A variational cluster approach to strongly correlated quantum systems out of equilibrium

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

TUG

Regensburg, 15.03.2013

itp cp

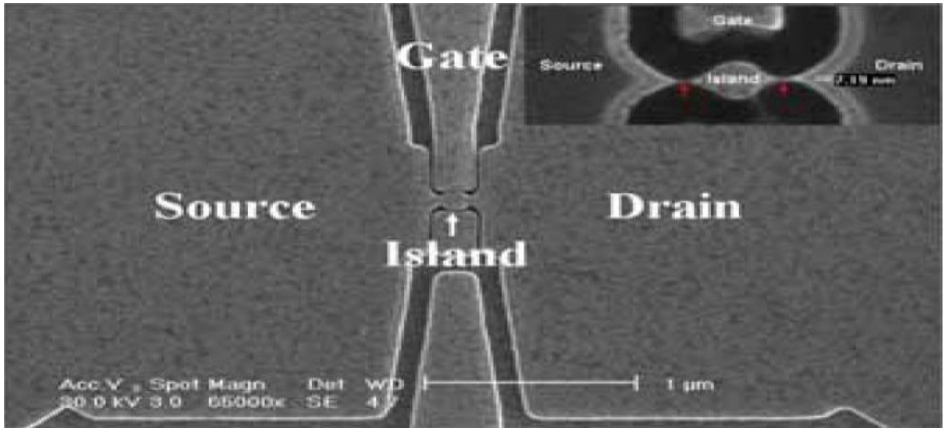
Agenda

I — correlated quantum systems out of equilibrium

II — non equilibrium variational cluster approach

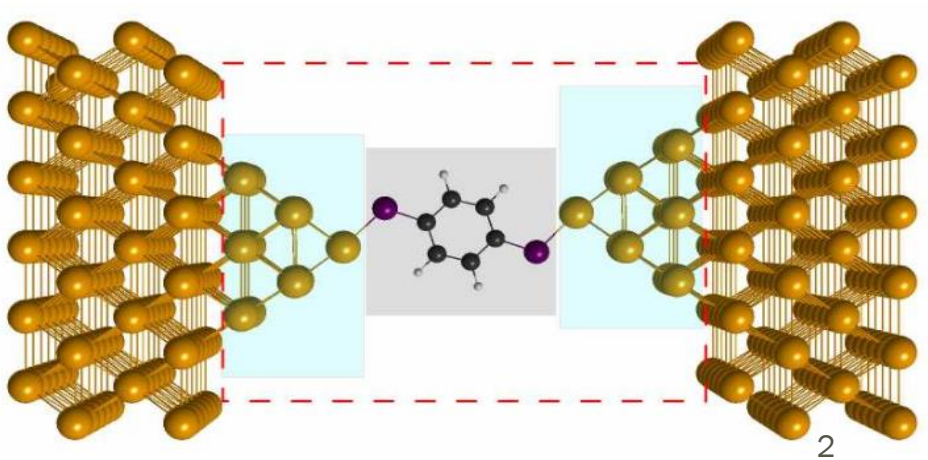
III — steady state results

1) single quantum dot



Wu etal (2010)

2) molecular ring junction

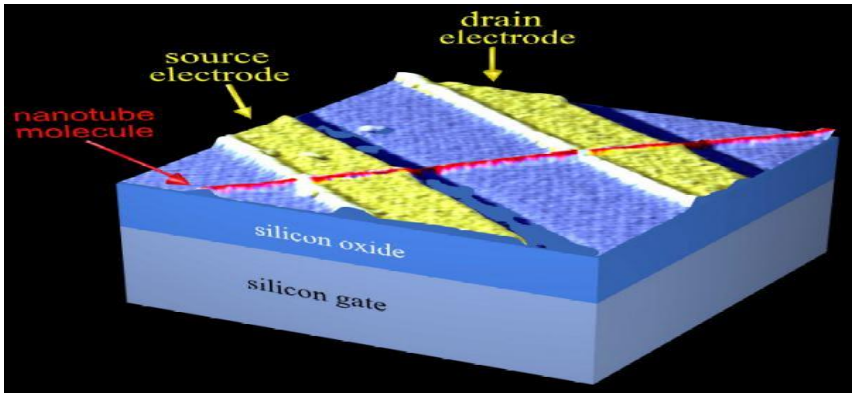


Ryndyk etal (2012)

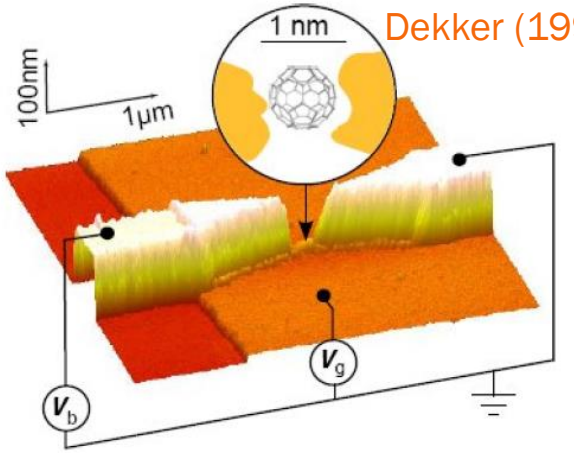
non equilibrium systems

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

this talk



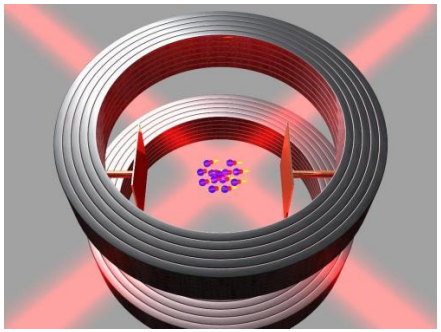
- transport through molecular junctions



Dekker (1998)

Yao (1999)

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



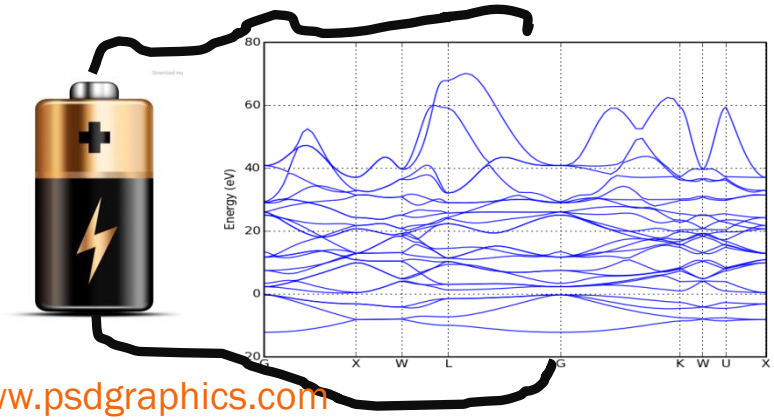
Modugno etal (2009)

- ultra fast pump probe spectroscopy

non equilibrium + many body interactions

non equilibrium

transient / dissipation / steady state



www.psdgraphics.com

+ manybody interactions

c Goscinny & Uderzo Ehapa

methods

- non equilibrium cluster perturbation theory
- non equilibrium variational cluster approach

} this talk

- non equilibrium dynamical mean field theory

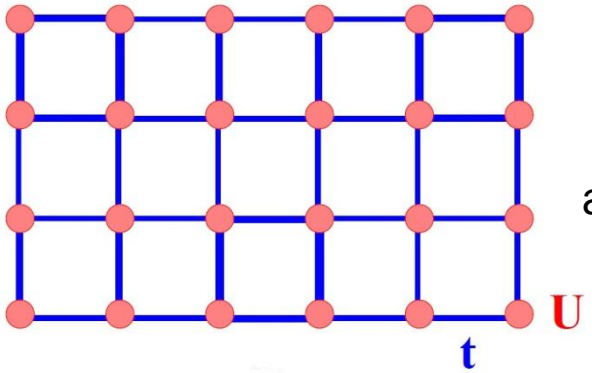
see E. Arrigoni's talk

- ...

non equilibrium variational cluster approach

15.03.2013

equilibrium many body cluster methods



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

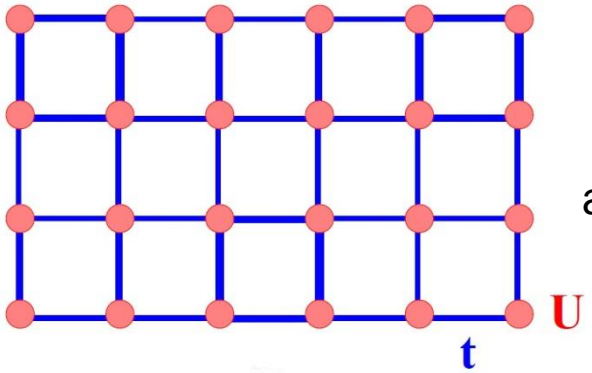
ask for G

in general unsolvable

Strategy ?

1) 2) 3) 4)

equilibrium many body cluster methods



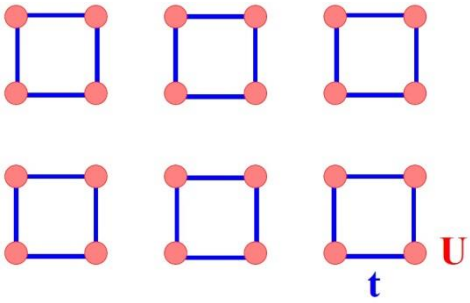
given $\hat{\mathcal{H}}$

ask for G

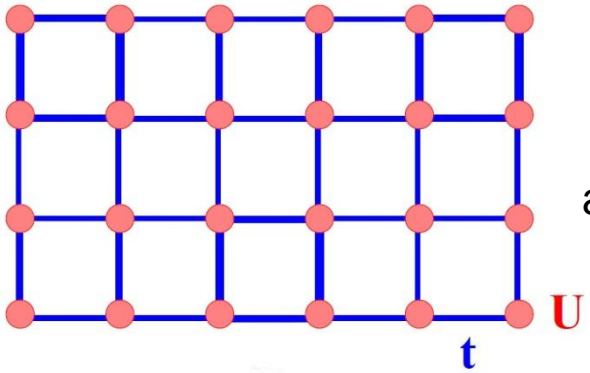
in general unsolvable

Strategy ?

1) CUT 2) 3) 4)



equilibrium many body cluster methods



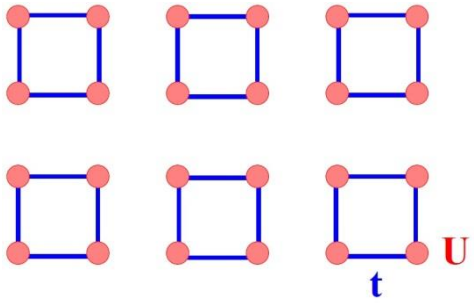
given $\hat{\mathcal{H}}$

ask for G

in general unsolvable

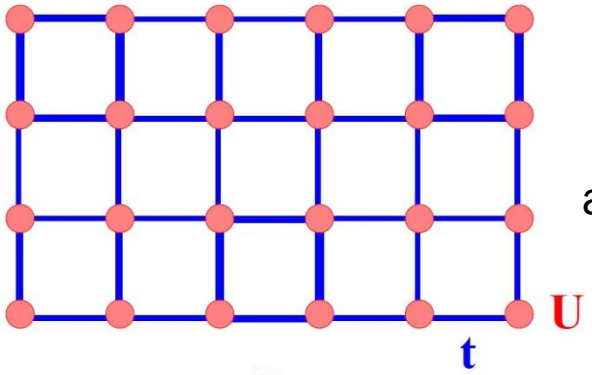
Strategy ?

