Quantum dots out of equilibrium

a non-equilibrium variational cluster approach

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

TUG

Ustron, 14.09.2012

itp[cp]

Agenda

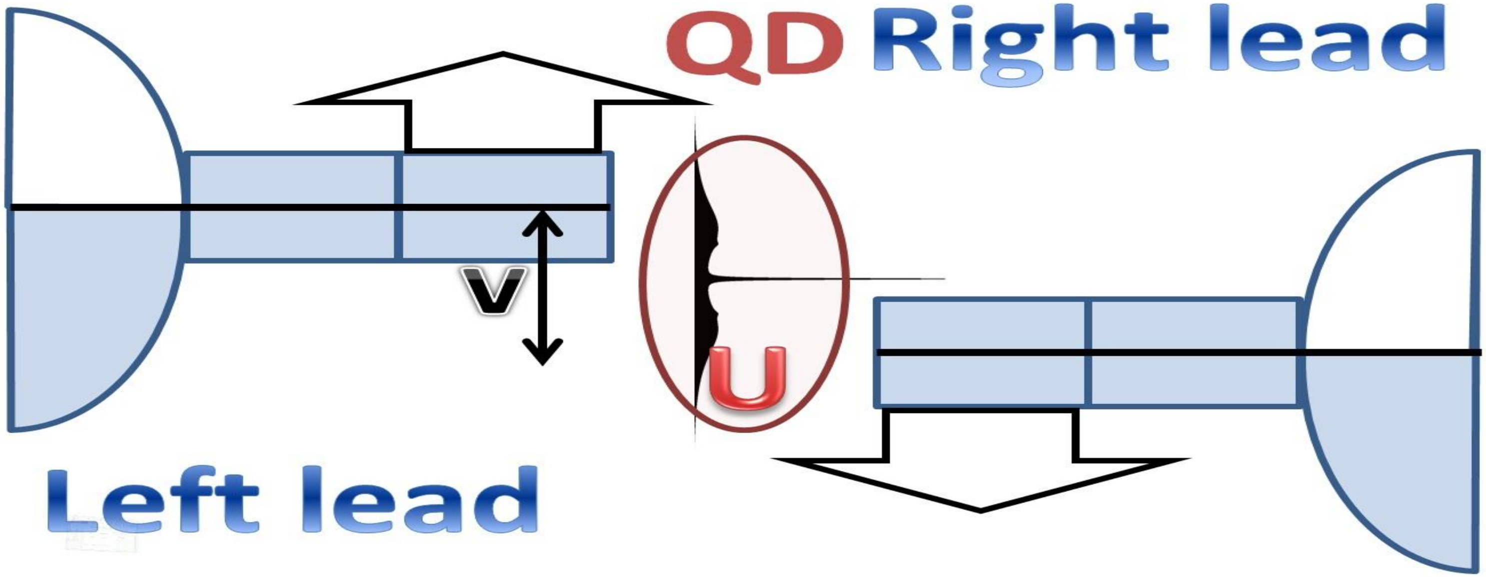
1. non-equilibrium phenomena - Quantum Dots
2. non-equilibrium Variational Cluster Approach
3. results: steady - state
4. (DMRG + TEBD time evolution)

Non-equilibrium phenomena – Quantum Dots

Transport through a strongly correlated object

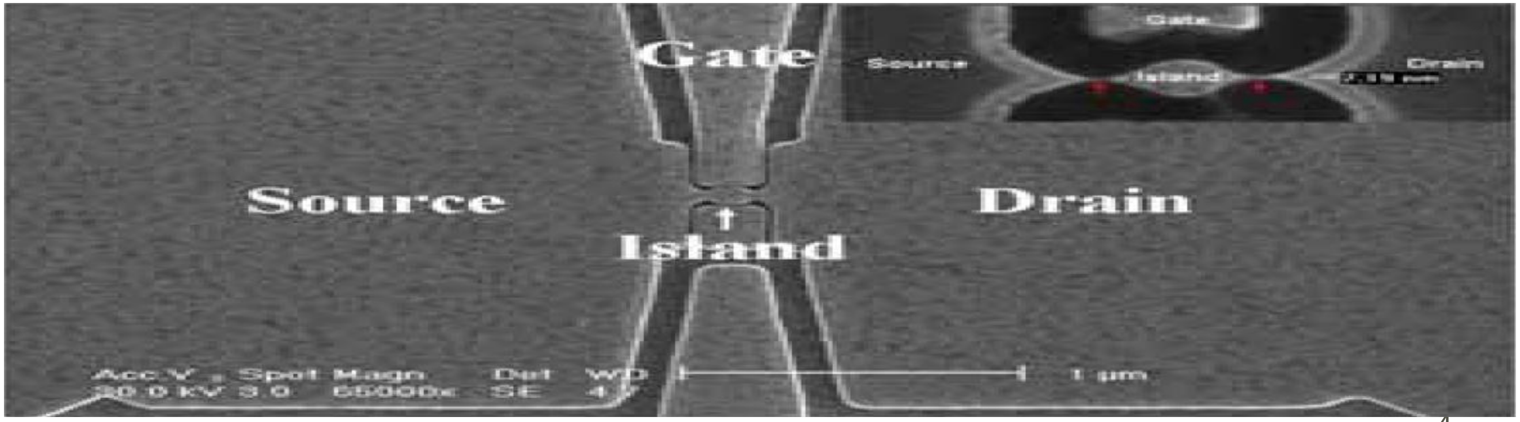
Single Impurity Anderson Model

P. W. Anderson (1961)



+

voltage bias



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

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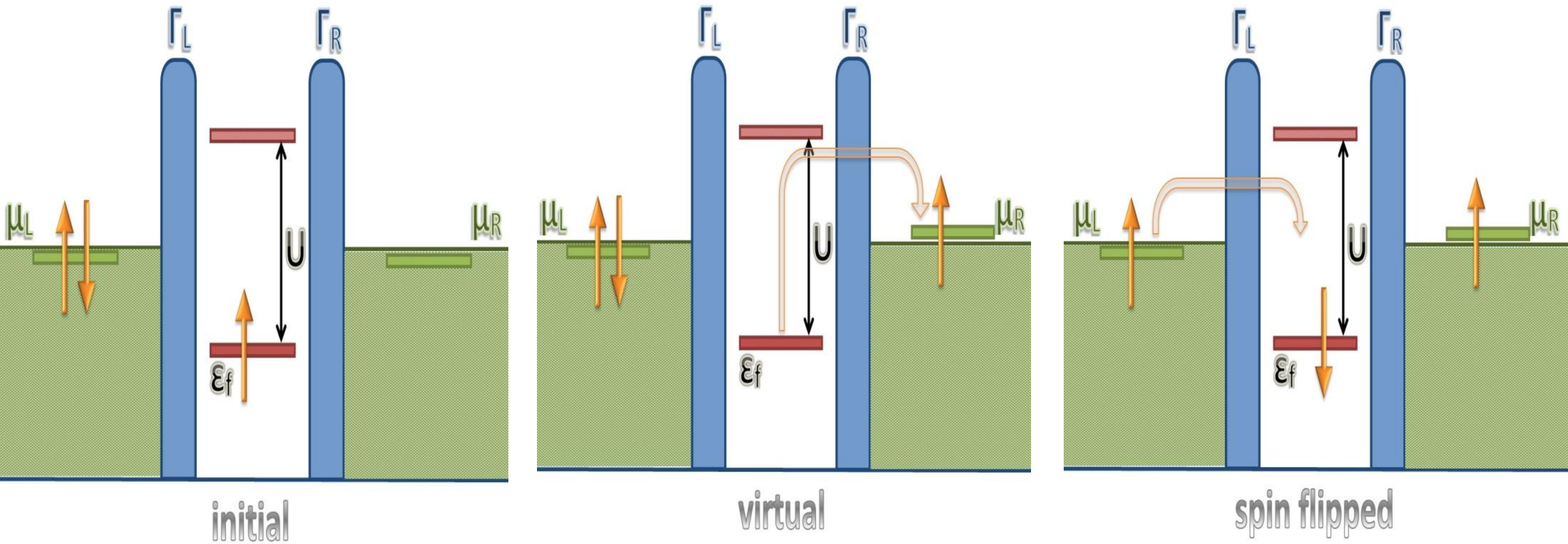
Transport through a strongly correlated object



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

need:

single particle Green's function G in Keldysh space

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

Non-equilibrium Variational Cluster Approach

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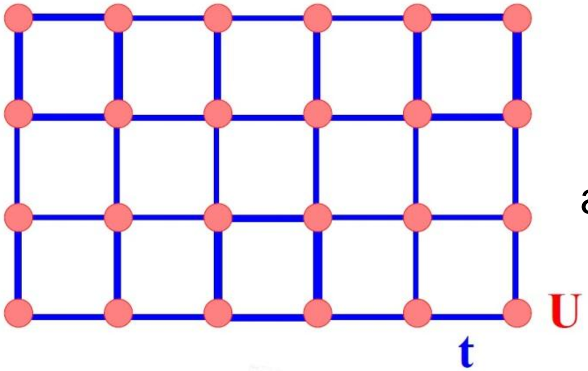
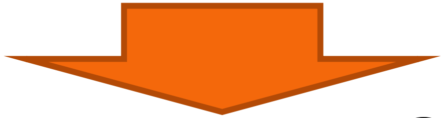
Many-Body cluster methods



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

ask for **G**

in general unsolvable



Strategy ?

