Strongly correlated quantum systems out of equilibrium

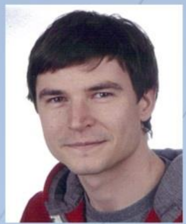
a non-equilibrium variational cluster approach

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

TUG

Ljubljana, 11.12.2012

itp^{cp}


Christoph Heil

Prof. Wolfgang von der Linden



Michael Knap

Prof. Enrico Arrigoni



Martin Nuss

non-equilibrium group at TUG

Prof. Hans Gerd Evertz


Martin Ganahl


Agenda

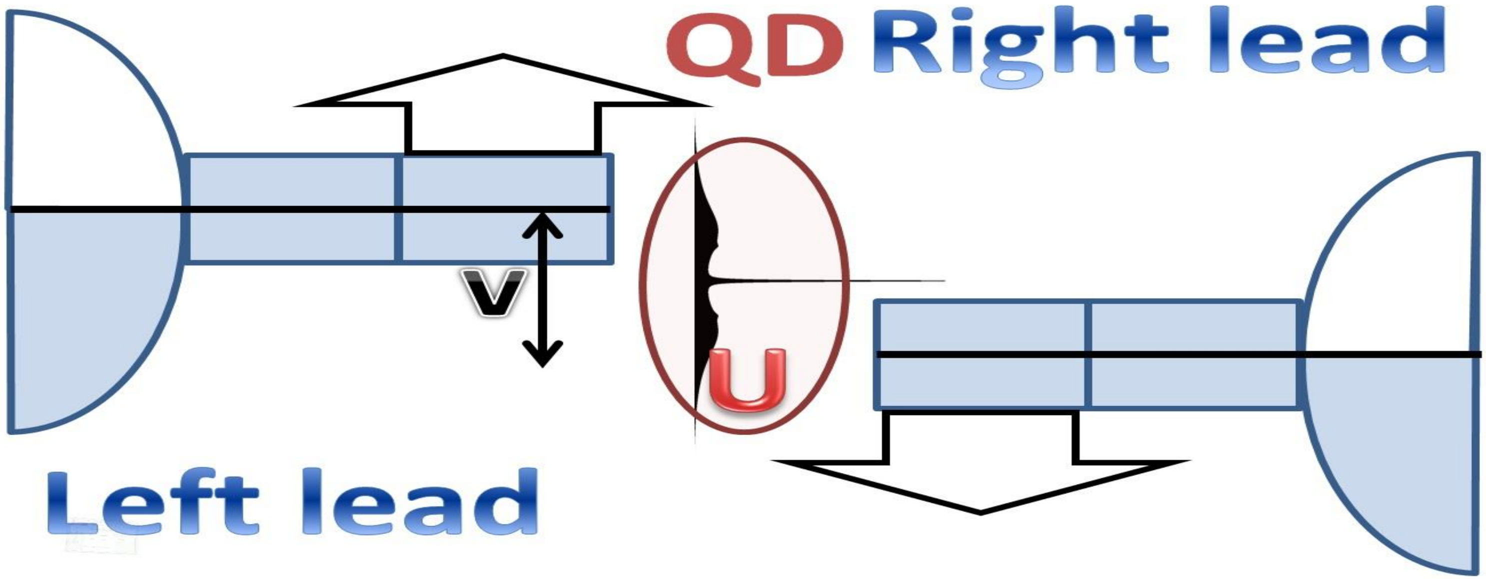
1. non-equilibrium phenomena - Quantum Dots
2. non-equilibrium Variational Cluster Approach
3. Matrix Product State time evolution
4. Results: steady – state
5. Results: time evolution

Non-equilibrium phenomena – Quantum Dots

Transport through a strongly correlated object

Single Impurity Anderson Model

P. W. Anderson (1961)

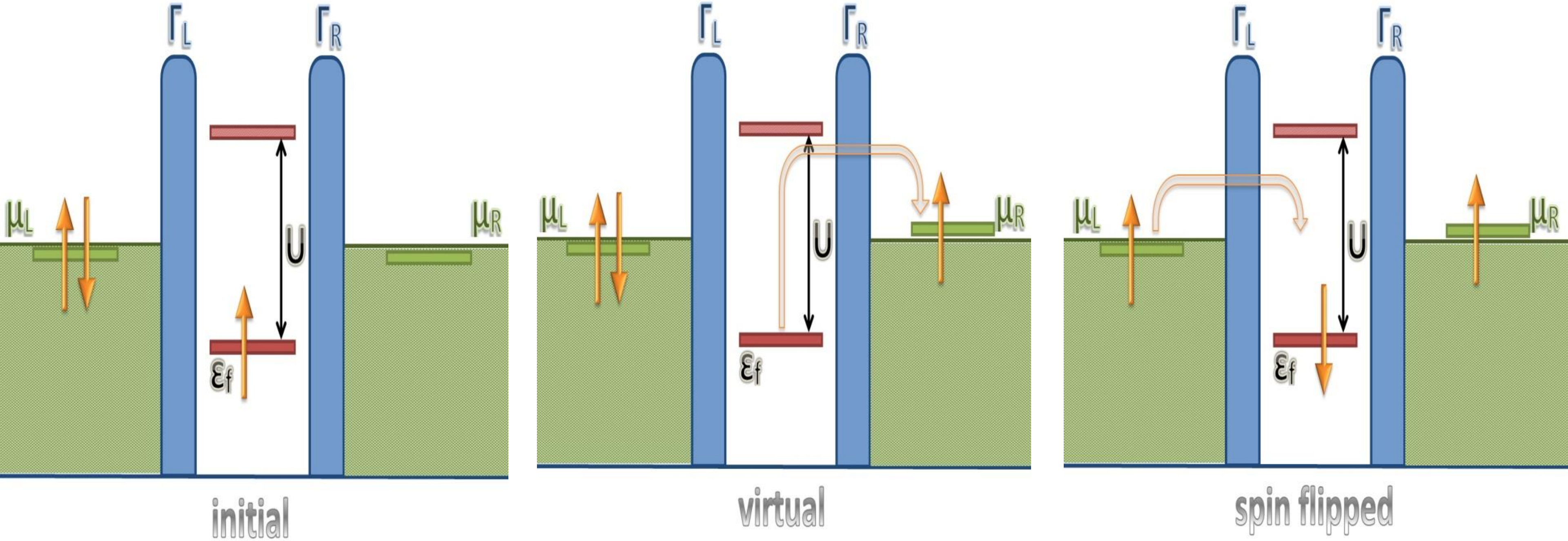


+

voltage bias

C. S. Wu, Y. Makiuchi, C. D. Chen, ed. M. Wang (2010)

Transport through a strongly correlated object



Y. Meir, N.S. Wingreen (1992)

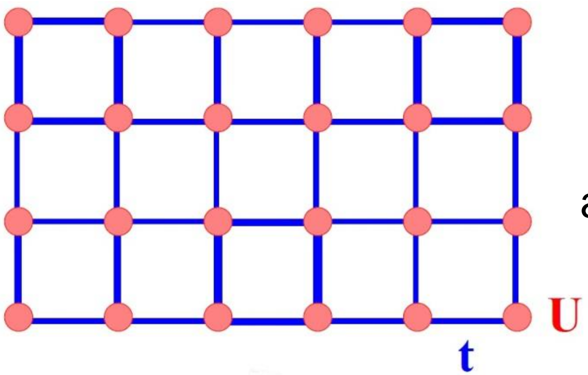
$$J = \frac{ie}{2h} \int d\epsilon \left(\mathrm{tr}\{[f_L(\epsilon)\Gamma^L - f_R(\epsilon)\Gamma^R](\mathbf{G}^r - \mathbf{G}^a)\} + \mathrm{tr}\{(\Gamma^L - \Gamma^R)\mathbf{G}^<\} \right)$$

need:

single particle Green's function G in Keldysh space

Non-equilibrium Variational Cluster Approach

Many-Body cluster methods



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

ask for **G**

in general unsolvable

Strategy ?

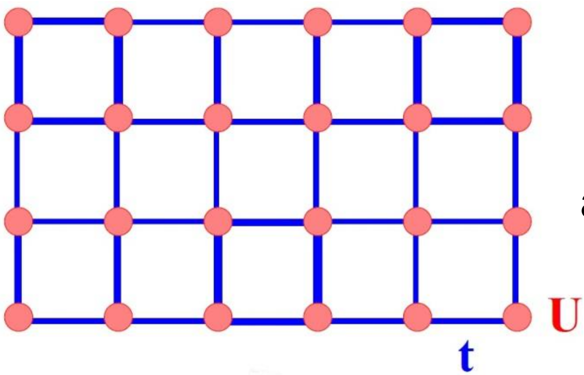
1) 

2) 

3) 

4) 

Many-Body cluster methods



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

ask for **G**

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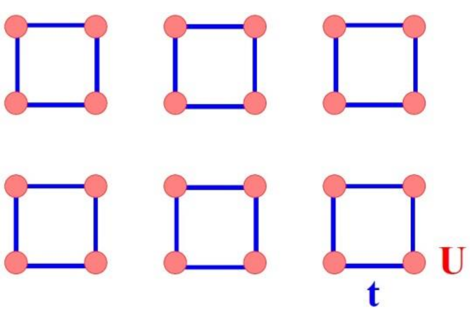
Strategy ?

1) CUT 2) 3) 4)



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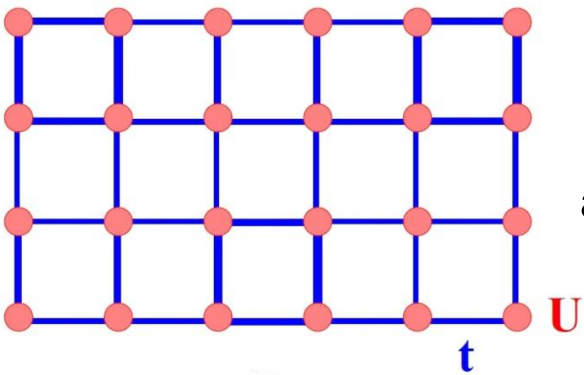
Many-Body cluster methods



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

ask for G

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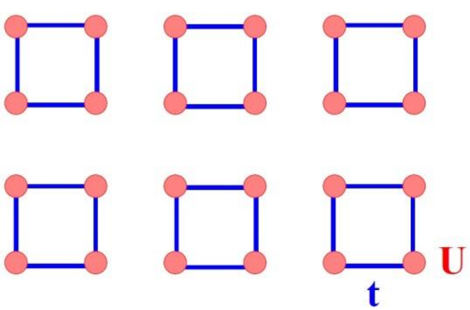
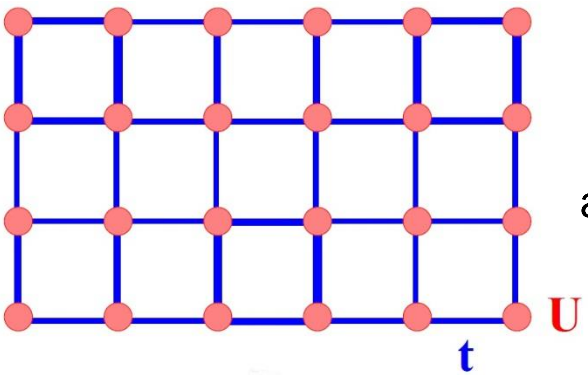
Strategy ?

1) CUT 2) SOLVE 3) 4)



$G_{cluster}$ = exactly solvable

Cluster Perturbation Theory (CPT)



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

ask for G

- **Cluster Perturbation Theory (CPT)**

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

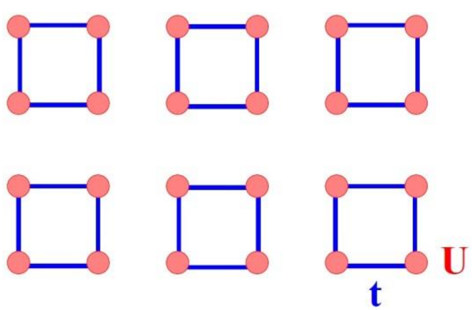
first order strong coupling perturbation theory

1) CUT

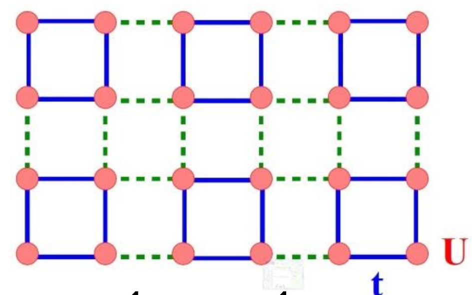
2) SOLVE

3) GLUE

4) $\Sigma = \Sigma_{cluster}$

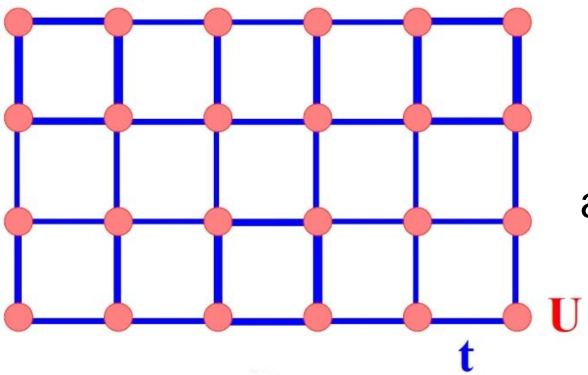


$G_{cluster}$ = exactly solvable



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

Variational Cluster Approach (VCA)

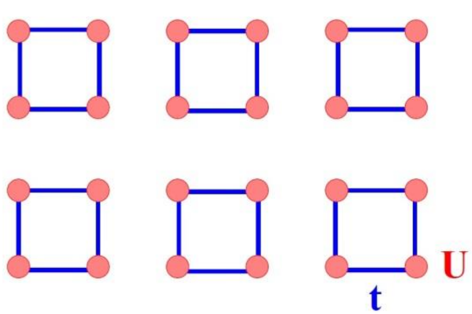


given $\hat{\mathcal{H}}$

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)

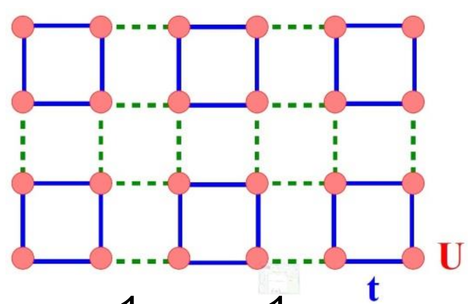
1) CUT



2) SOLVE

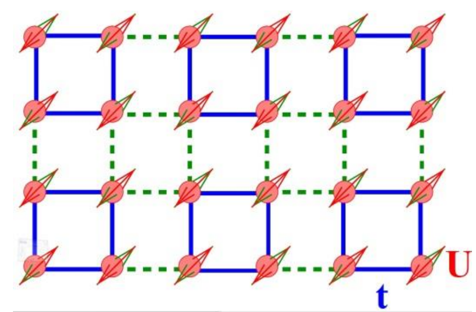
$G_{cluster}$ = exactly solvable

3) GLUE



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

4) ADD FIELDS



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

M. Potthoff (2003)

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

Equilibrium Theory

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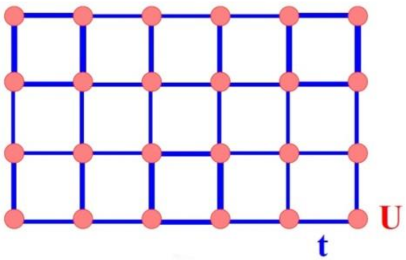
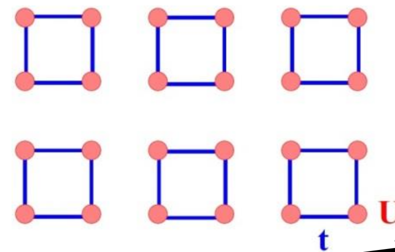
Motivation for CPT



$$G^{-1} = G_0^{-1} - \Sigma$$



$$G_{cluster}^{-1} = G_{0,cluster}^{-1} - \Sigma_{cluster}$$

non interacting

$$G^{-1} = G_0^{-1} - \Sigma$$

approximate $\Sigma := \Sigma_{cluster}$

$$G^{-1} \approx G_0^{-1} - \Sigma_{cluster}$$

$$G^{-1} \approx G_0^{-1} - (G_{0,cluster}^{-1} - G_{cluster}^{-1})$$

$$G^{-1} \approx G_{cluster}^{-1} - (G_{0,cluster}^{-1} - G_0^{-1})$$

$$G^{-1} \approx G_{cluster}^{-1} - T$$

→ CPT equation

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Cluster Perturbation Theory in practice I

requires: 1) (numerically) exact $G_{cluster}(z,k)$

- Analytic
- Exact Diagonalization (Band) Lanczos
  - real frequency data
  - Limited system size (~20 Fermionic orbitals)
- Quantum Monte Carlo
- Dynamic Density Matrix Renormalization Group
- ...

