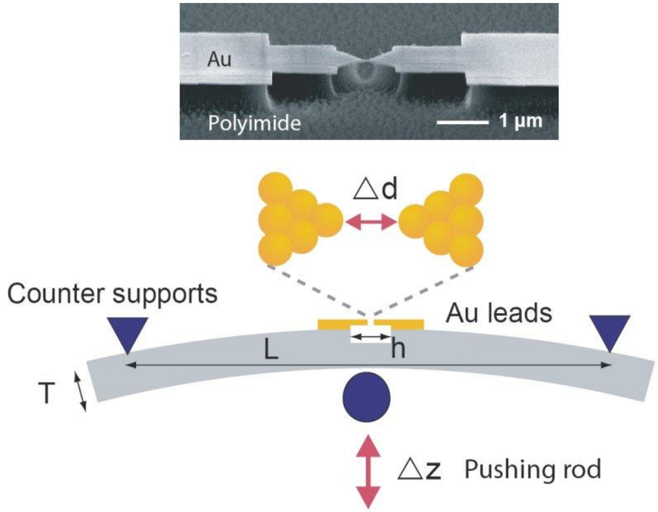


nVCA

$$G = g_{eff} + (T_{eff} + \Delta\Sigma)\,G$$

Molecular junctions

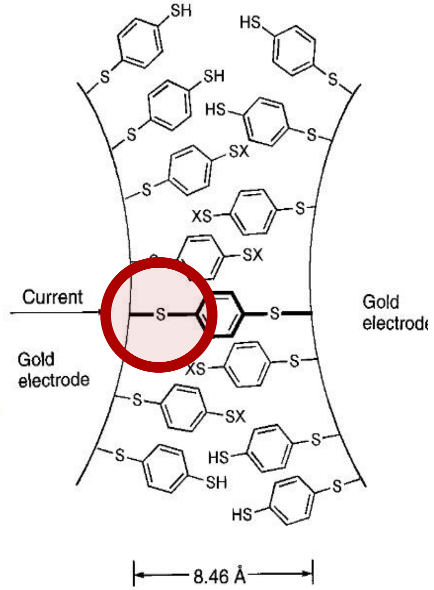
1) Mechanically controlled break junction (MCBJ)



© Dep. Physics, Nanoelectronics , Univ. Basel

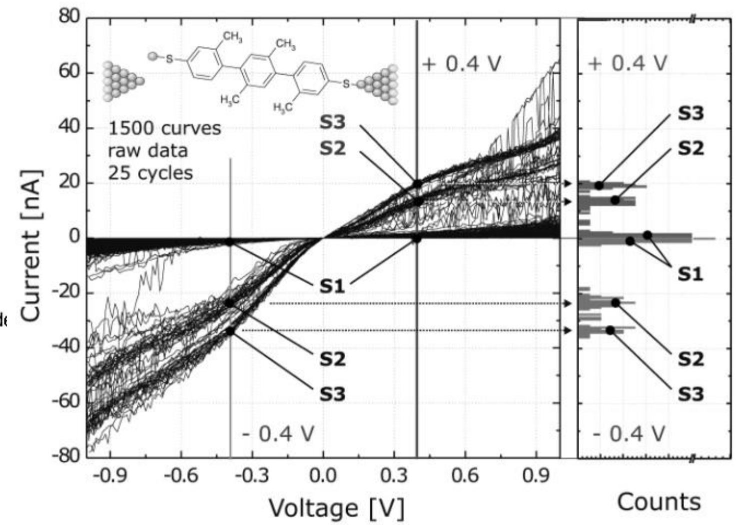
Agrait *etal*. Phys. Rep. **377** 81 (2003)

2) Anchor groups



Reed *etal*. Science **278**, 5336 (1997)

3) Statistical measurements



Lörtscher *etal*. PRL **98**, 176807 (2007)

4) Typical theoretical approach: Density Functional Theory + non equilibrium Green's functions (DFT+NEGF)

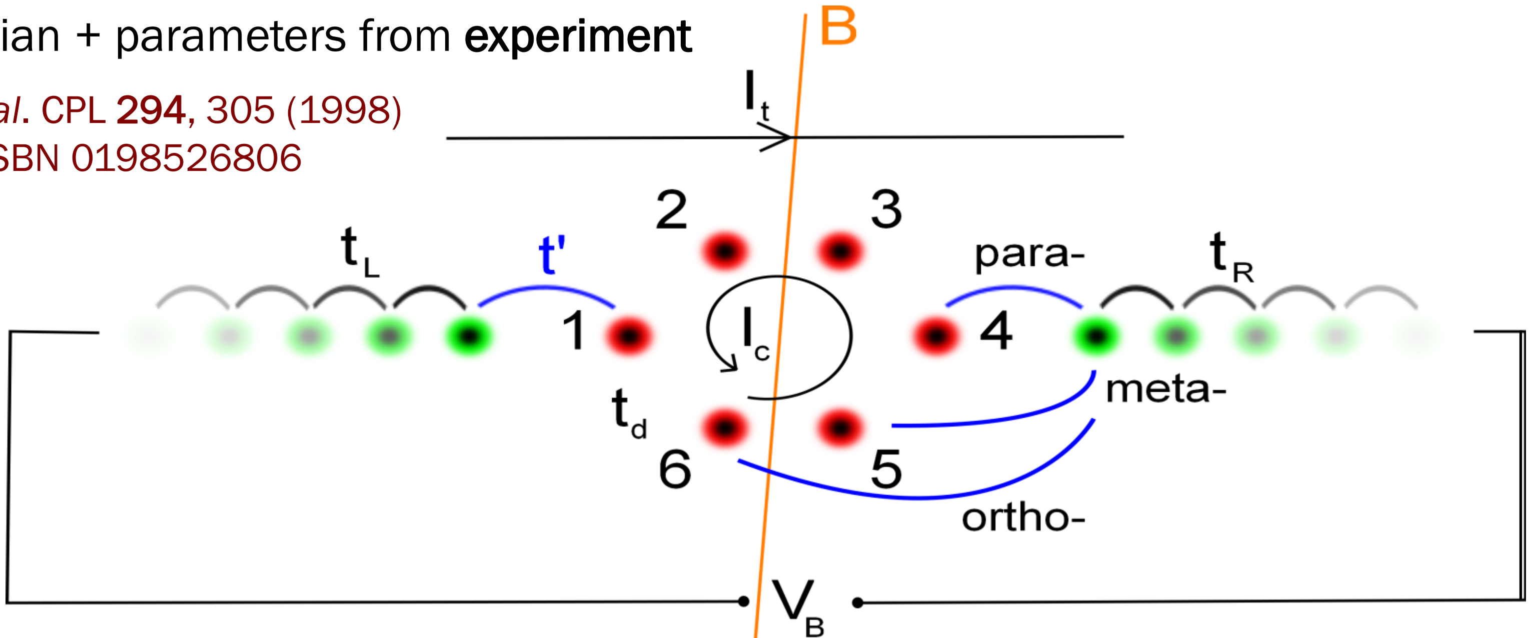
BUT: agreement between experiment and theory often poor – improve on electronic correlations – suitable methods ?

Dzhioev *etal*. J. Chem. Phys. **134** 044121 (2011);Toher *etal*. PRL **95**, 146402 (2005)

Metal - „Benzene“ - metal junction

model hamiltonian + parameters from **experiment**

Bursill *etal*. CPL **294**, 305 (1998)
Barford ISBN 0198526806



- 6 electronic orbitals + **e^- - e^- interaction**
- perpendicular **magnetic field B**, Peierls + Zeeman
- left + right **metallic leads + bias voltage V_B**
- **3 setups:** para, meta, ortho