1) 

2) 

3) 

4) 

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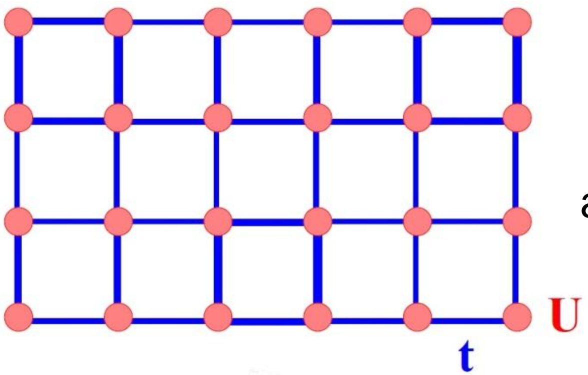
Many-Body cluster methods



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

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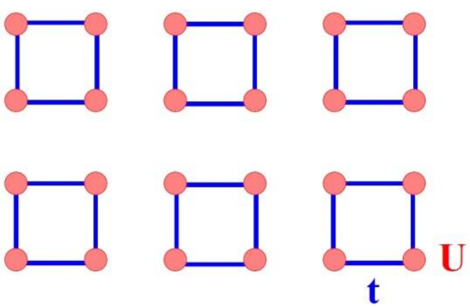
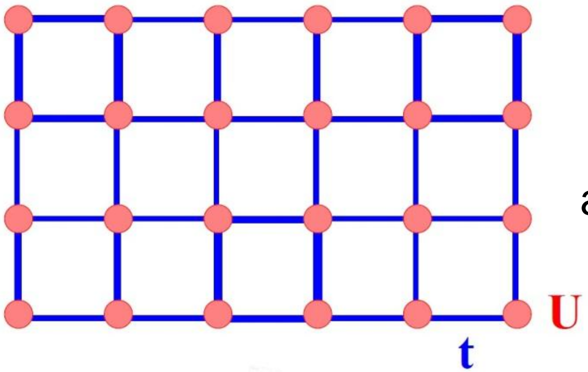
Strategy ?

1) CUT 2) 3) 4)



Many-Body cluster methods



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

ask for G

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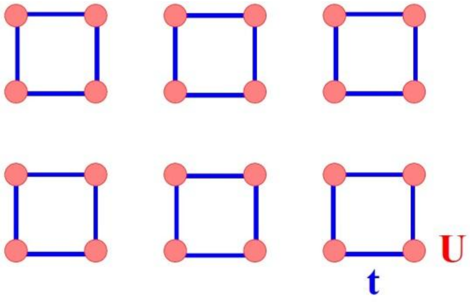
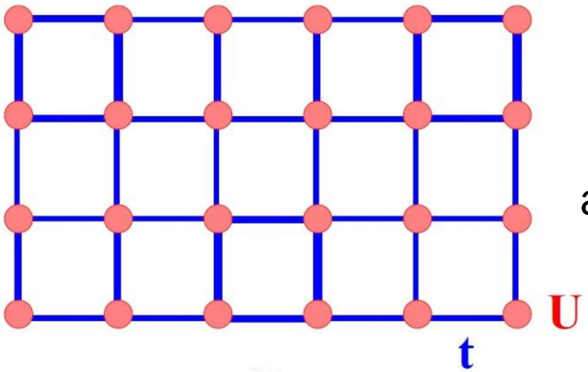
Strategy ?

1) CUT 2) SOLVE 3) 4)



$G_{cluster}$ = exactly solvable

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)

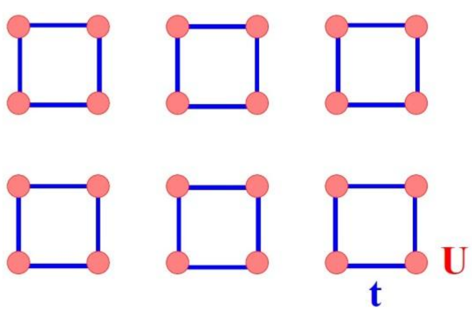
first order strong coupling perturbation theory

1) **CUT**

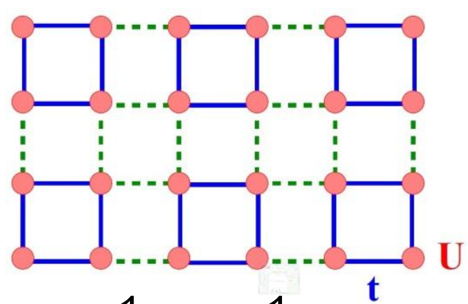
2) **SOLVE**

3) **GLUE**

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



G_{cluster} = exactly solvable



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

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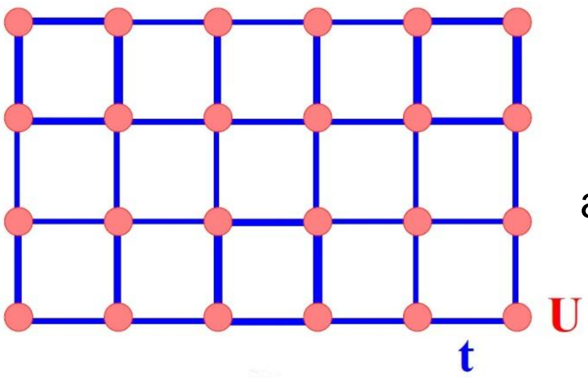
Many-Body cluster methods

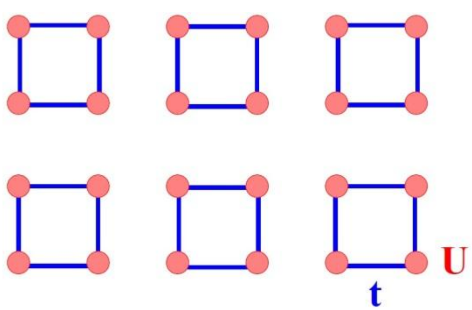


given $\hat{\mathcal{H}}$

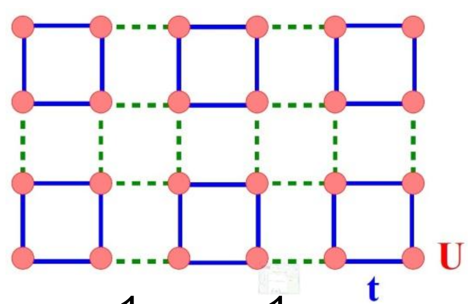
ask for **G**

- **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)

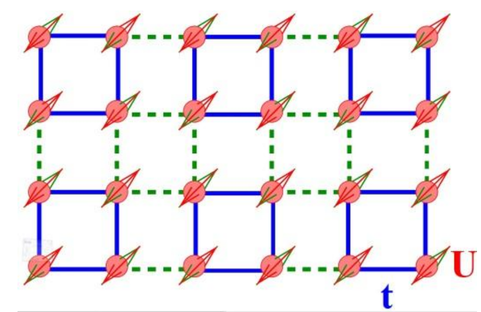
1) CUT   2) SOLVE   3) GLUE   4) ADD FIELDS



$G_{cluster}$ = exactly solvable



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



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

M. Potthoff (2003)

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

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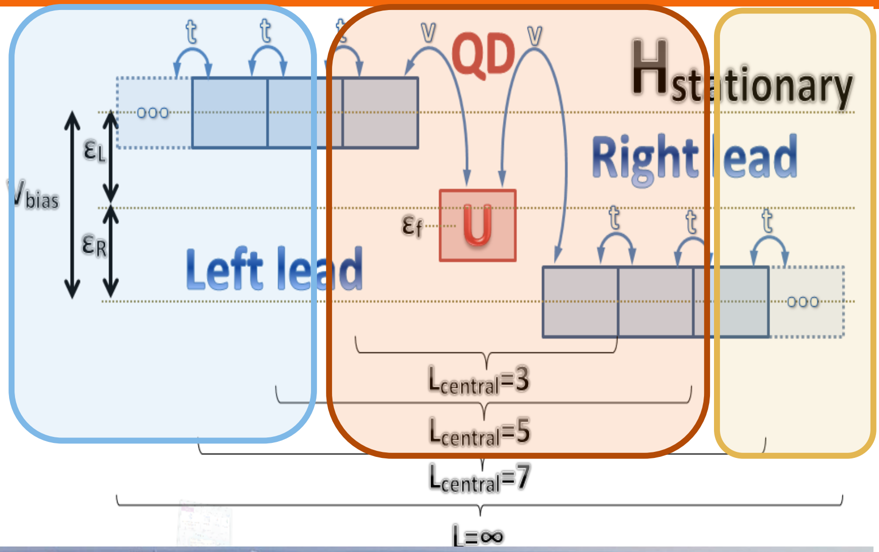
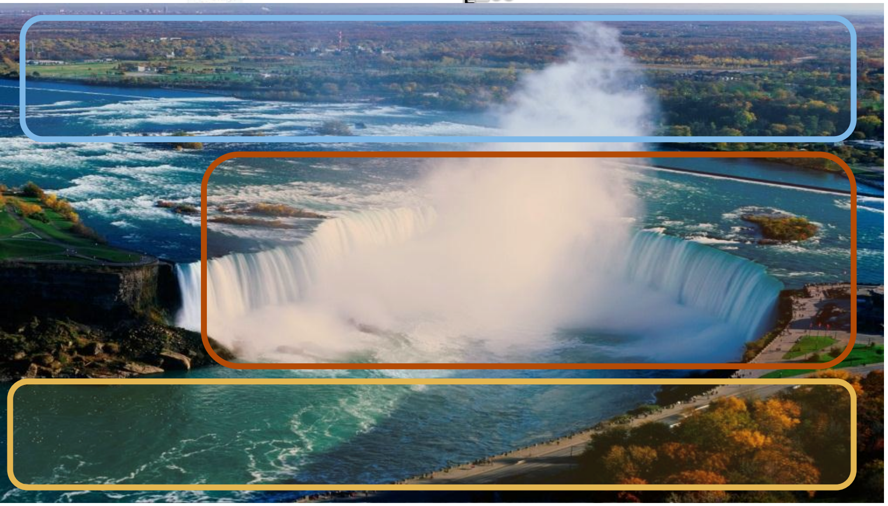
Non-equilibrium Variational Cluster Approach