1) CUT 2) SOLVE 3) 4)



$G_{cluster}$ = exactly solvable

equilibrium many body cluster methods



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

ask for G

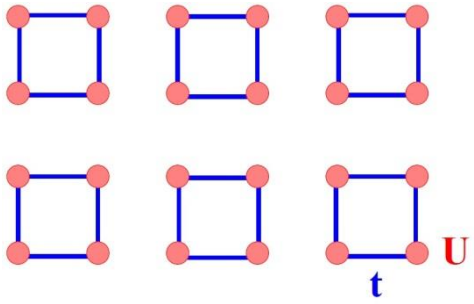
- **Cluster Perturbation Theory (CPT)**

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

first order strong coupling perturbation theory

$$\sum = \sum_{\text{cluster}}$$

1) CUT 2) SOLVE 3) GLUE 4)



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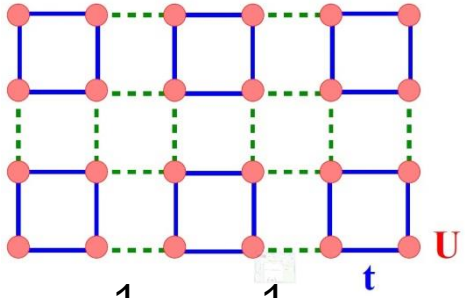
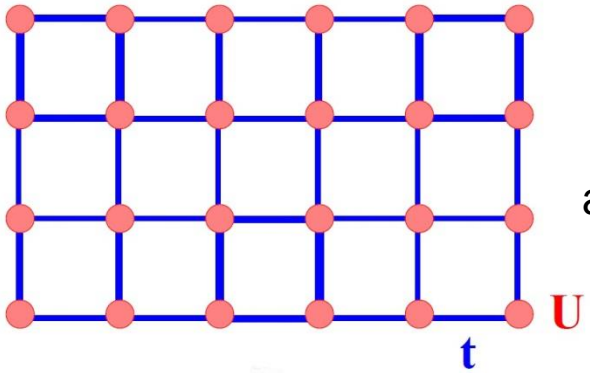


$G = G_{cluster}^{-1} - T^{-1}$

equilibrium many body cluster methods

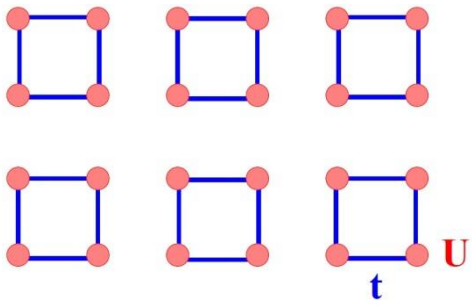


given $\hat{\mathcal{H}}$

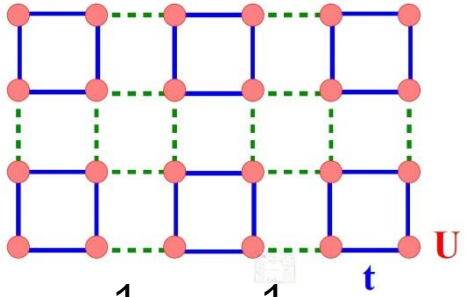
ask for **G**

- **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



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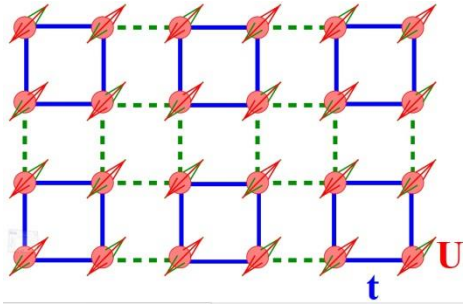
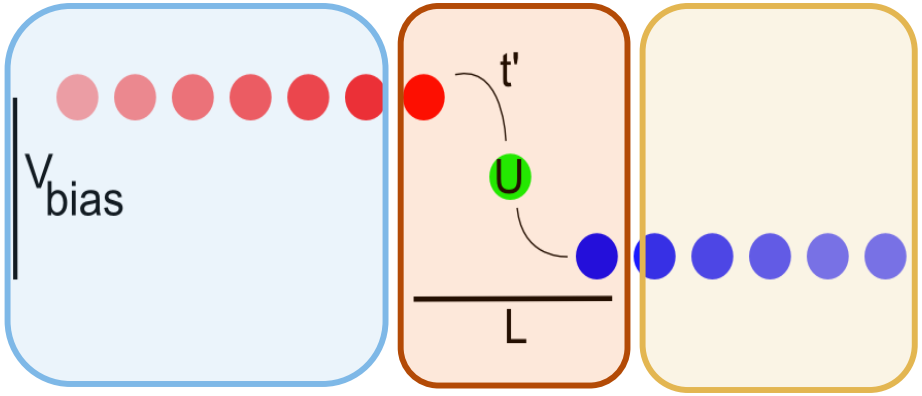


$\sum = \sum_{cluster}(x)$

M. Potthoff (2003)

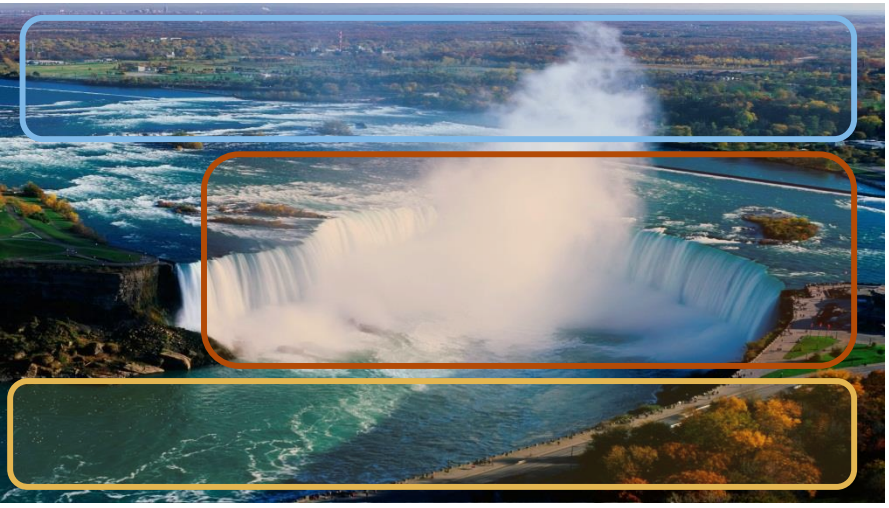
+ Variational principle to fix **x** : Self-energy Functional Approach

non equilibrium Variational Cluster Approach



$$\hat{\mathcal{H}} = \hat{h} + \theta(\tau - \tau_0)\,\mathrm{T}$$

$\tau < \tau_0$ 3 decoupled systems: $\hat{h}$



http://www.niagarafallslive.com

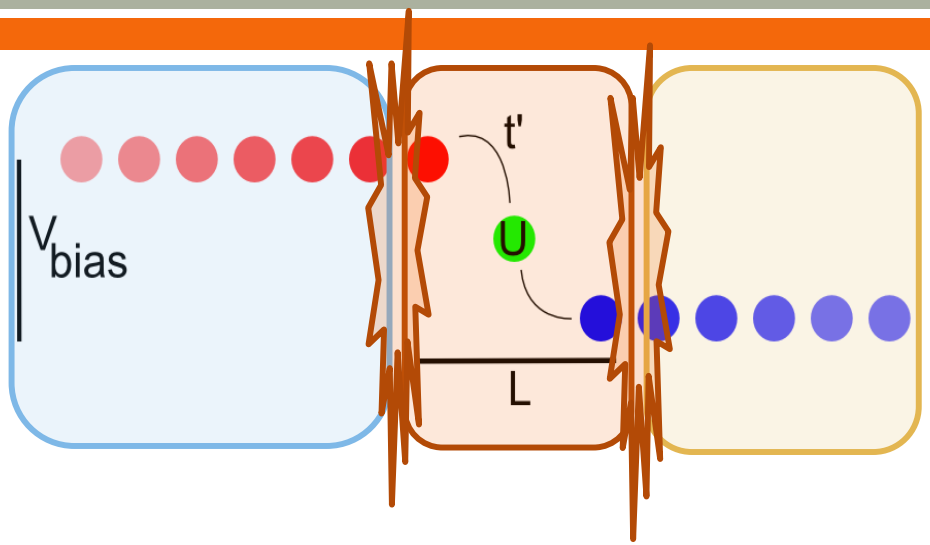
CPT time evolution

M. Balzer, M. Potthoff (2011)

VCA steady state

M. Knap, W. von der Linden, E. Arrigoni (2011)

non equilibrium Variational Cluster Approach

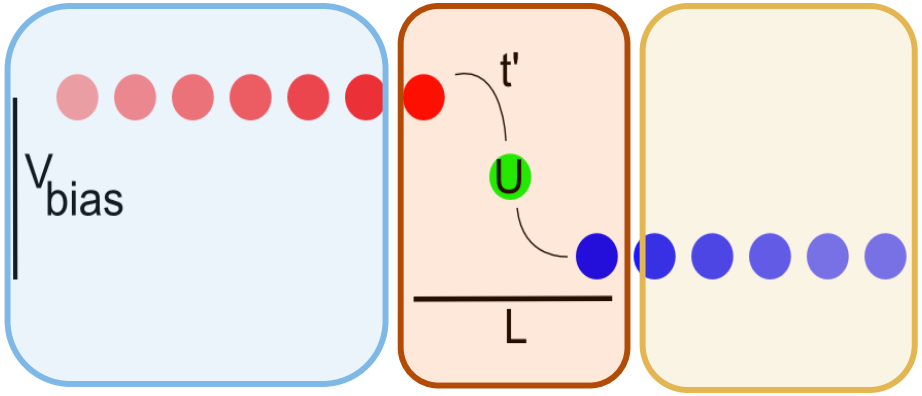


$$\hat{\mathcal{H}} = \hat{h} + \theta(\tau - \tau_0)\hat{T}$$

$\tau < \tau_0$ 3 decoupled systems: $\hat{h}$

@ τ_0 cpl. $\hat{T}$ switched on

non equilibrium Variational Cluster Approach



$$\hat{\mathcal{H}} = \hat{h} + \theta(\tau - \tau_0)\,T$$

$\tau < \tau_0$ 3 decoupled systems: $\hat{h}$

@ τ_0 cpl. T switched on

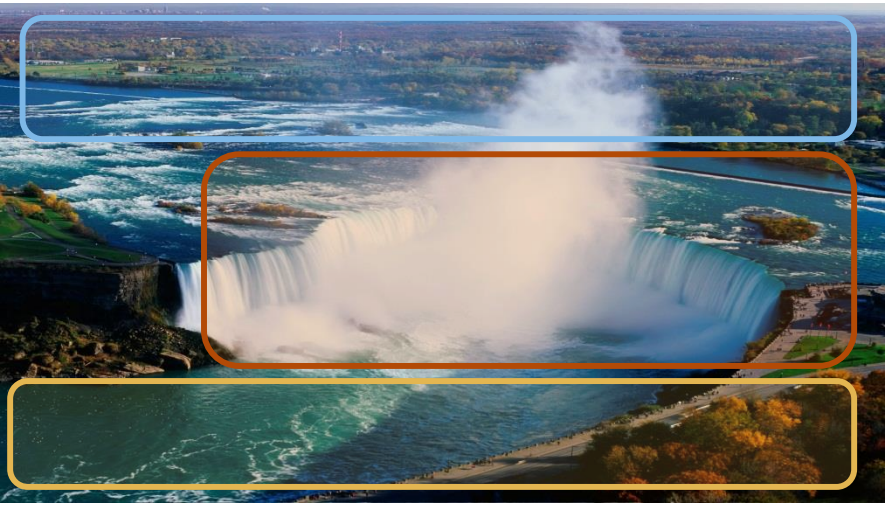
$\tau \to \infty$ steady state $\tau - \tau' \to \omega$