- **transmission** current

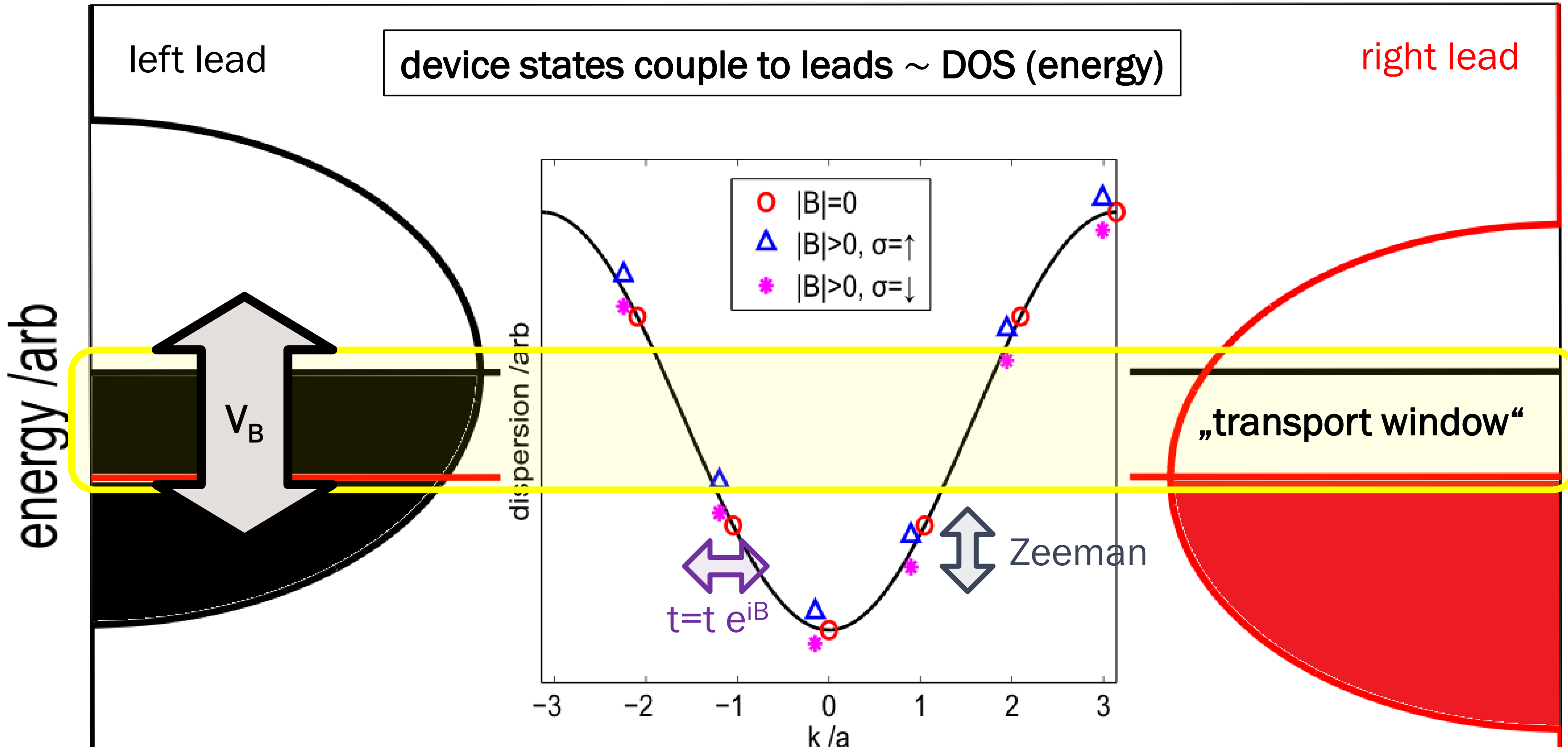
$$j_t = \bar{j}_2 - \bar{j}_1$$

- **circular** current

$$j_c = \frac{(\bar{j}_1 L_1 + \bar{j}_2 L_2)}{6}$$

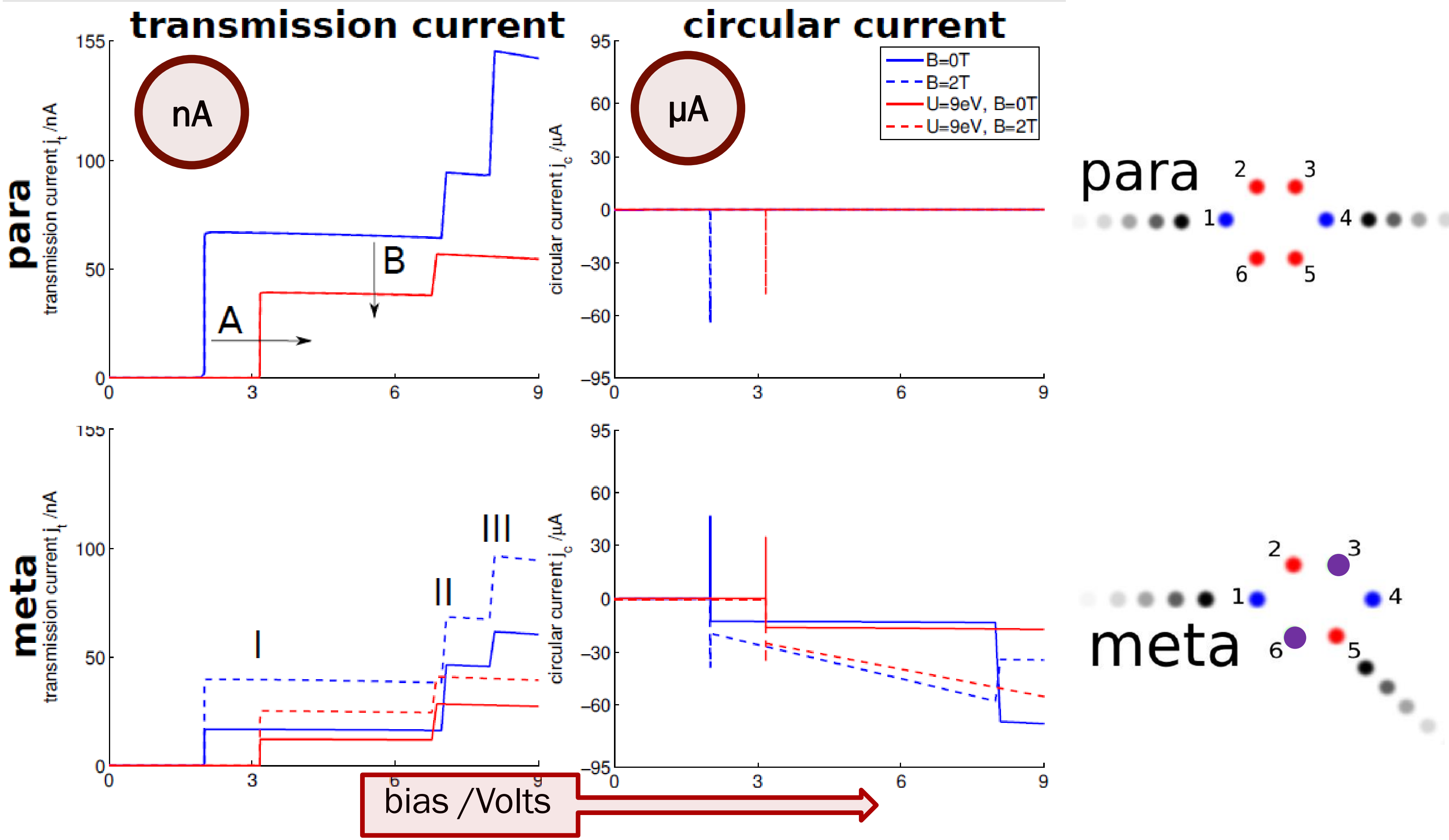
Rai *etal*. PhysChemC **114**, 20583 (2010)

Lead DOS effects

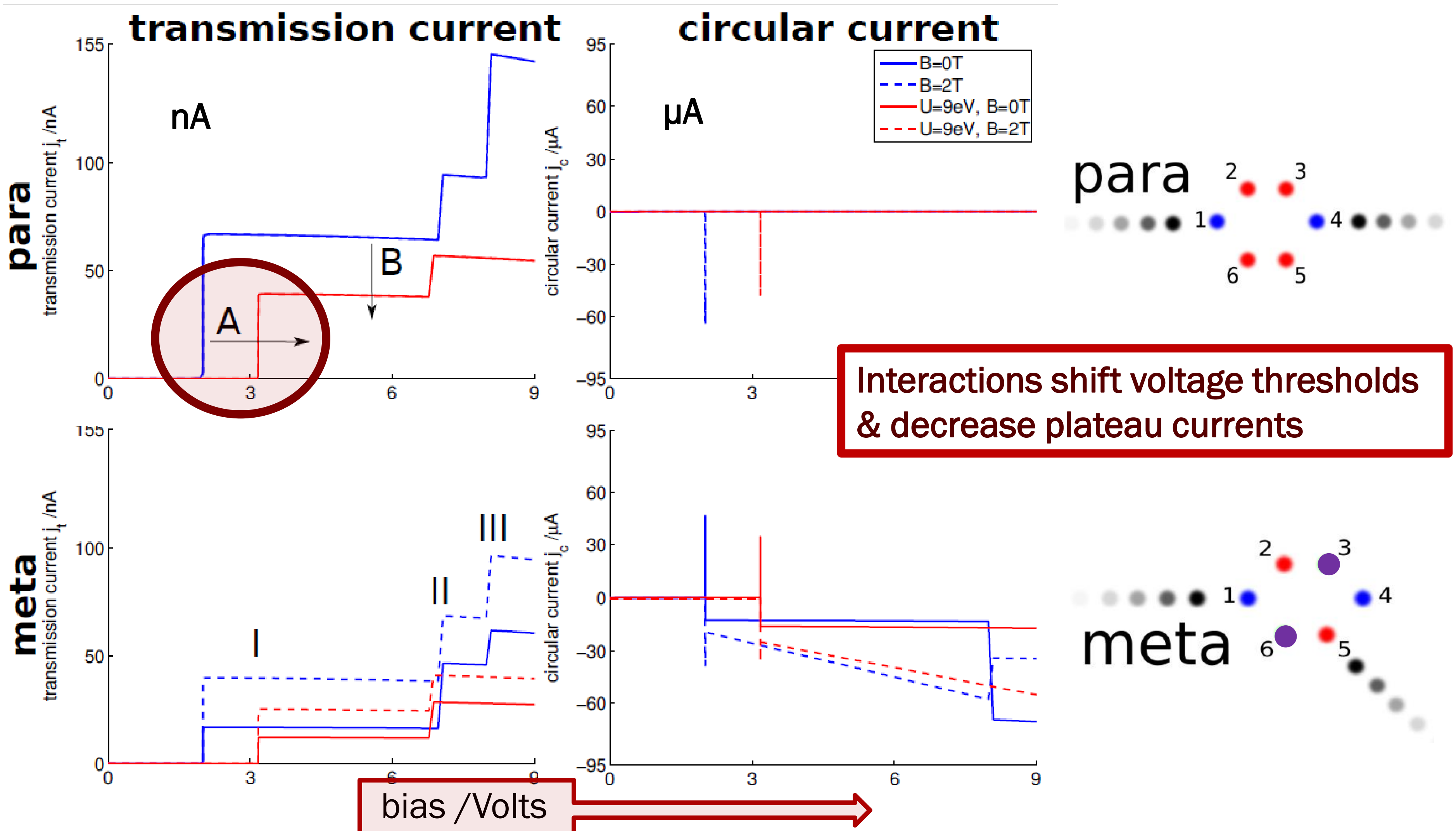


population imbalance of k=+/- $\frac{2\pi}{3}$ states (= counter propagating)

II. Current-voltage overview

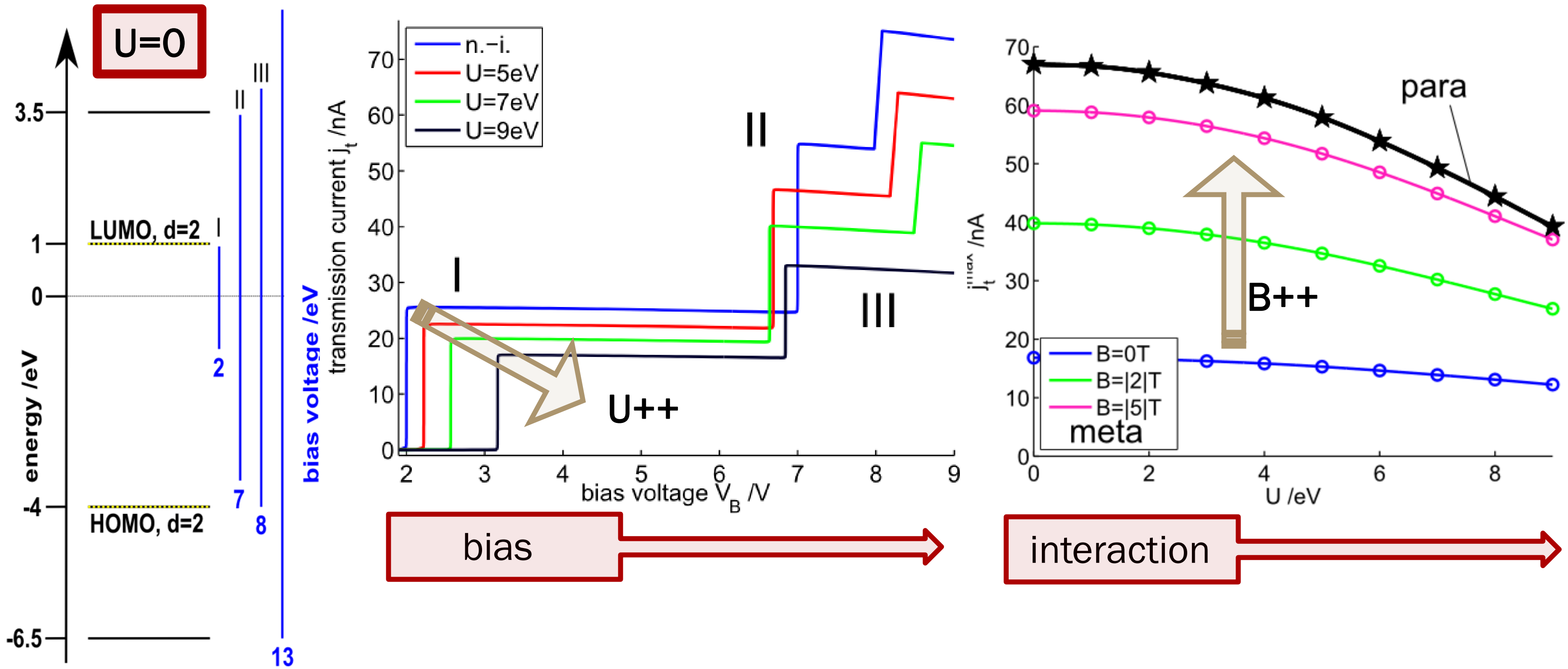


II. Current-voltage overview



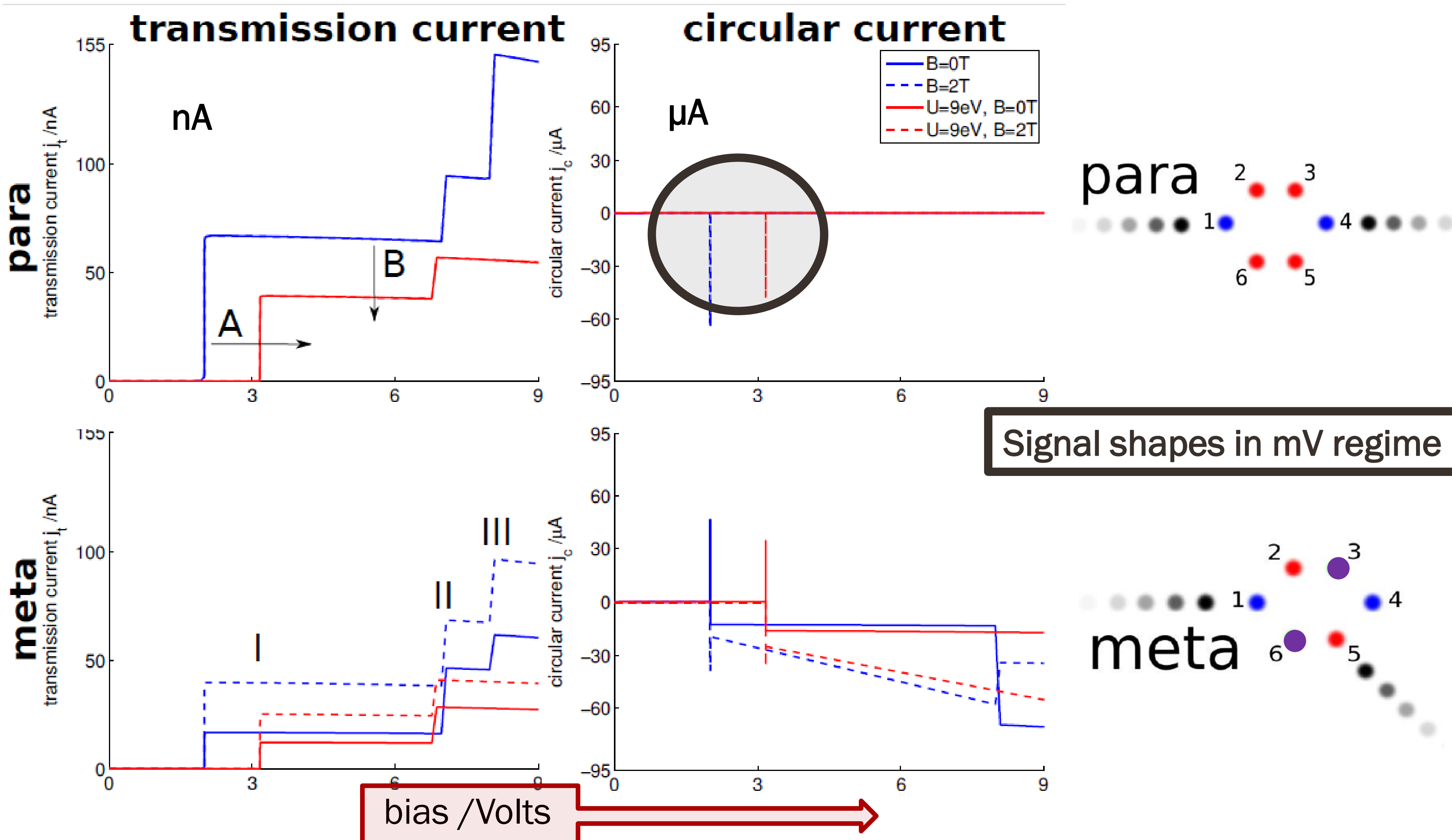
Interactions shift voltage thresholds & decrease plateau currents