2) superlattice wavevector transformed T

$$T_{RR'}(k) = \sum_x e^{ik.x}\, T_{Rr'} \qquad \text{with} \qquad r' = x+R'$$

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Cluster Perturbation Theory in practice II

exact limits:

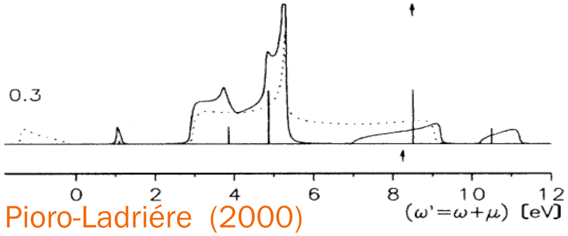
- U=0
- $U/t \longrightarrow \infty$
- cluster size $L \longrightarrow \infty$

performance:

- relatively simple, once Gcluster(z,k) is obtained
- quality may depend strongly on L
- improve starting point: VCA

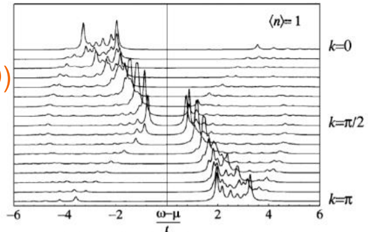
C. Gros, R. Valenti (1993)

CuO_2 planes



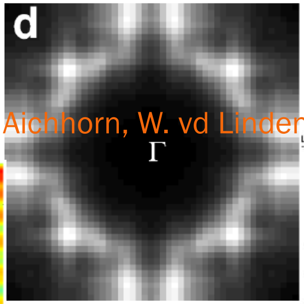
D. Sénéchal, D. Perez, M. Pioro-Ladriére (2000)

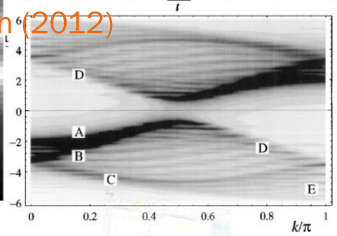
stripes in AFM



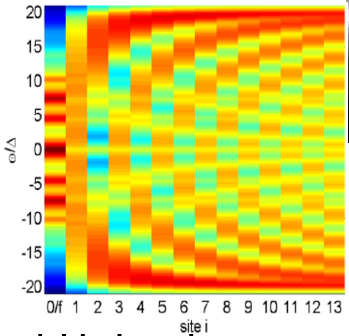
M. G. Zacher, R. Eder, E. Arrigoni, W. Hanke (2000)

single impurity

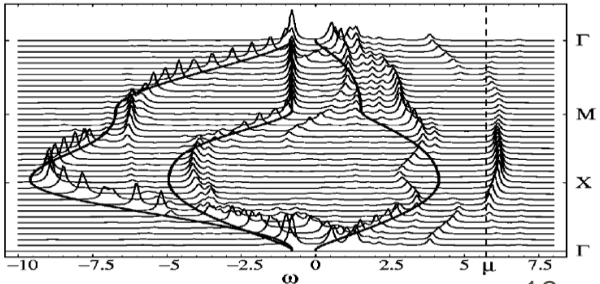




M. Nuss, E. Arrigoni, M. Aichhorn, W. vd Linden (2012)

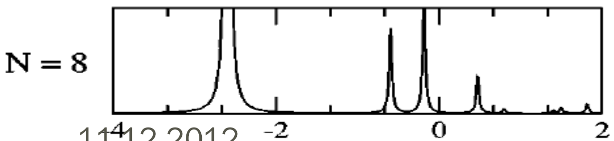


D. Sénéchal, D. Perez, D. Plouffee (2002)

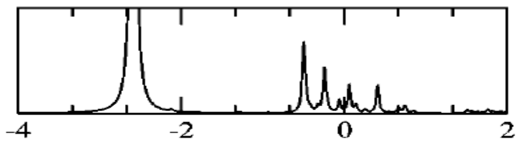


M. Hohenadler, M. Aichhorn, W. vd Linden (2003)

Hubbard-Holstein



ED



CPT

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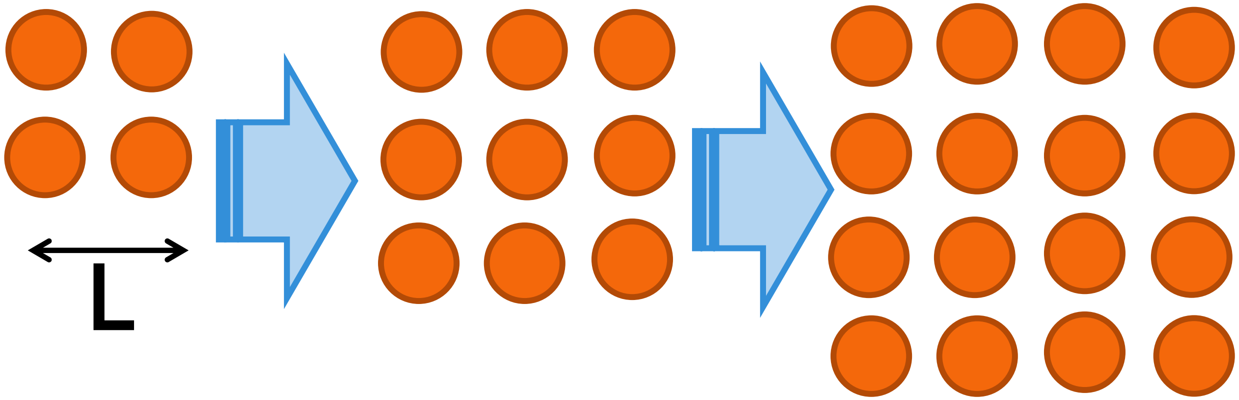
improving Cluster Perturbation Theory



CPT improves

$\Sigma_{cluster}(L)$

already a very fancy tractor

but just one steering wheel

Variational cluster approach

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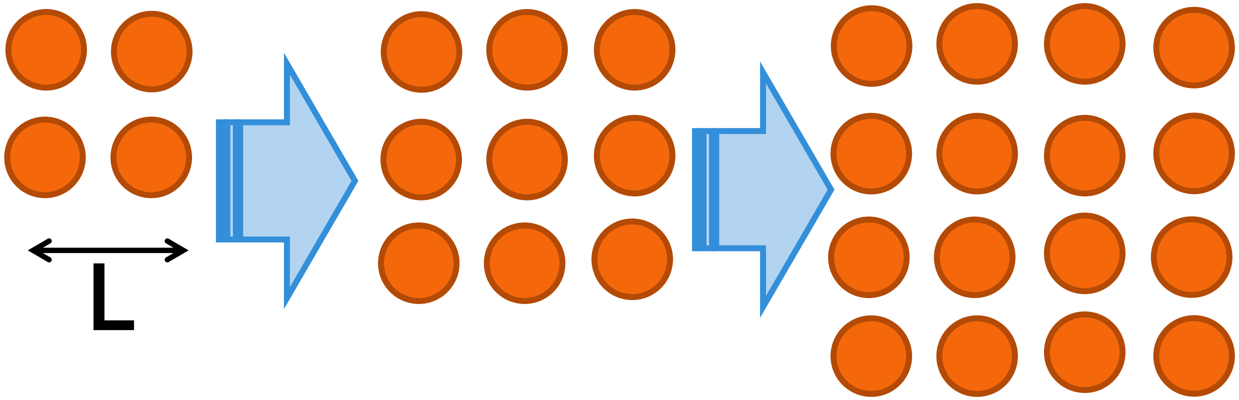
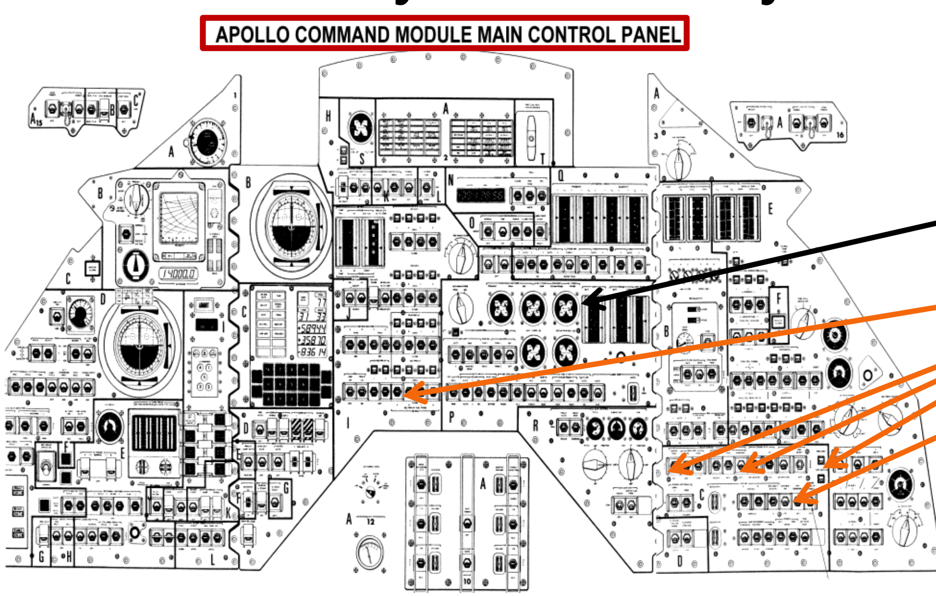


CPT improves

$\Sigma_{cluster}$ (L)

now

if you want to land on the moon you need many more knobs to turn



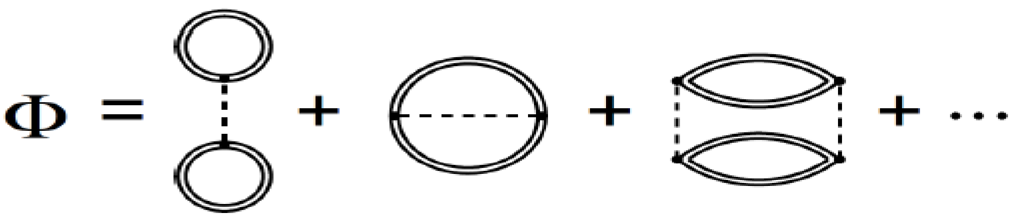
$\Sigma_{VCA}(L, \Delta_1, \Delta_2, \ldots, \Delta_n)$

Variational cluster approach

the Apollo command module however is a little bit more complicated than the fancy tractor

VCA may be develped within the Self Energy Functional Approach M. Potthoff (2003)

$$\Omega[G] = \Phi[G] - \mathrm{Tr}\left\{ \left(G_0^{-1} - G^{-1} \right) G \right\} + \mathrm{Tr}\left\{ \ln\left(-G \right) \right\}$$



$$\frac{\delta \Phi[G]}{\delta G} = \Sigma$$

$$\frac{\delta \Omega[G]}{\delta G} = \frac{\delta \Phi[G]}{\delta G} - \frac{\mathrm{Tr}\left\{ \left(G_0^{-1} - G^{-1} \right) G \right\}}{\delta G} + \frac{\mathrm{Tr}\left\{ \ln\left(-G \right) \right\}}{\delta G}$$

$$= \Sigma - G_0^{-1} + G^{-1} \overset{!}{=} 0$$

$$\Rightarrow G^{-1} = G_0^{-1} - \Sigma$$

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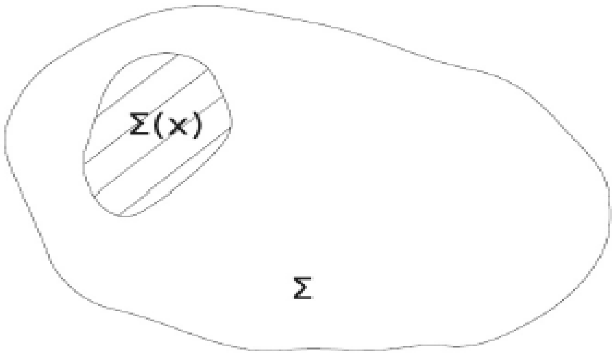
Variational cluster approach

limit domain of avaialbe Σ's



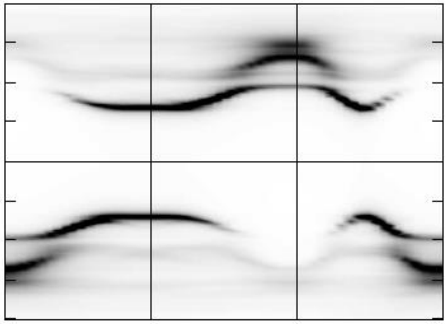
1) $\Omega(x') = \Omega'(x') + \mathrm{Tr}\left\{\ln\left(-G(x')\right)\right\} - \mathrm{Tr}\left\{\ln\left(-G'(x')\right)\right\}$

2) $\nabla_{x'}\Omega(x') \overset{!}{=} 0$

VCA

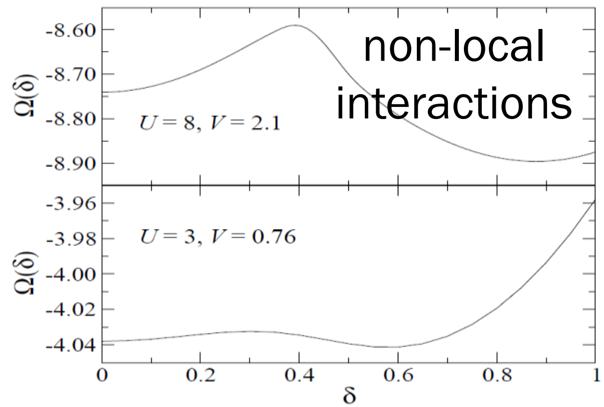
3) $G^{-1} = G'^{-1} - T$ CPT

equilibrium Variational cluster approach

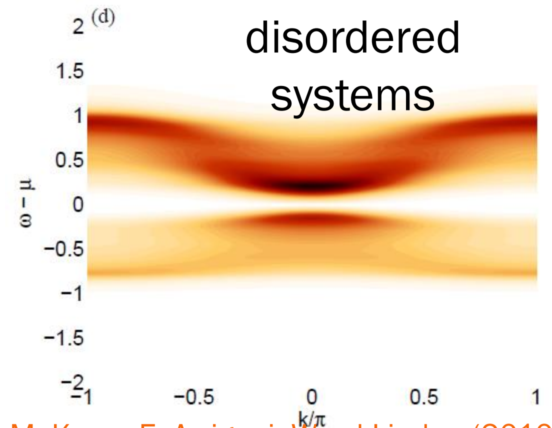


spont. symmetry breaking

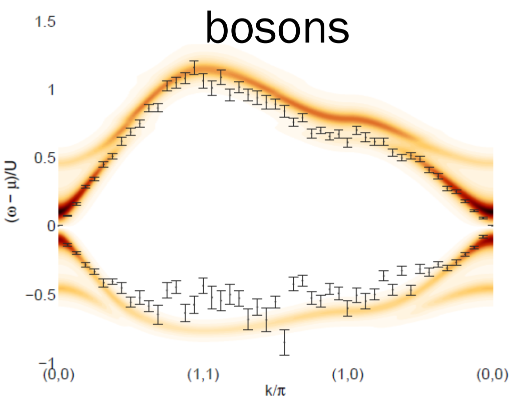
C. Dahnken, M. Aichhorn, W. Hanke, E. Arrigoni, M. Potthoff, (2004)



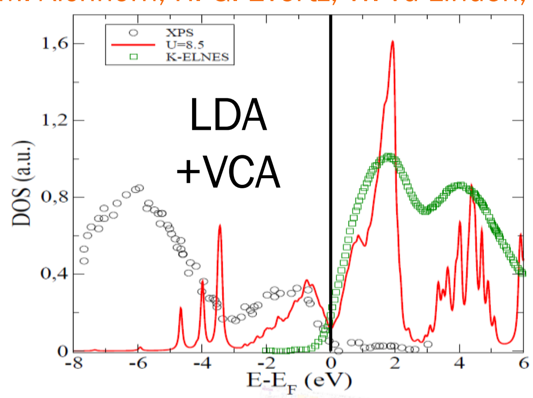
M. Aichhorn, H. G. Evertz, W. vd Linden, M. Potthoff (2004)



M. Knap, E. Arrigoni, W. vd Linden (2010)

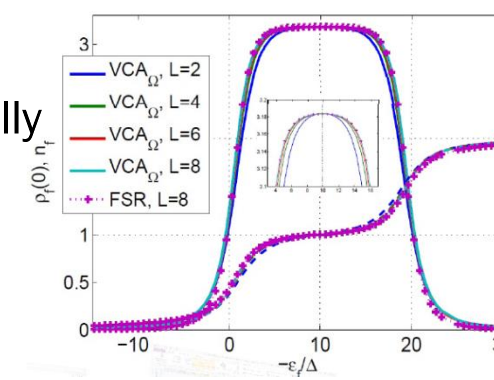


E. Arrigoni, M. Knap, W. vd Linden (2011)



H. Allmaier, L. Chioncel, E. Arrigoni (2009)

non-translationally invariant systems



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

for reviews see:

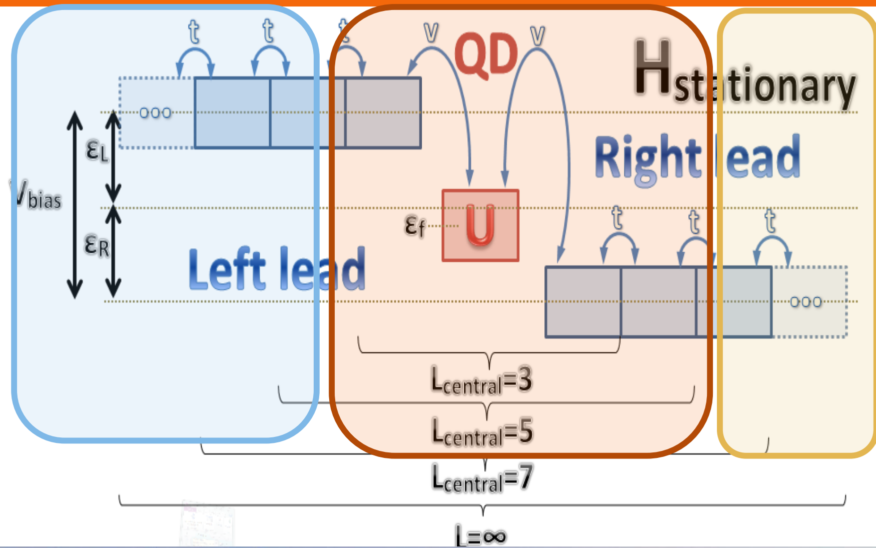
D.Sénéchal, arXiv.org/0806.2690 (2008)

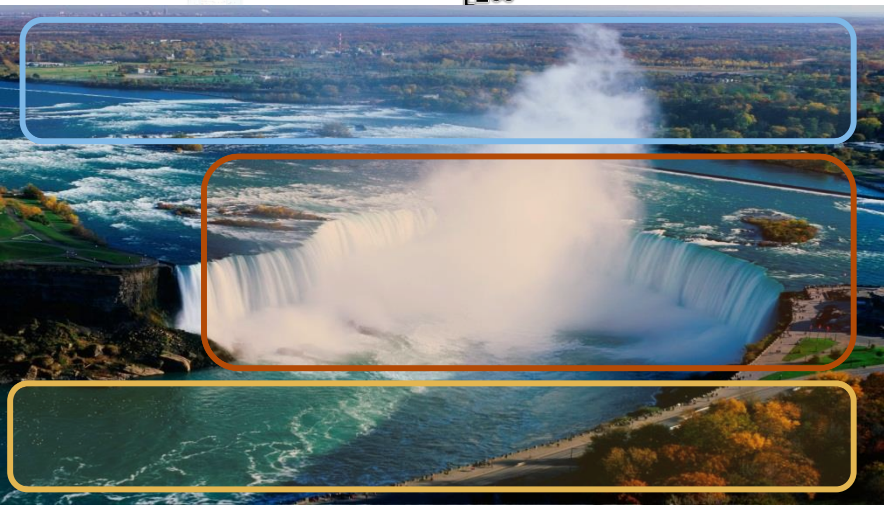
M. Potthoff, arXiv/1108.2183 (2010)