Keldysh

$$\widetilde{G}(\omega) = \begin{pmatrix} G^R(\omega) & G^K(\omega,\mu) \\ 0 & G^A(\omega) \end{pmatrix}$$

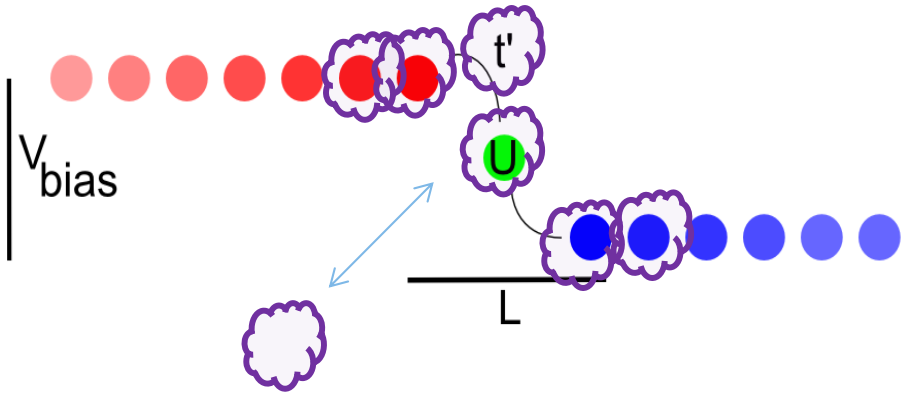
CPT

$$\widetilde{G}^{-1} = \widetilde{g}^{-1} - \widetilde{T}$$



see cf L. V. Keldysh (1965), Rammer+Smith '86

non equilibrium Variational Cluster Approach



non unique decomposition

$$\hat{\mathcal{H}} = \hat{h} + \theta(\tau - \tau_0)\,\mathsf{T}$$

CPT approximation

$$\Sigma_{\hat{\mathcal{H}}} \overset{!}{=} \Sigma_{\hat{h}}$$

optimize initial state: VCA

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

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

flexible self-energy $\Sigma(x)$

variational principle

$$\langle \hat{\Delta}_i \rangle_{\text{initial-state}} \overset{!}{=} \langle \hat{\Delta}_i \rangle_{\text{steady-state}}$$

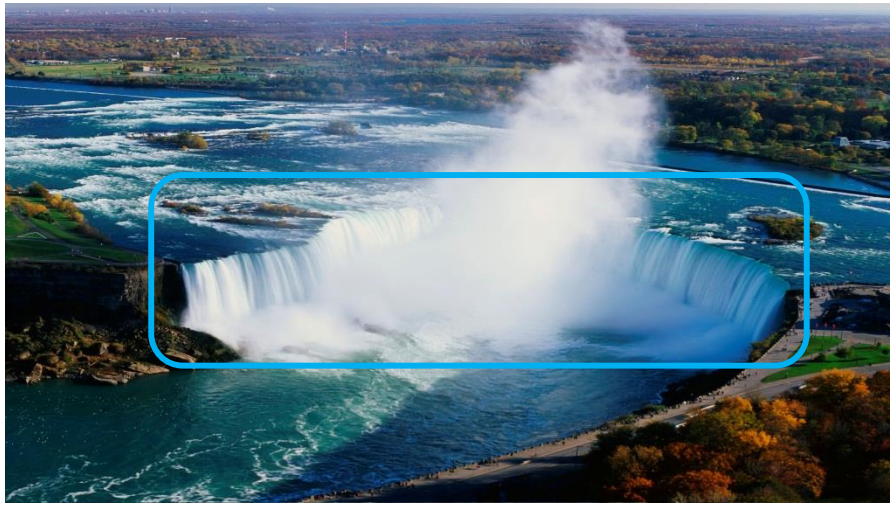
non equilibrium Variational Cluster Approach

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

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

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

$\cong$

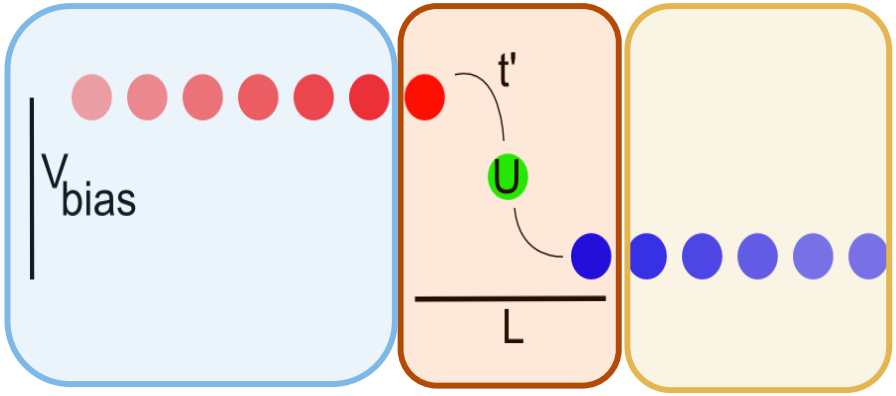


initial reference system *as similar as possible to* the steady-state system

non equilibrium Variational Cluster Approach

full Dyson

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

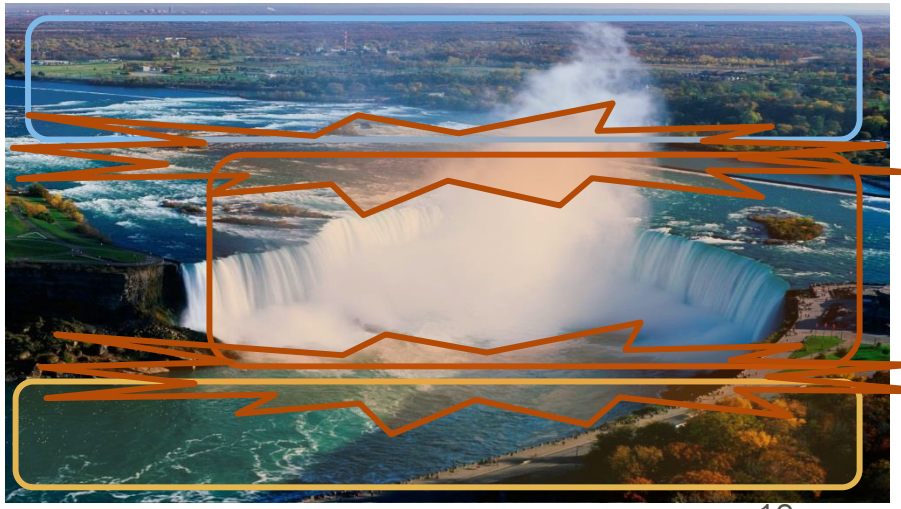


nCPT („Hubbard I type“)