e⁻ - e⁻ interactions / transmission current



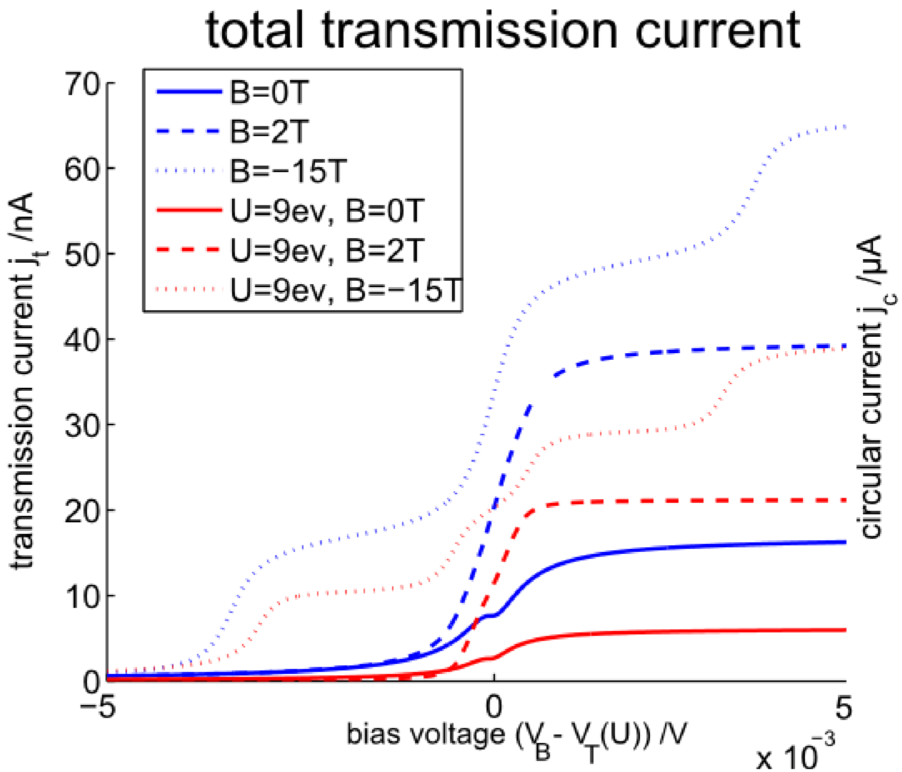
- threshold renormalization beyond mean-field
- plateau current renormalized by U, B