Non-quilibrium Theory

2 - B

Non-equilibrium Variational Cluster Approach





http://www.niagarafallslive.com

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

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

CPT time evolution

M. Balzer, M. Potthoff (2011)

VCA steady-state

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

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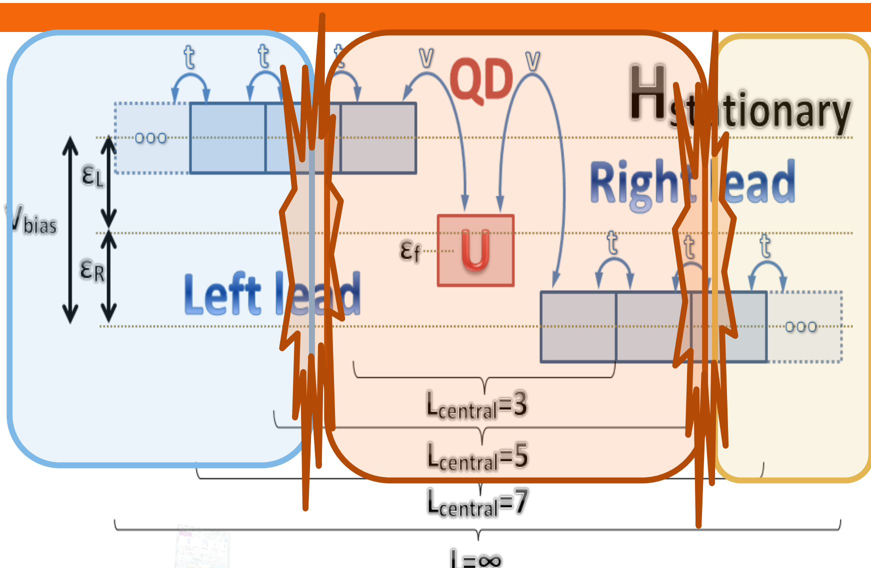
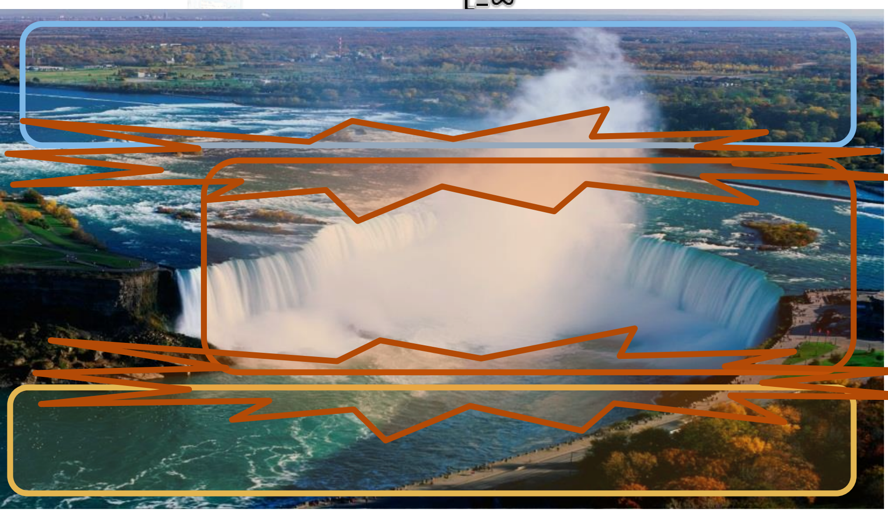
Non-equilibrium Variational Cluster Approach





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

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

@ τ_0 cpl. T switched on

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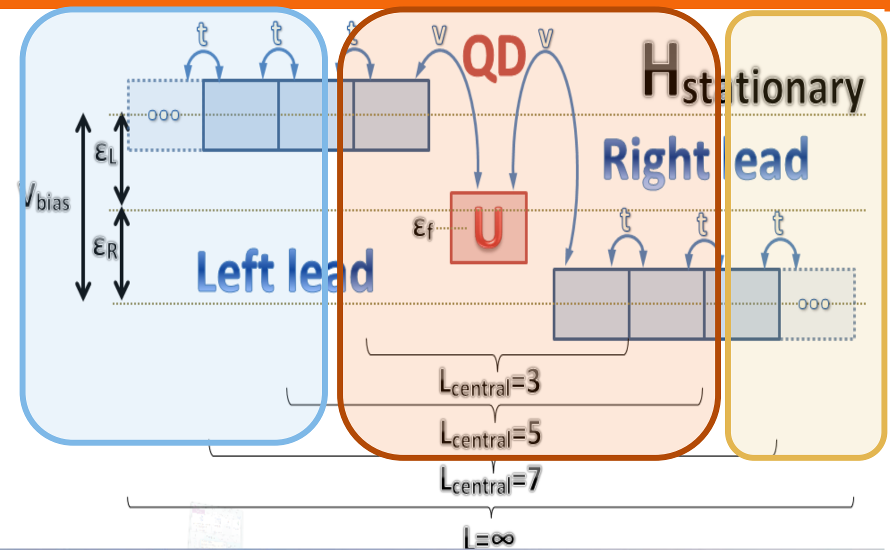
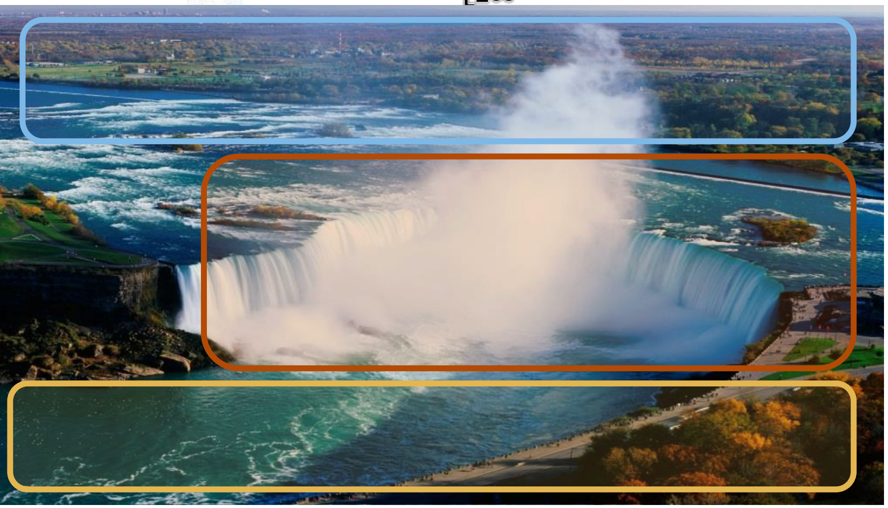
Non-equilibrium Variational Cluster Approach





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

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

@ τ_0 — cpl. T switched on

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

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

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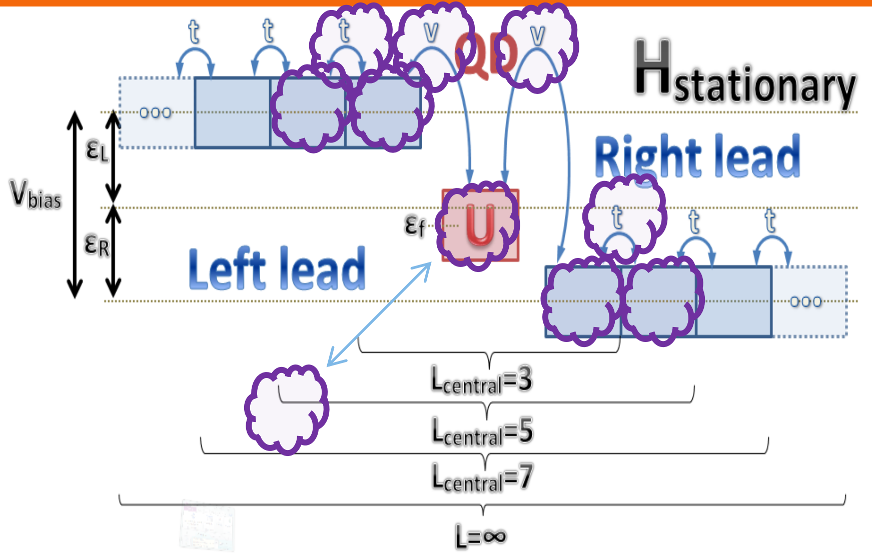
Non-equilibrium Variational Cluster Approach



non unique decomposition

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

CPT approximation

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

optimize initial state: VCA

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

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

flexible self-energy $\Sigma(x)$

variational principle

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

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Non-equilibrium Variational Cluster Approach

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

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

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

$\cong$

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

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Non-equilibrium Variational Cluster Approach

full Dyson

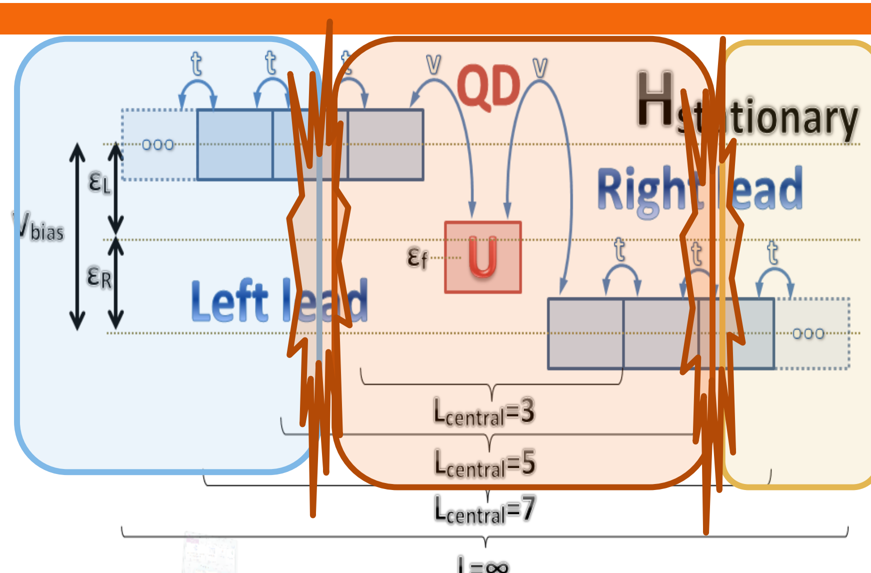
$$G = g + (T + \Delta\Sigma)\, G$$

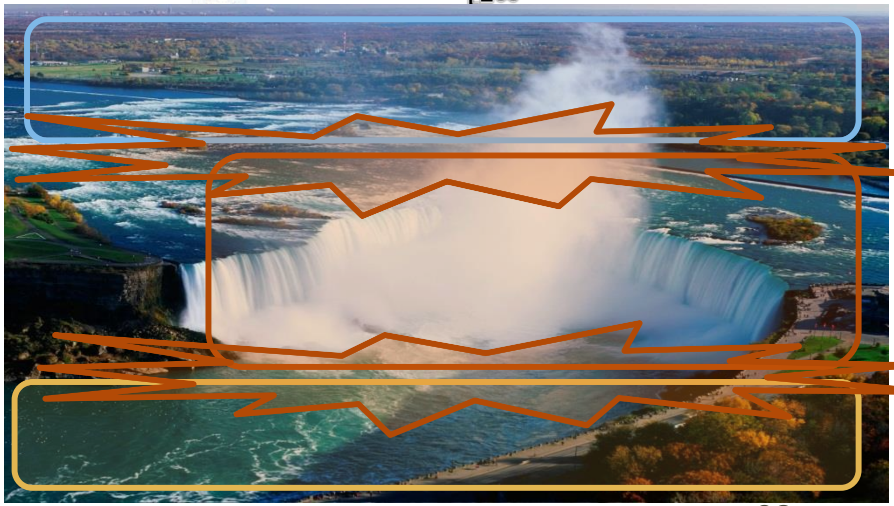
CPT („Hubbard I type")

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

VCA

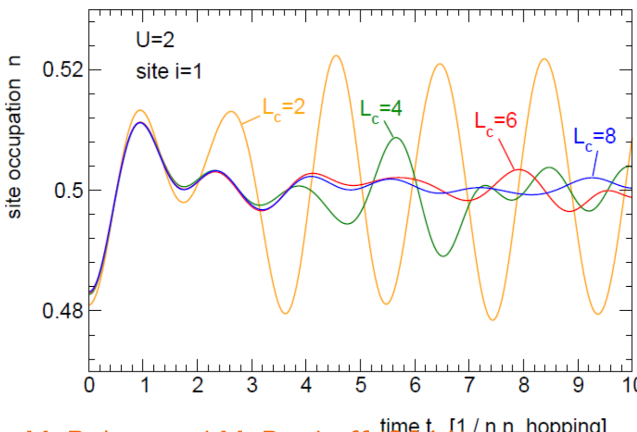
$$G = g_{eff} + (T_{eff} + \cancel{\Delta\Sigma})\, G$$





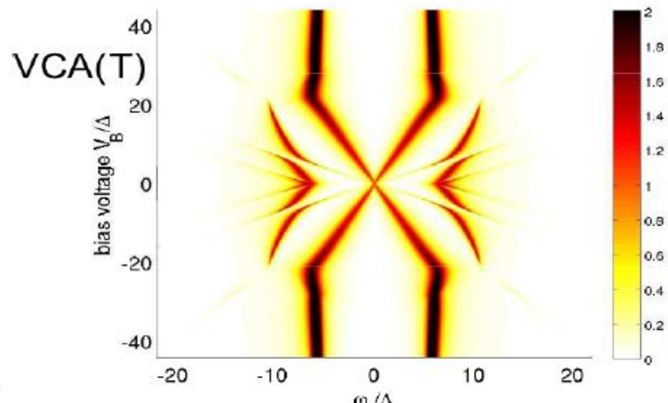
Non-equilibrium Variational Cluster Approach

Time evolution by CPT



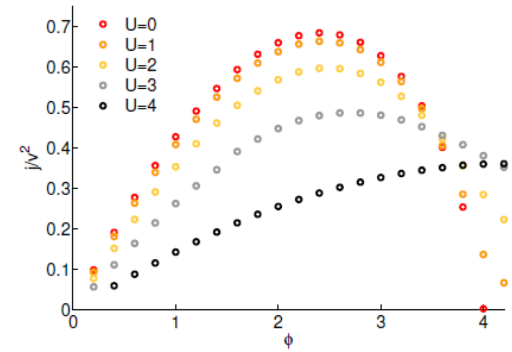
M. Balzer and M. Potthoff (2011)

Steady state of quantum dots



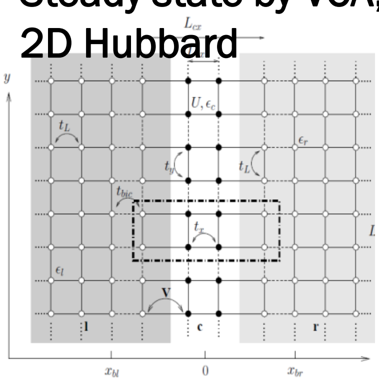
M. Nuss, C. Heil, M. Ganahl, M. Knap, H. G Evertz, E. Arrigoni, W. vd Linden (2012)

non equilibrium DMFT



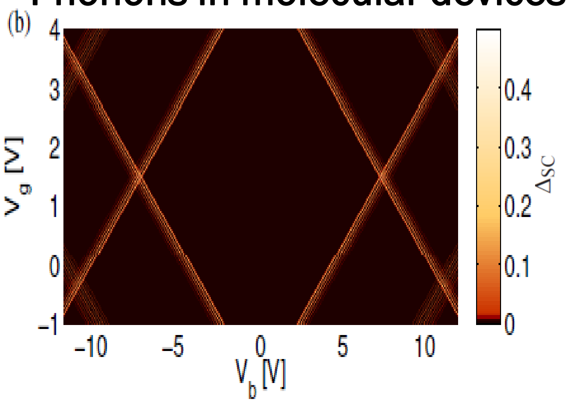
E. Arrigoni, M. Knap, W. vd Linden (2012)

Steady state by VCA, 2D Hubbard



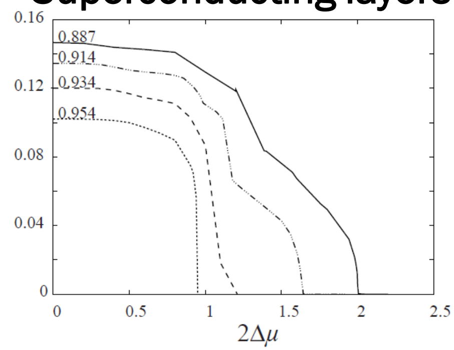
M. Knap, W. vd Linden, E. Arrigoni (2011)

Phonons in molecular devices



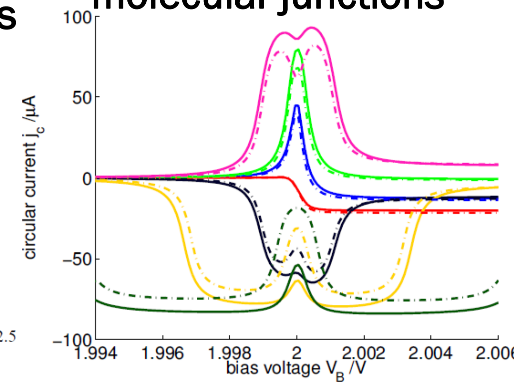
M. Knap, E. Arrigoni, W. von der Linden (2012)