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

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

CPT time evolution

M. Balzer, M. Potthoff (2011)

VCA steady-state

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

http://www.niagarafallslive.com

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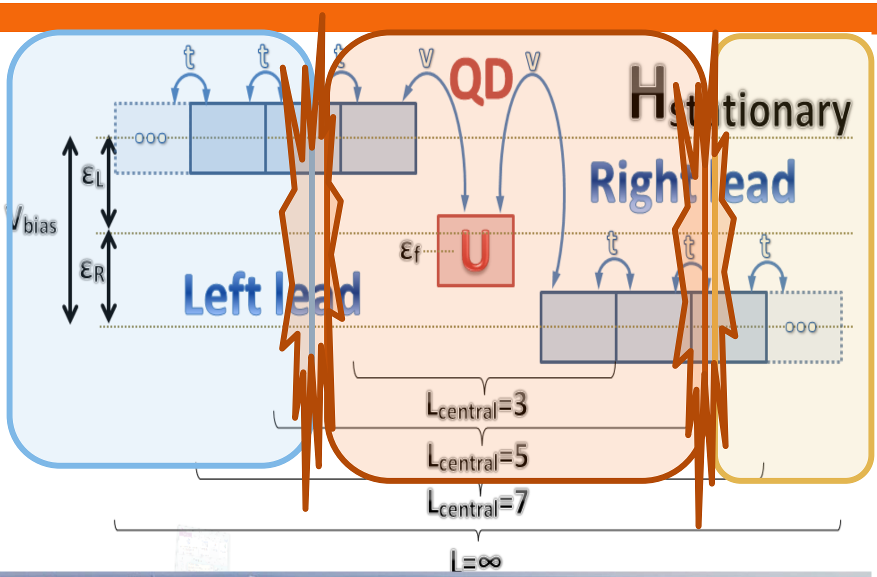
Non-equilibrium Variational Cluster Approach



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

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

@ τ_0 cpl. T switched on

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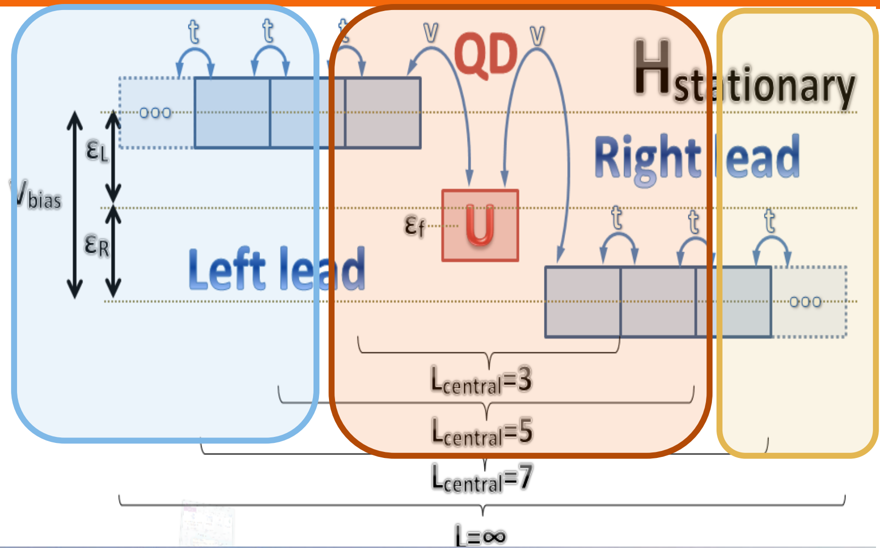
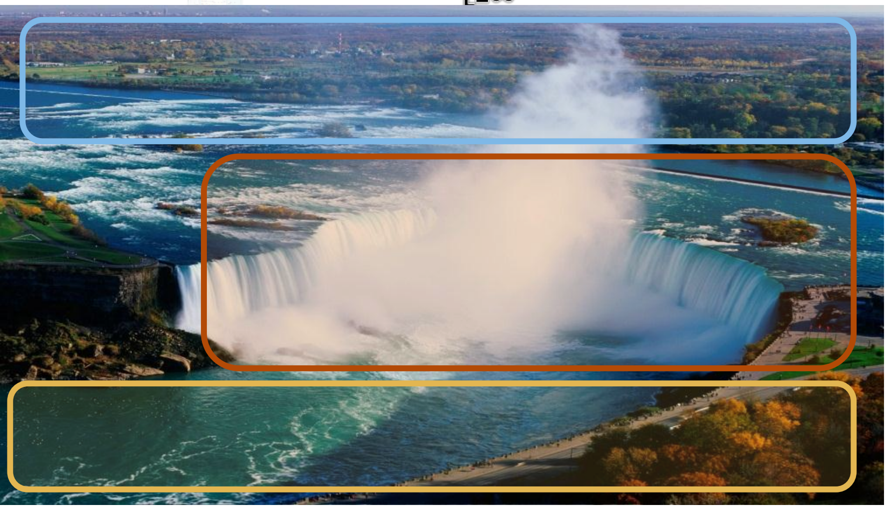
Non-equilibrium Variational Cluster Approach





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

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

@ τ_0 — cpl. T switched on

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

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

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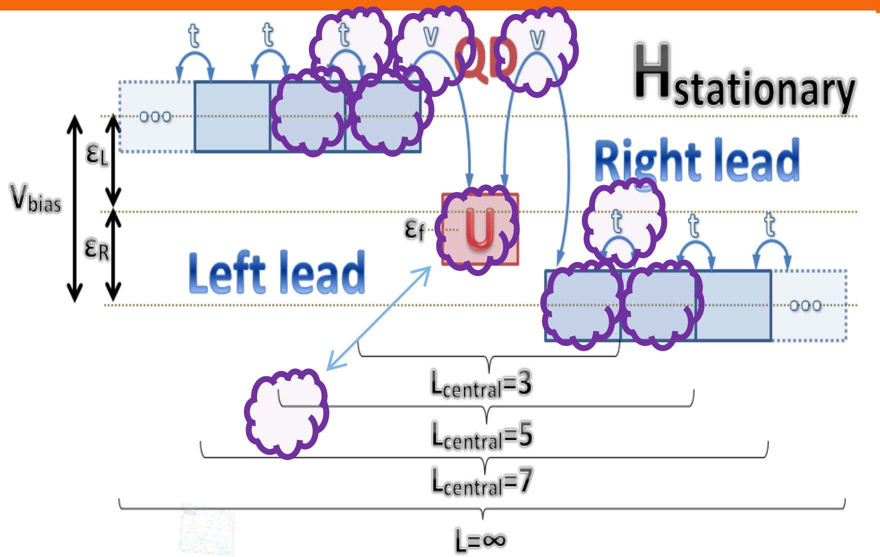
Non-equilibrium Variational Cluster Approach



non unique decomposition

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

CPT approximation

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

optimize initial state: VCA

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

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

flexible self-energy $\Sigma(\mathrm{x})$

variational principle

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

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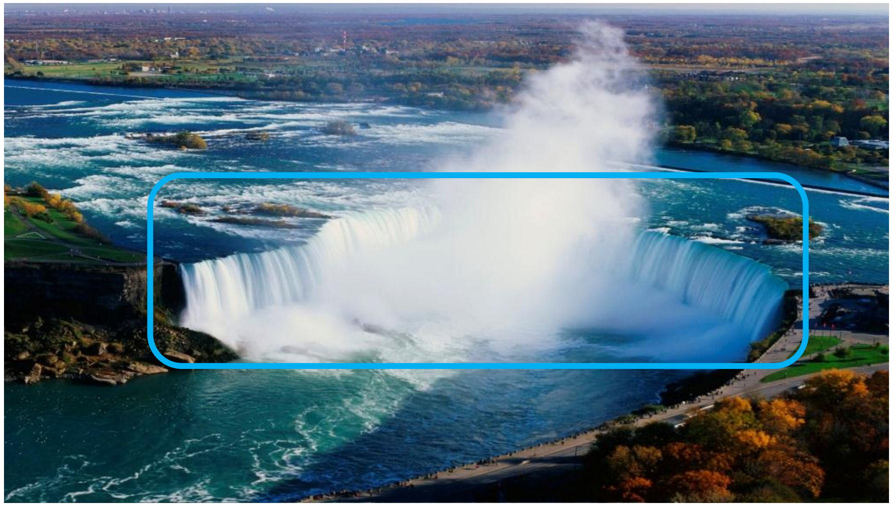
Non-equilibrium Variational Cluster Approach

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

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

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

$\cong$

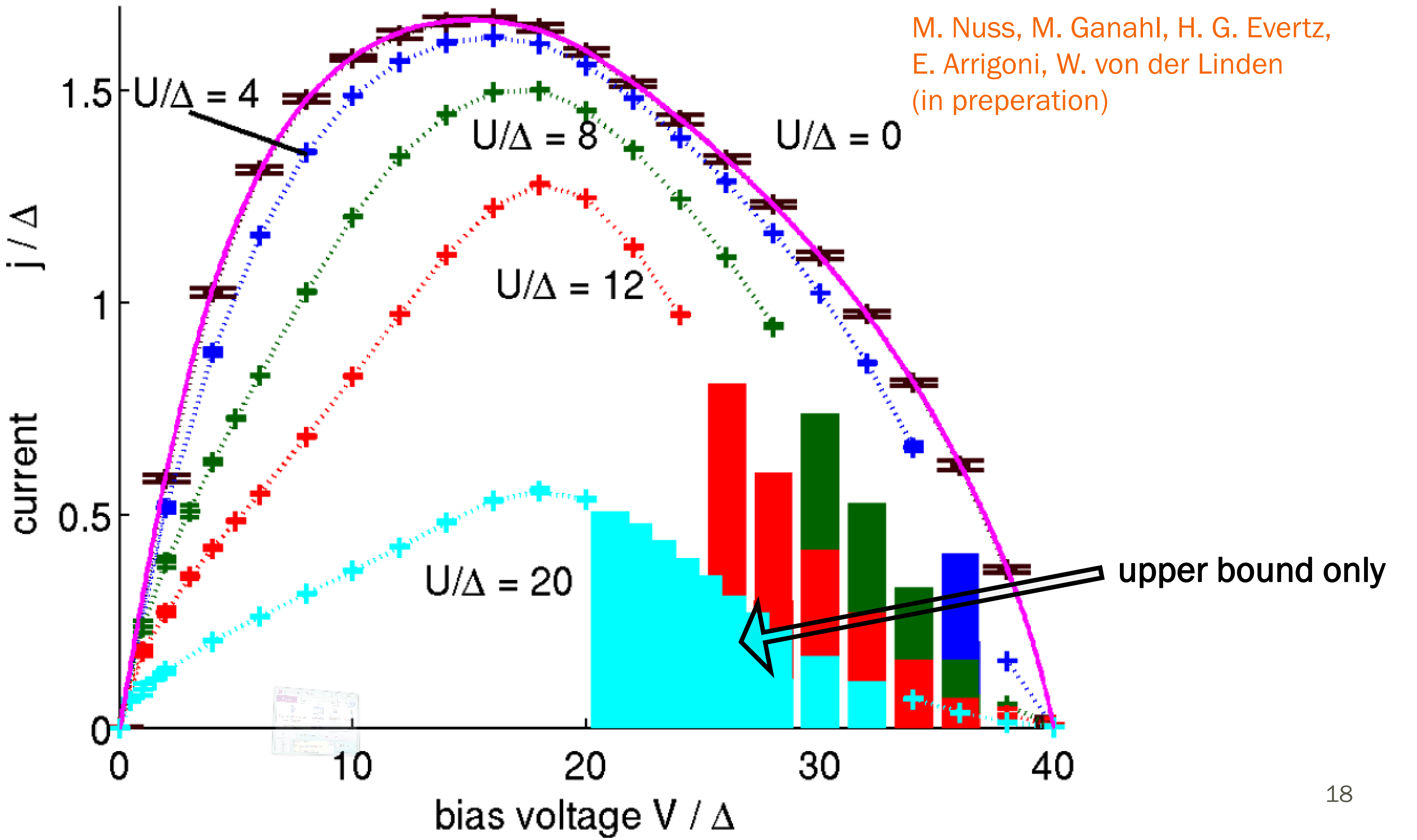


initial reference **system** *as similar as possible to* **the steady-state system**