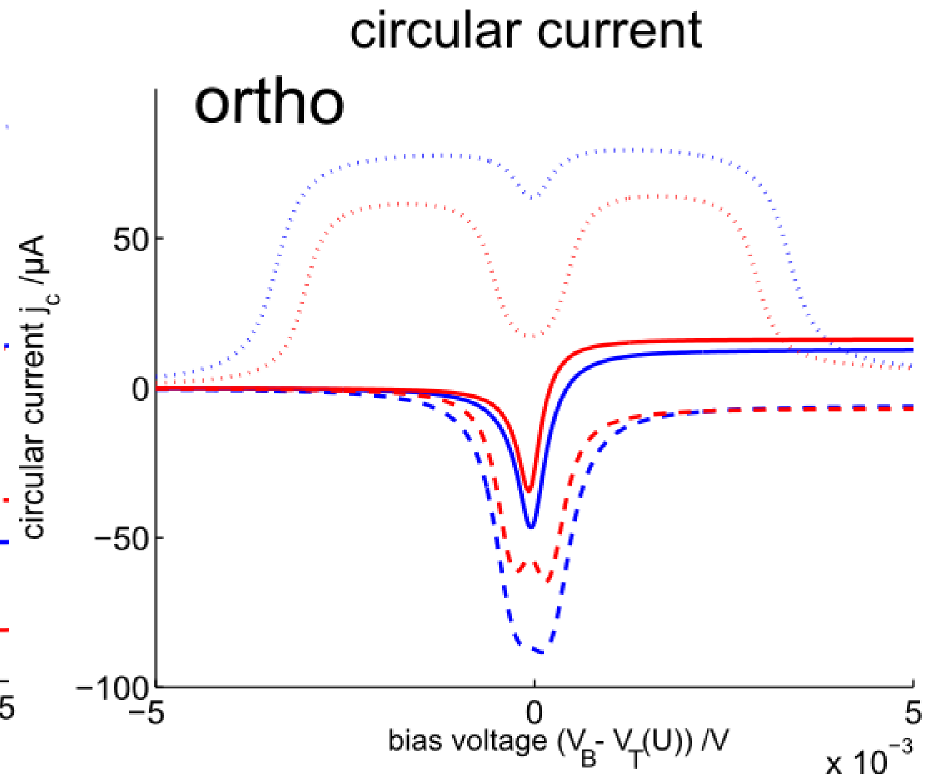
II. Current-voltage overview



Signal shapes in mV regime

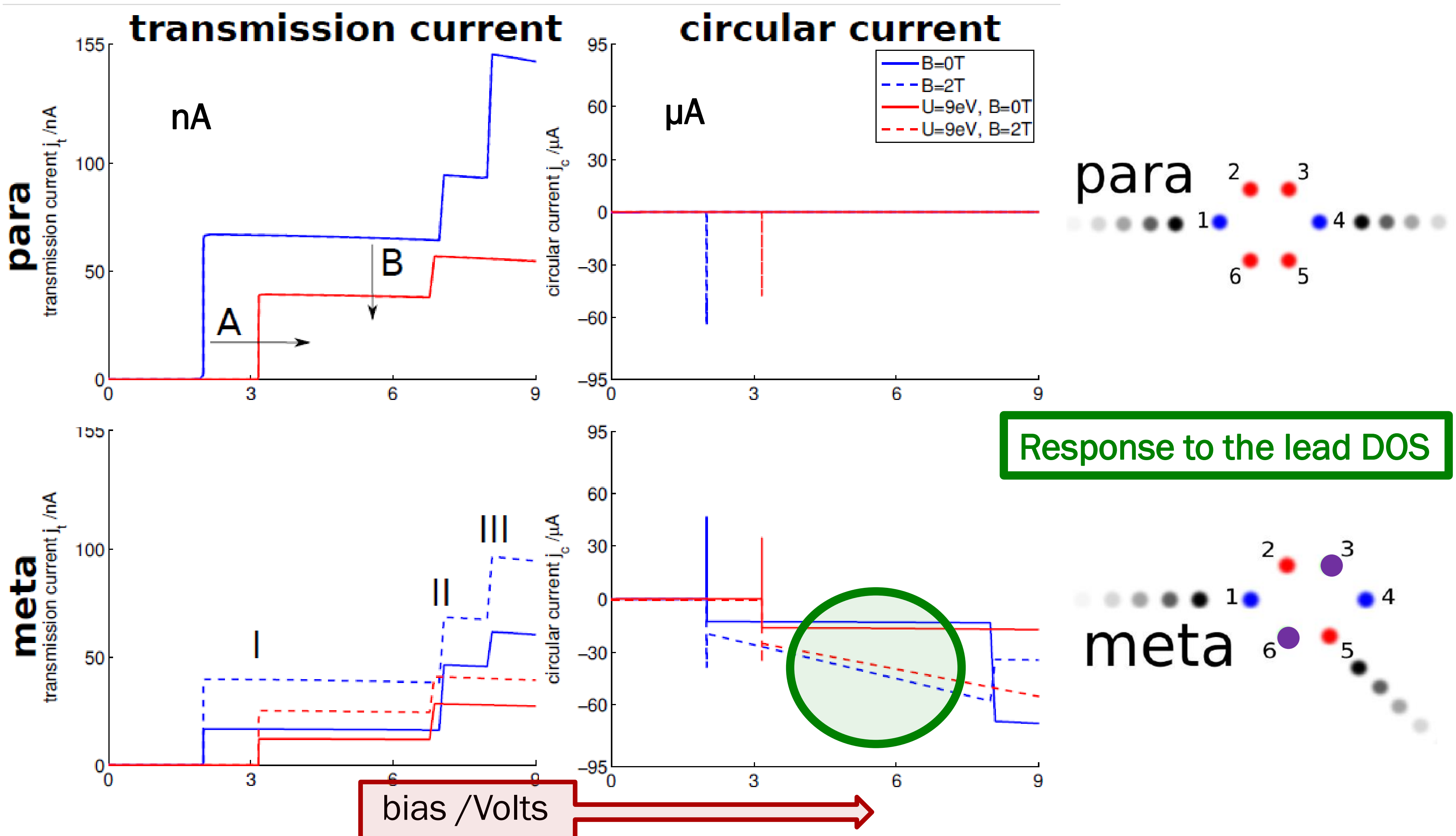
Current-voltage signals



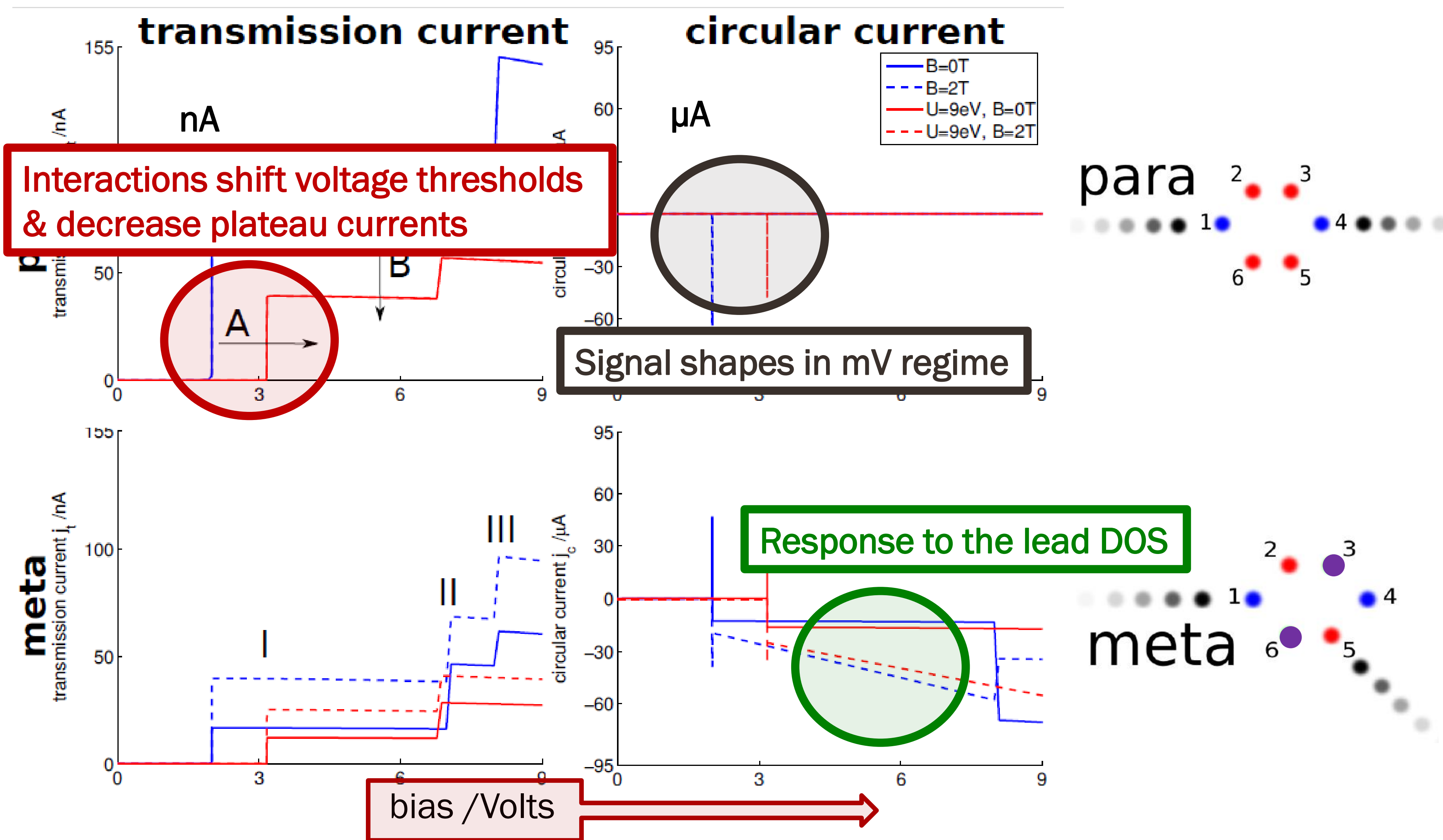


- Lenz rule
- Zeemann splitting

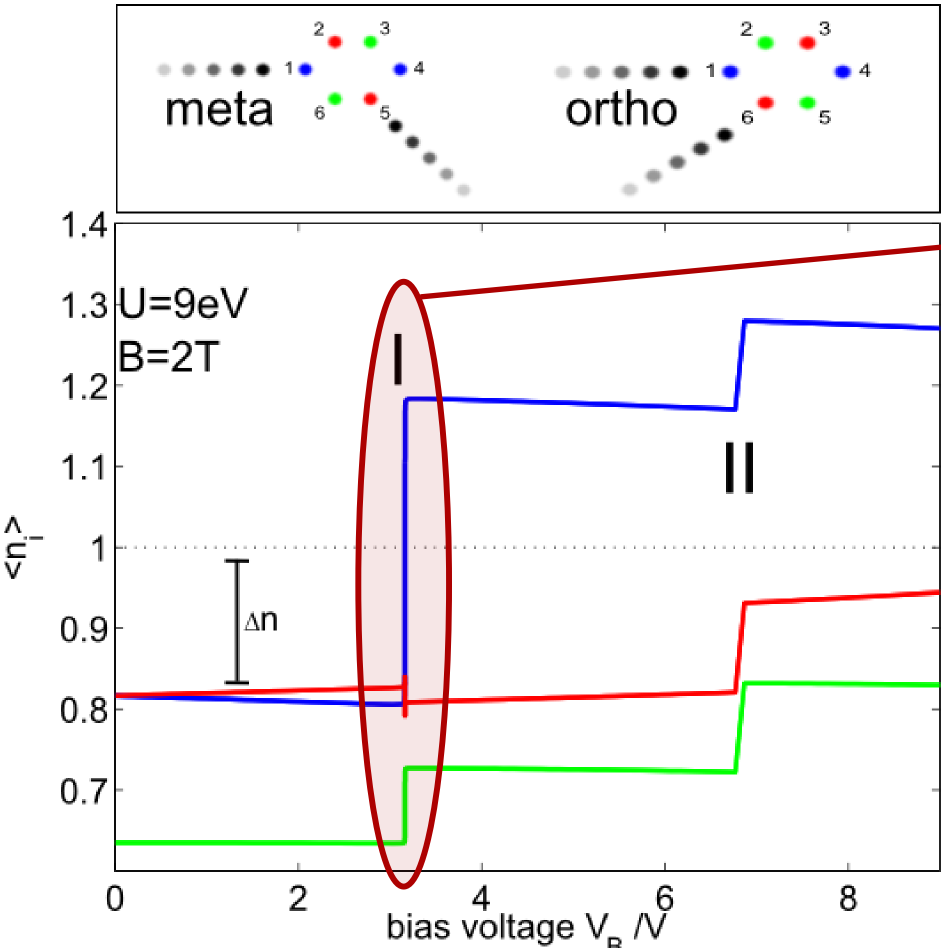
II. Current-voltage overview



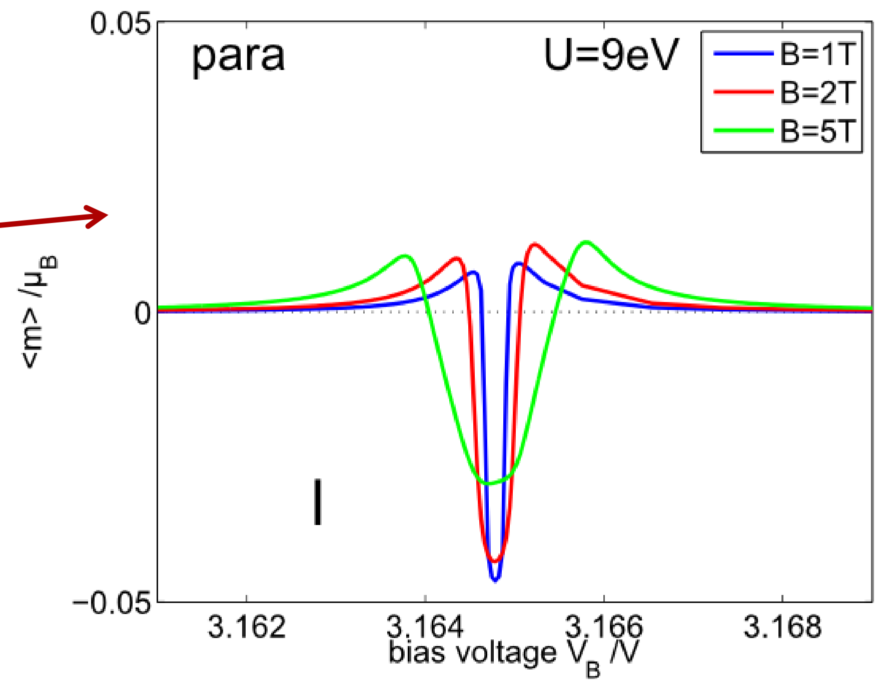
II. Current-voltage overview



III. Charge distribution + magnetization



Volts



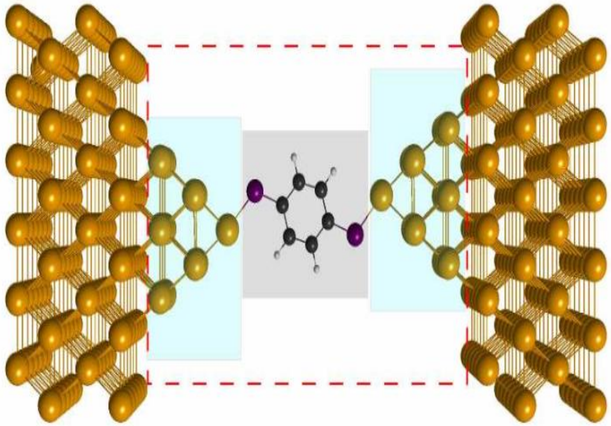
milli Volts

- <n> substantially renormalized
- <m> signals due to Zeeman

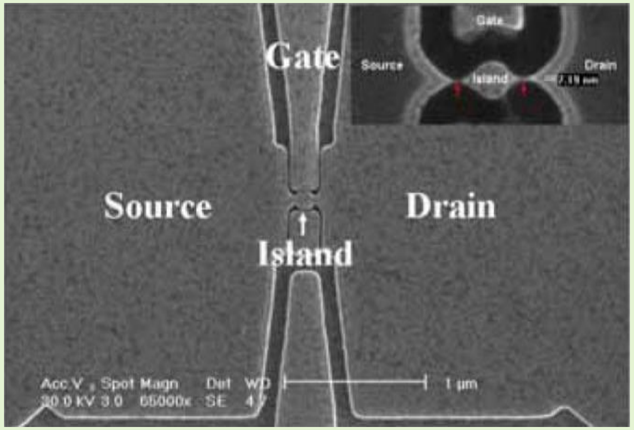
Overview

1) $Li_{0.9}Mo_6O_{17}$

2) molecular ring junction

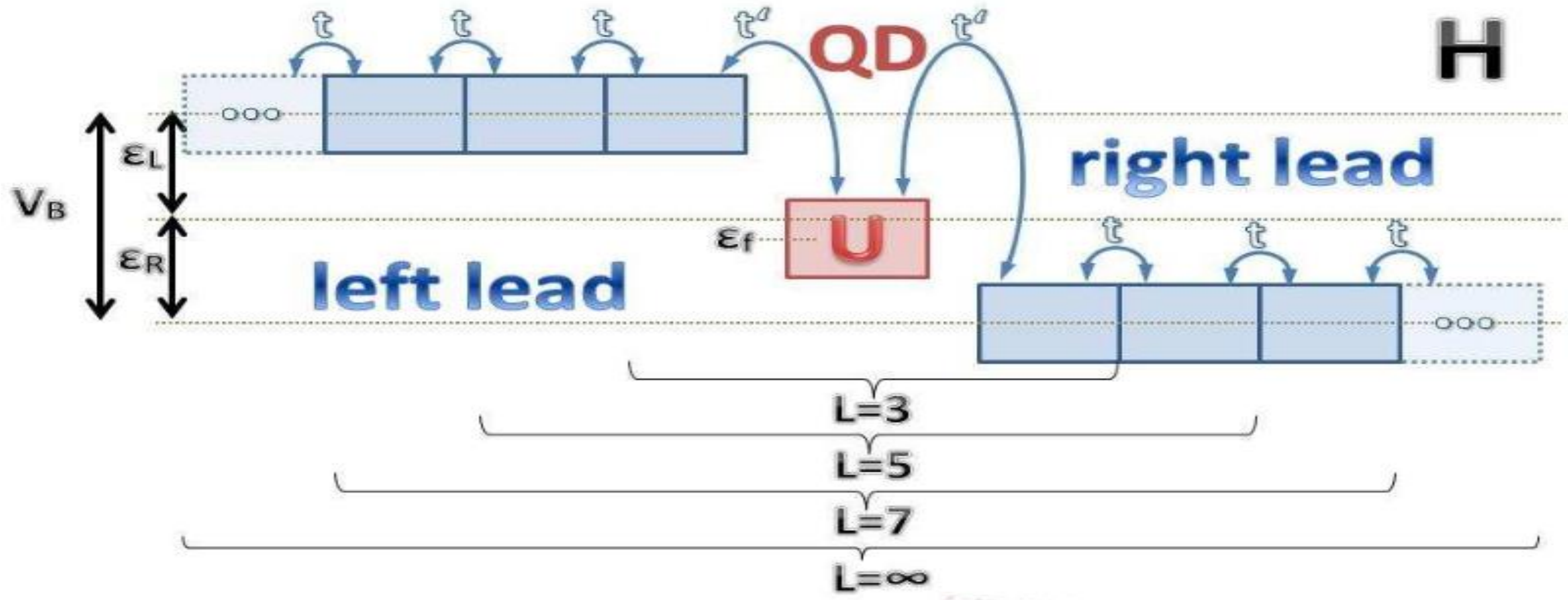


3) single quantum dot



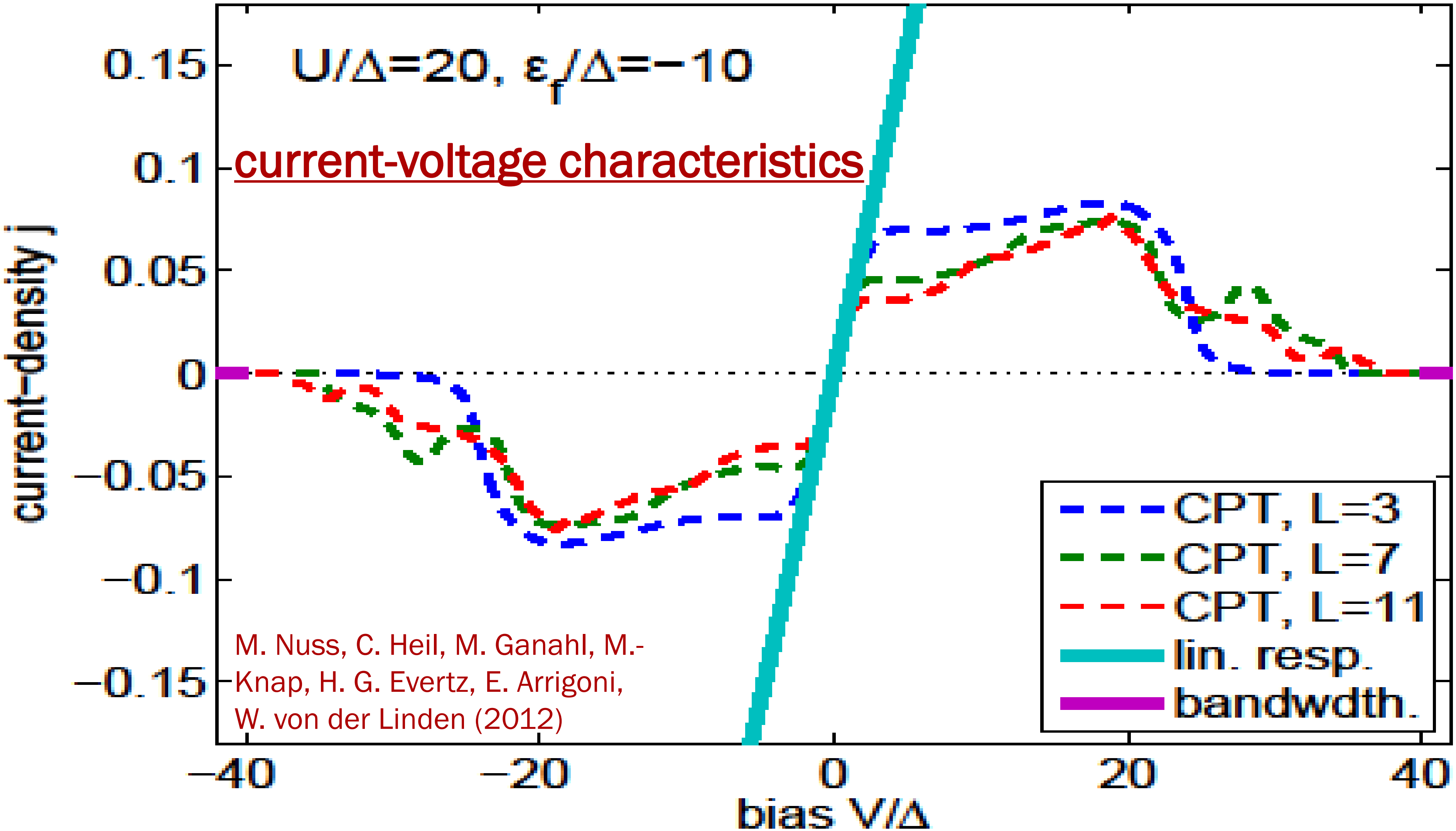
- Non equilibrium **V**ariational **C**luster **A**pproach
- Time evolution using **M**atrix **P**roduct **S**tates