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

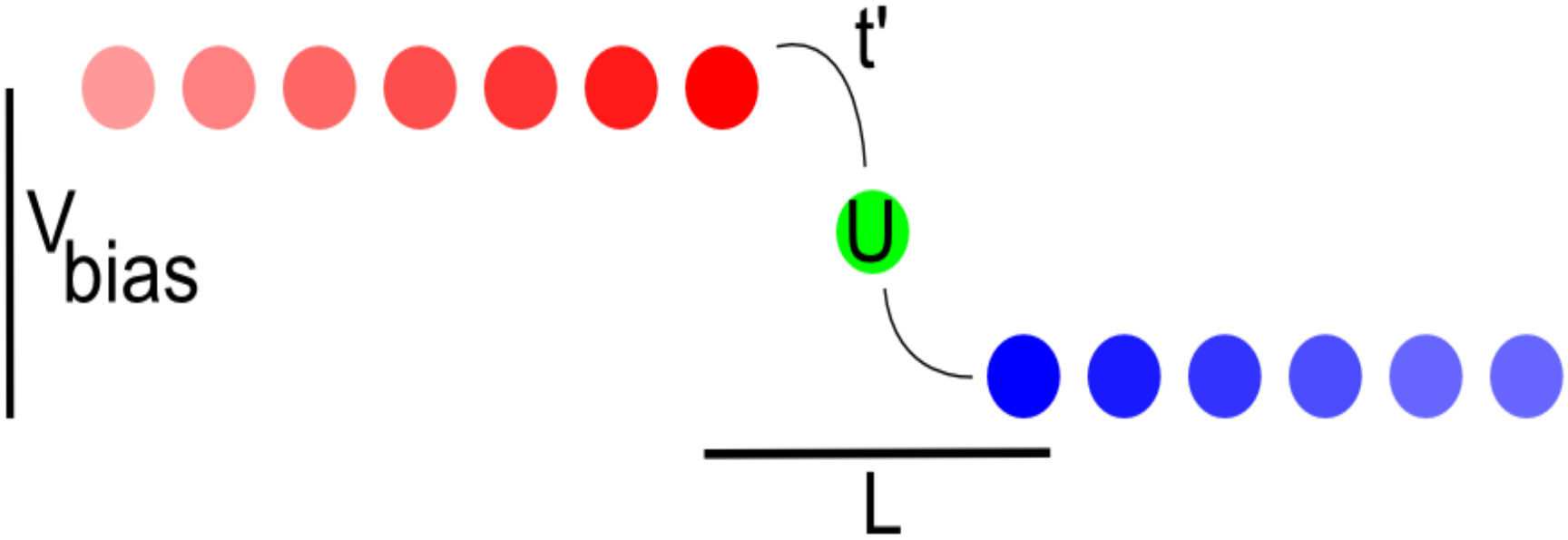
nVCA

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



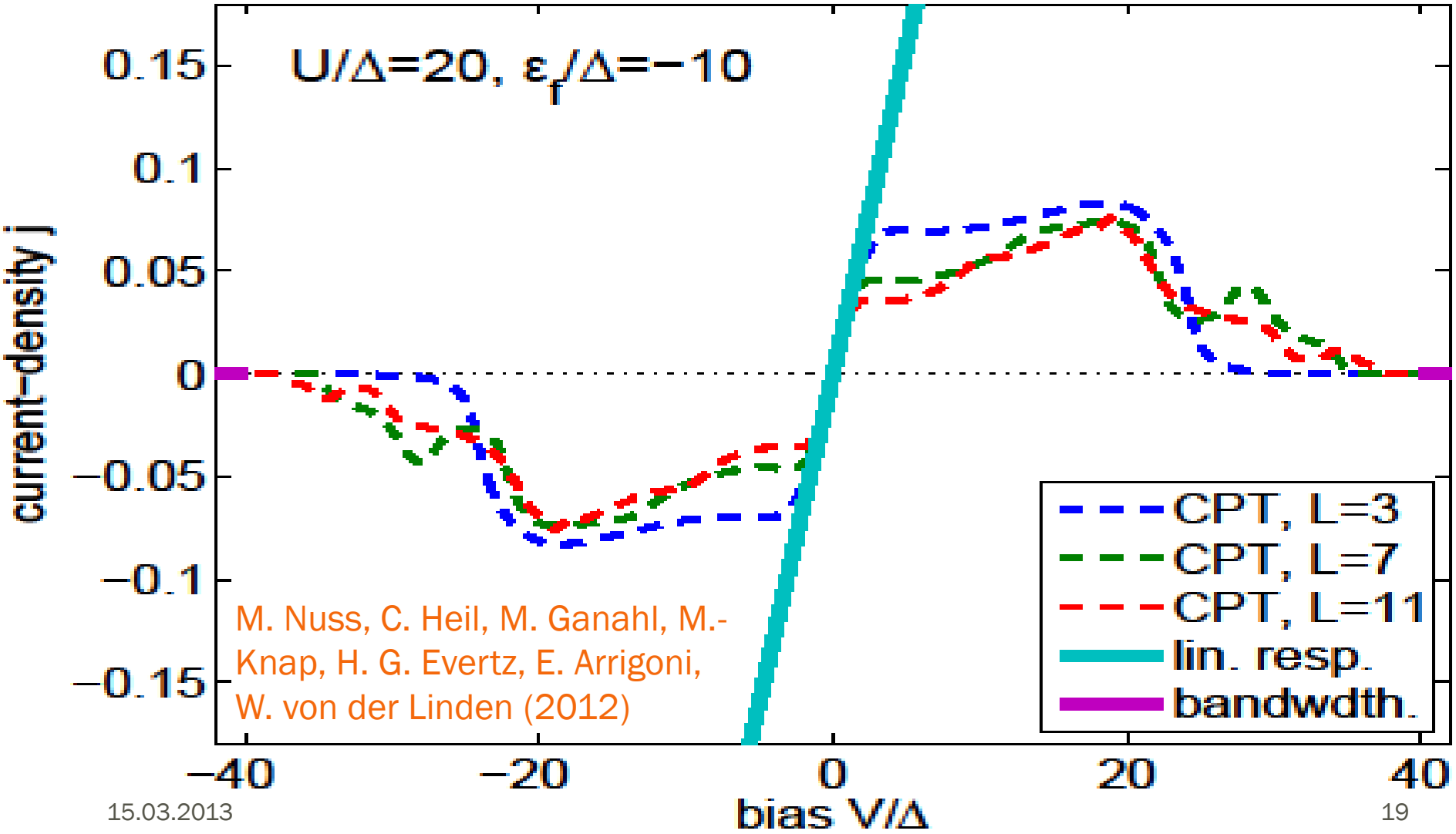
steady state results

single impurity Anderson model



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

I. current voltage characteristics



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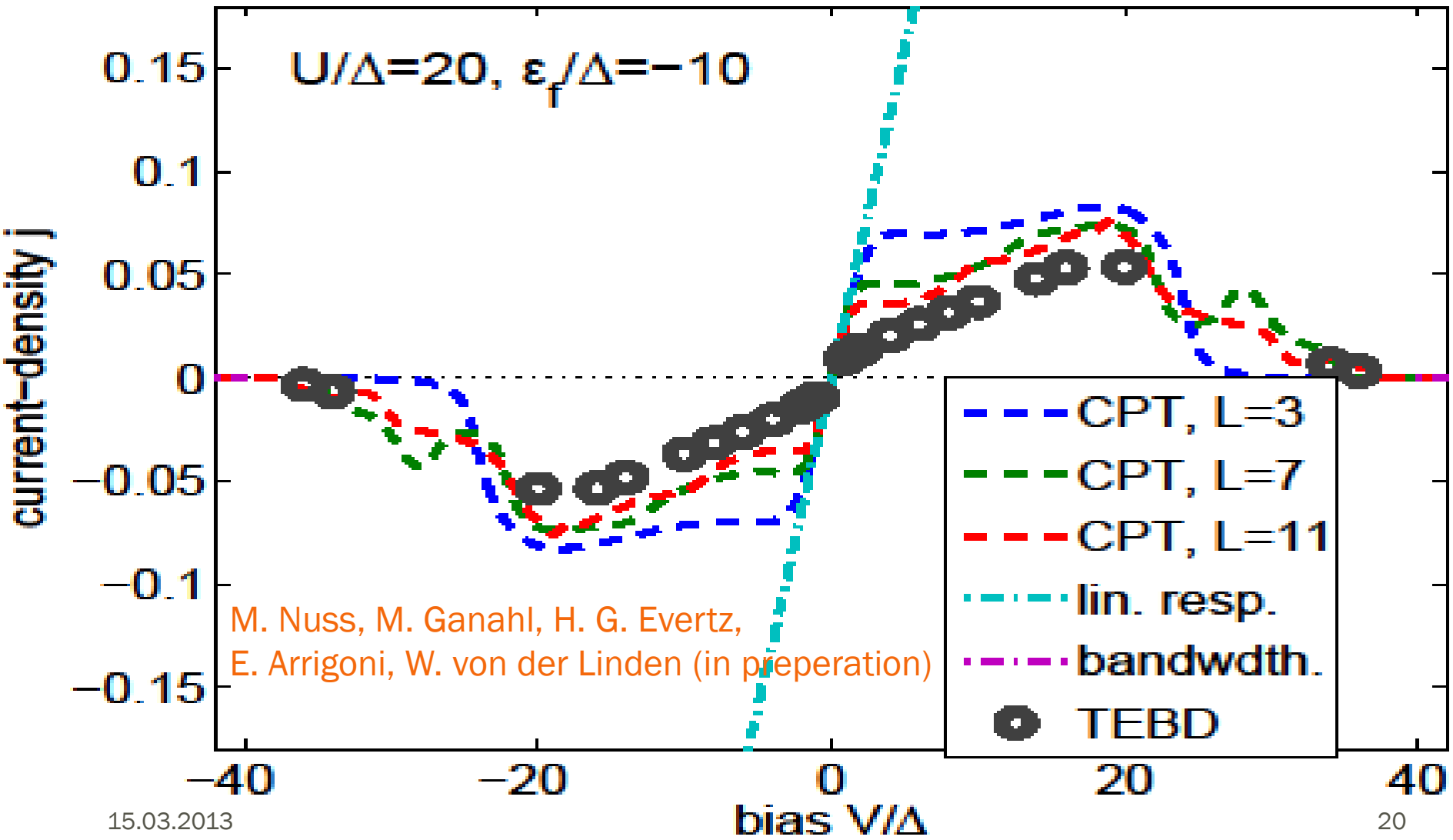

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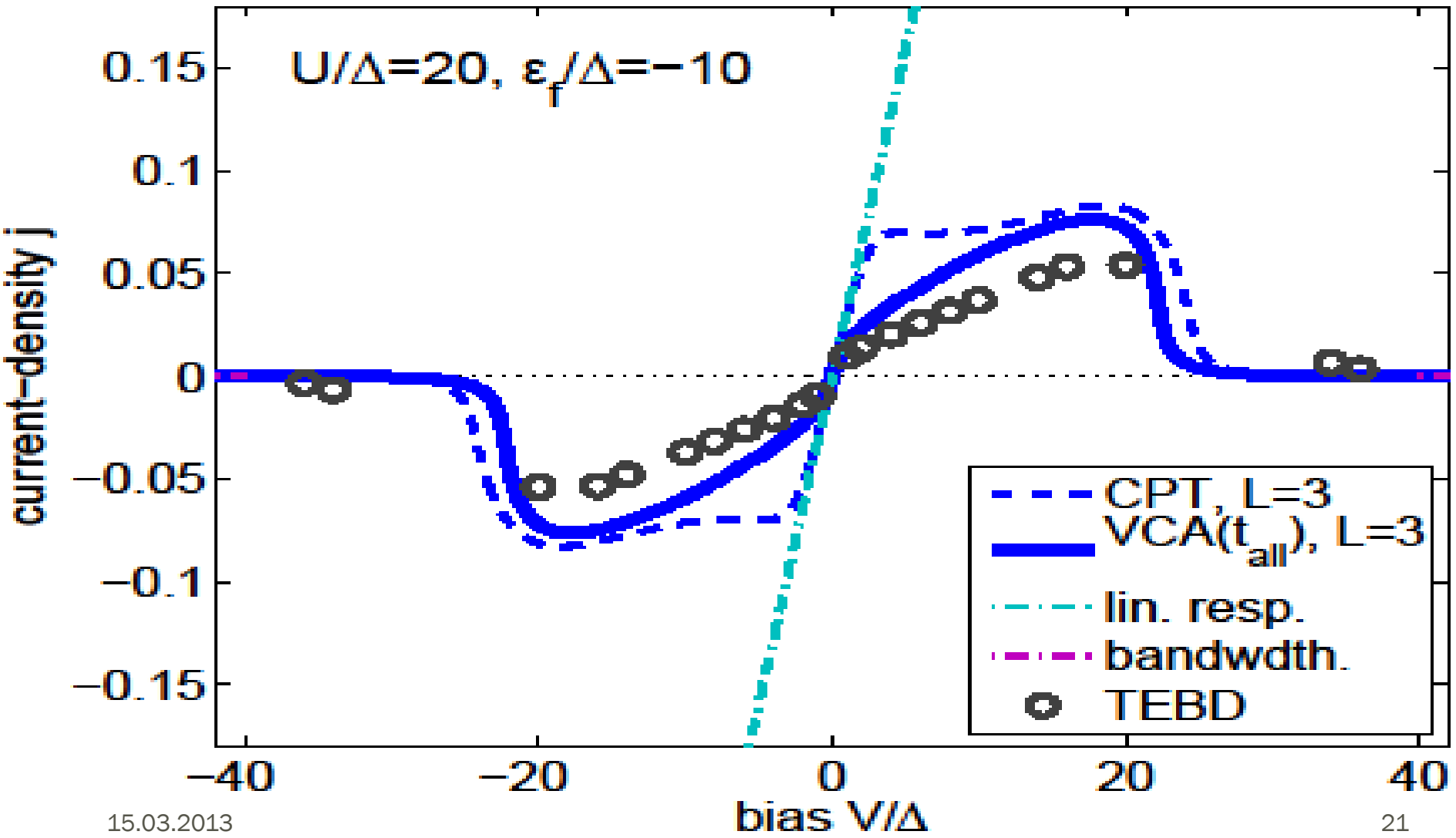