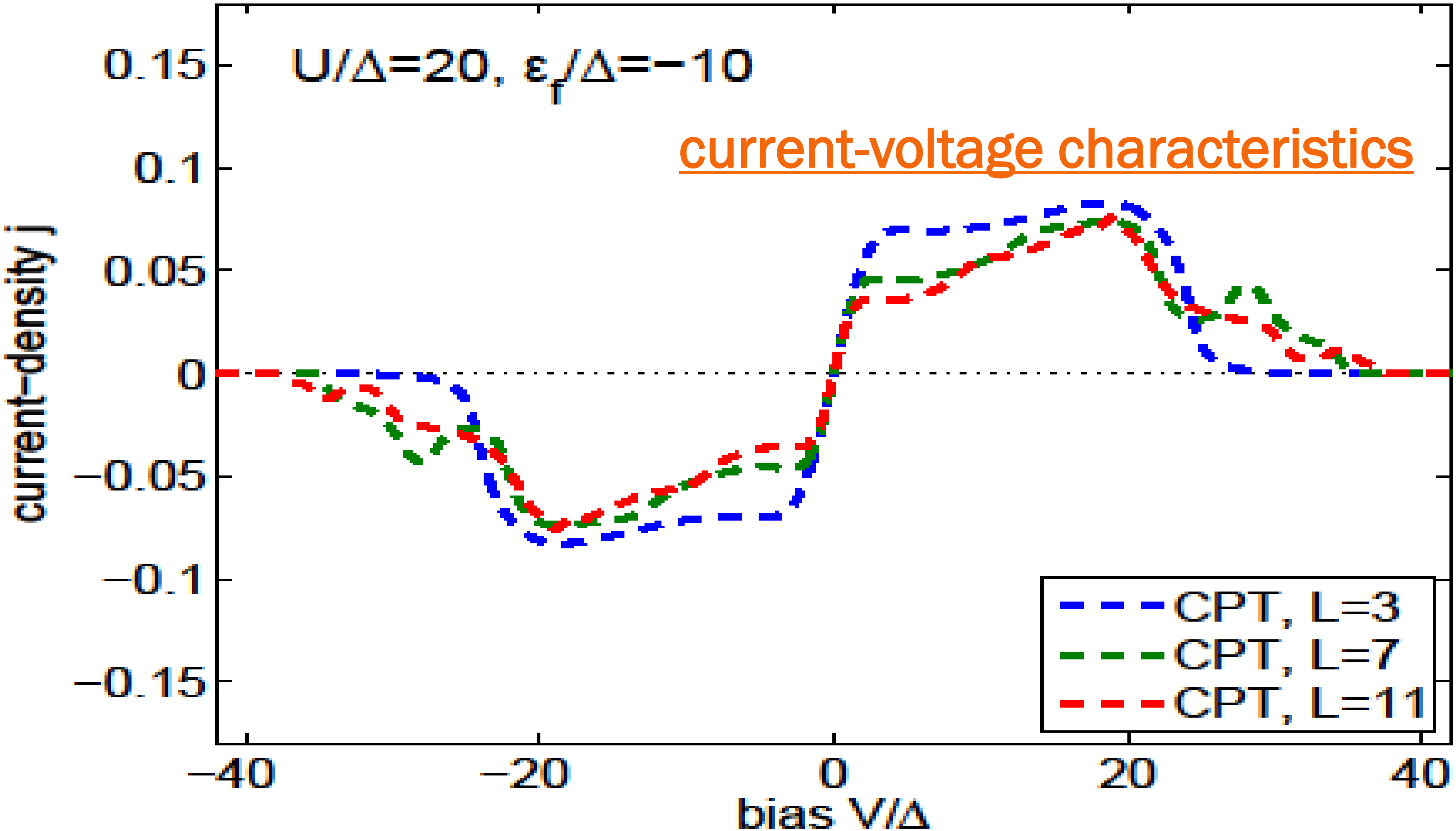
Steady-state properties of a quantum dot

DMRG+TEBD current-voltage characteristics

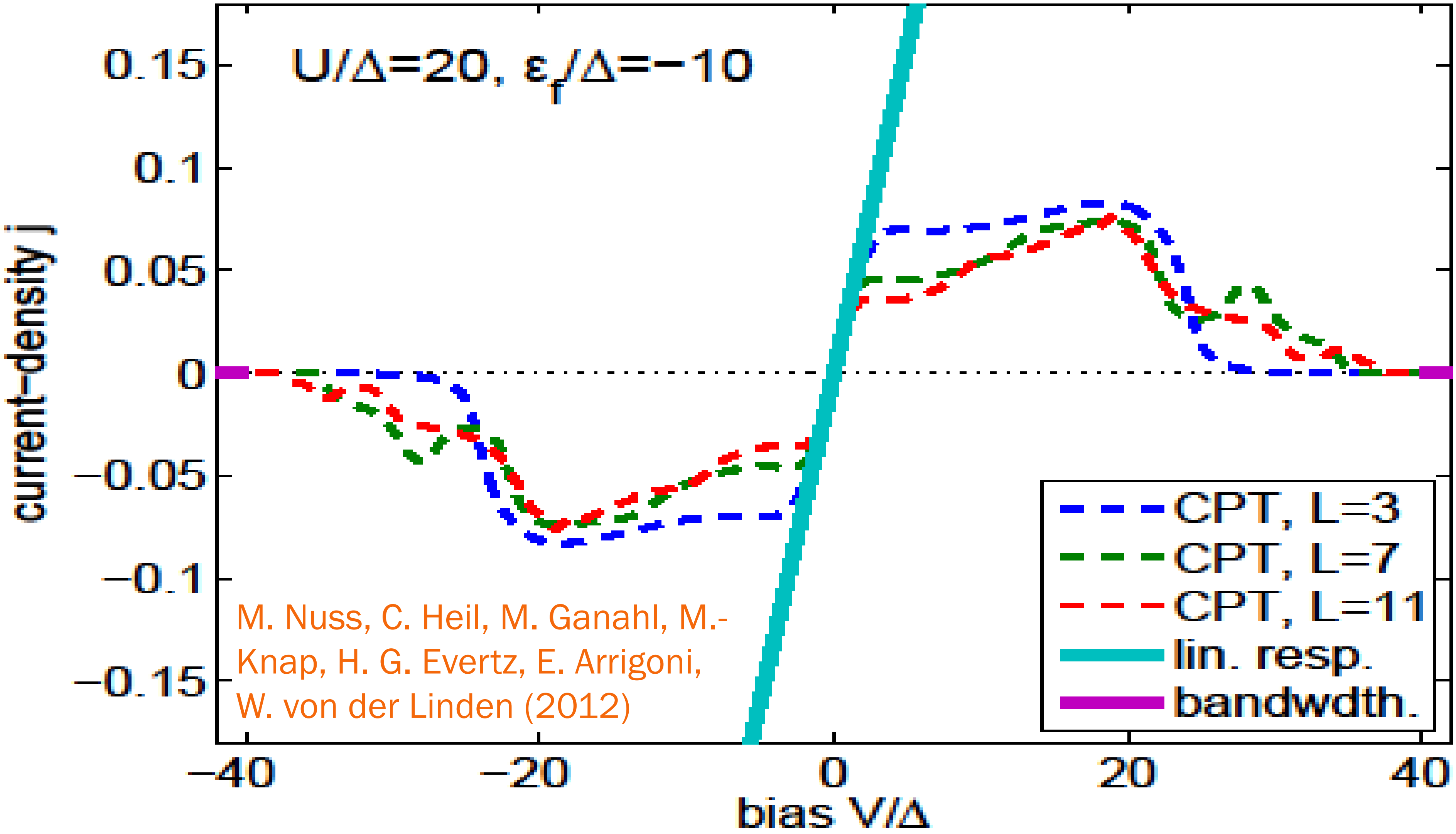
M. Nuss, M. Ganahl, H. G. Evertz,
E. Arrigoni, W. von der Linden
(in preperation)