Superconducting layers



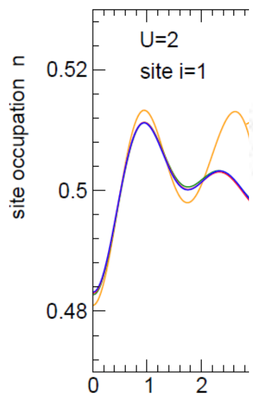
A. Fulterer, E. Arrigoni (2012)

Magnetic effects in molecular junctions



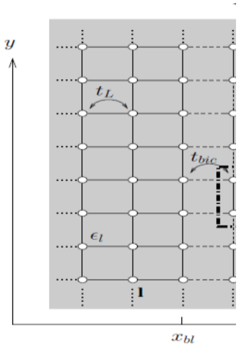
M. Nuss, E. Arrigoni, W. vd Linden (2012)

Steady state of quantum dots



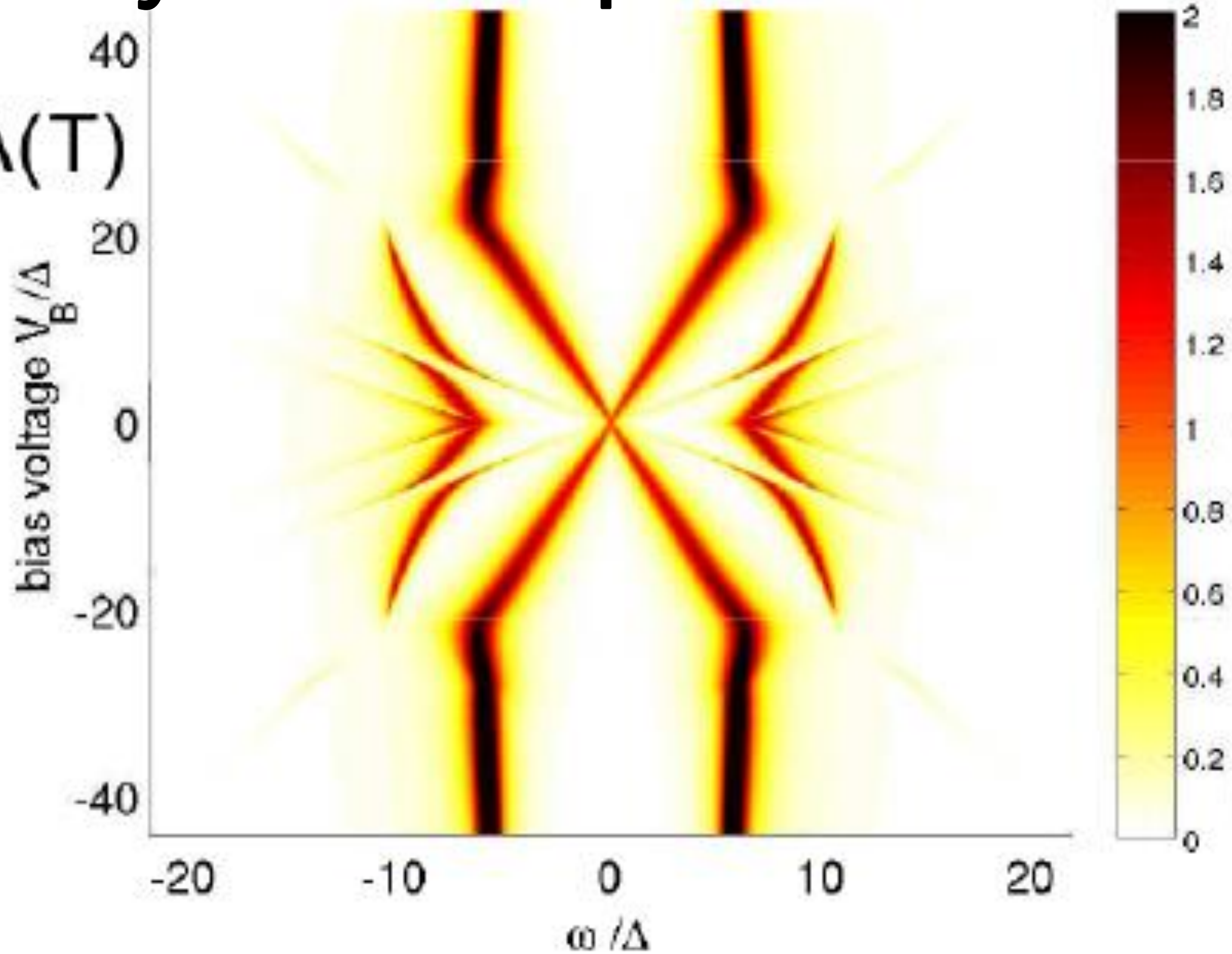
M. Balzer and M

Steady state



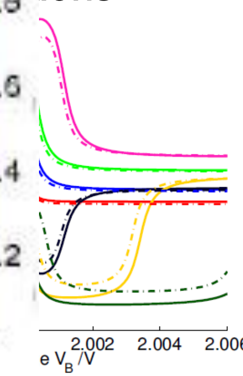
M. Knap, W. vd L

VCA(T)



, W. vd Linden

s in
ions



W. vd Linden

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

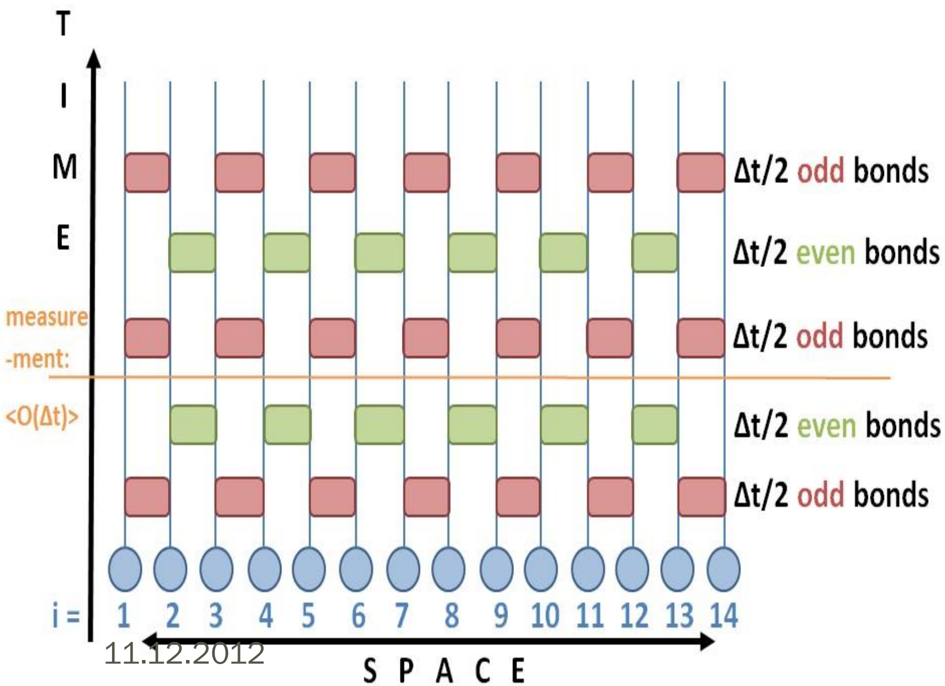
Matrix Product State time evolution

Martin Nuss

Time evolution with Matrix Product States

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

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



S. R. White (1993)

1) DMRG($H_0(t_0)$) $\longrightarrow$ Ψ_0

2) @ t_x quench: $H_0 \longrightarrow H_>$

3) TEBD(Ψ_0) $\longrightarrow$ $\Psi(t)$

G. Vidal (2004)

Martin Nuss

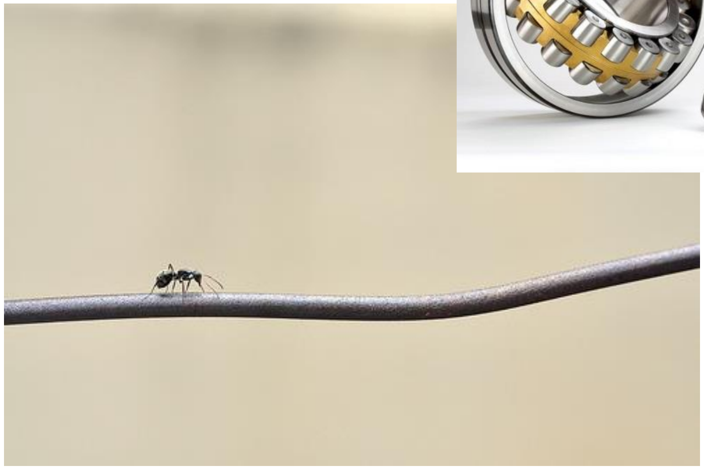
Time evolution with Matrix Product States

quasi exact / high precision

most powerful in 1D

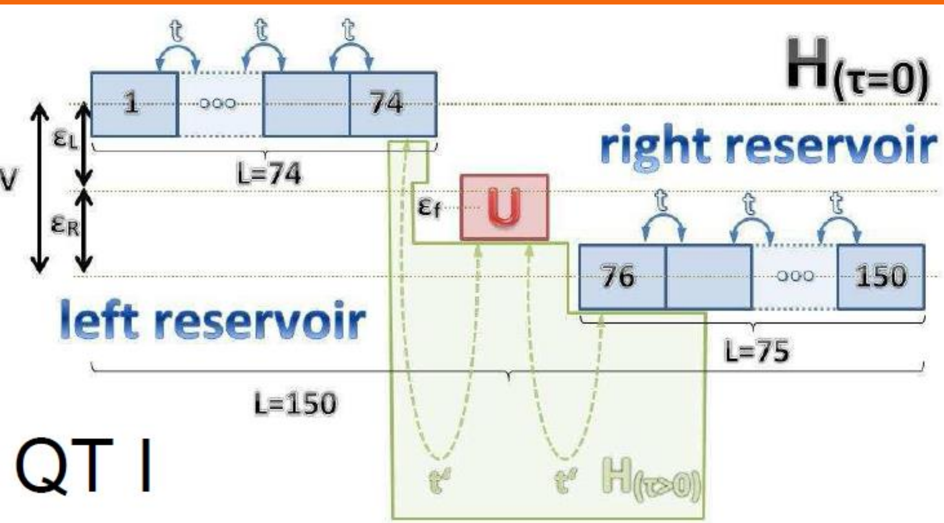
limited system size

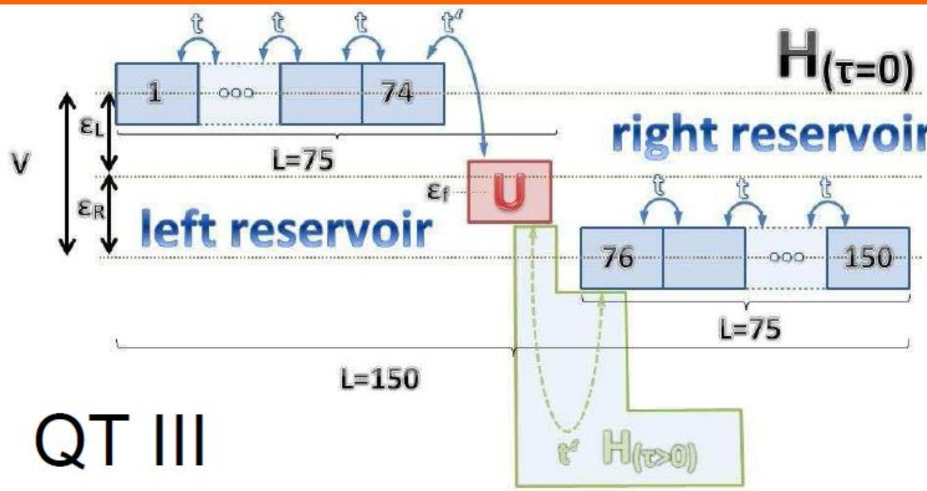
limited simulation time

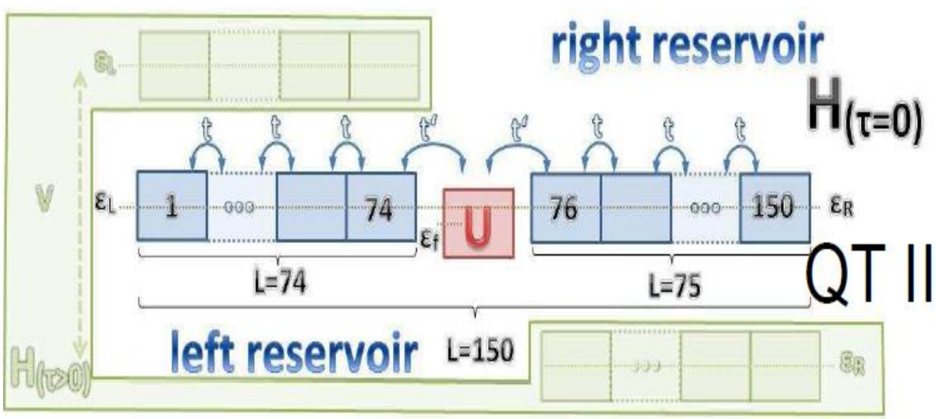


Martin Nuss

Time evolution after a quantum quench







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

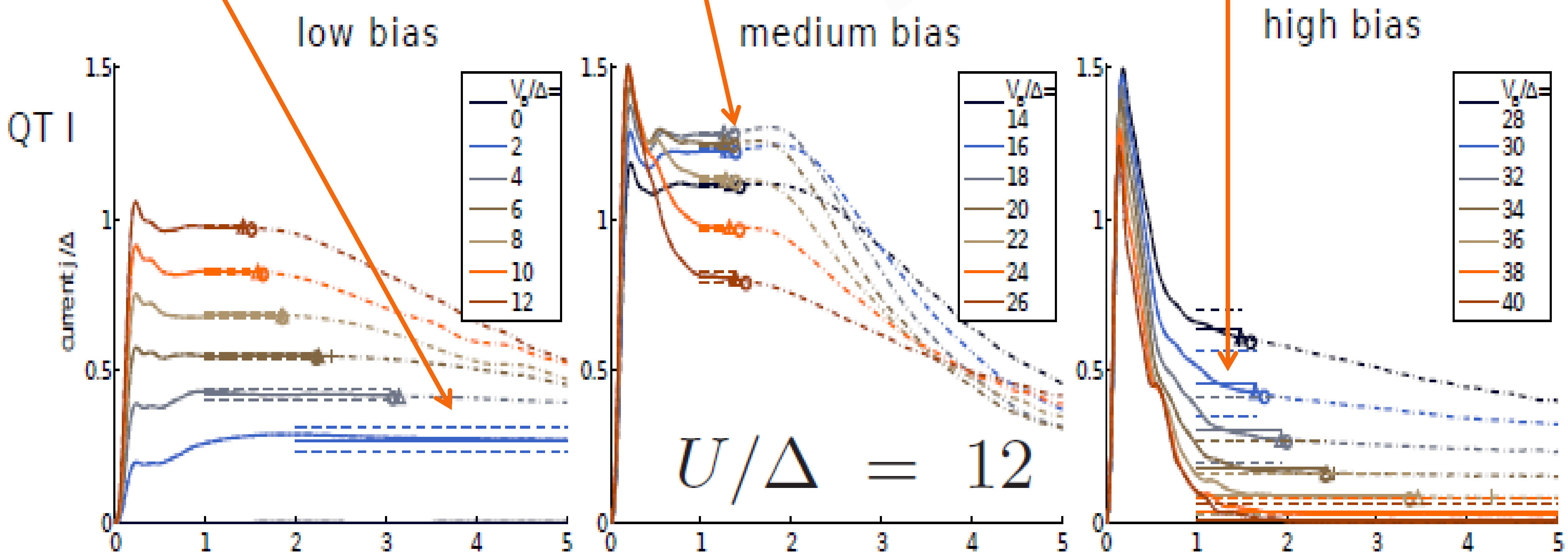
M. Nuss, M. Ganahl, H. G. Evertz,
E. Arrigoni, W. von der Linden
(in preperation)

Can the steady state be reached?

