Strongly correlated quantum dot out of equilibrium

A variational cluster approach

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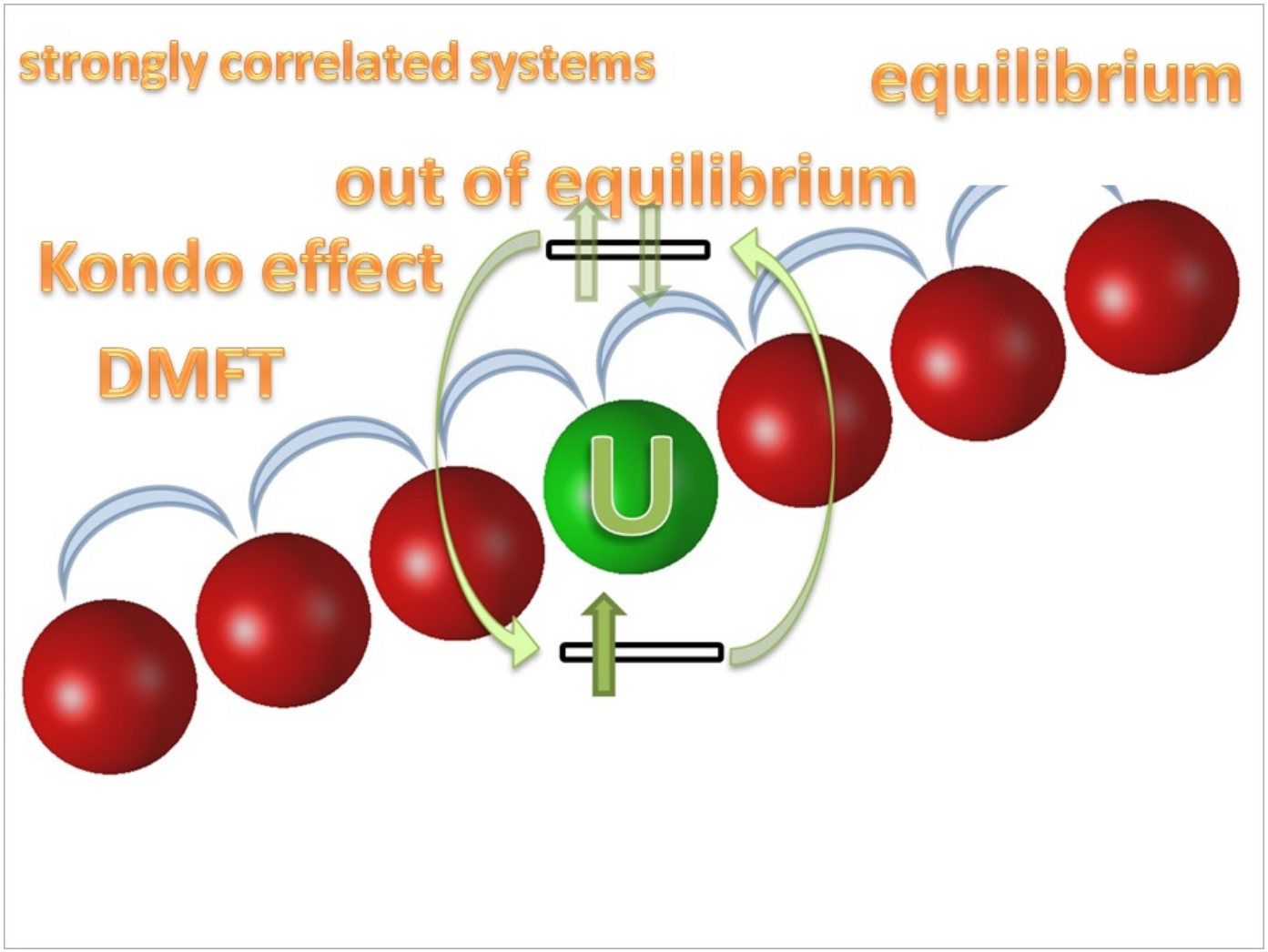
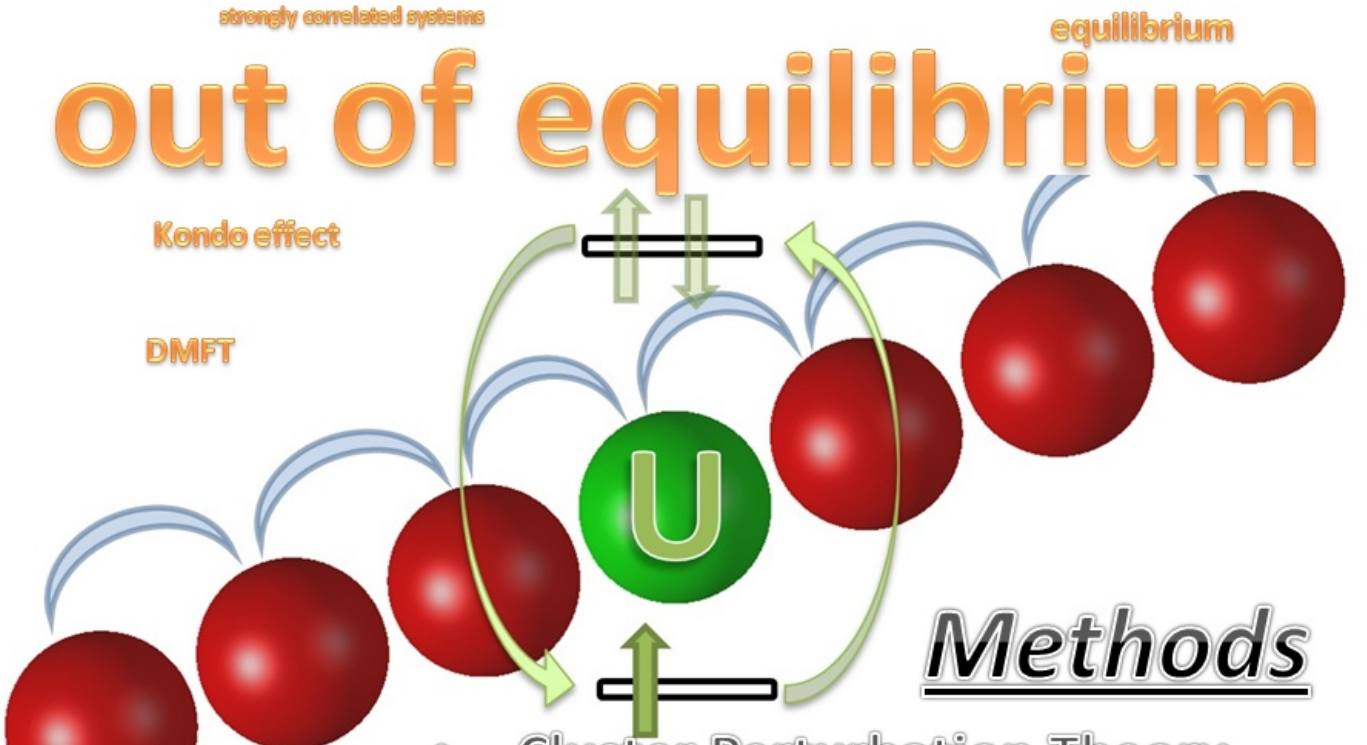
[1] cooperation of ViCoM P03 and P04