Single impurity Anderson model

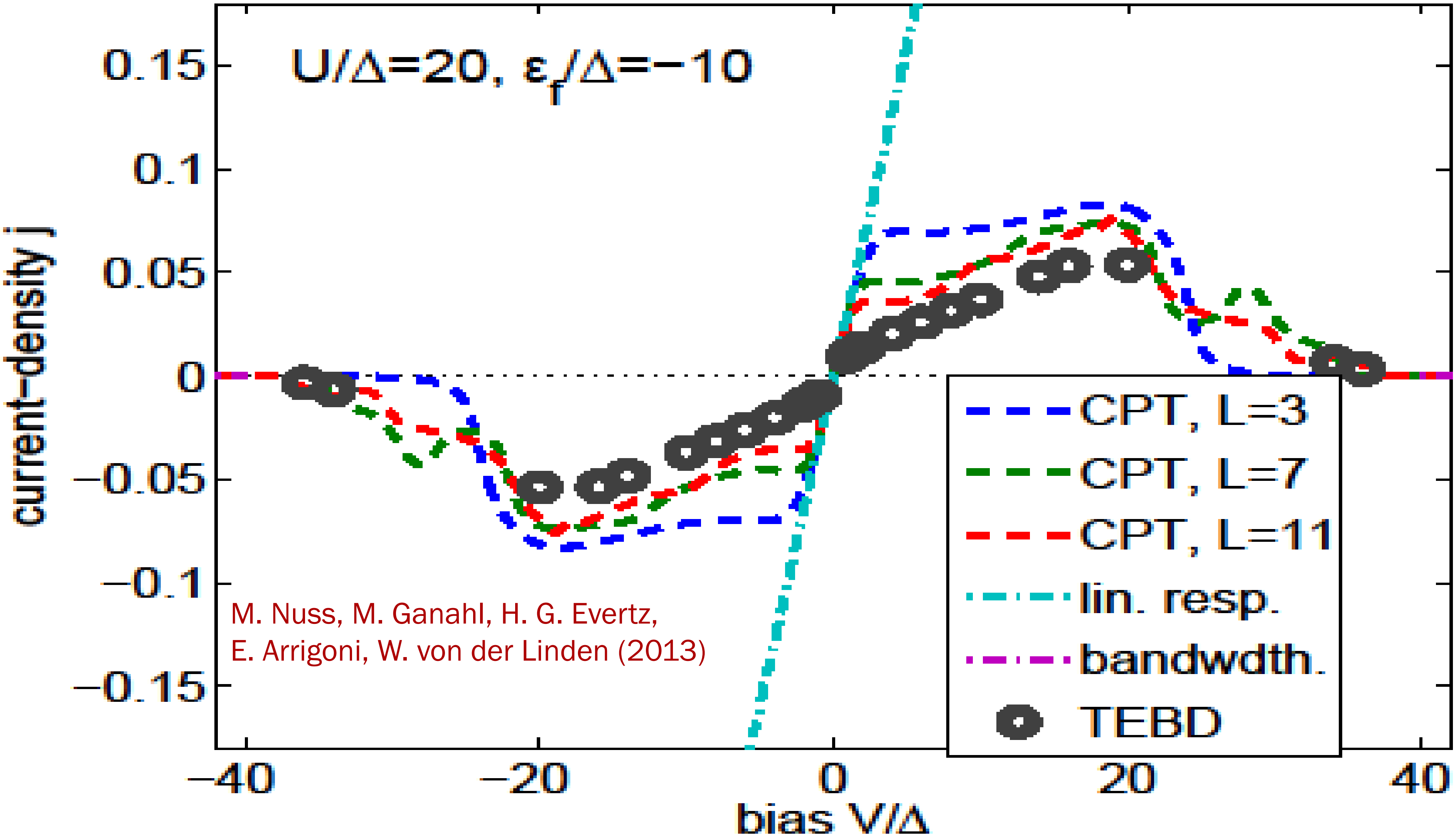


- one orbital with on-site interaction
- bias voltage
- infinite system

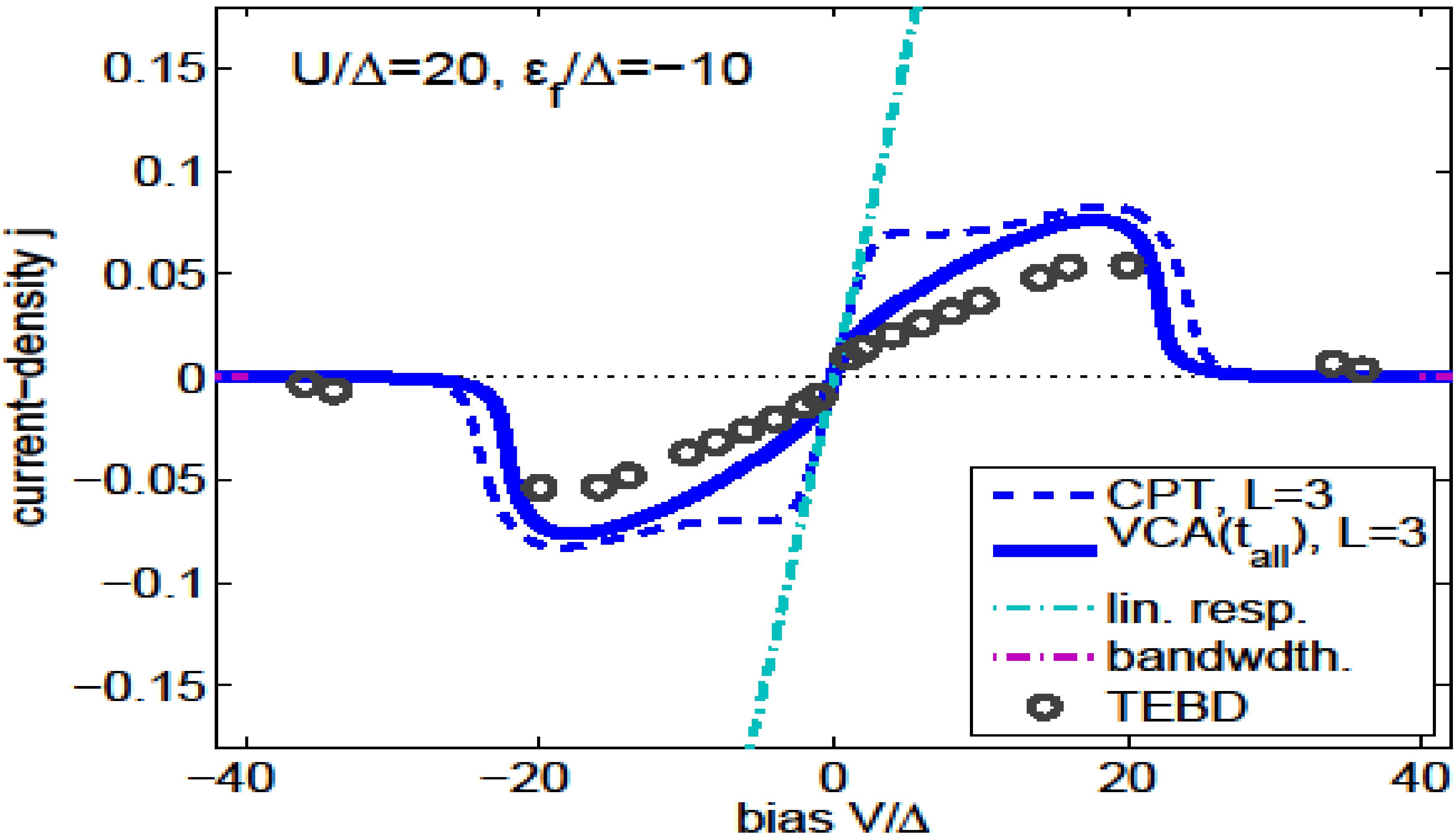
Non equilibrium Cluster Perturbation Theory