entanglement

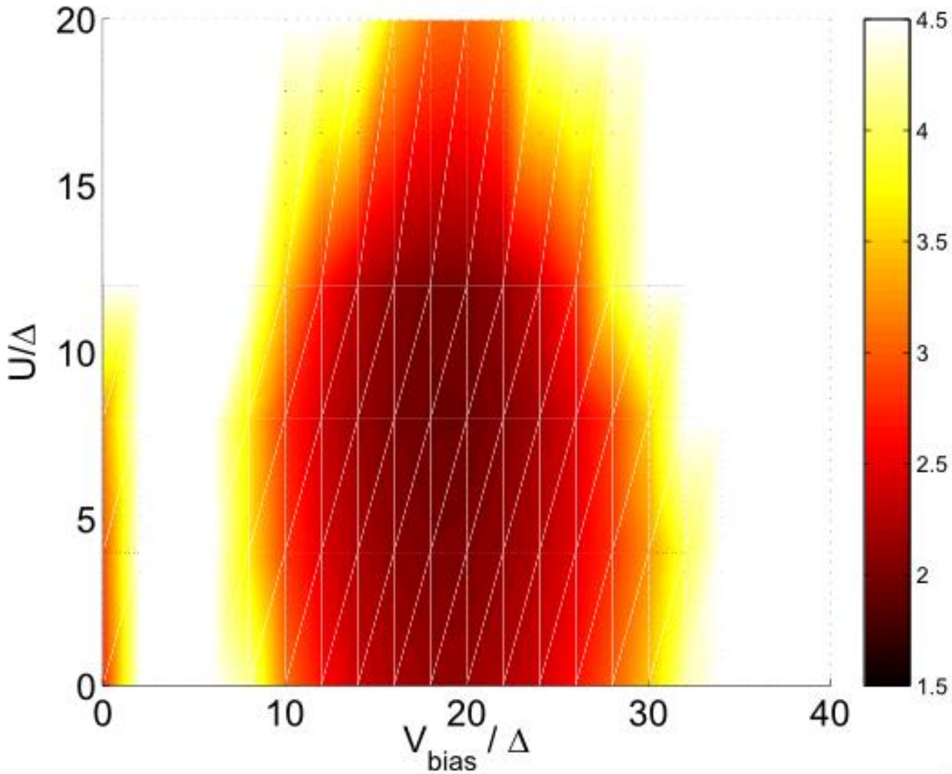
steady-state ✓

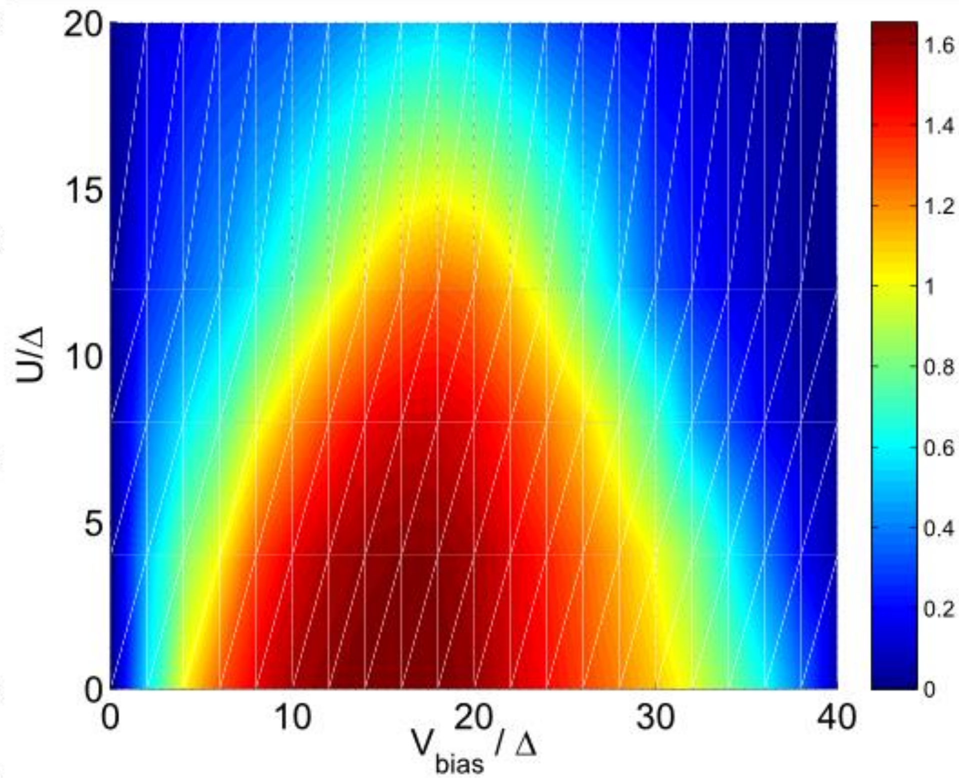
steady-state ✗



time t / Δ^{-1}

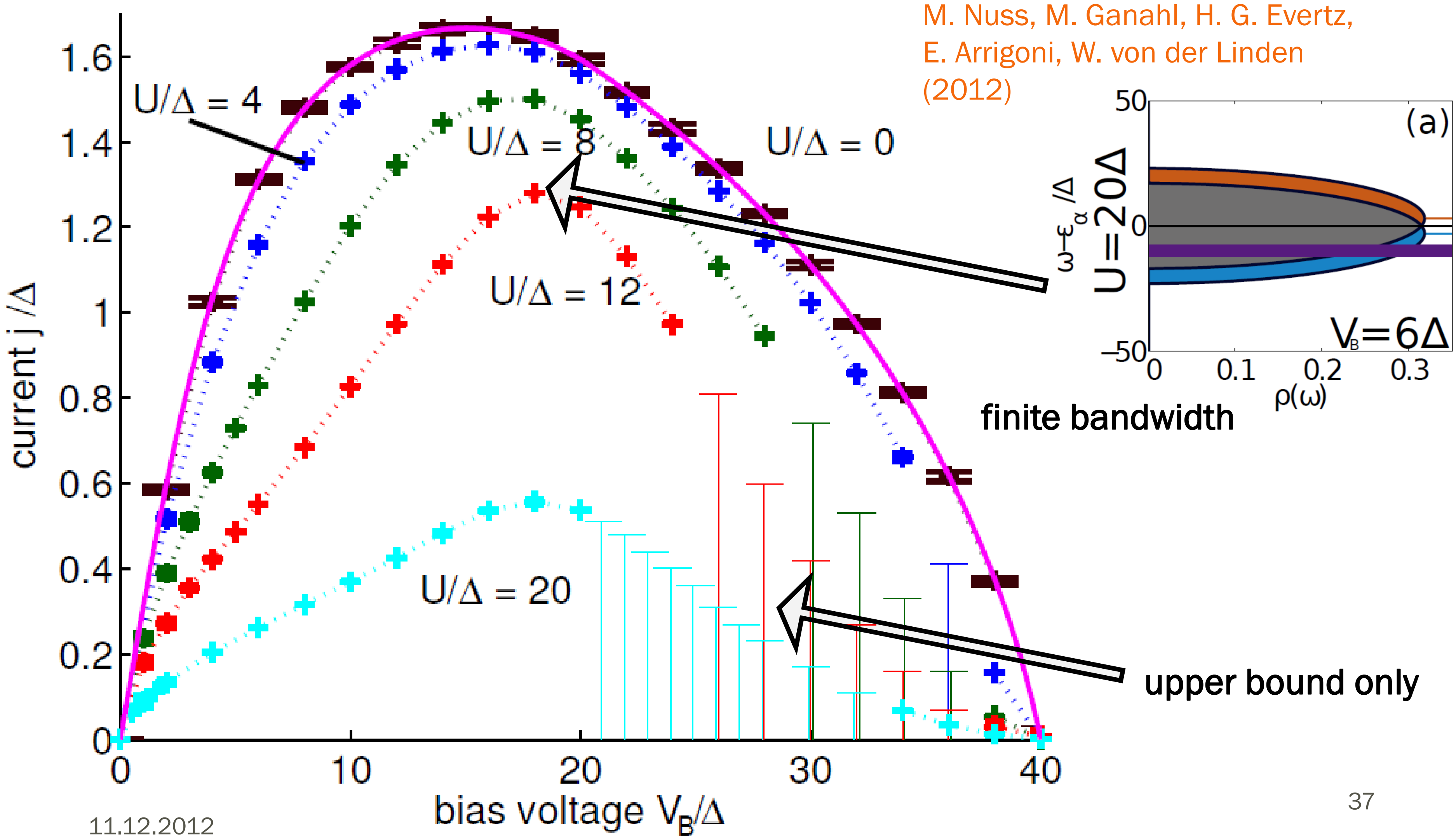
entanglement ⟷ current





DMRG+TEBD current-voltage characteristics

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



Steady-state properties of a quantum dot

Martin Nuss

equilibrium cluster theory for SIAM

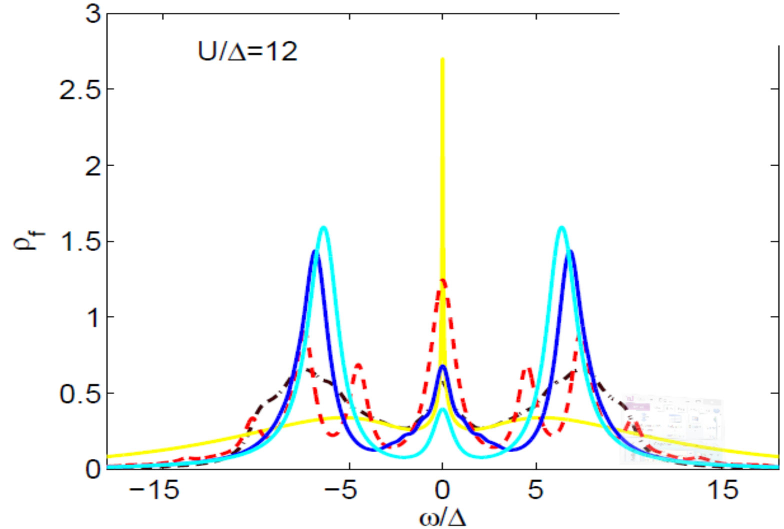
much more accurate methods, c.f. NRG, ...

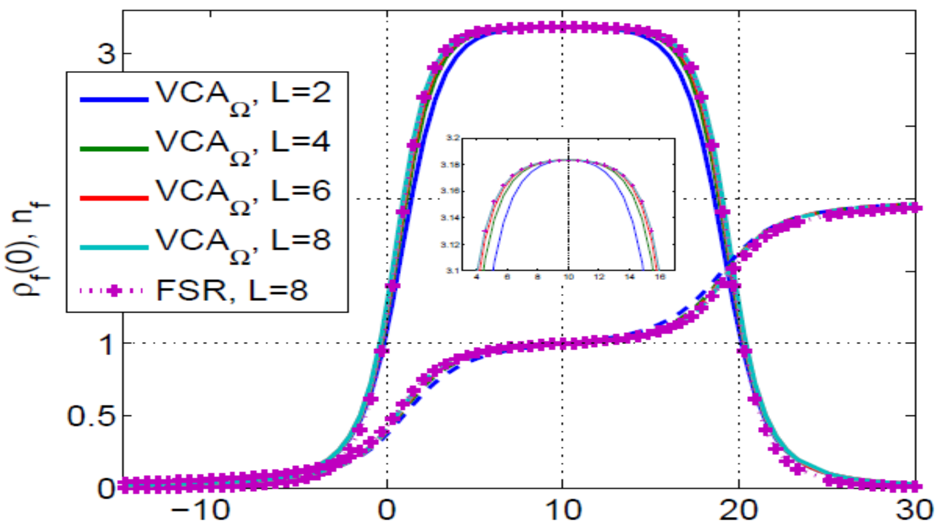
exponentially large Kondo singlet (Bethe Ansatz)

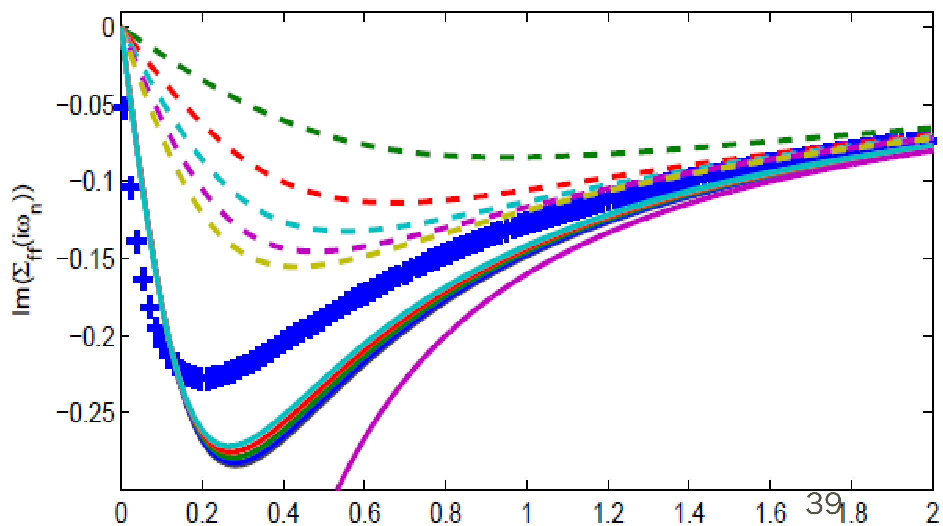
$$T_K = \sqrt{\frac{\Delta U}{2}}\, e^{-\gamma \frac{\pi}{8\Delta} U}\ ,\quad \gamma = 1 \qquad (\text{VCA}) = 0.651$$

Friedel sum rule

$$\rho_f(0) = \frac{1}{\pi\Delta}\ \sin^2\left(\frac{\pi\langle n^f\rangle}{2}\right)$$