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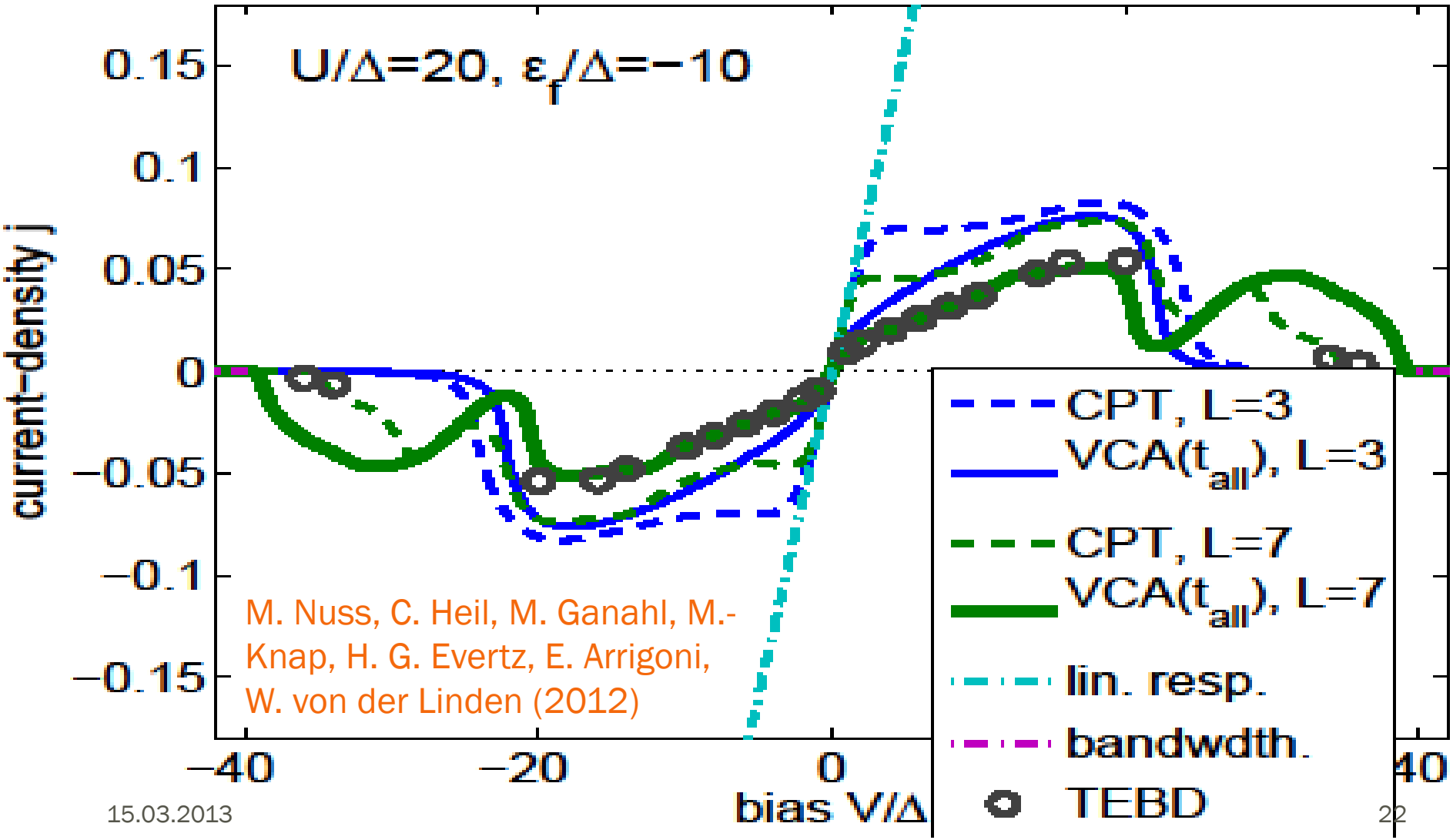
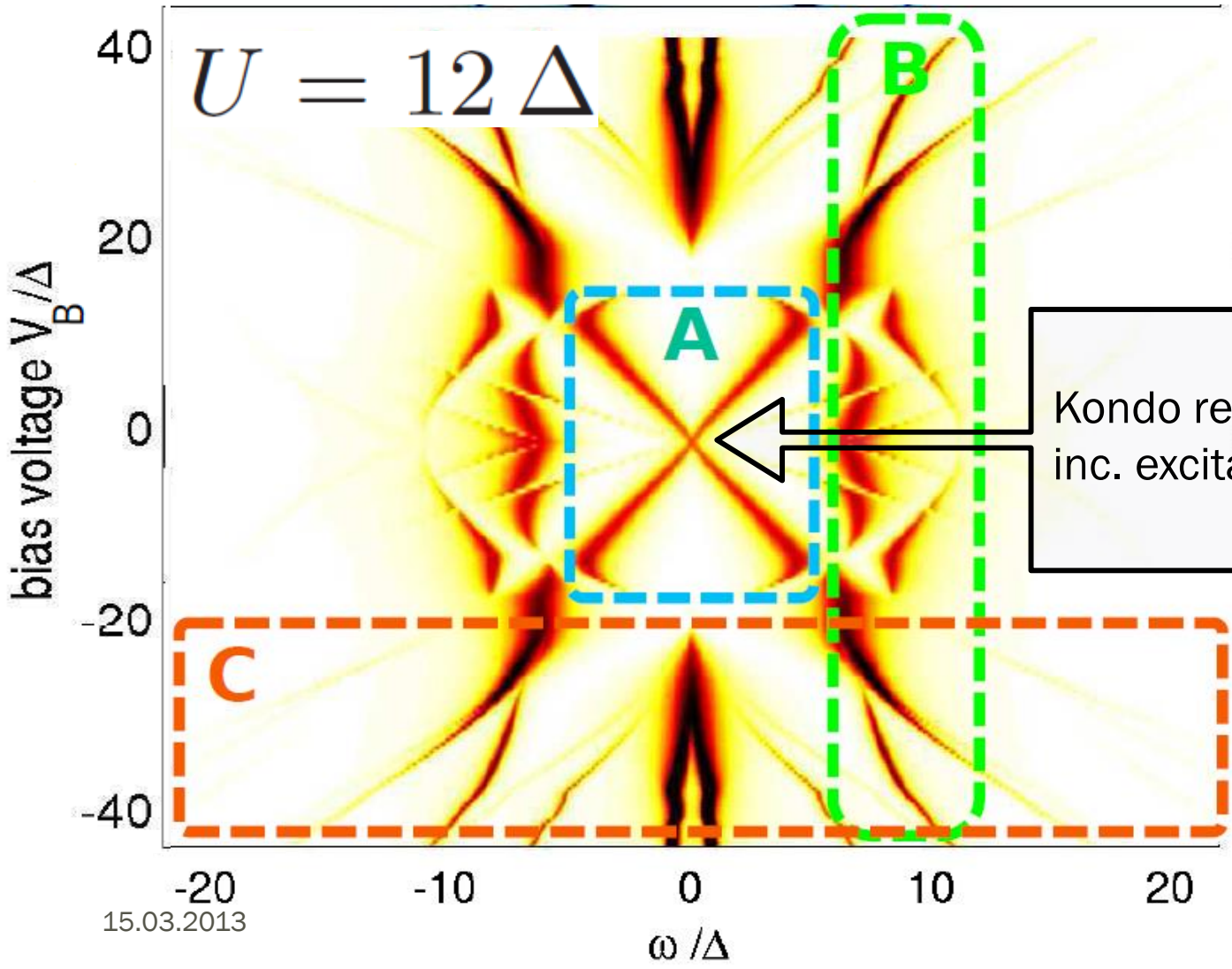