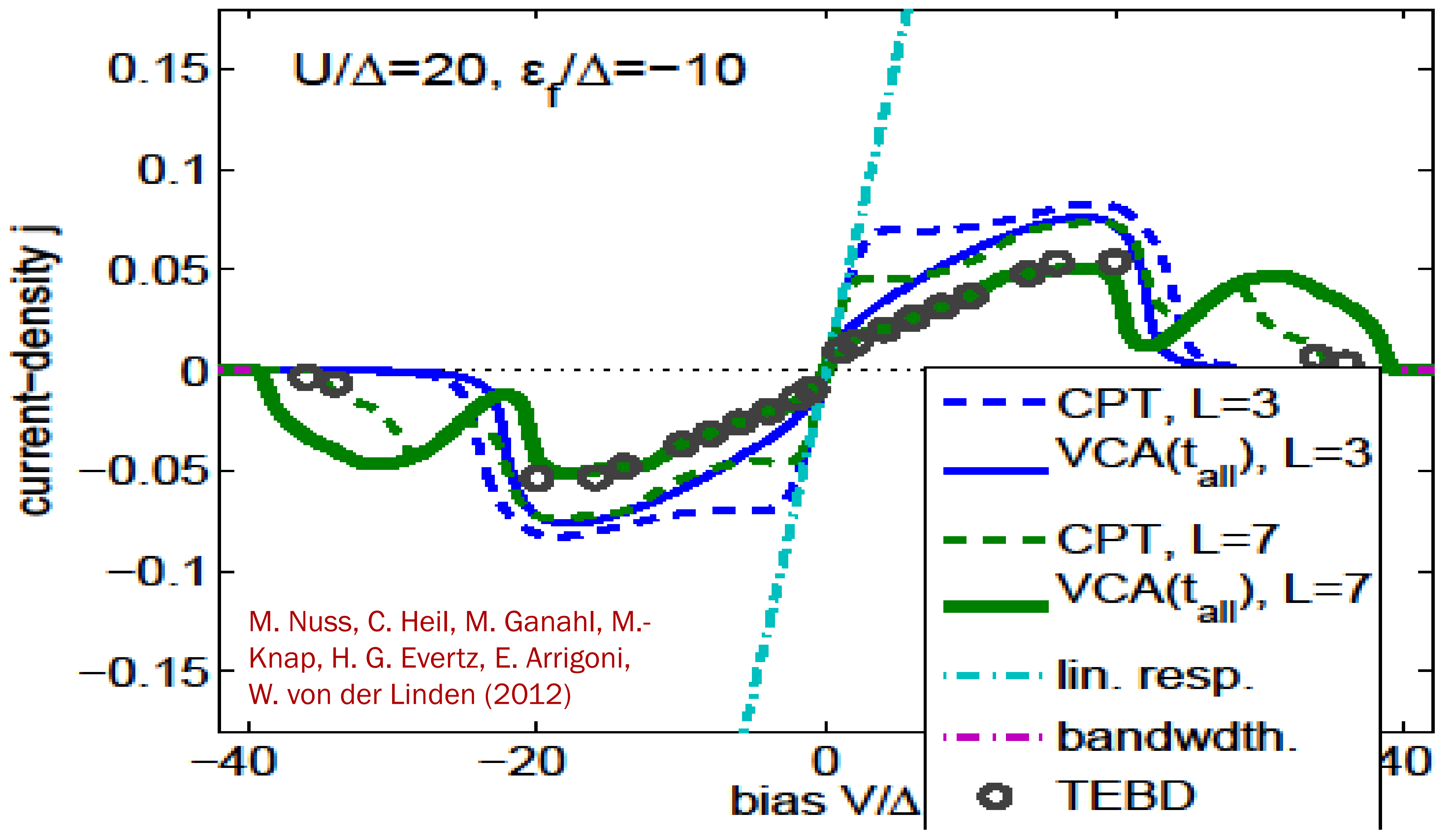
Quasi exact DMRG+TEBD



Non equilibrium Variational Cluster Approach

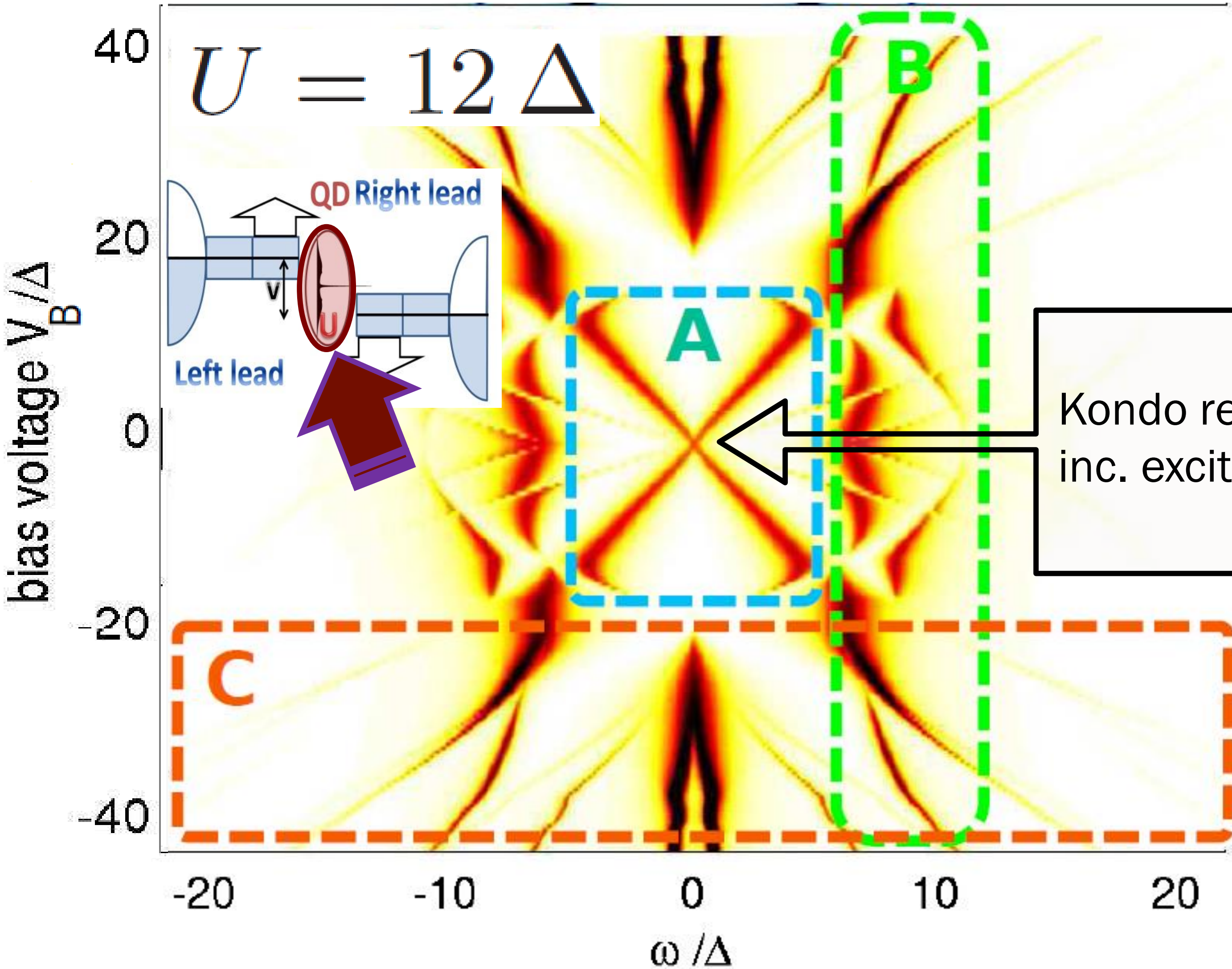


Non equilibrium Variational Cluster Approach



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

Non equilibrium local density of states



A: splitting of Kondo resonance: *linear* + *U dep.*

Equilibrium

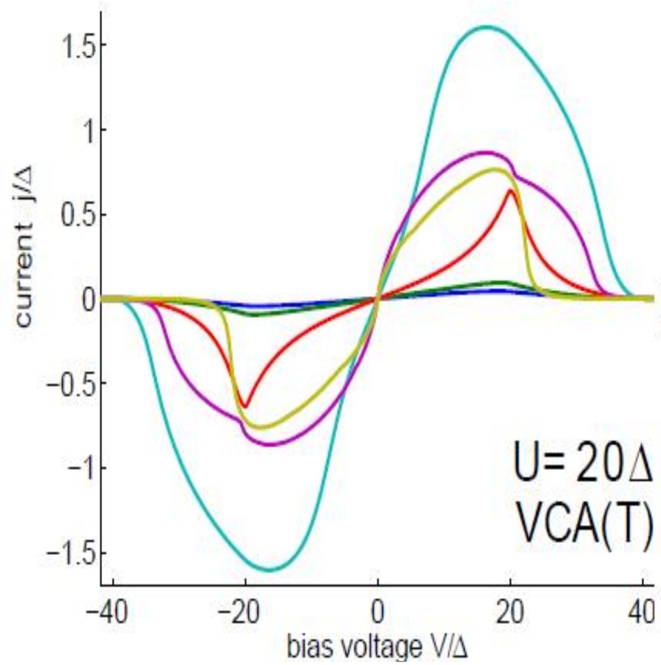
Kondo resonance @ $\omega = 0$

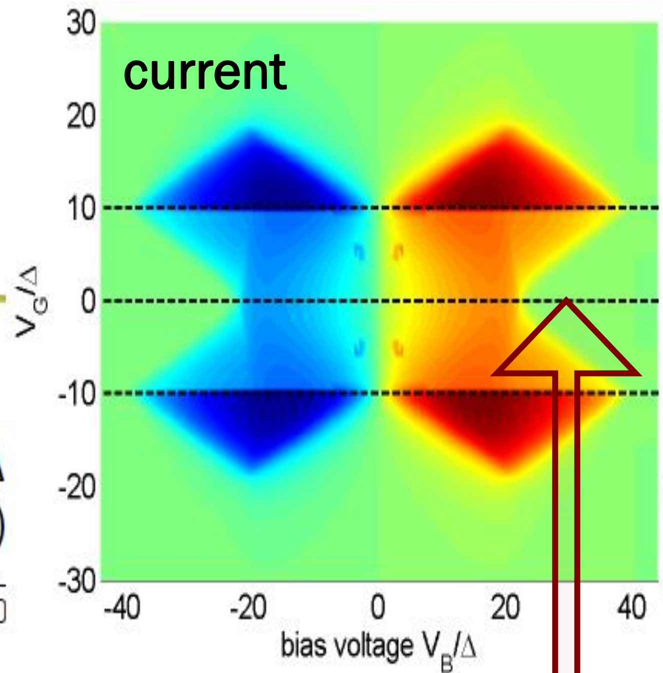
inc. excitations @ $\omega \cong \pm \frac{U}{2}$

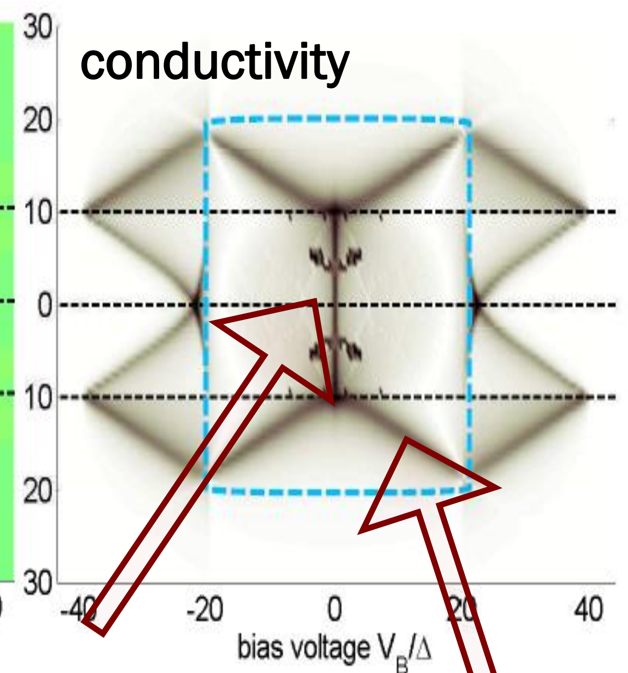
B: finite size eff. in Hubbard band

C: lead-band effects

Applying a gate voltage



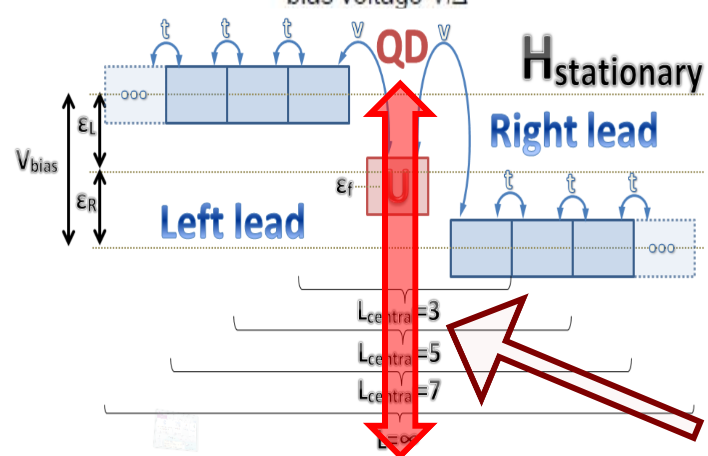




Kondo

Coulomb blockade

results from previous slides Vgate=0

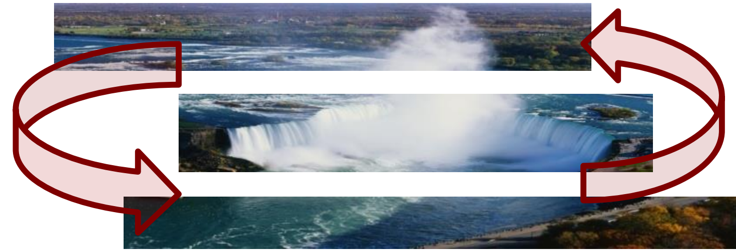


gate V: U=fixed

Conclusions + outlook

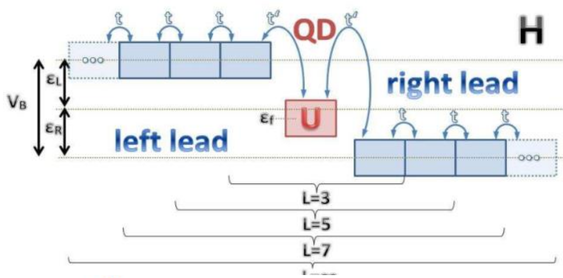
- non equilibrium Variational Cluster Approach
  - fast
  - versatile
  - self consistent feedback

Arrigoni *etal.* (2011)
Knap *etal.* (2011)



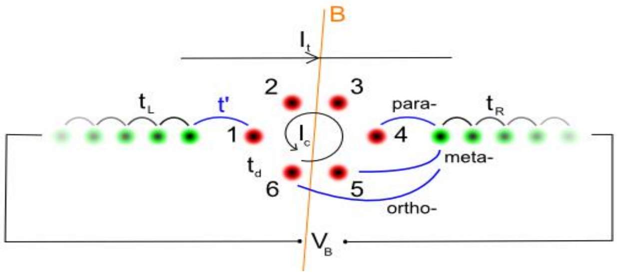
- quantum dot
  - current density up to intermediate U
  - TEBD benchmark
  - linear U dep. splitting of Kondo resonance
  - Kondo regime + Coulomb blockade
  - nVCA >> nCPT: variational feedback crucial

Nuss *etal.* PRB **86**, 245119 (2012
Nuss *etal.* AIPcp. **1485** (2012)
Nuss *etal.* PRB **85**, 235107 (2012)
Nuss *etal.* PRB **88**, 045132 (2013)



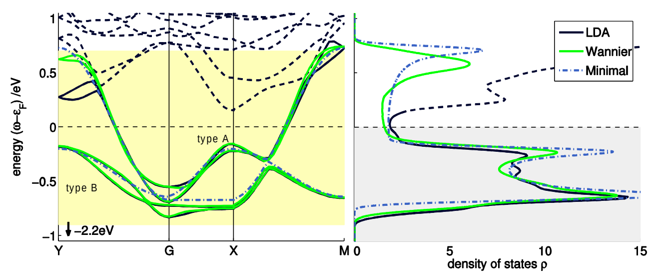
- molecular ring junction
  - interaction effects
  - magnetic fields
  - broadening effects

Nuss *etal.* arXiv (2013)



- transport in 1D materials
  - ab-initio + correlations
  - linear response transport

Nuss *etal.* arXiv (2013)

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Thank you!

maybe some day:

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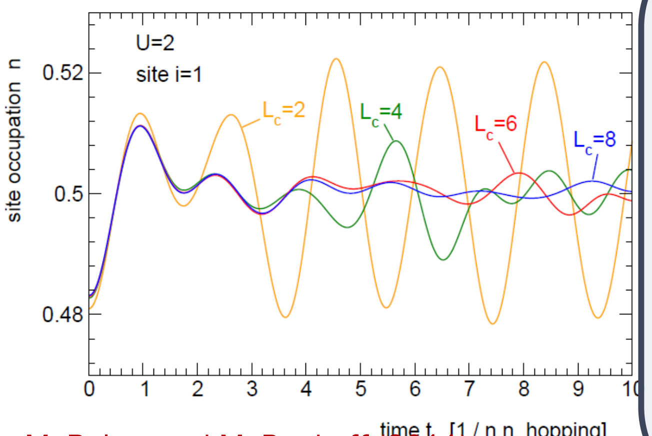
We gratefully acknowledge support from the Austrian Science Fund (FWF) P24081-N16 as well as the Vienna Scientific Cluster (VSC).