Single quantum impurity model



Single quantum impurity model



Non-equilibrium Group at Technical University Graz

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Outline

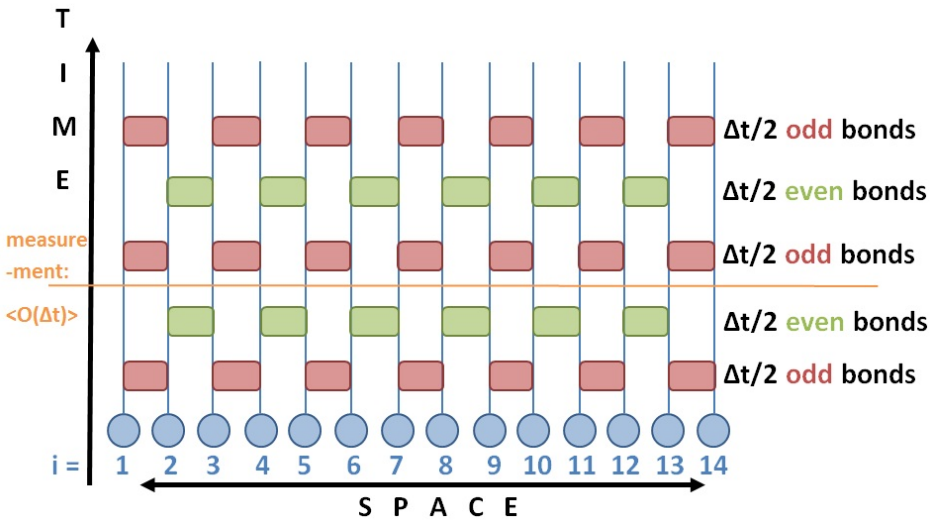
Generic lattice model

$$\hat{\mathcal{H}} = \sum_{ij} t_{ij}\, c_i^\dagger\, c_j + \sum_{ijkl} U_{ijkl}\, c_i^\dagger\, c_j^\dagger\, c_k\, c_l$$
$$= \hat{\mathcal{H}}_I(t) + \hat{\mathcal{H}}_{II}(U)$$

Time Evolution using Matrix Product States

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

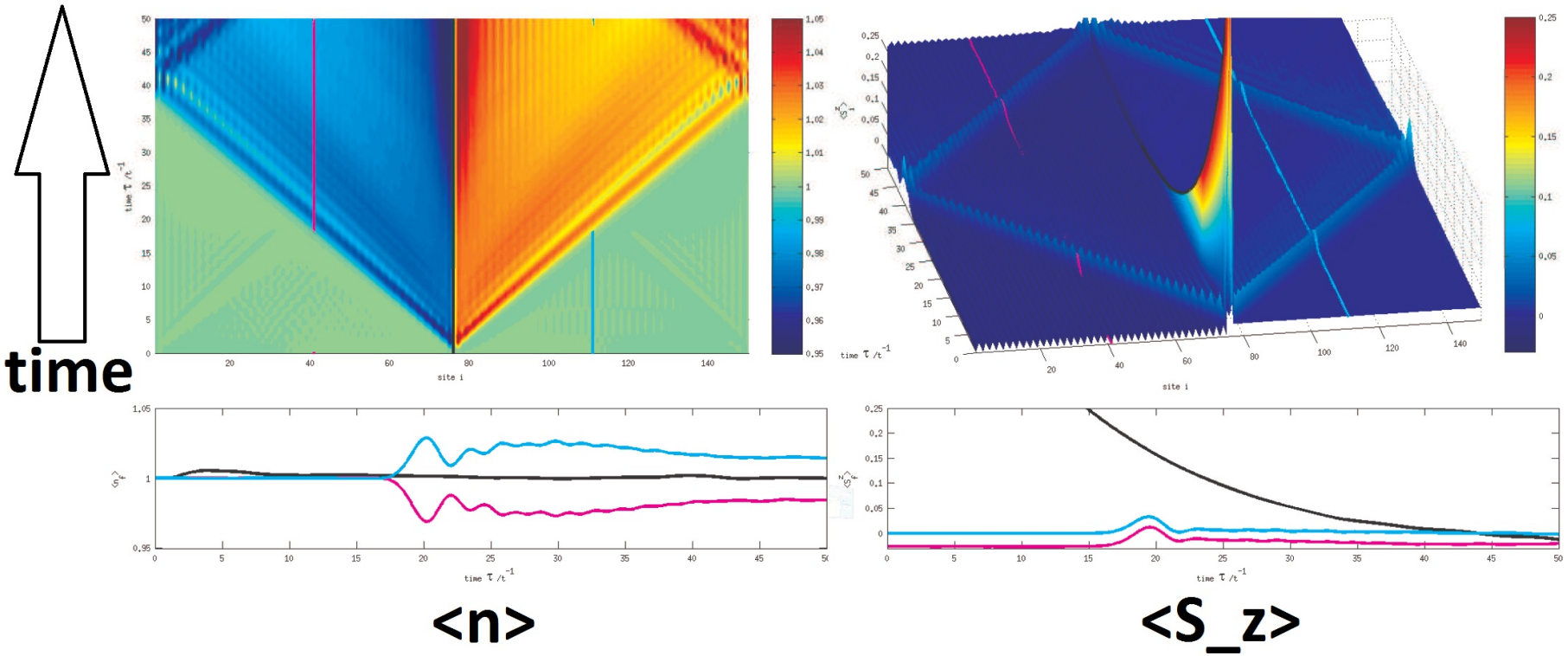
$$= \sum_{\{s_1,\ldots,s_L\}} \sum_{\{\alpha_1,\ldots,\alpha_L\}} A^{[1]s_1}_{\alpha_1} \, A^{[2]s_2}_{\alpha_1\alpha_2} \, \ldots \, A^{[L-1]s_{L-1}}_{\alpha_{L-2}\alpha_{L-1}} \, A^{[L]s_L}_{\alpha_{L-1}} \, |s_1, \ldots, s_L\rangle$$