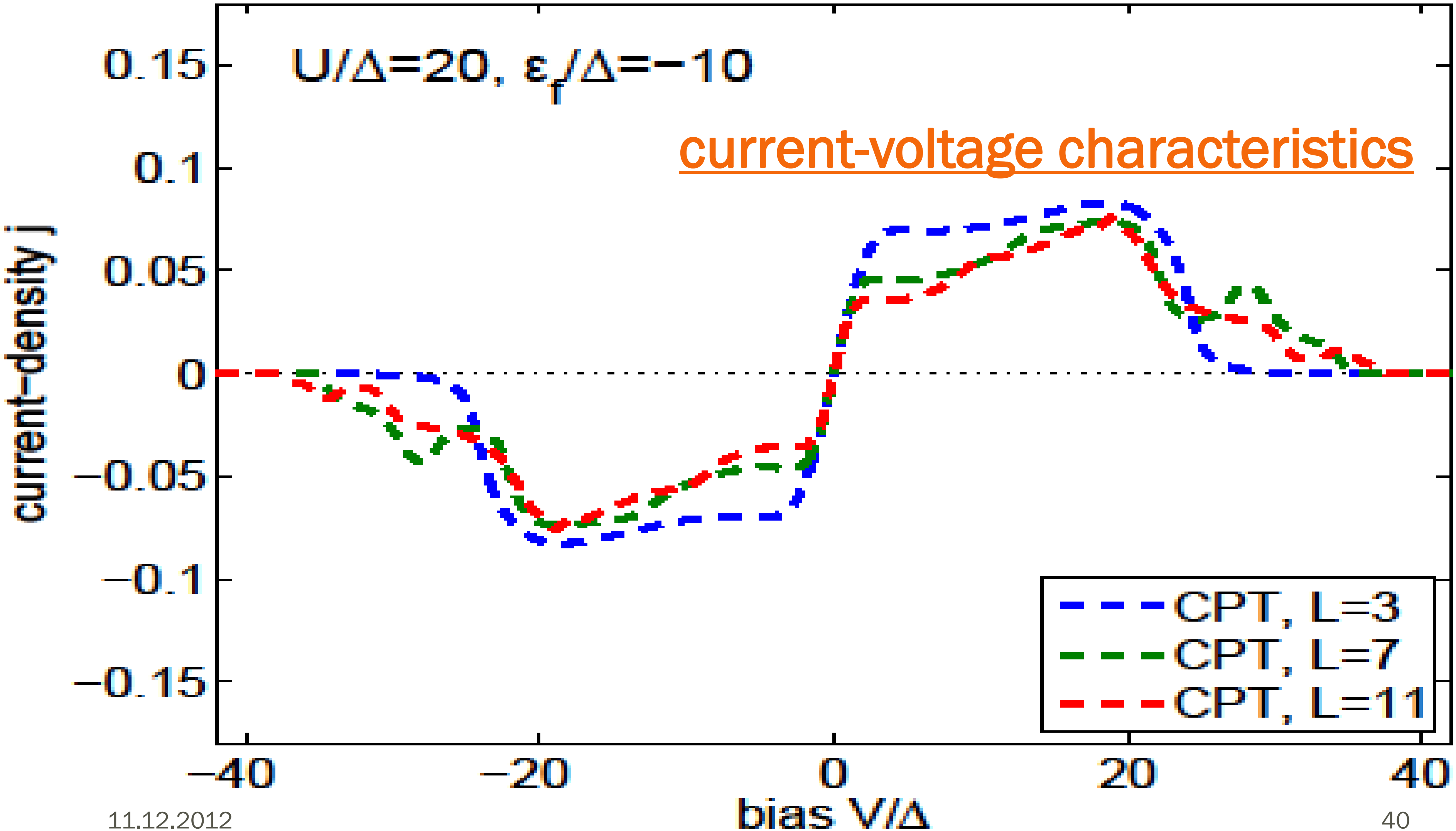




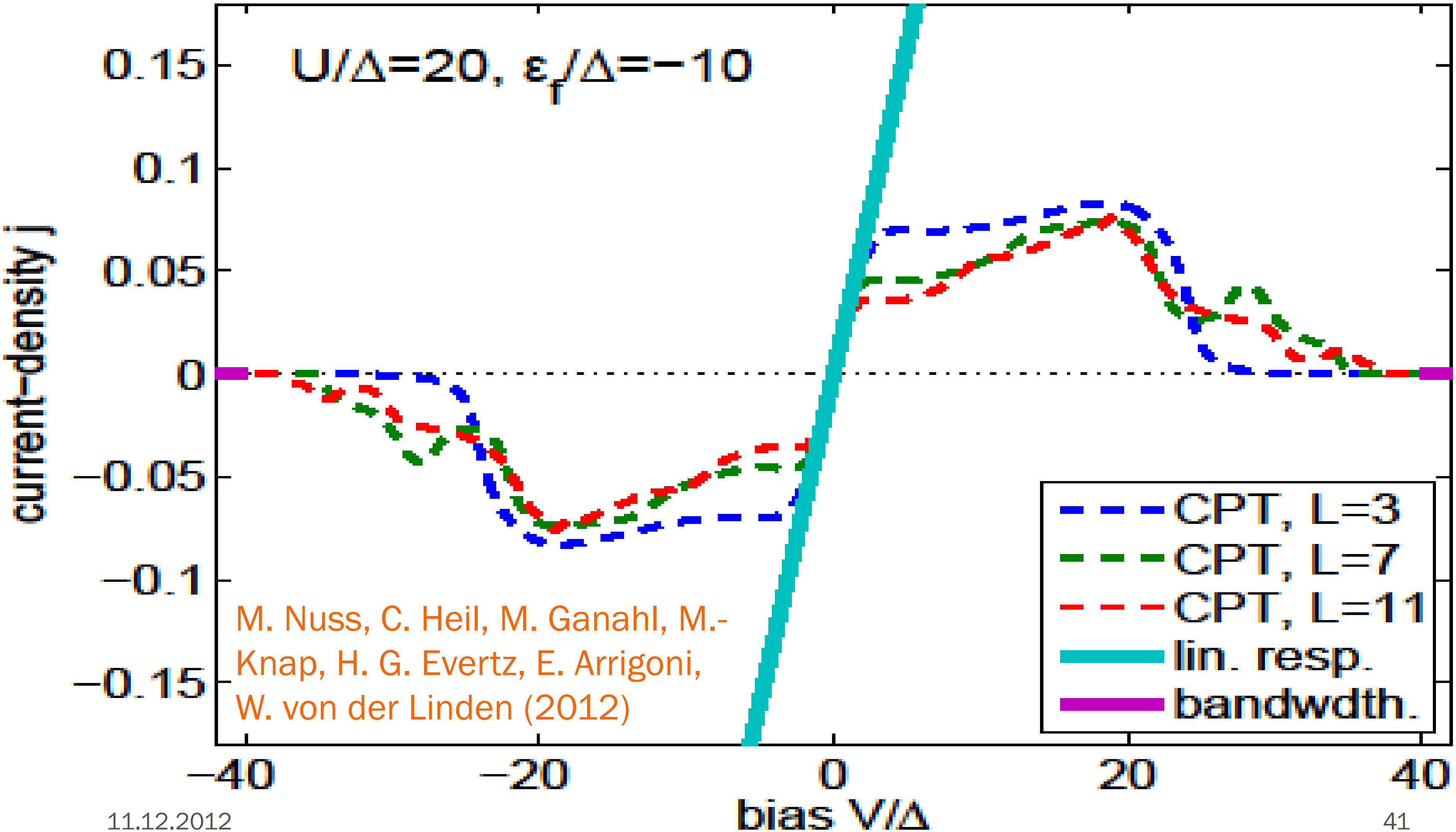


Martin Nuss

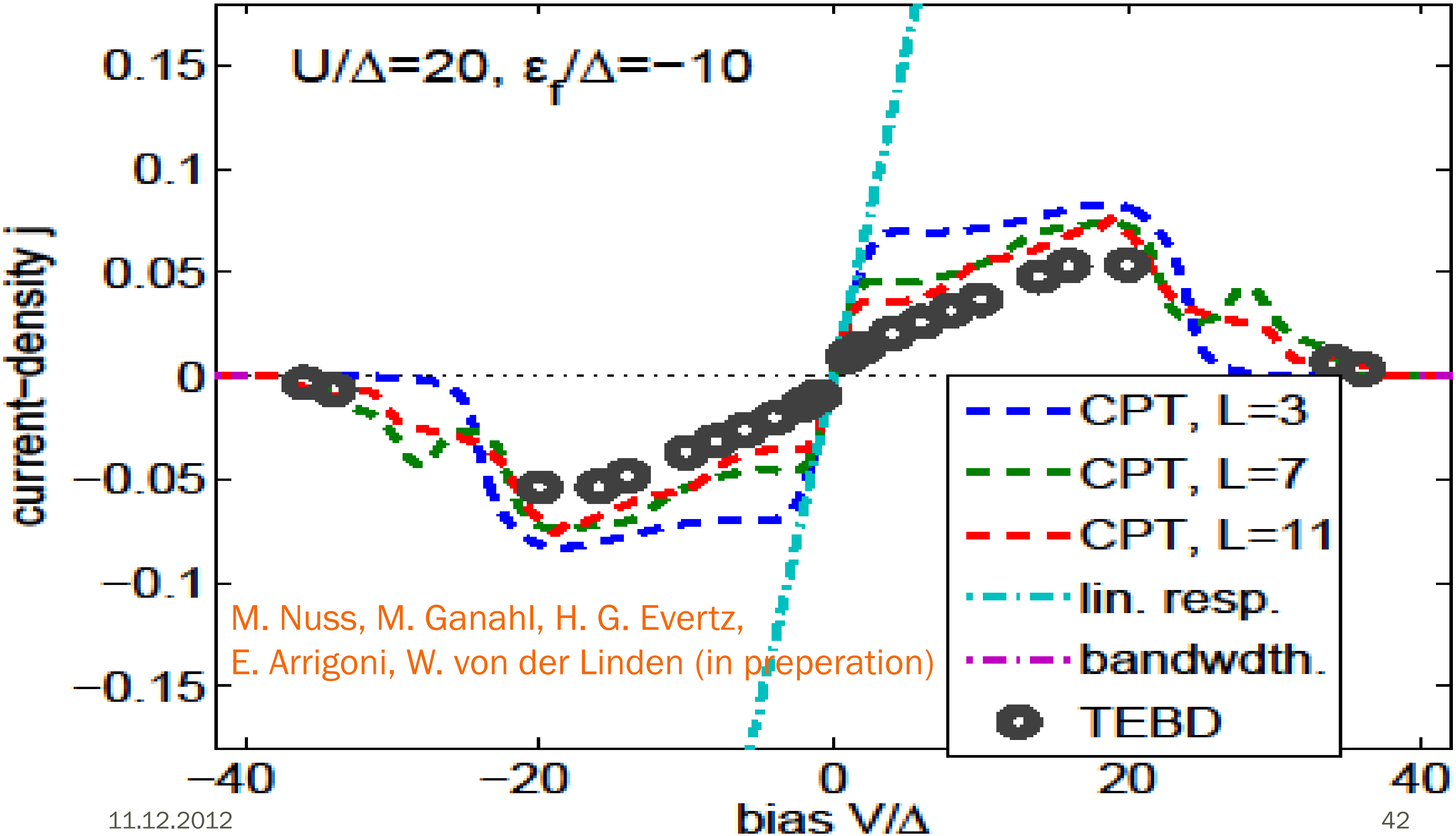
non-equilibrium CPT



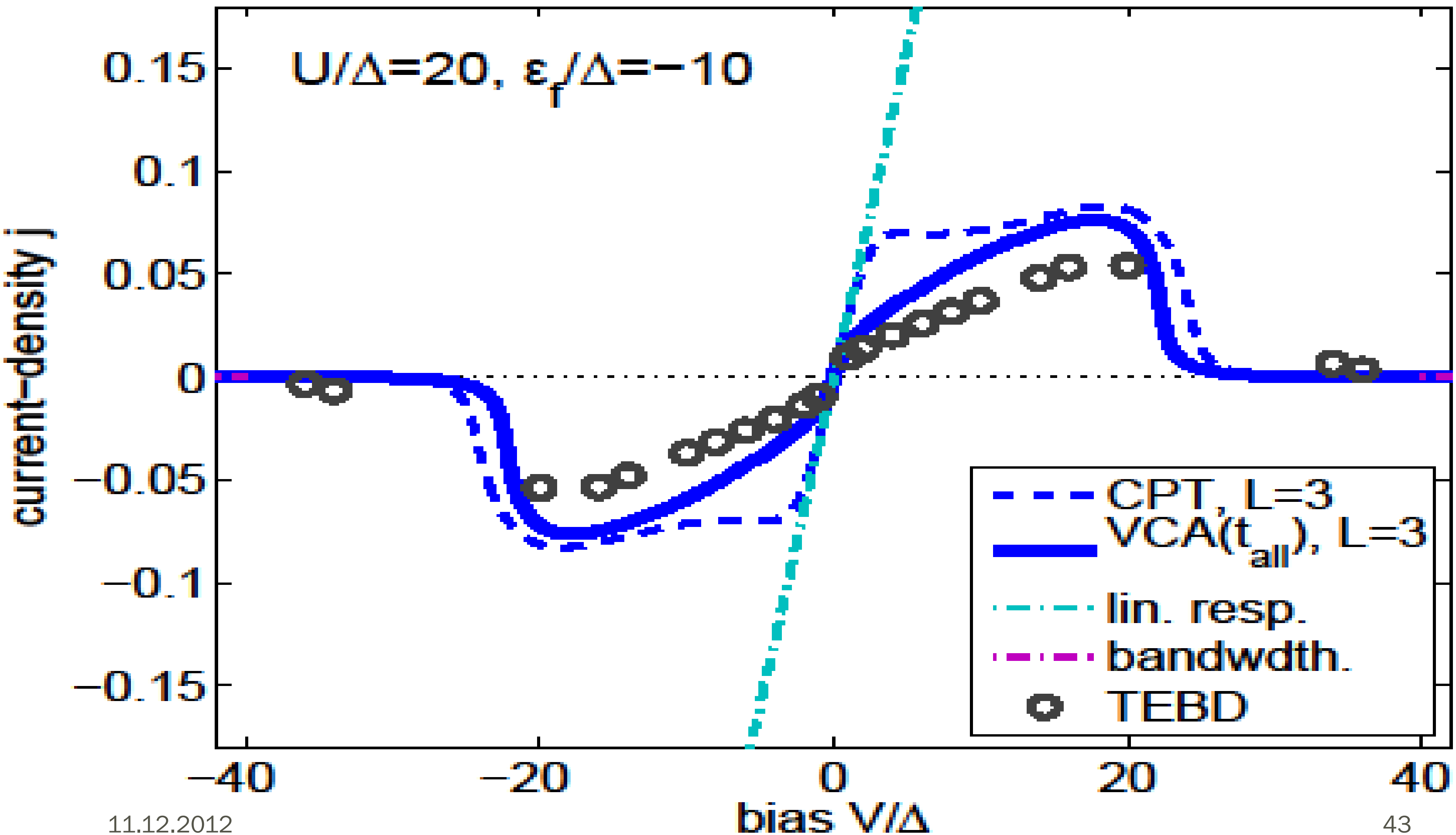
exact limits



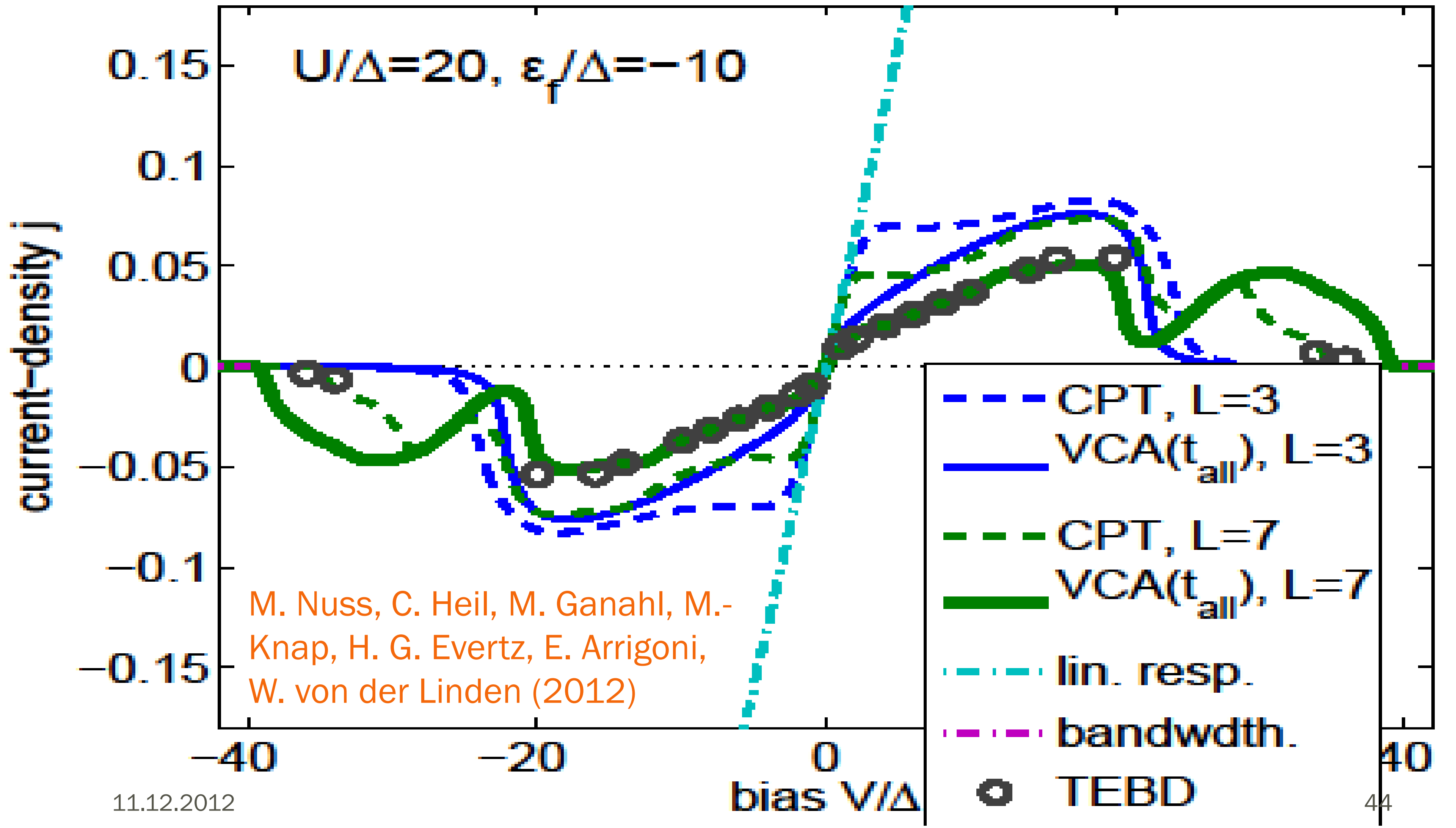
quasi-exact DMRG+TEBD



non-equilibrium VCA



non-equilibrium VCA



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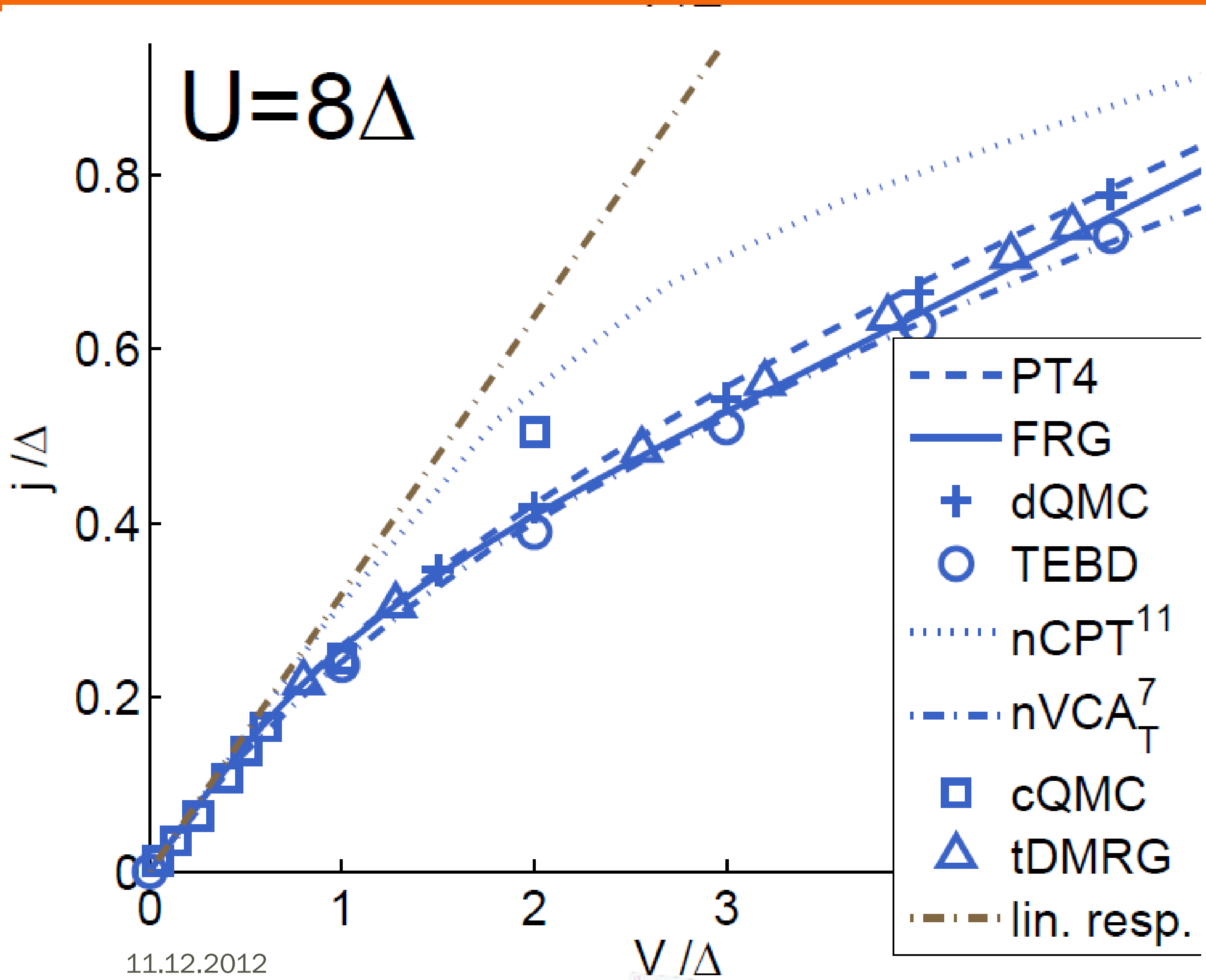
comparison in low bias regime



PT IV: T. Fujii,K. Ueda (2003)

ISPI: S. Weiss, J. Eckel, M. Thorwart, and R. Egger (2008)

tDMRG: F. Heidrich-Meisner, A. E.-Feiguin, E. Dagotto (2009)

dQMC: P. Werner, T. Oka, M. Eckstein, A. J. Millis (2010)

FRG: S. G. Jakobs, M. Pletyukhov, H. Schoeller (2010)

PT II: L. Mühlbacher, D.F. Urban, A.-Komnik (2011)