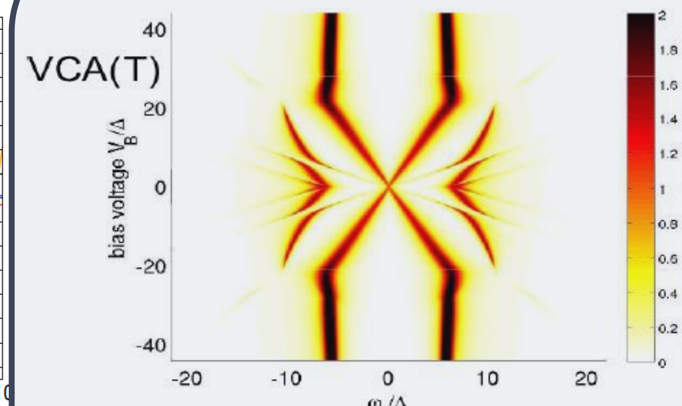
Non equilibrium Variational Cluster Approach

time evolution by CPT



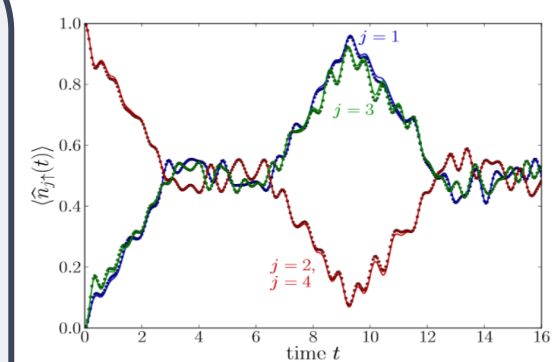
M. Balzer and M. Potthoff (2011)

steady state of quantum dots



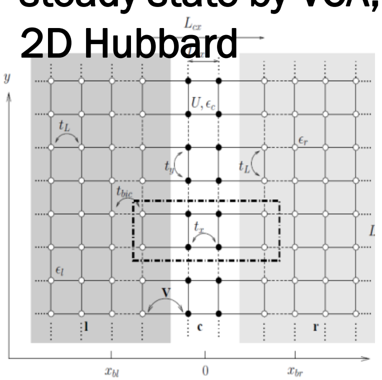
M. Nuss, C. Heil, M. Ganahl, M. Knap, H. G Evertz, E. Arrigoni, W. vd Linden (2012)

dynamical symmetry in 2D



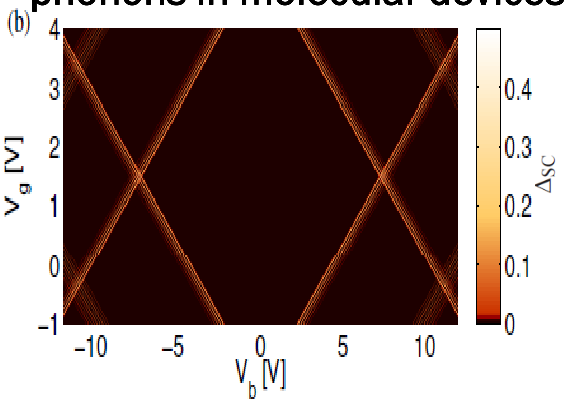
P. Jurgenowski and M. Potthoff (2013)

steady state by VCA, 2D Hubbard



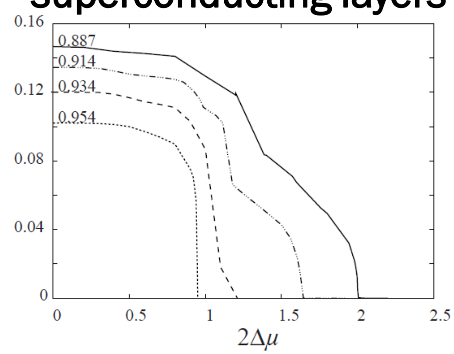
M. Knap, W. vd Linden, E. Arrigoni (2011)

phonons in molecular devices



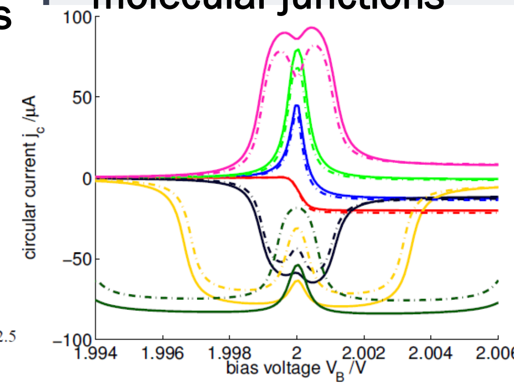
M. Knap, E. Arrigoni, W. von der Linden (2012)

superconducting layers



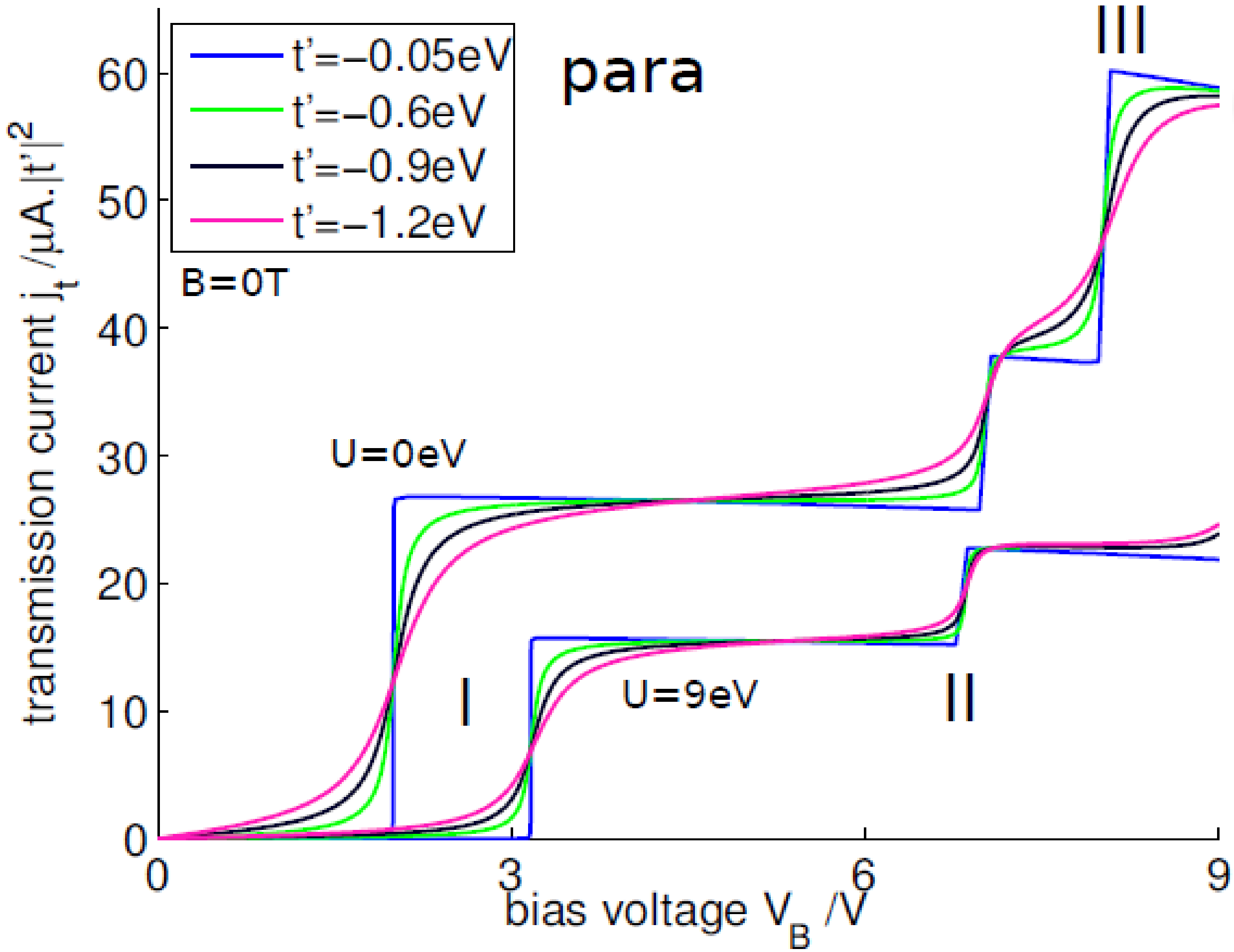
A. Fulterer, E. Arrigoni (2012)

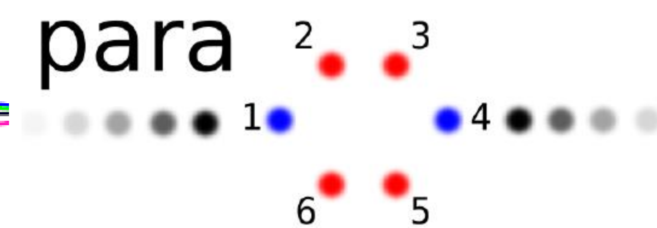
magnetic effects in molecular junctions



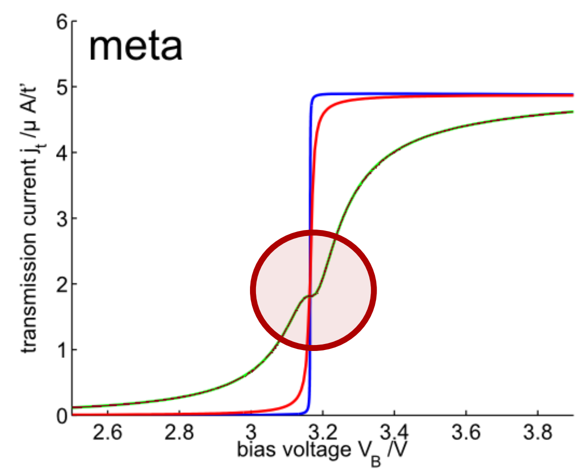
M. Nuss, E. Arrigoni, W. vd Linden (2012)

I. Transmission current voltage characteristics





- interaction U
- broadening t'

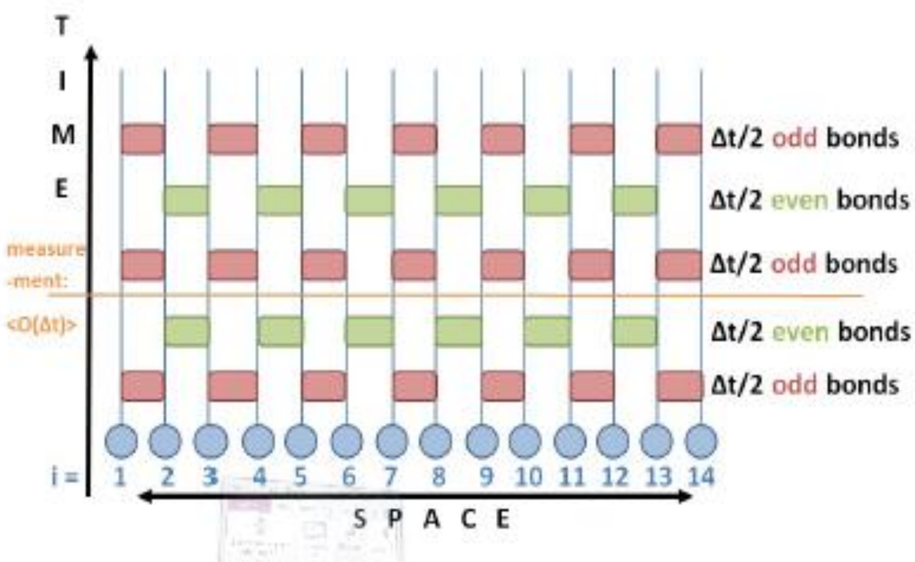


M. Nuss, W. von der Linden and E. Arrigoni (2013)

Real time evolution with matrix product states

$$|\Psi\rangle = \sum_{\{s_1,s_2,\ldots,s_L\}} c_{s_1,s_2,\ldots,s_L} \left|s_1, s_2, \ldots, s_L\right\rangle$$