II. non equilibrium local density of states



A: Kondo

Equilibrium

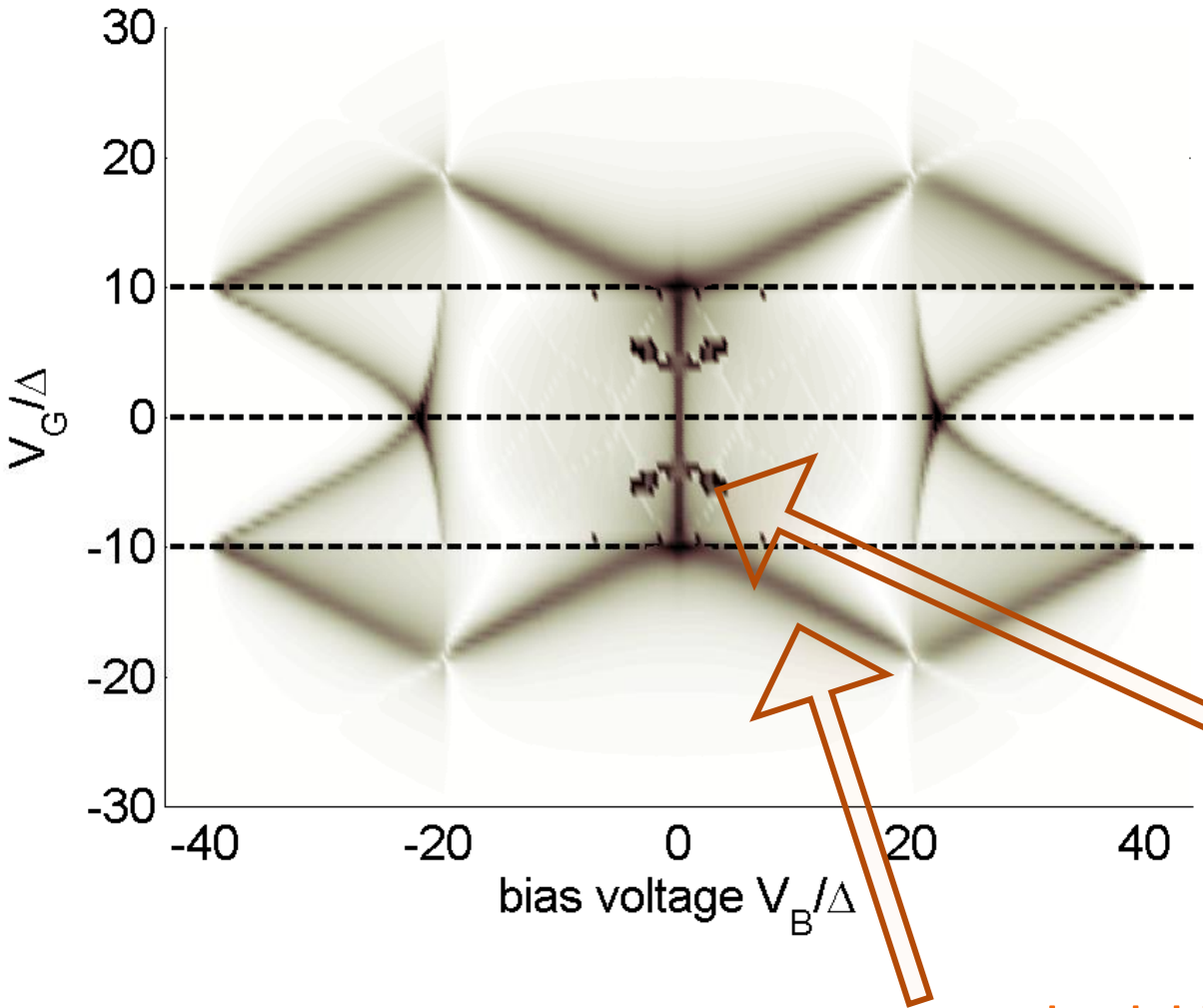
Kondo resonance @ $\omega = 0$

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

B: Hubbard band

C: lead-band

III. conductivity + gate voltage

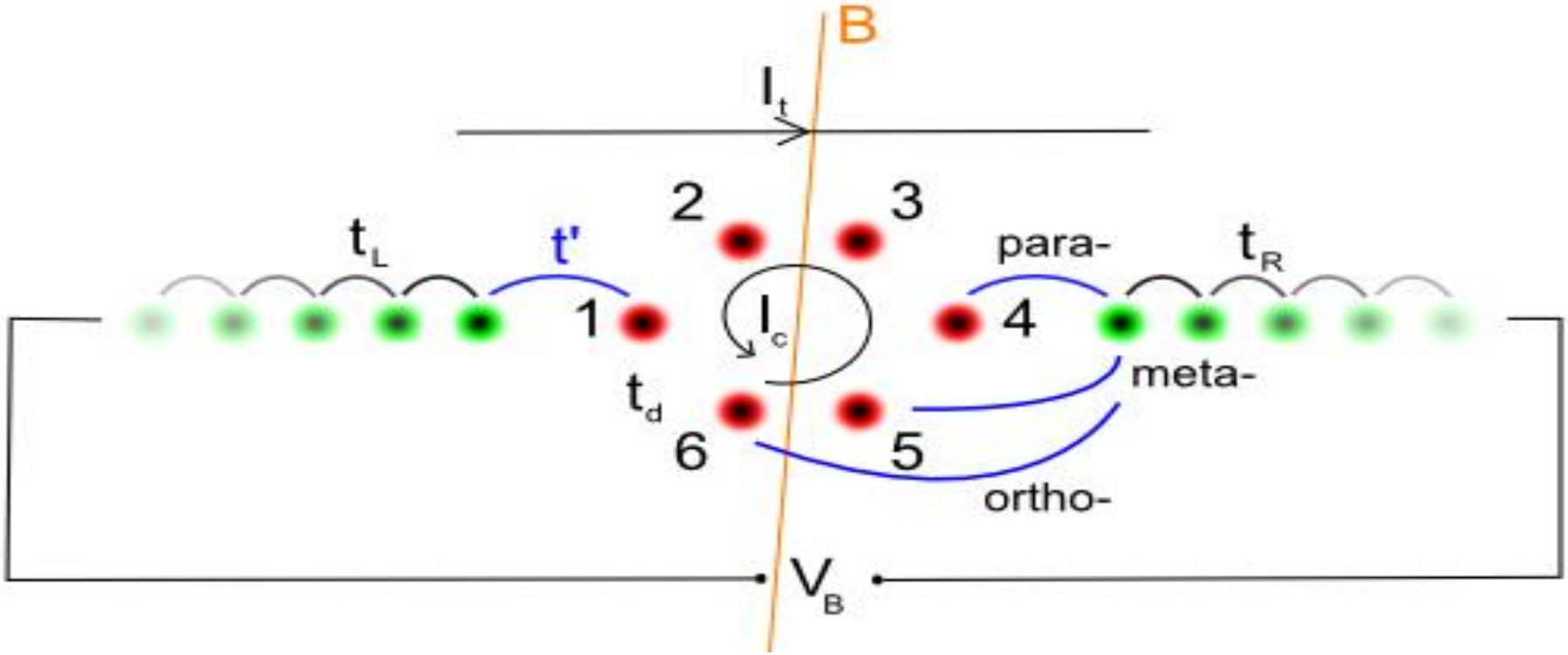


previous slides Vgate=0

Kondo

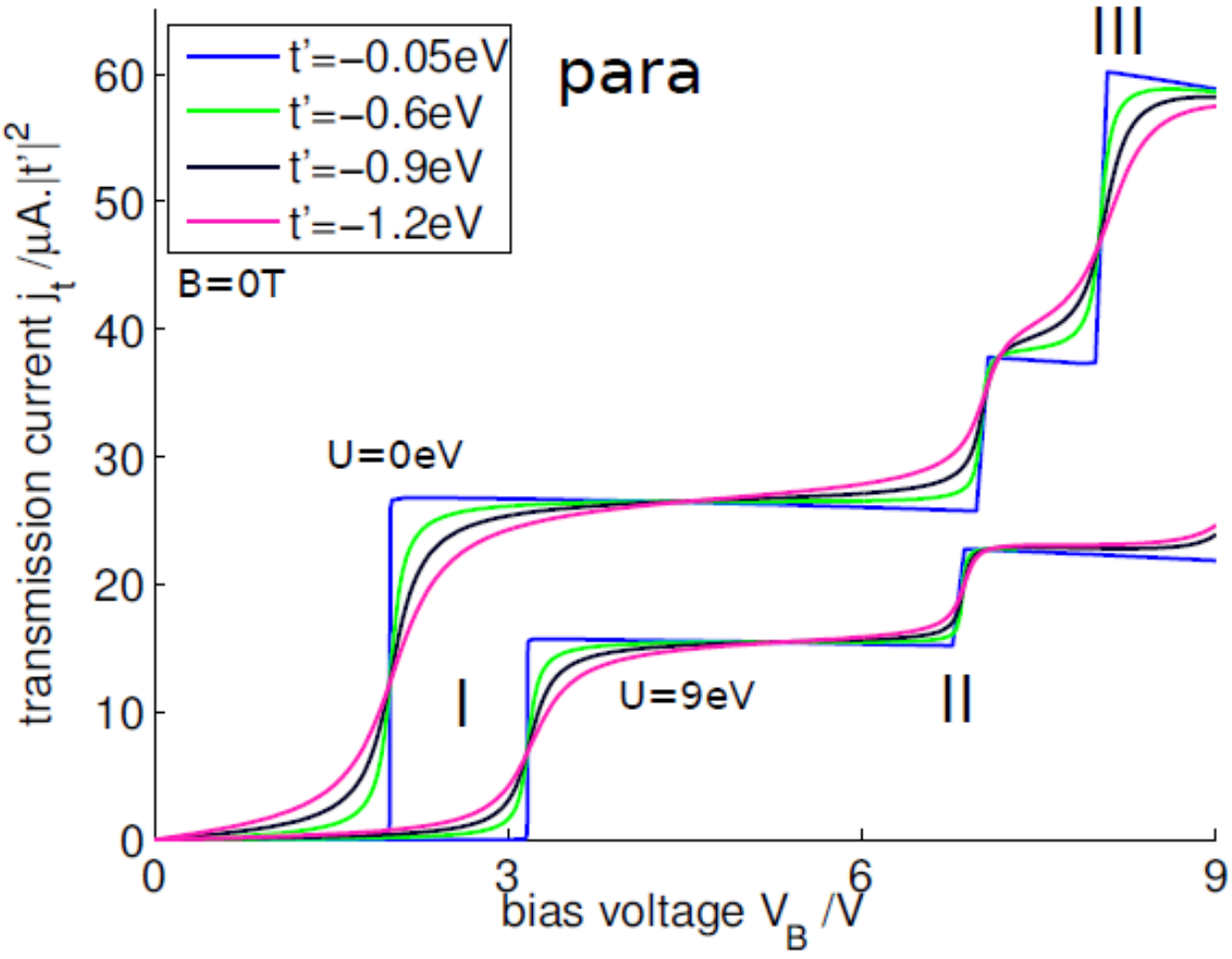
coulomb blockade

molecular ring junction

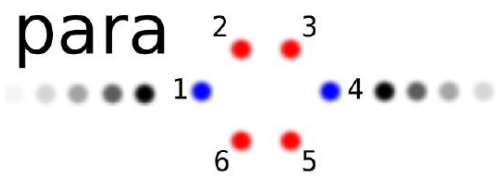


- simple model for benzene: six „interacting“ carbon pz orbitals
- bias voltage
- magnetic field
- infinite system

I. transmission current voltage characteristics



- interaction U
- broadening t‘



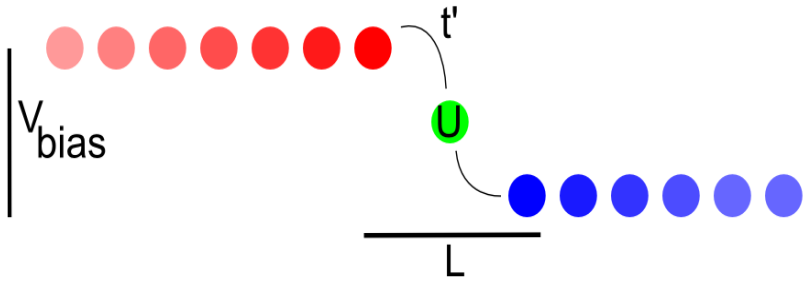
M. Nuss, W. von der Linden, E. Arrigoni (2013)

conclusions + outlook

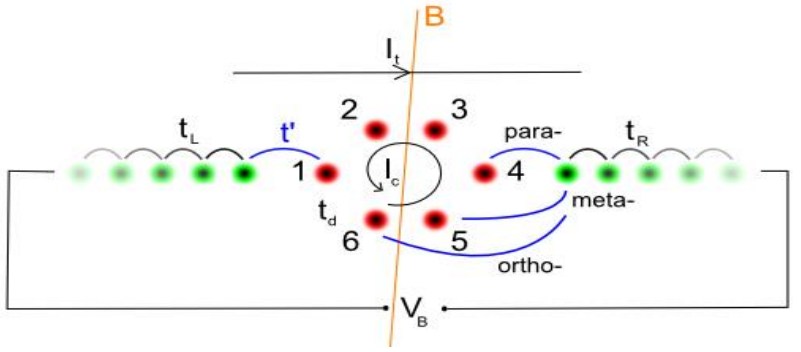
- non equilibrium

Variational Cluster Approach

- quantum dot



- molecular ring junction



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Martin Ganahl

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Thank you!

maybe some day:

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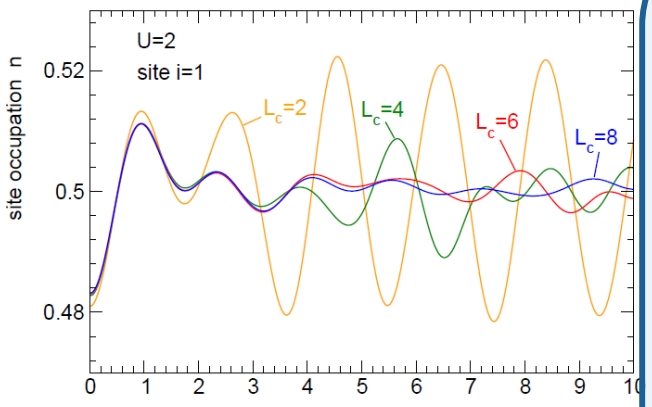
TUG

itp cp

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

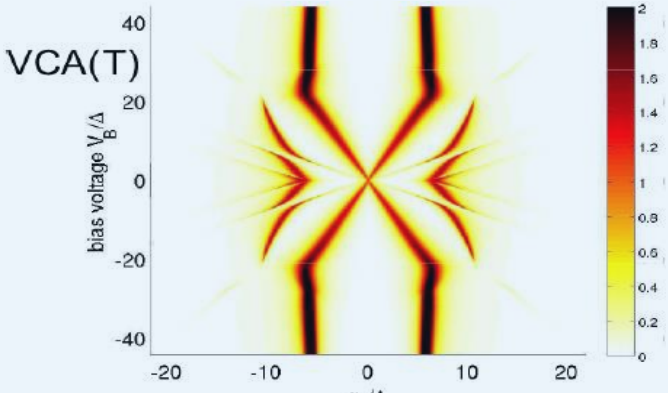
non equilibrium Variational Cluster Approach

time evolution by CPT



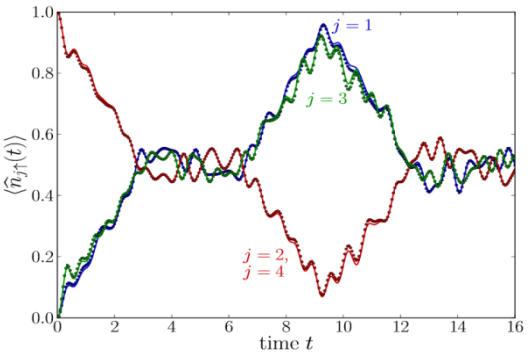
M. Balzer and M. Potthoff (2011)