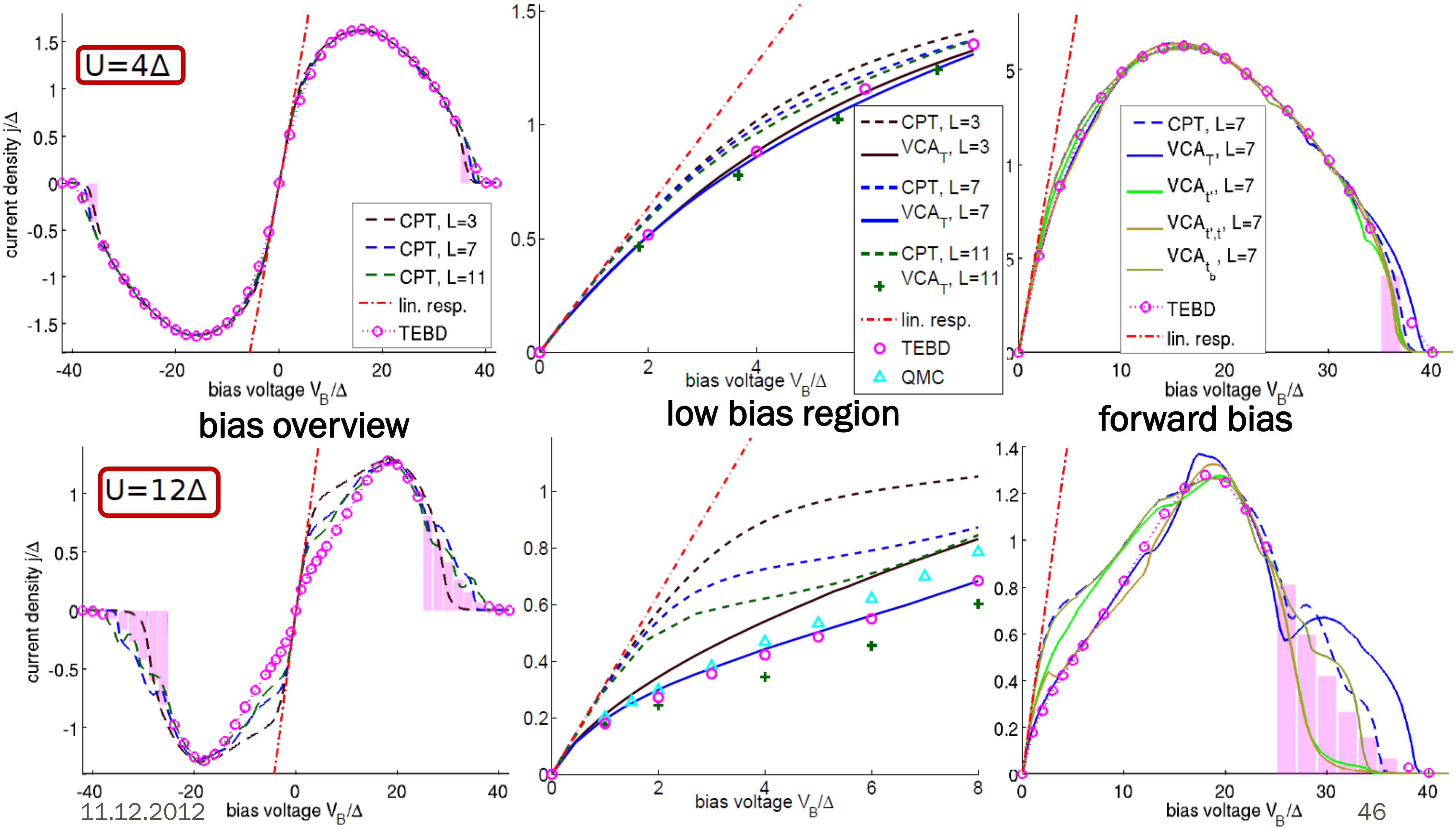
cmp: J. Eckel, F. Heidrich-Meisner, S. G. Jakobs, M. Thorwart, M.-Pletyukhov, R. Egger (2010)

cQMC: A. Dirks, J. E. Han, M. Jarrell, T. Pruschke (2012)

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

current voltage performance

Martin Nuss



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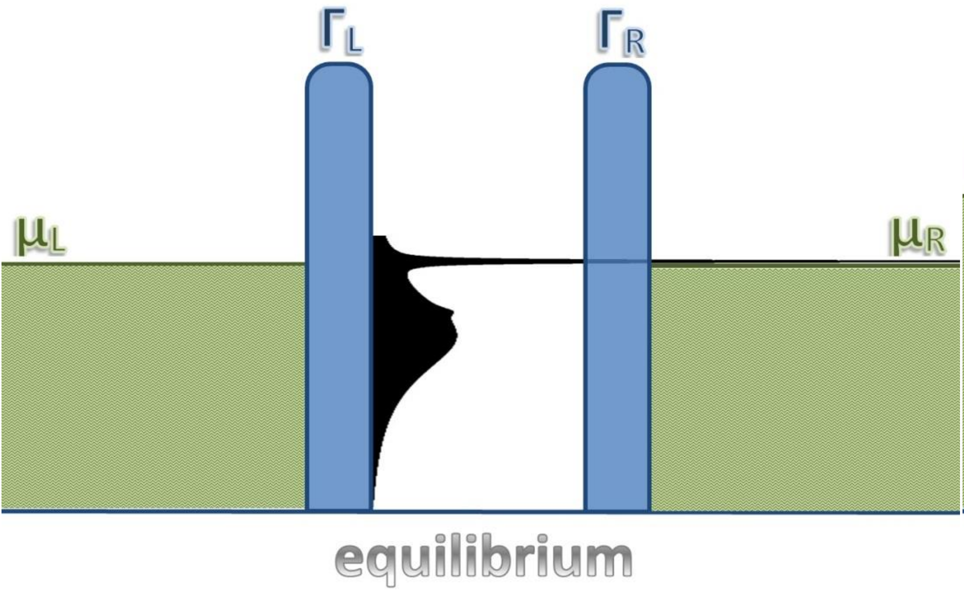
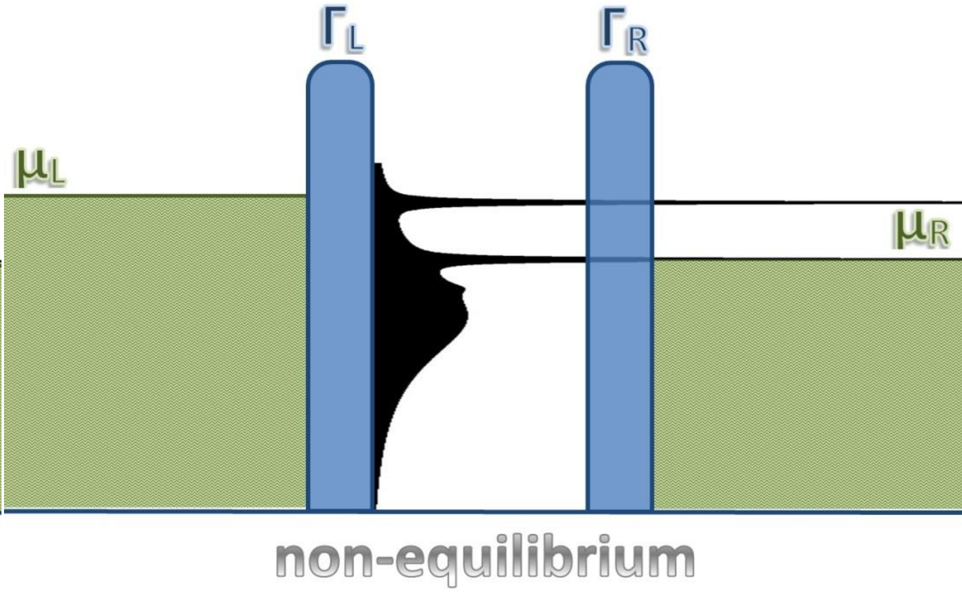
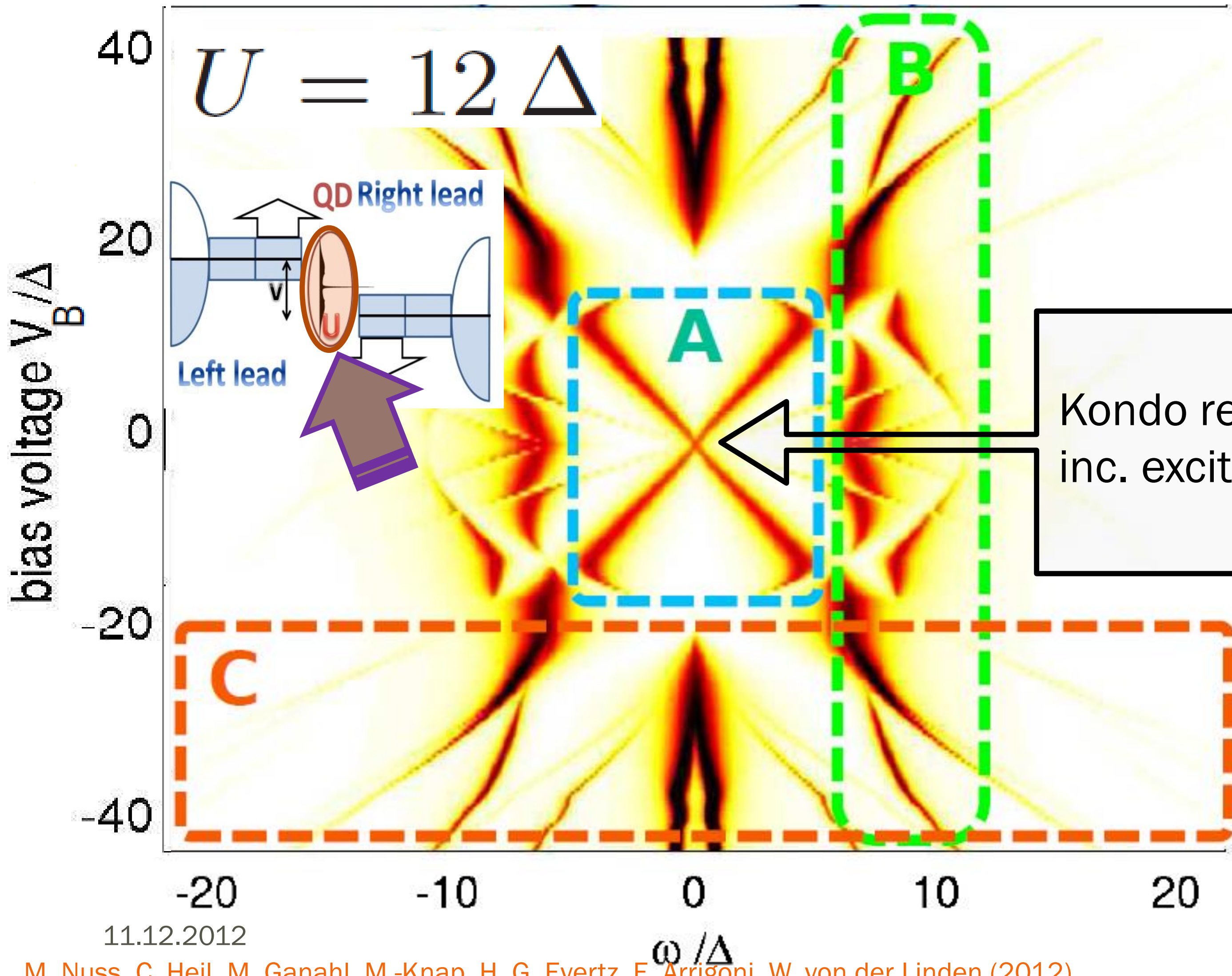
non-equilibrium local density of states