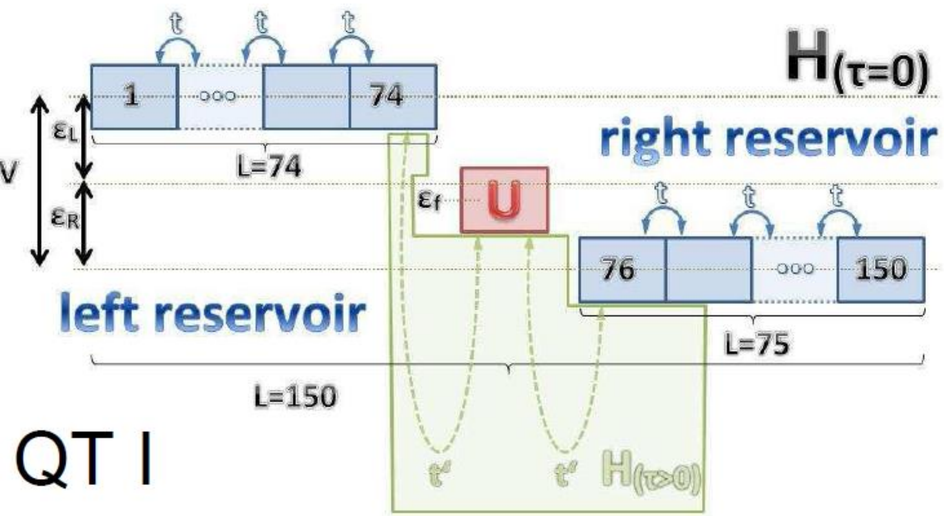
$$= \sum_{\{s_1,\ldots,s_L\}} \sum_{\{\alpha_1,\ldots,\alpha_L\}} A^{[1]s_1}_{\alpha_1} A^{[2]s_2}_{\alpha_1\alpha_2} \ldots A^{[L-1]s_{L-1}}_{\alpha_{L-2}\alpha_{L-1}} A^{[L]s_L}_{\alpha_{L-1}} \left|s_1, \ldots, s_L\right\rangle$$

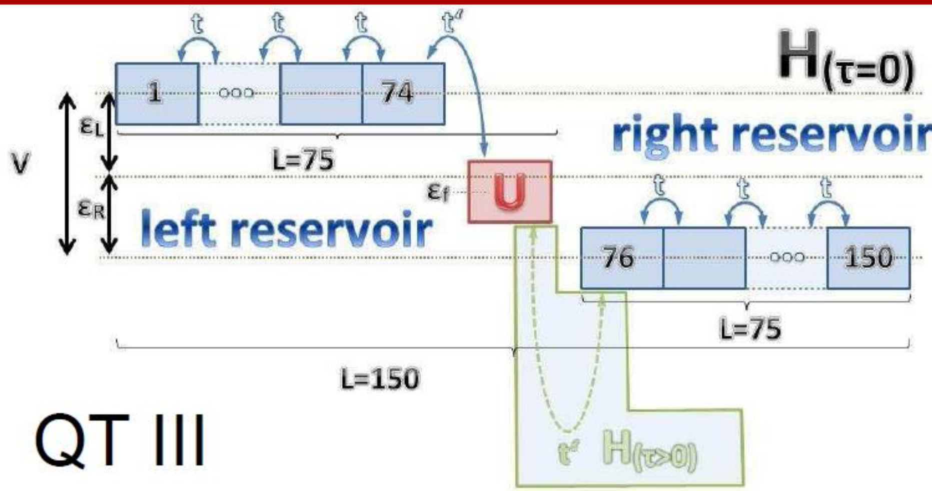


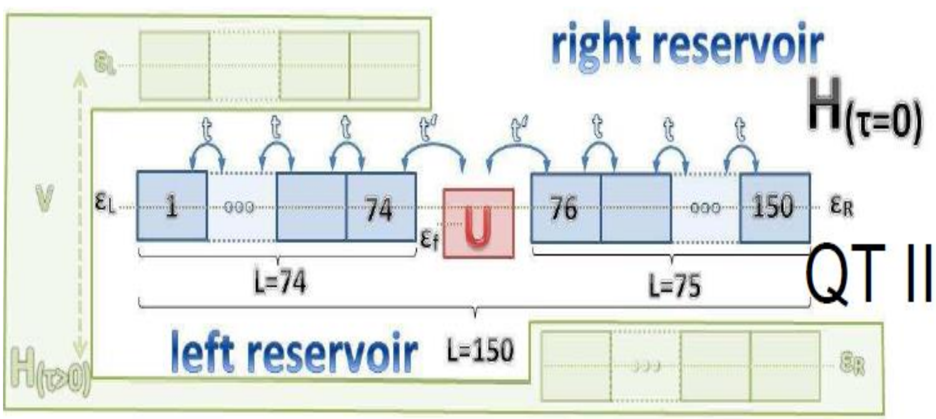
1. S. R. White (1993)
   DMRG$(\hat{\mathcal{H}}(t_0)) \Rightarrow |\Psi\rangle_0$
2. quench
3. evolve $|\Psi\rangle_0$ with $\hat{\mathcal{H}}(t > 0)$ by TEBD

G. Vidal (2004)

3 different quneches



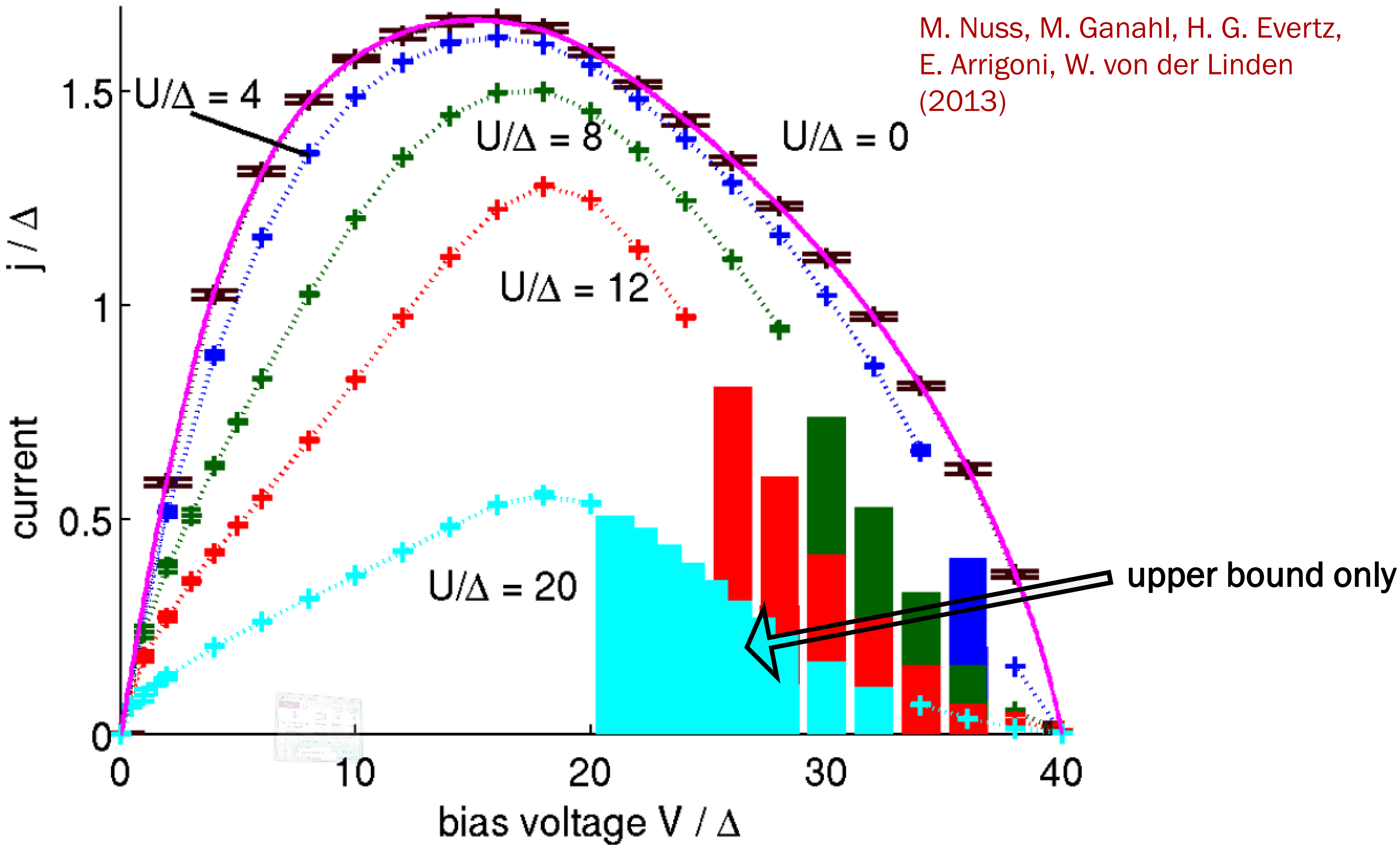




comparison of short time quench dynamics
+ quasi-steady-state

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

DMRG+TEBD current-voltage characteristics



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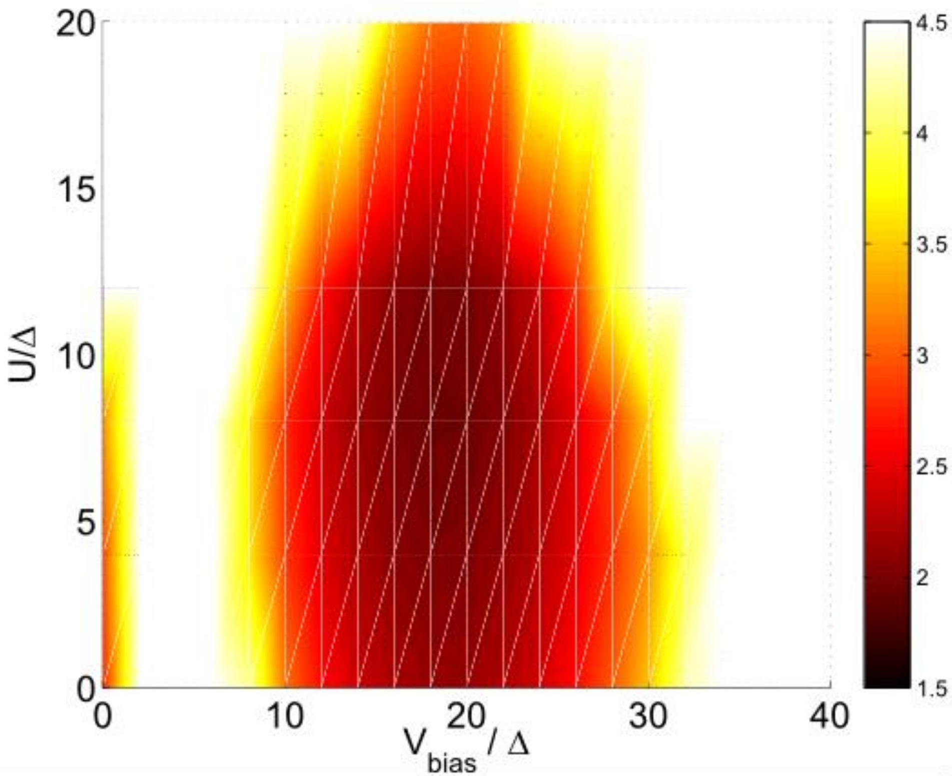
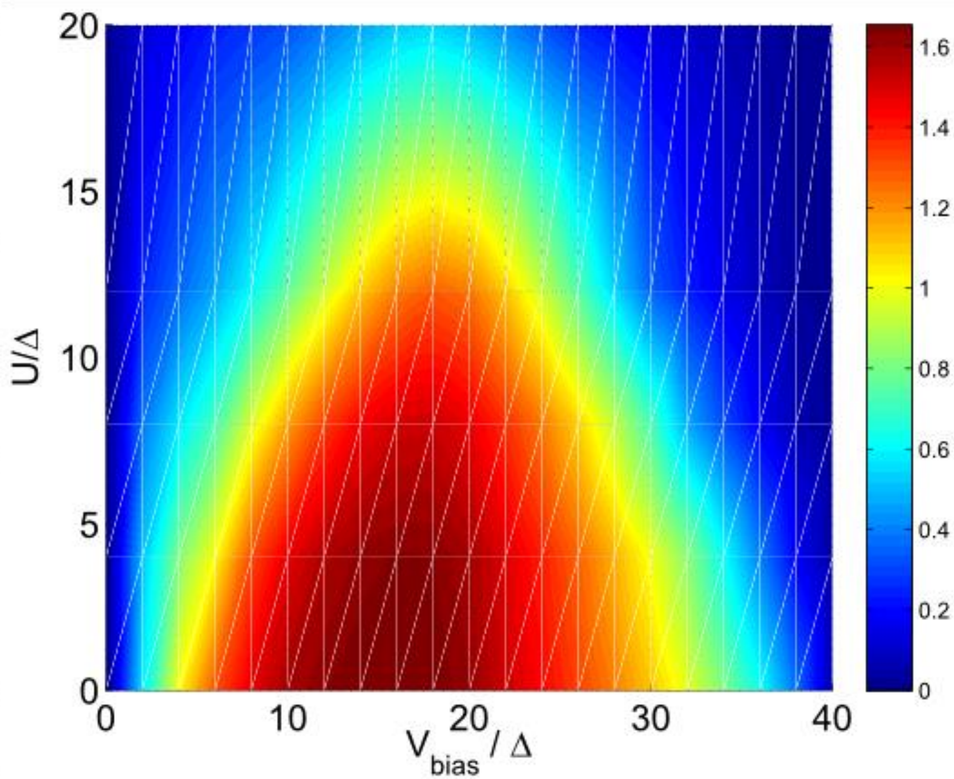
Entanglement ⟷ current





Time evolution of current