non-equilibrium CPT



exact limits



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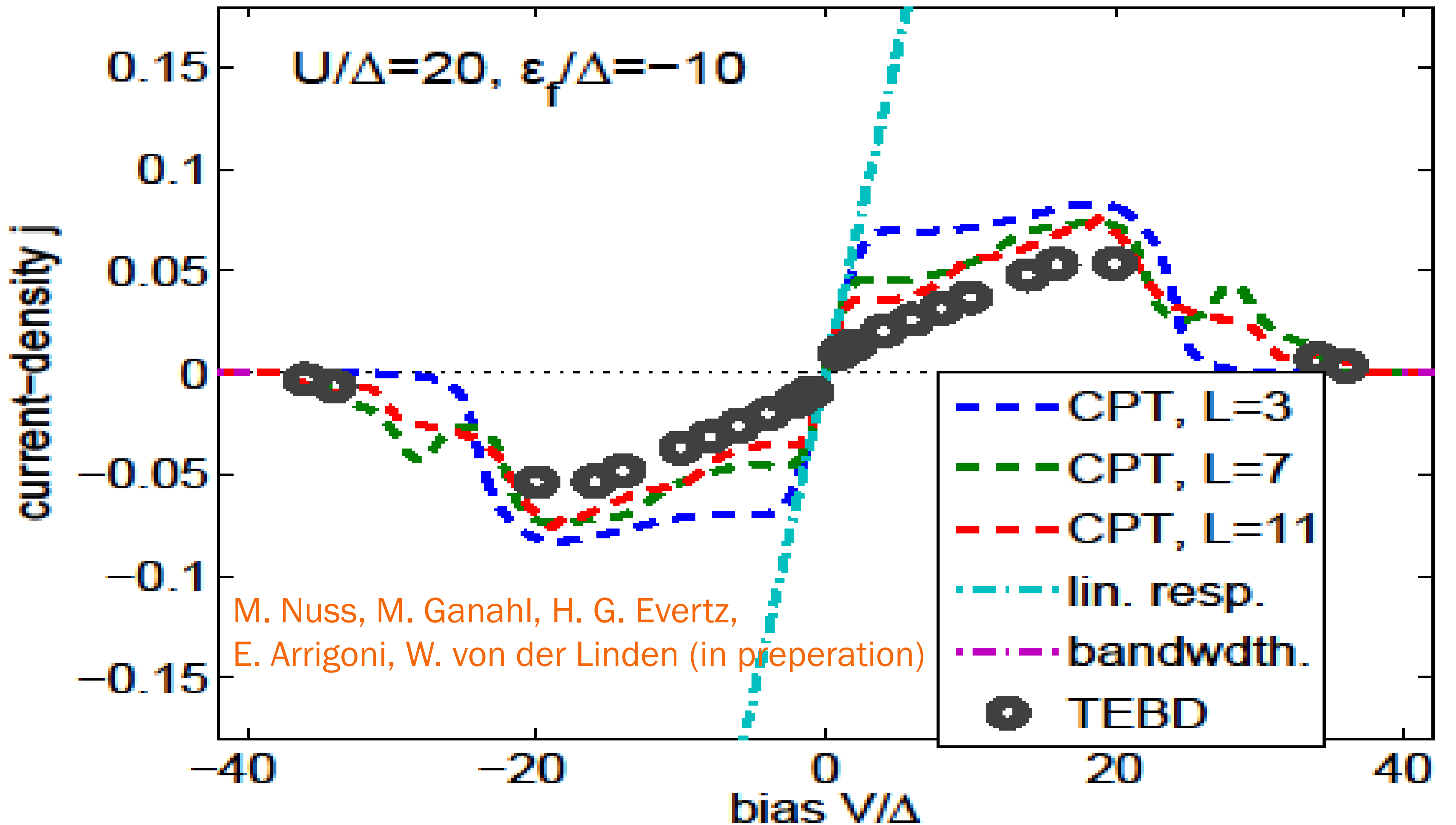
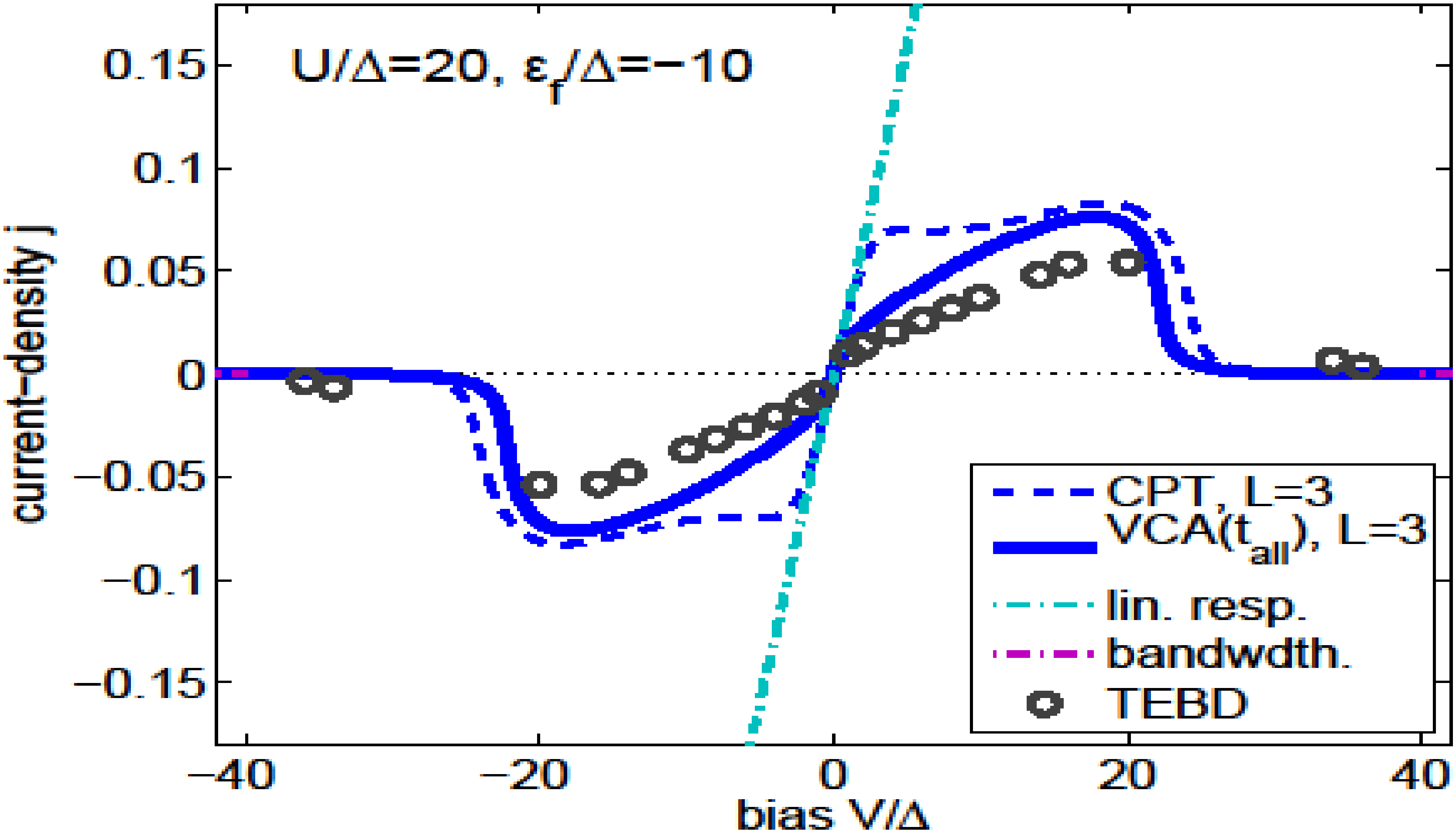
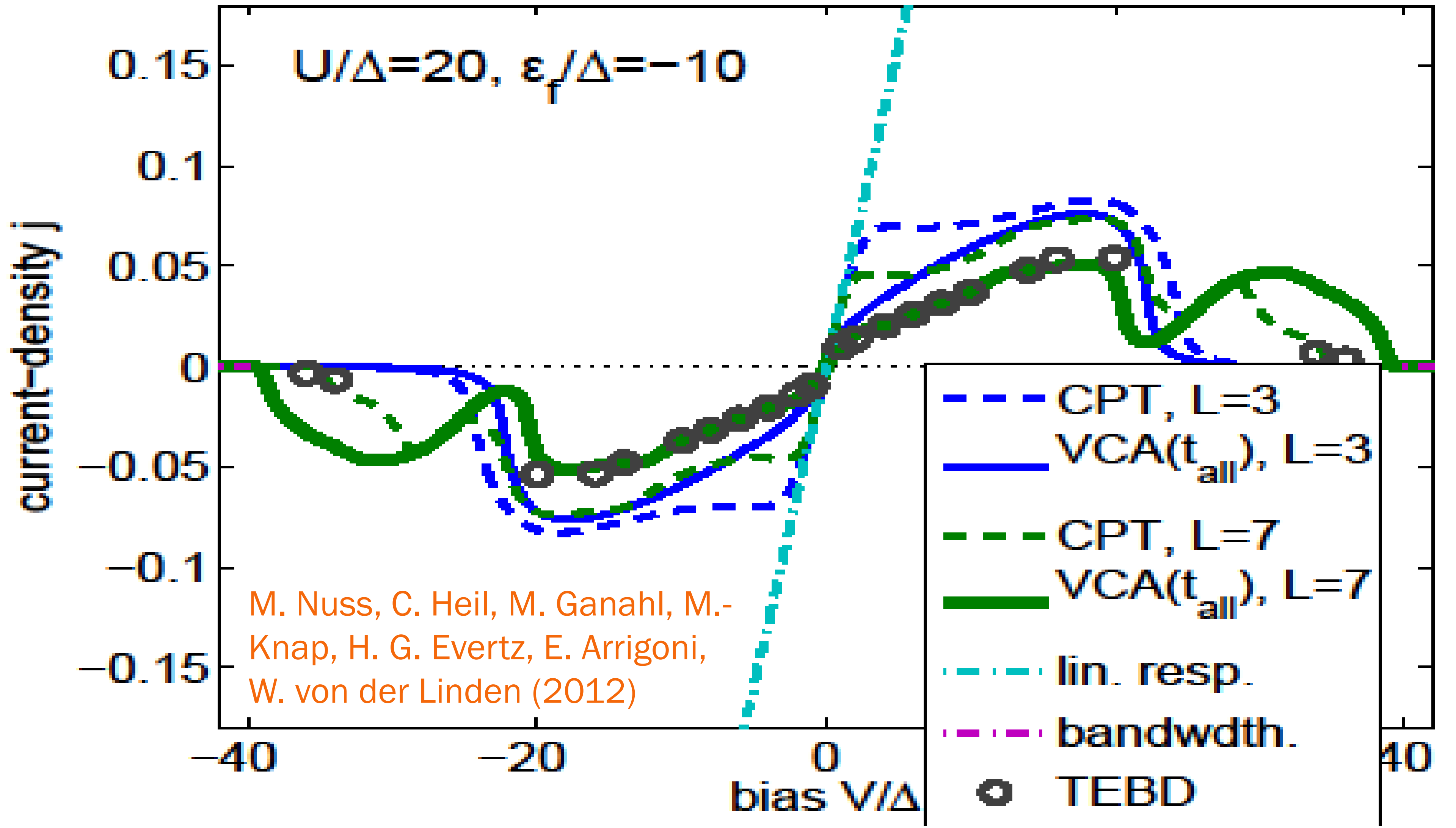
quasi-exact DMRG+TEBD