steady state of quantum dots



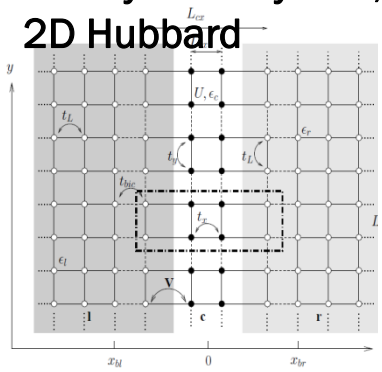
M. Nuss, C. Heil, M. Ganahl, M. Knap, H. G Evertz, E. Arrigoni, W. vd Linden (2012)

dynamical symmetry in 2D



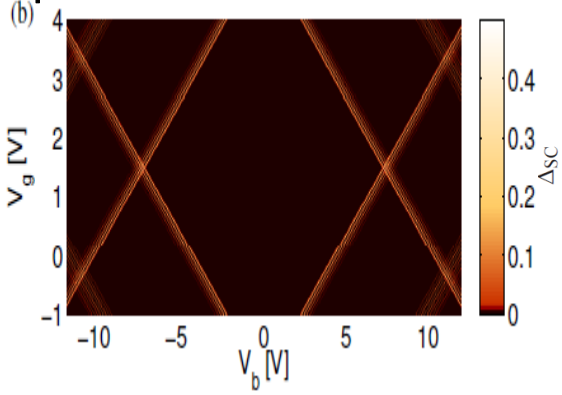
P. Jurgenowski and M. Potthoff (2013)

steady state by VCA, 2D Hubbard



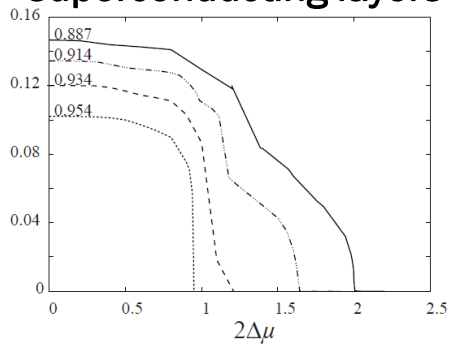
M. Knap, W. vd Linden, E. Arrigoni (2011)

phonons in molecular devices



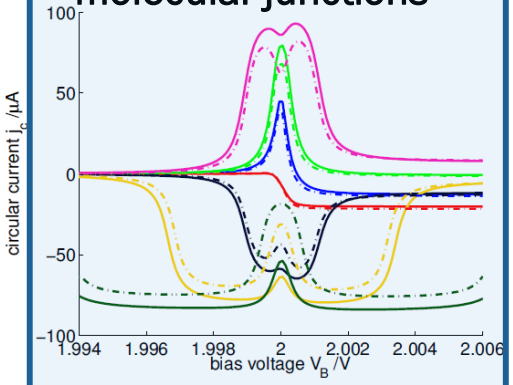
M. Knap, E. Arrigoni, W. von der Linden (2012)

superconducting layers



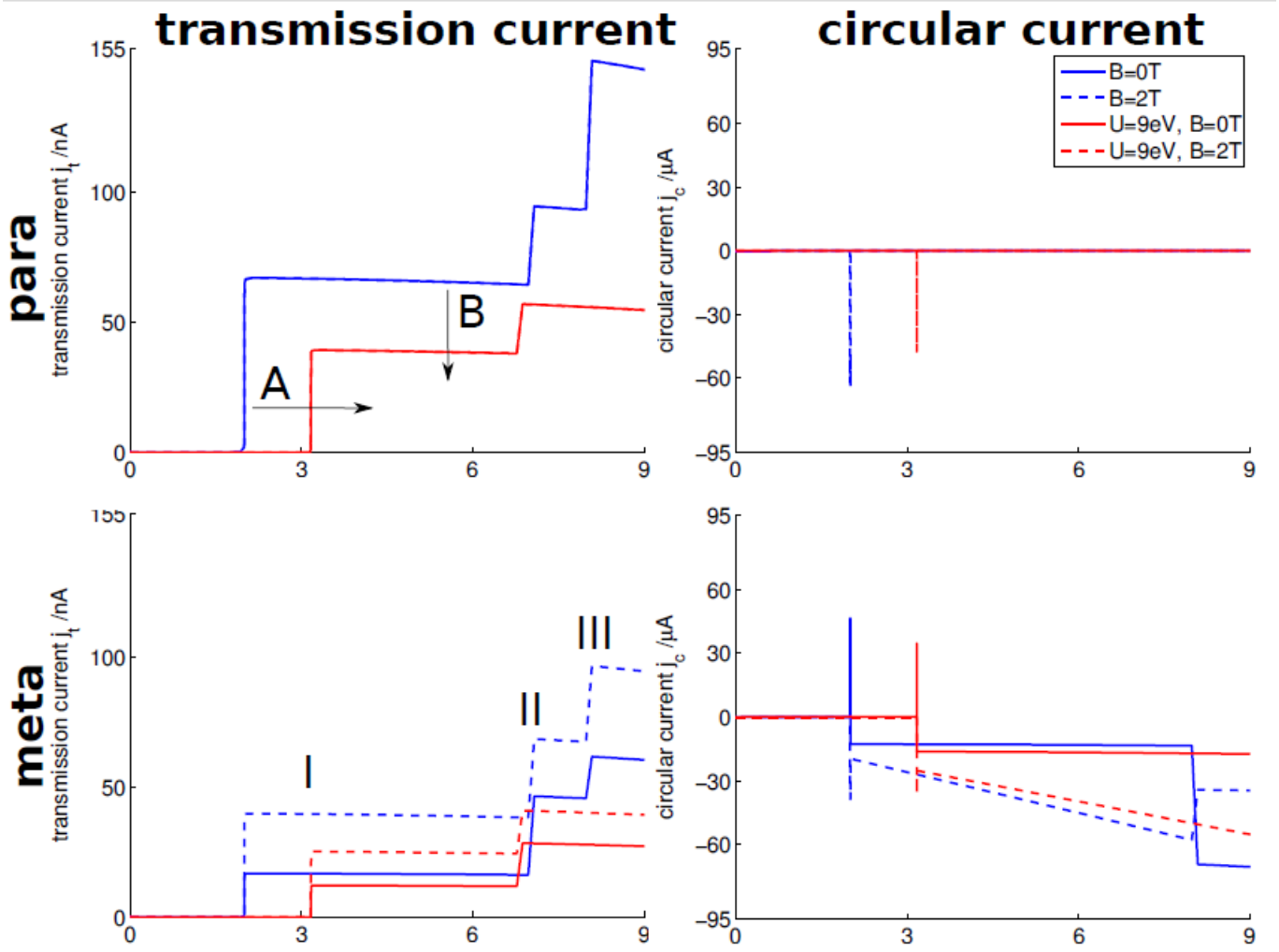
A. Fulterer, E. Arrigoni (2012)

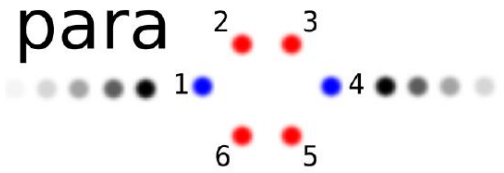
magnetic effects in molecular junctions

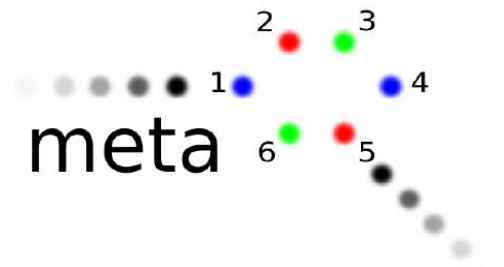


M. Nuss, E. Arrigoni, W. vd Linden (2012)

molecular ring junction







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

Time evolution after a quench of a quantum dot

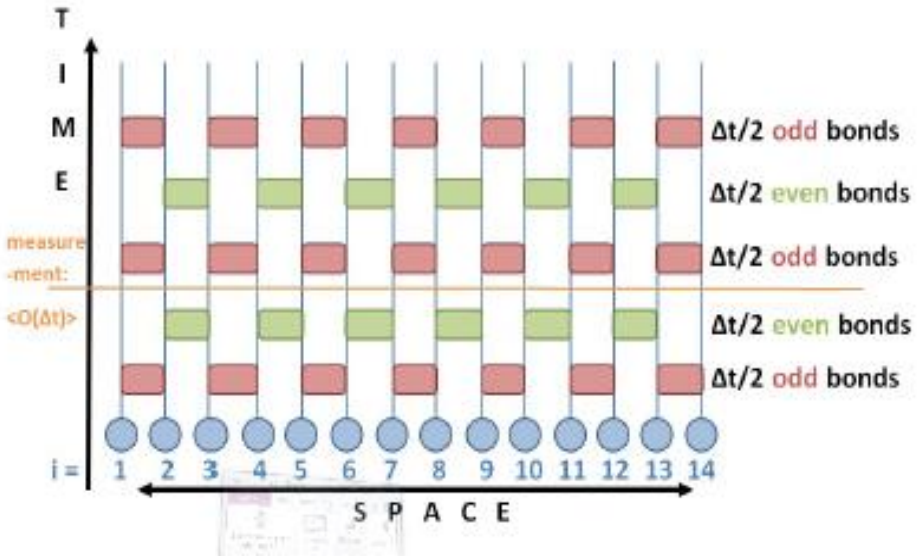
IV

15.03.2013

Real time evolution with matrix product states

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

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



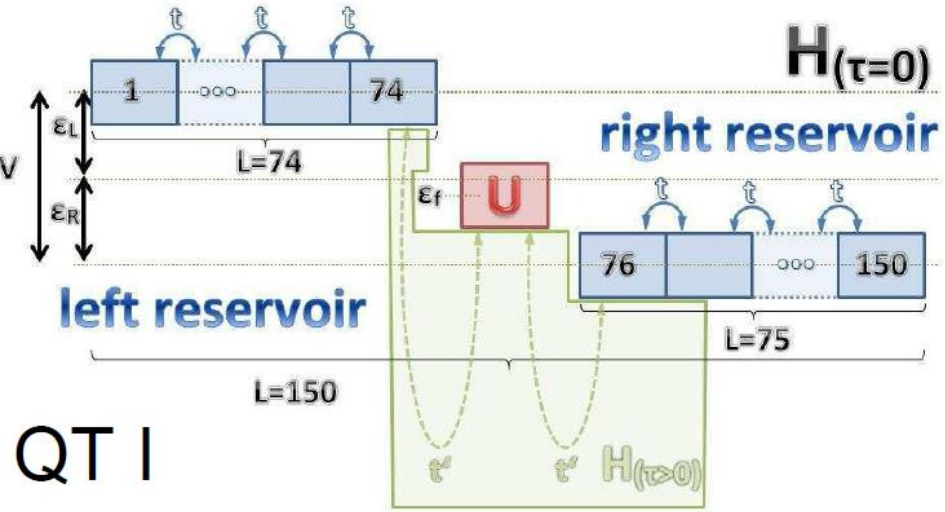
1. S. R. White (1993)