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

Short time TEBD dynamics: particle number and spin

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



- established, quasi-exact method in 1 dimension
- dynamic quantities are more difficult to obtain

Outline

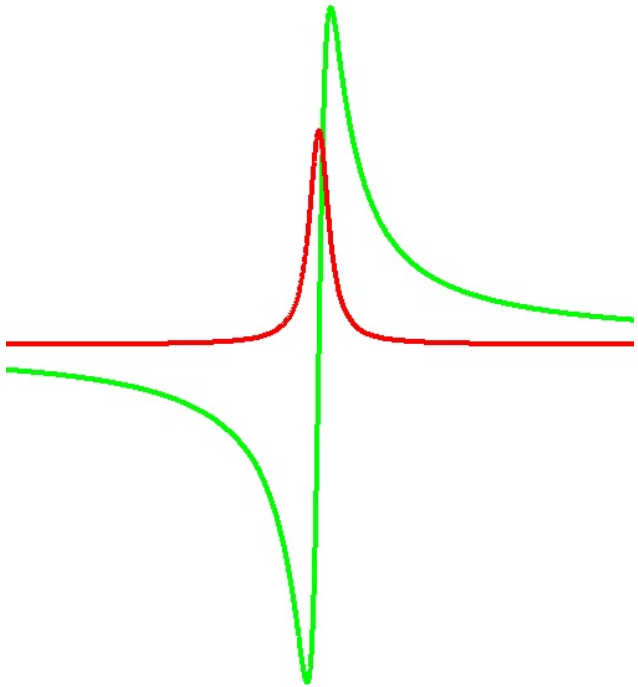
Generic lattice model

$$\hat{\mathcal{H}} = \sum_{ij} t_{ij}\, c_i^\dagger\, c_j + \sum_{ijkl} U_{ijkl}\, c_i^\dagger\, c_j^\dagger\, c_k\, c_l$$
$$= \hat{\mathcal{H}}_I(t) + \hat{\mathcal{H}}_{II}(U)$$

To apply a perturbative method one has to expand in some parameter. Usually the hopping (strong coupling) or the interaction (weak coupling) are considered.