non-equilibrium VCA

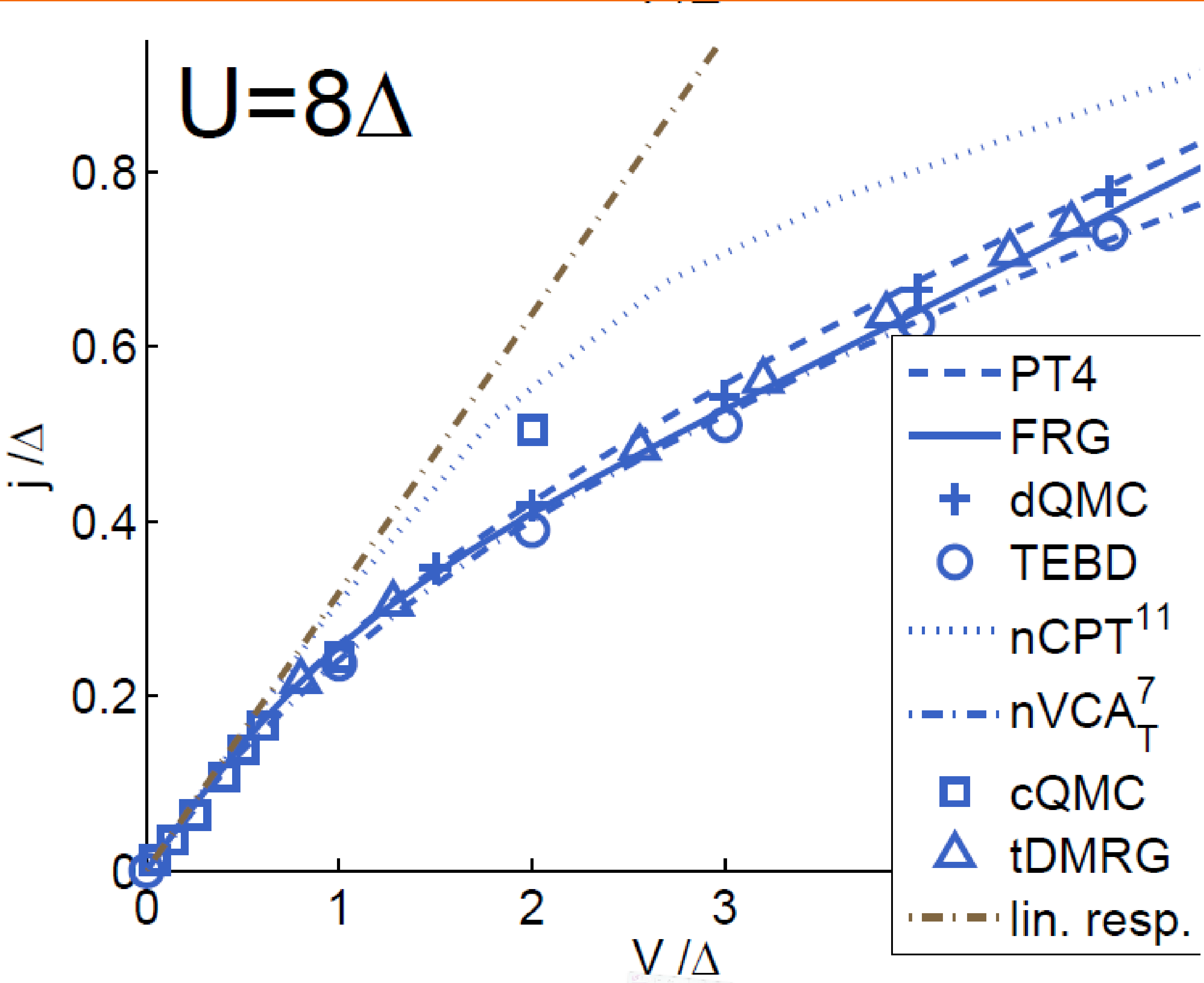


non-equilibrium VCA



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

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)

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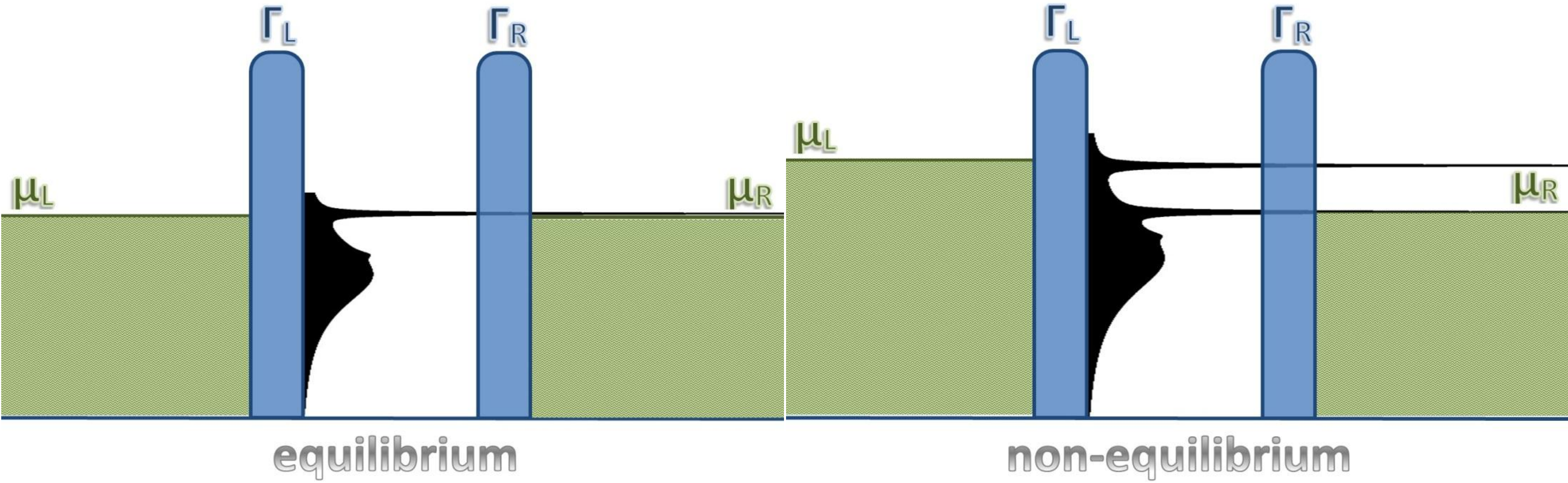
non-equilibrium local density of states



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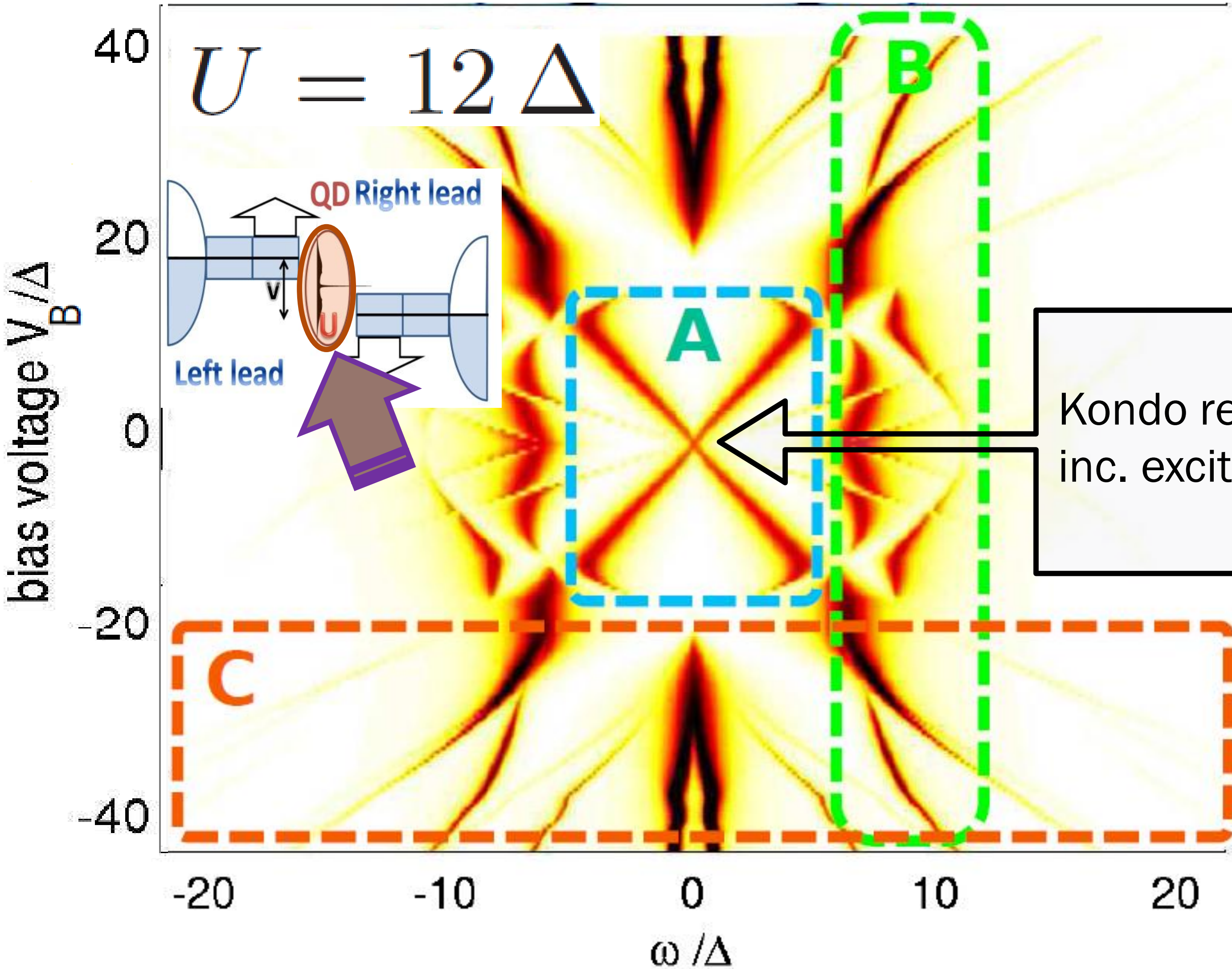
non-equilibrium local density of states