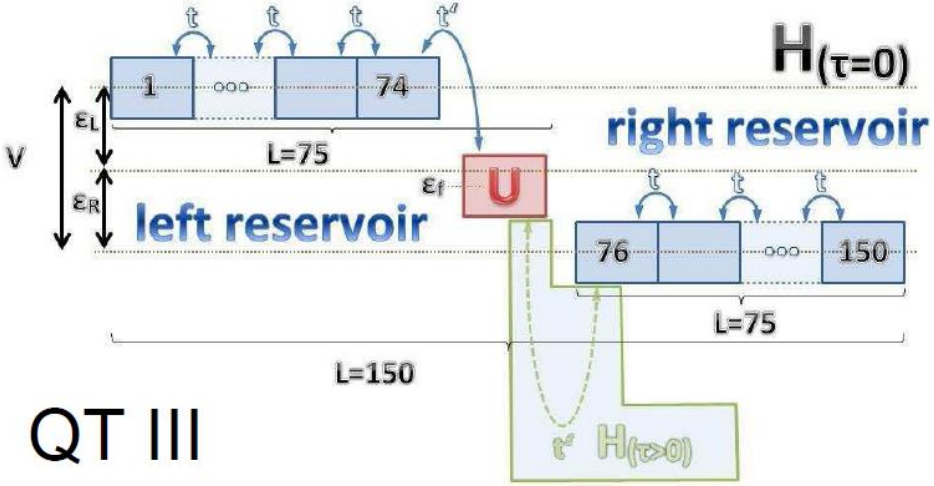
   $\mathrm{DMRG}(\hat{\mathcal{H}}(t_0)) \Rightarrow |\Psi\rangle_0$

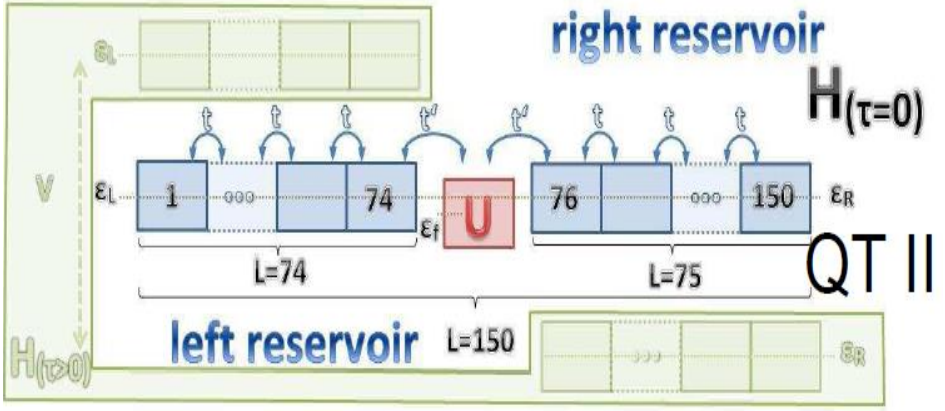
2. quench
3. evolve $|\Psi\rangle_0$ with $\hat{\mathcal{H}}(t > 0)$ by TEBD

G. Vidal (2004)

3 different quneches





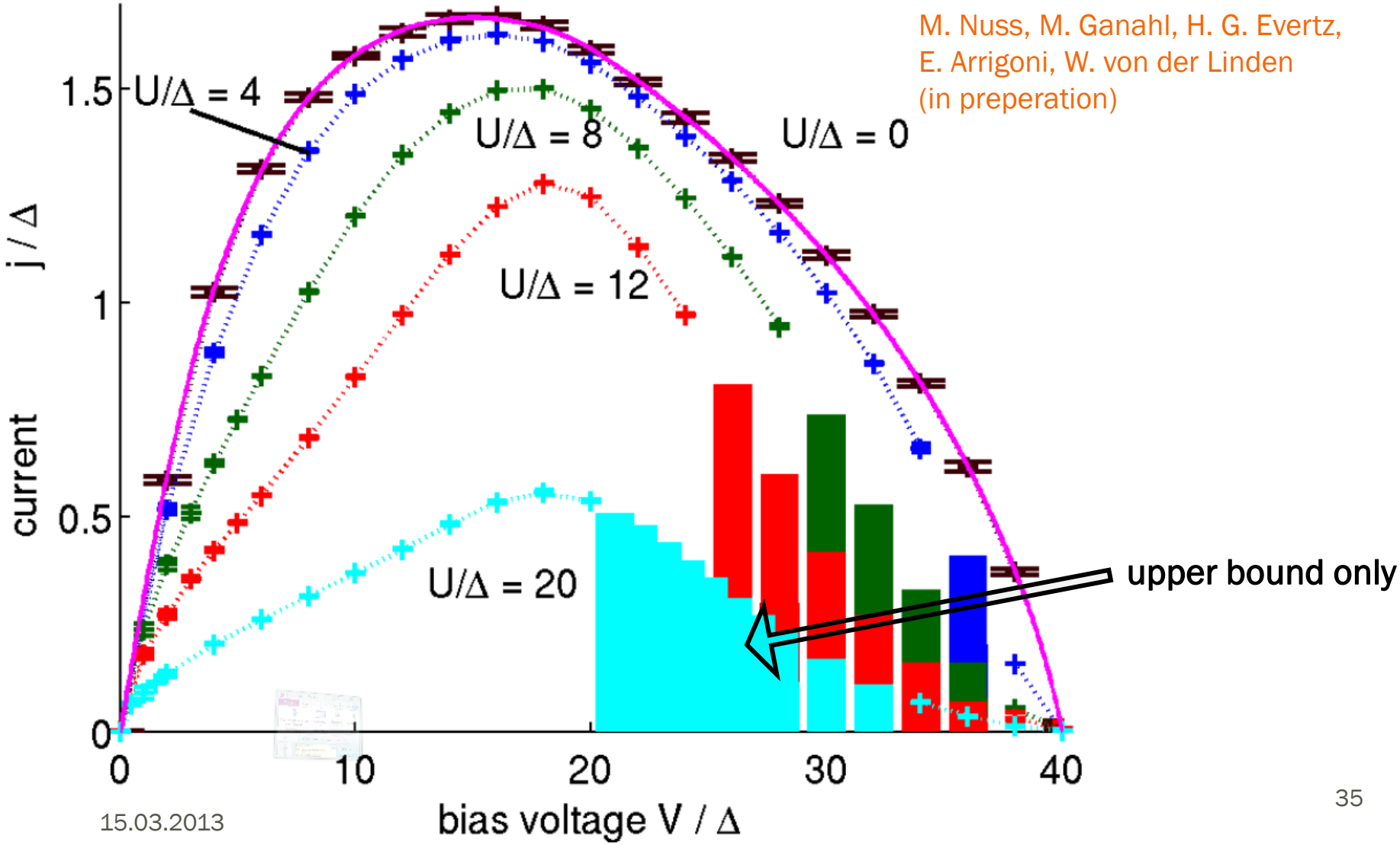


comparison of short time quench dynamics
+ quasi-steady-state

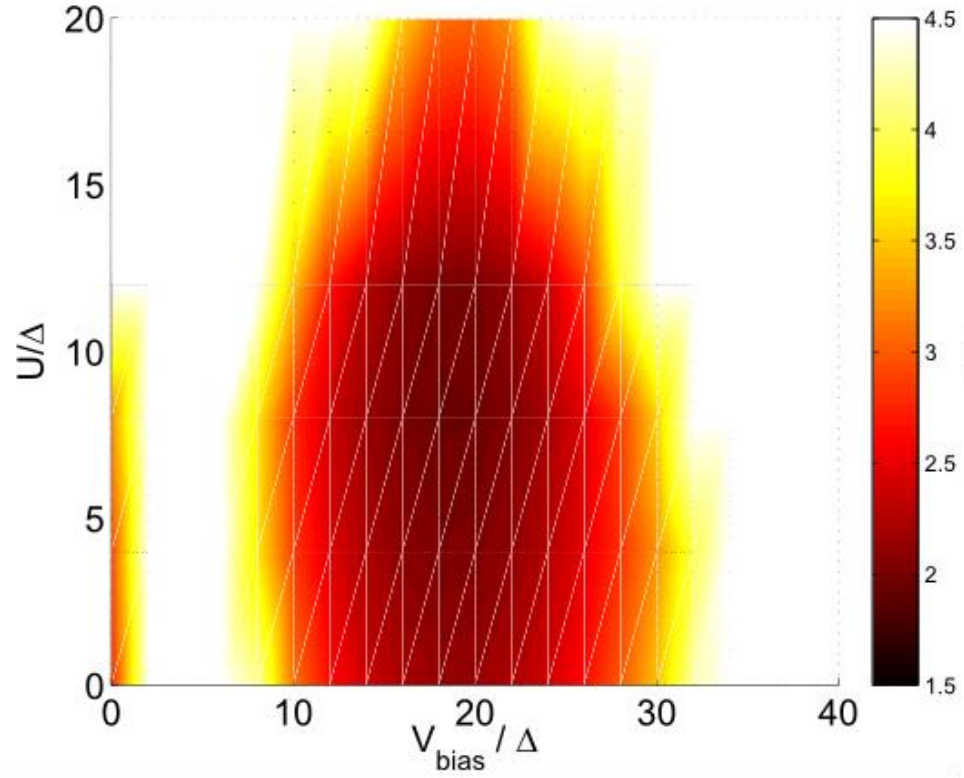
M. Nuss, M. Ganahl, H. G. Evertz,
E. Arrigoni, W. von der Linden
(in preperation)

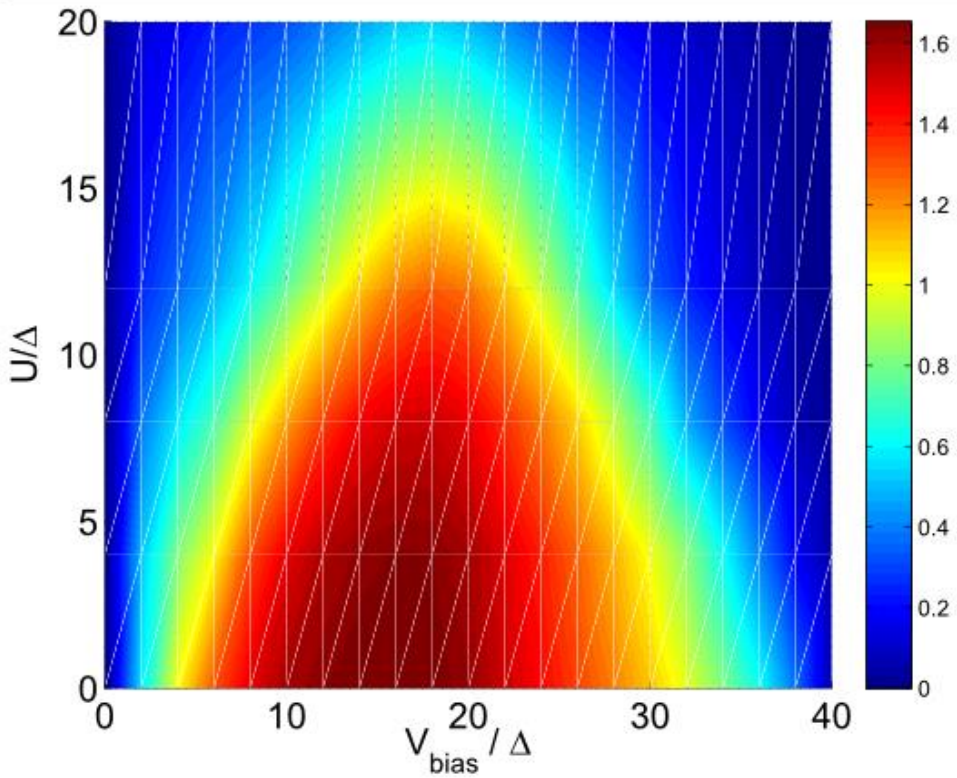
DMRG+TEBD current-voltage characteristics

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



entanglement ⟺ current





time evolution of current