non-equilibrium local density of states



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

Equilibrium

Kondo resonance @ $\omega = 0$

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

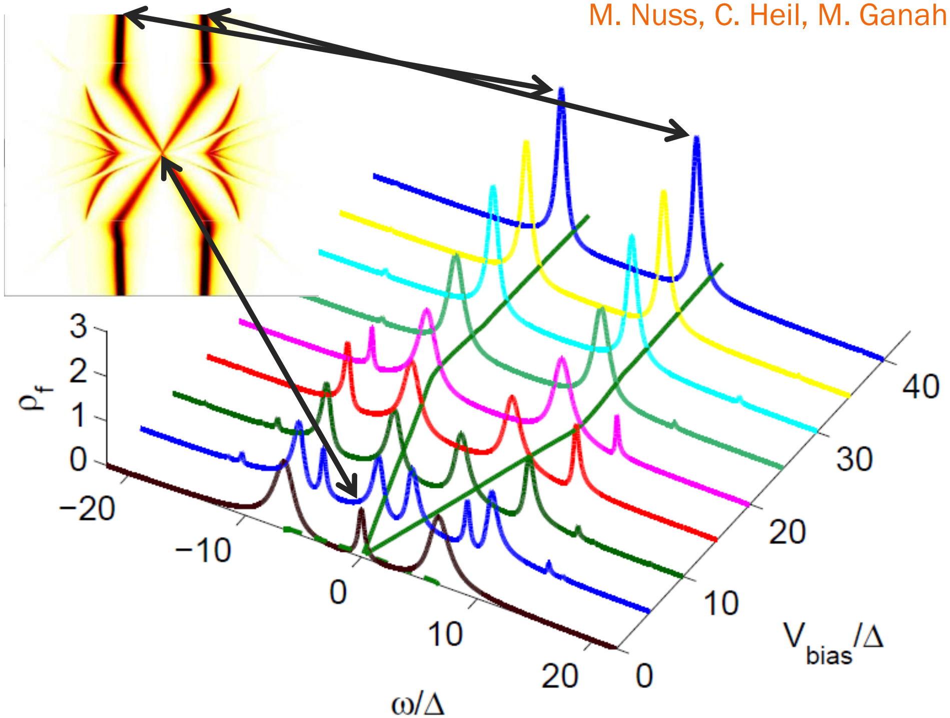
B: finite size eff. in Hubbard band

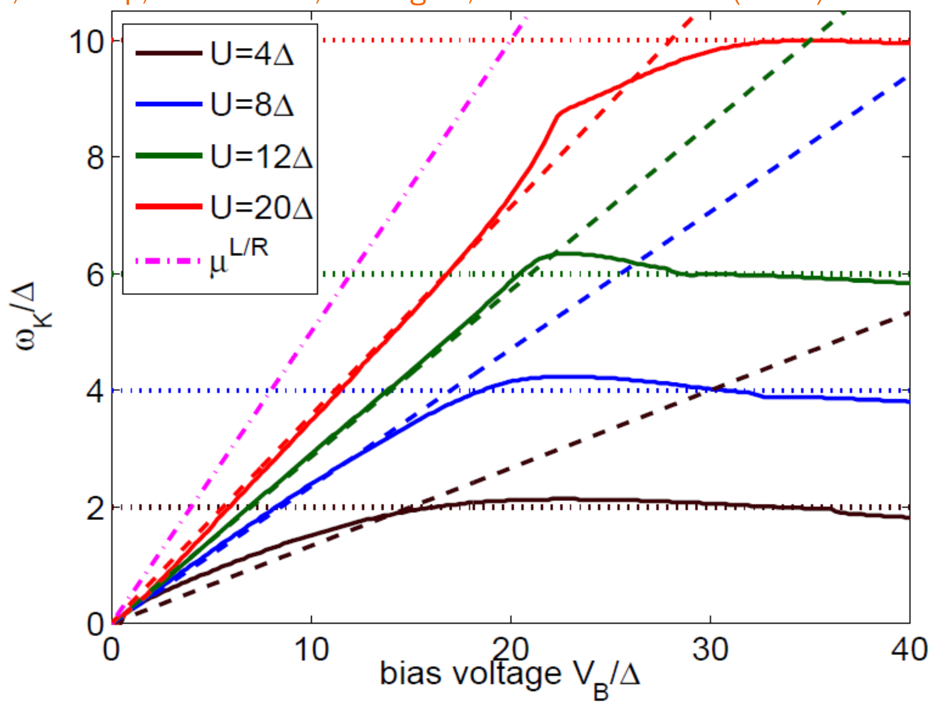
C: lead-band effects

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

Kondo resonance under bias

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

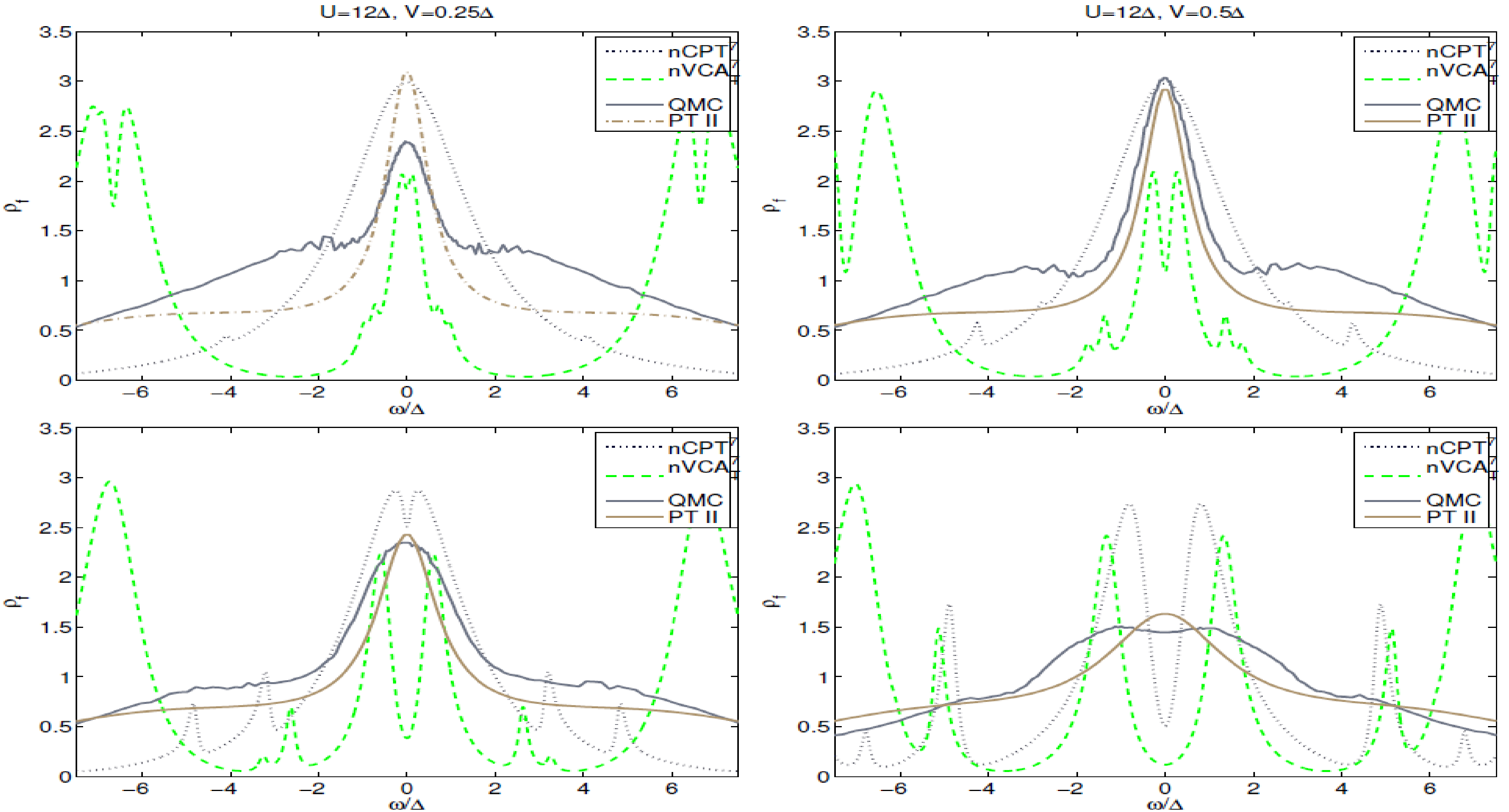




VCA: immediate linear splitting

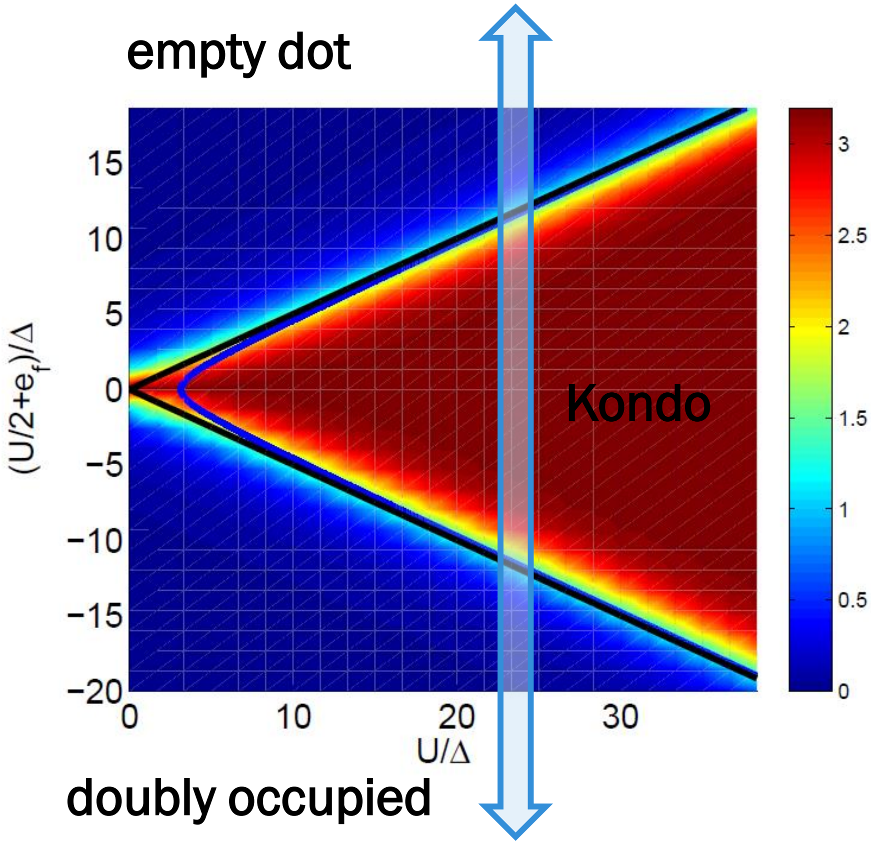
pinning not exactly at chemical potential but U dependent

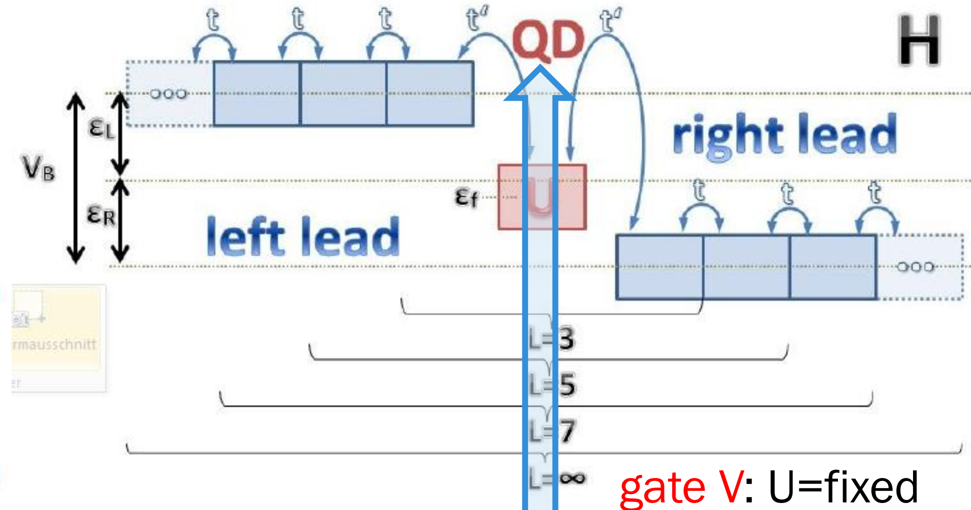
Kondo resonance under bias



A. Dirks, J. E. Han, M. Jarrell, T. Pruschke (2012)
M. Nuss, C. Heil, M. Ganahl, M.-Knap, H. G. Evertz, E. Arrigoni, W. von der Linden (2012)

applying a gate voltage

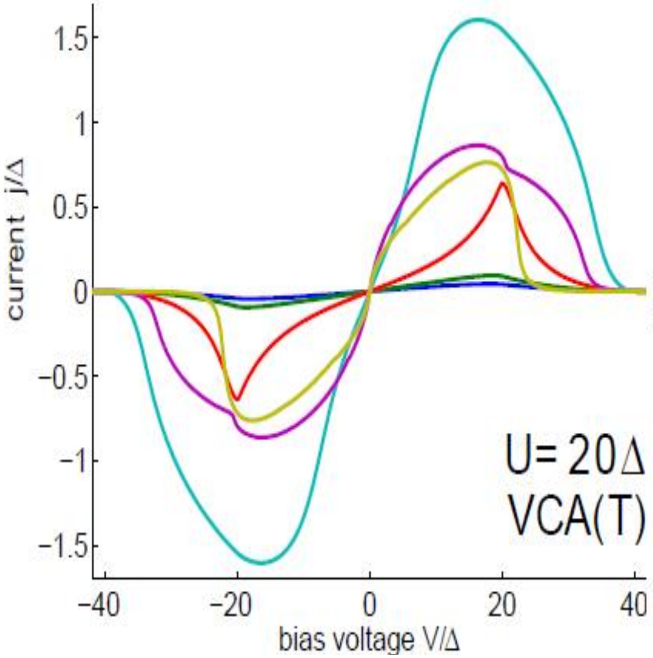


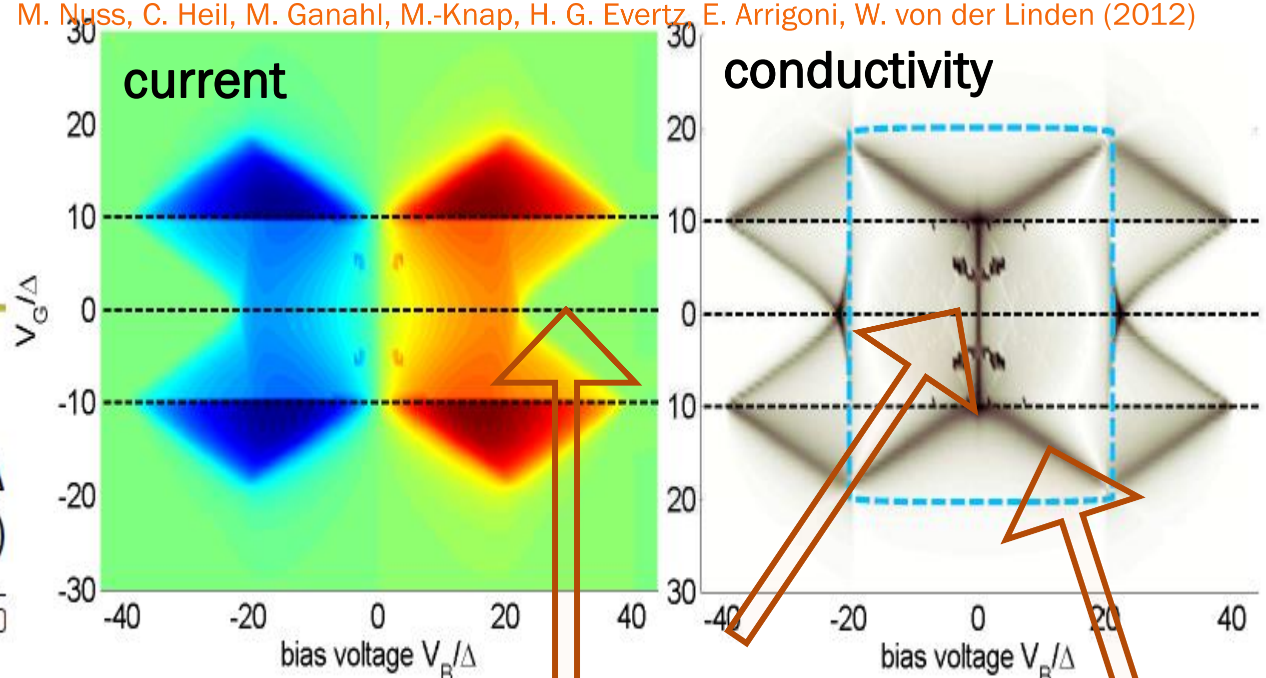


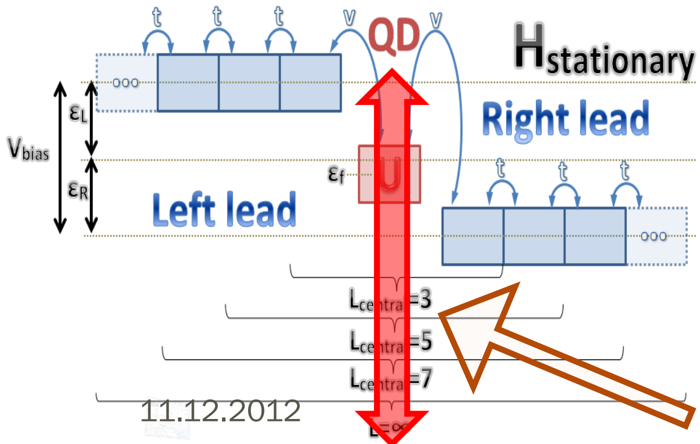
M. Nuss, E. Arrigoni, M. Aichhorn, W. vd Linden (2012)

applying a gate voltage

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







Kondo

coulomb blockade

results from previous slides Vgate=0

gate V: U=fixed

Conclusions + Outlook

- steady-state: Quantum Dot
  - good current density up to intermediate U
  - agrees with TEBD benchmark
  - linear U dep. splitting of Kondo resonance
  - Kondo regime + Coulomb blockade
  - nVCA >> nCPT: variational feedback crucial

- non-equilibrium Variational Cluster Approach
  - applicable to any fermionic bosonic lattice Hamiltonian
  - benchmark on SIAM good
  - more complex models, interactions, versatile and flexible
  - dynamic quantities out of equilibrium (real)
  - realistic materials: combine with ab-initio

Thank you!

maybe some day:

martin.nuss@student.tugraz.at

TUG

itp[cp]

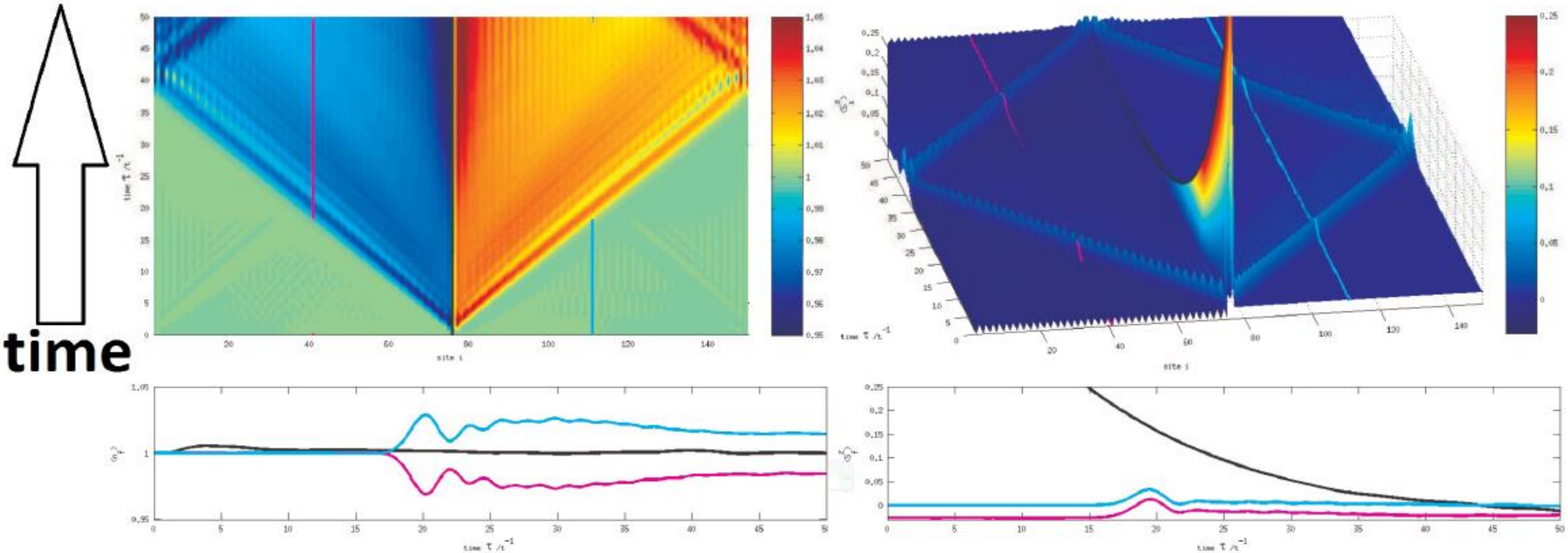
We gratefully acknowledge support from the Austrian Science Fund (FWF) P24081-N16 as well as the Vienna Scientific Cluster (VSC).

Time evolution of a quantum dot

particle number and spin projection

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

$$L = 150, U = 20\Delta, V_{\text{bias}} = 14\Delta$$

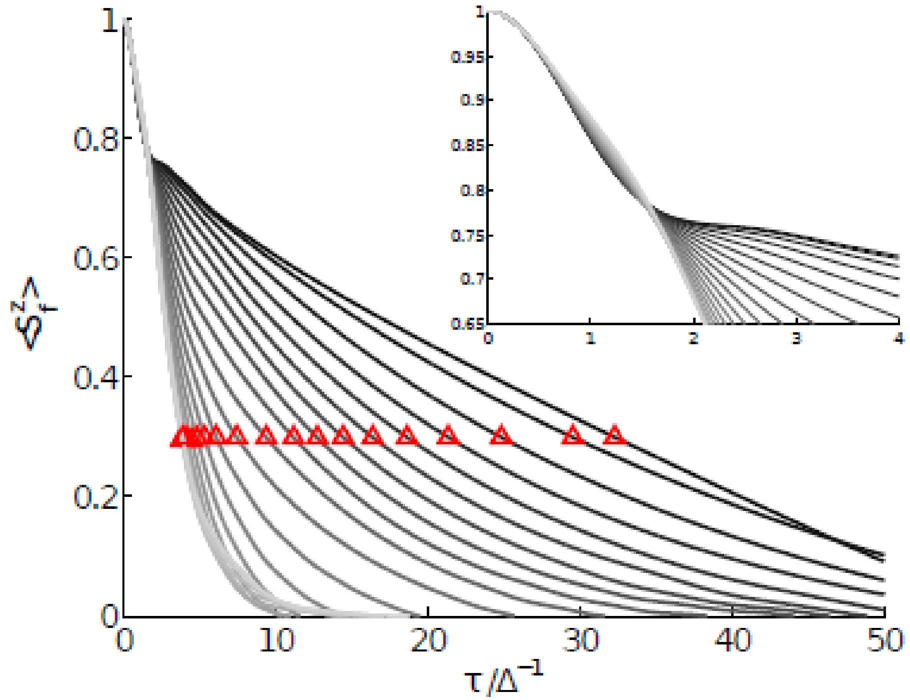


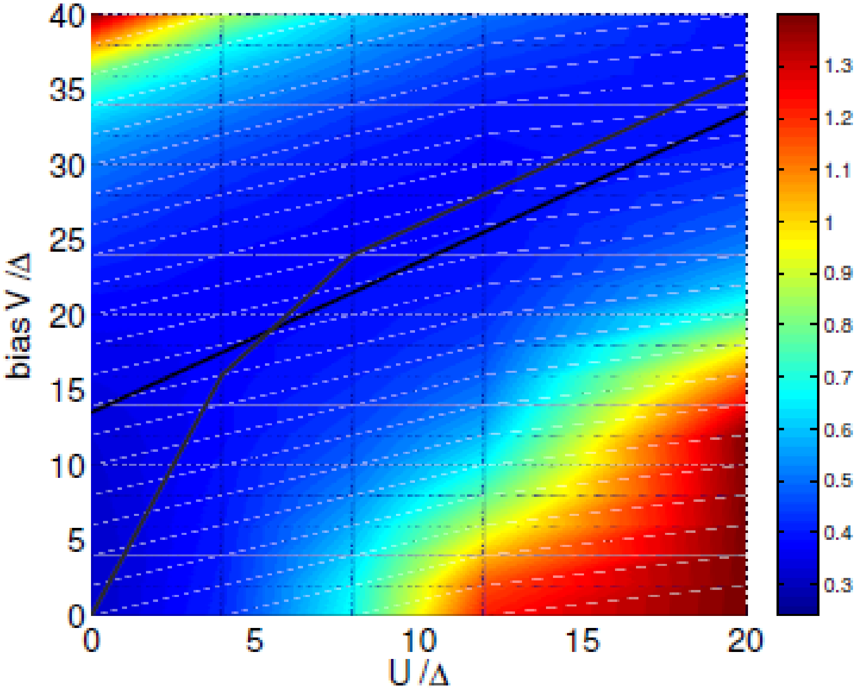
<n>

<S_z>

Spin relaxation

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





Entanglement

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