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

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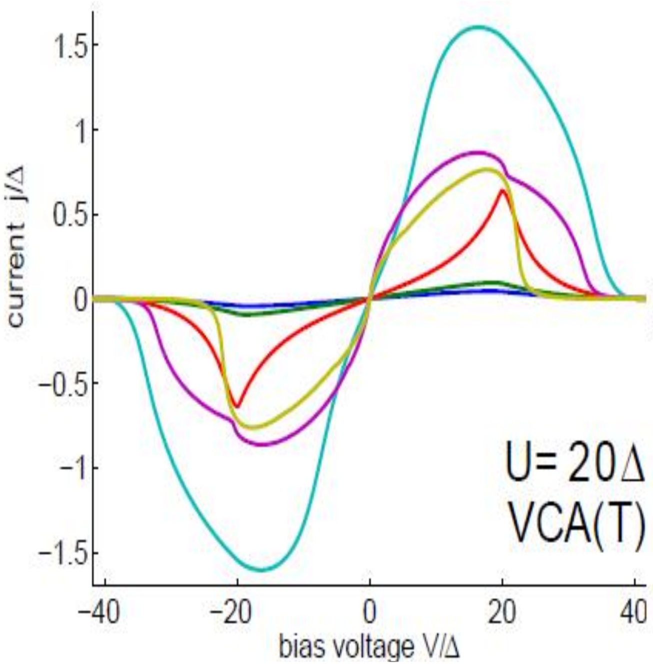
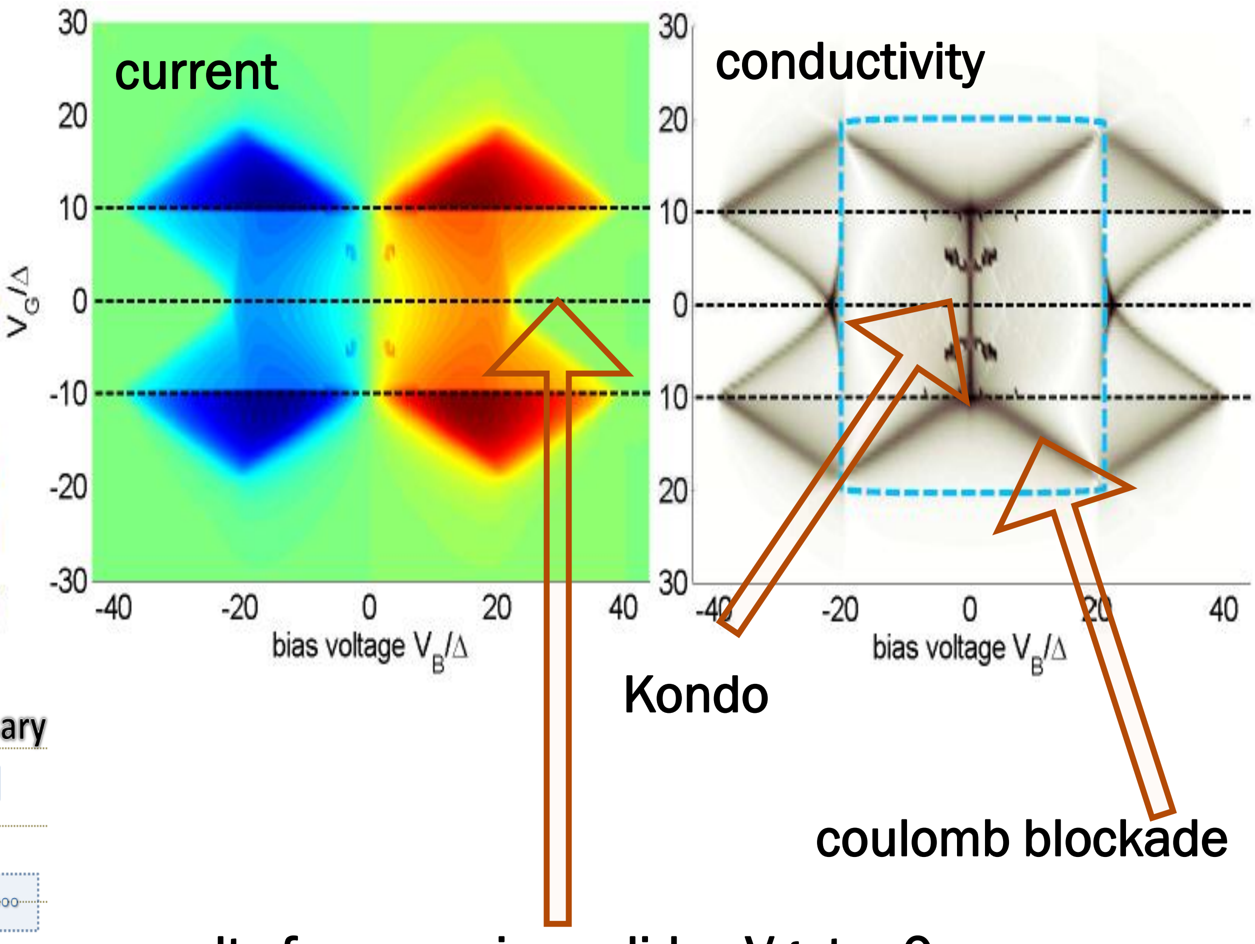
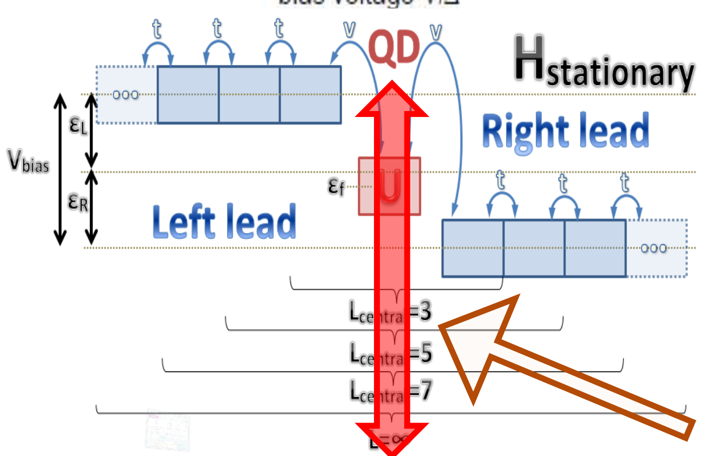
applying a gate voltage







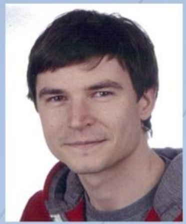
results from previous slides Vgate=0

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
  - realistic materials: combine with ab-initio



Christoph Heil

Michael Knap

Martin Nuss

Prof. Wolfgang von der Linden

Prof. Enrico Arrigoni

non-equilibrium group at TUG

Prof. Hans Gerd Evertz

Martin Ganahl

Martin Nuss

Thank you!

maybe some day:

martin.nuss@student.tugraz.at

TUG

itp^cp

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Time evolution after a quench of a quantum dot

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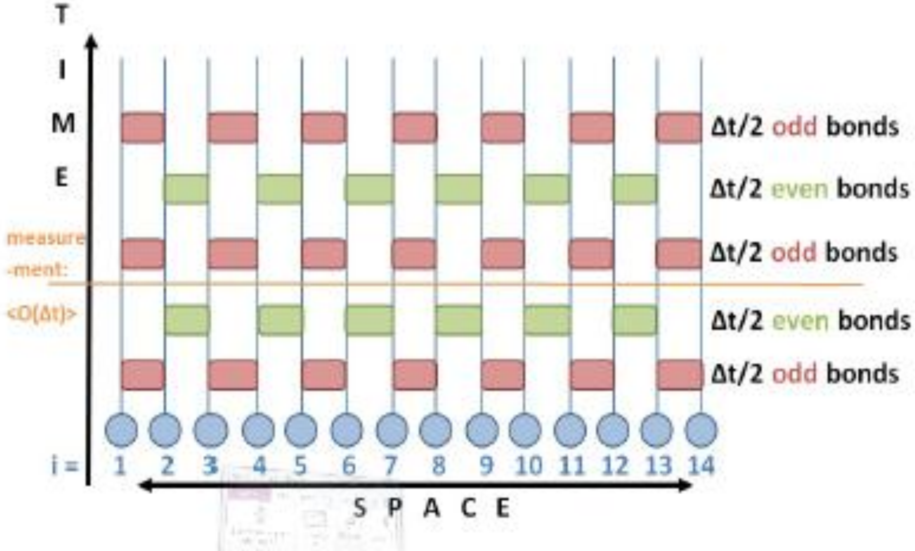
Real time evolution with matrix product states

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

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



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)

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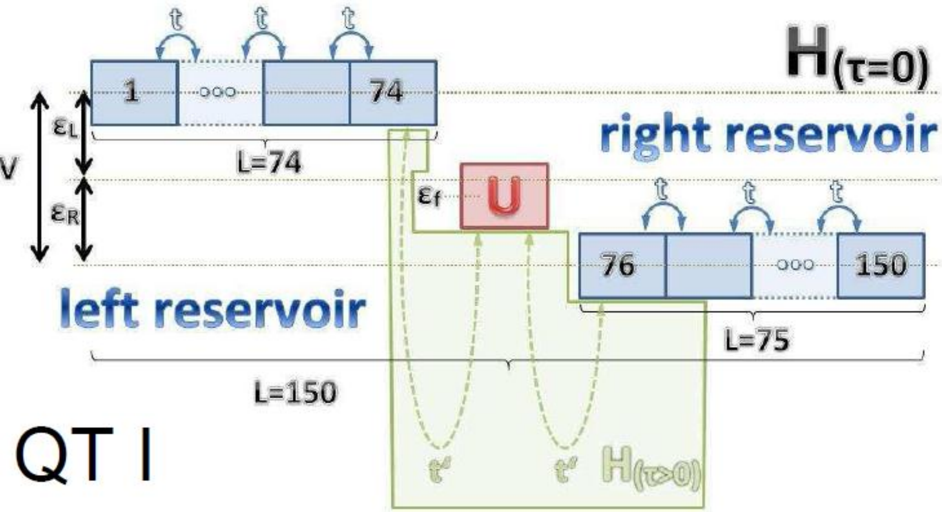
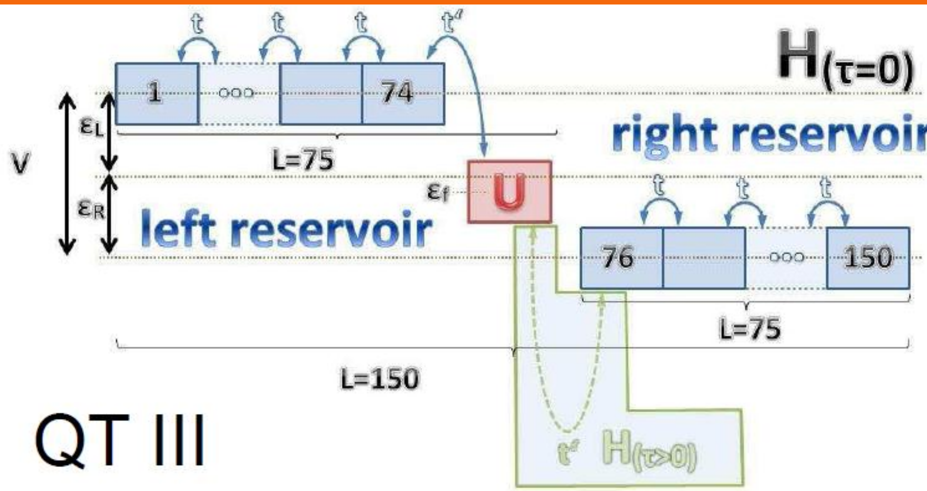
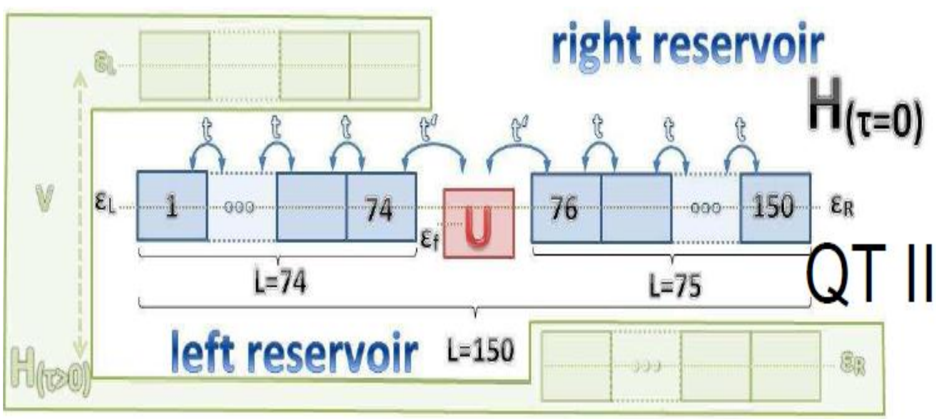
3 different quneches



QT I



QT III



QT II

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
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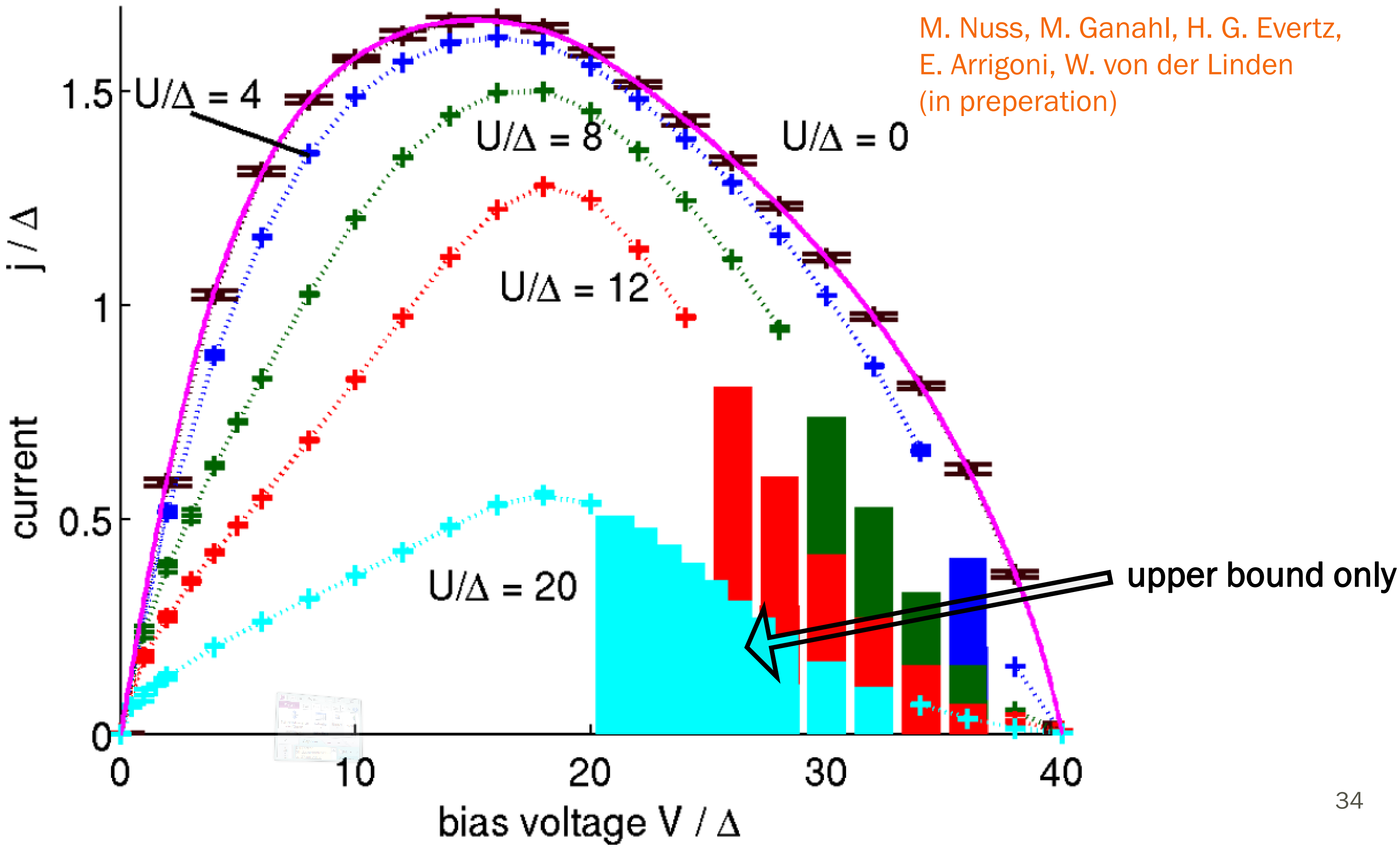
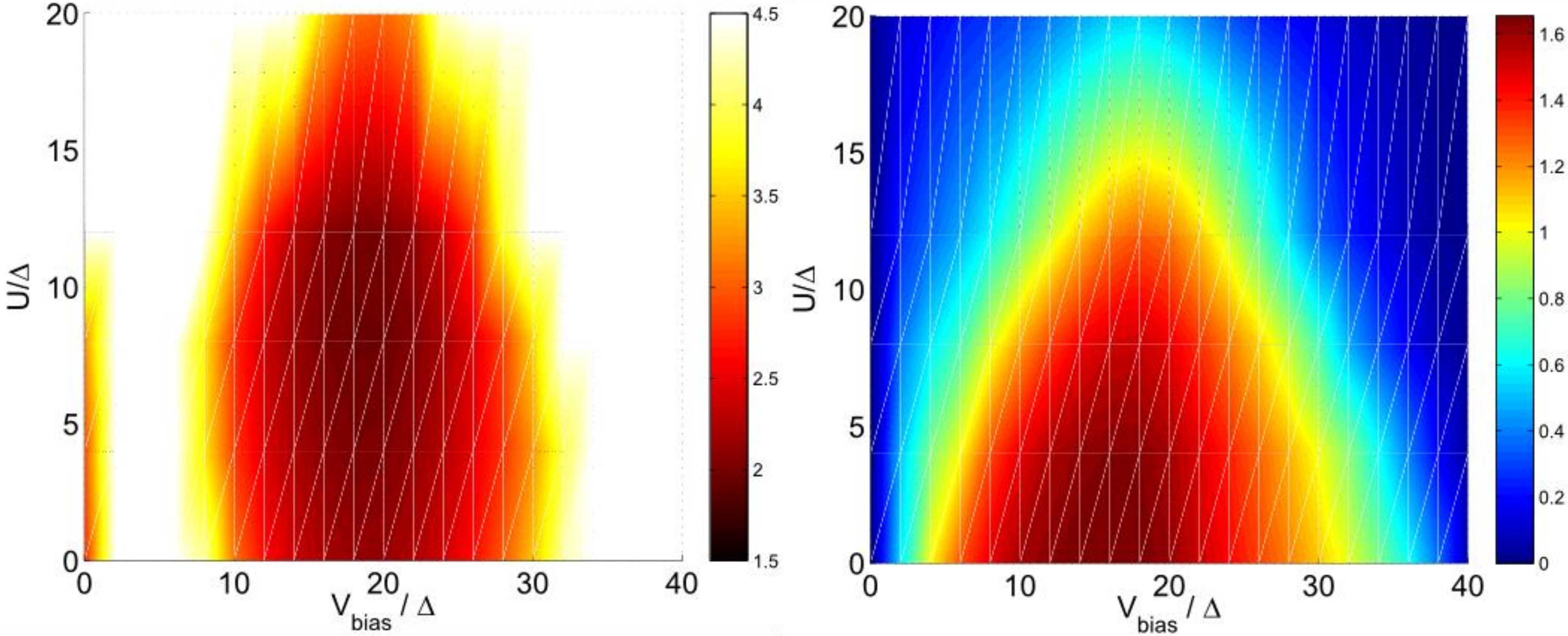


entanglement ⟺ current



time evolution of current