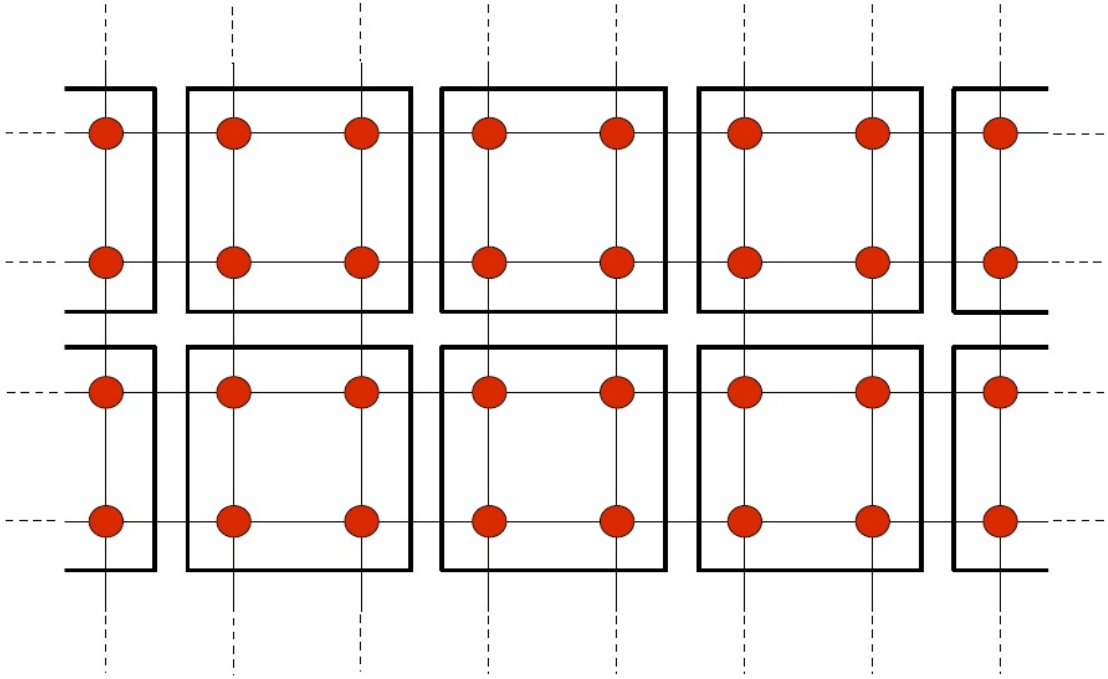
Atomic limit

$$G(z;t,U) = \left\langle \frac{1}{z - \hat{\mathcal{H}}(t,U)} \right\rangle$$



- strong coupling perturbation theory (in hopping t)
- consider G$(t = 0)$ as starting point

Manybody Cluster Methods

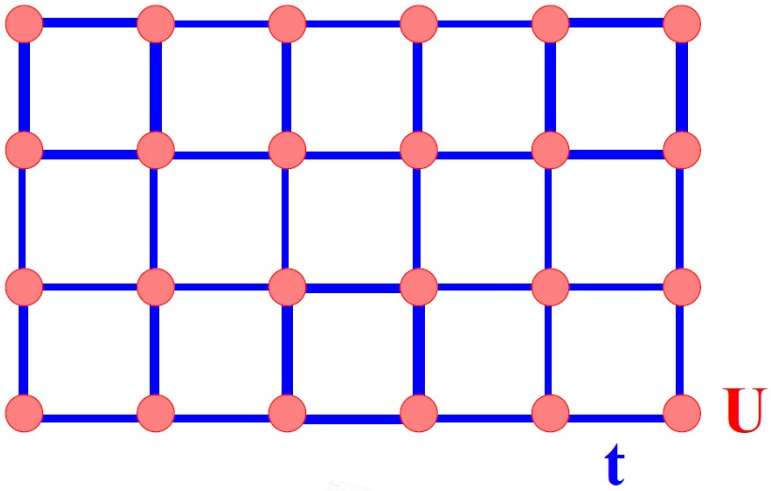


Extrapolate cluster to thermodynamic limit:

- Cluster Perturbation Theory (**CPT**)
- Variational Cluster Approach (**VCA**)
- Cluster/Cellular Dynamical Mean-Field Theory (**CDMFT**)
- Dynamical Cluster Approximation (**DCA**)

Illustration of Cluster Perturbation Theory

Correlated lattice model



given: Hamiltonian e.g. Hubbard model

$\hat{\mathcal{H}}$

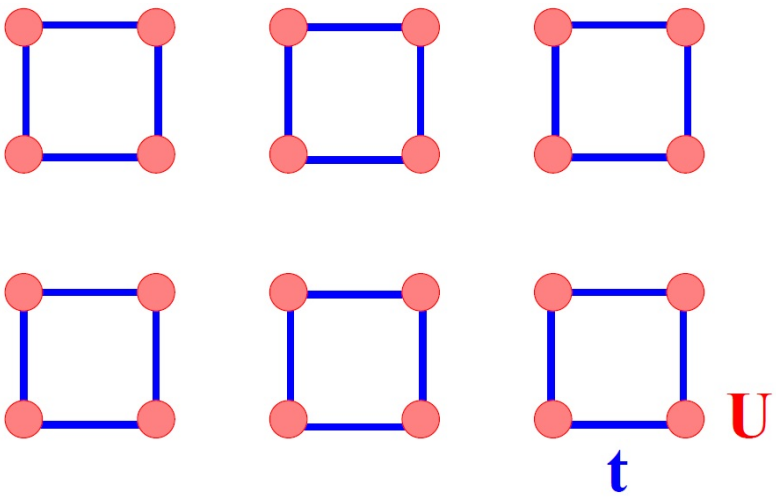
ask for: Green's function

$\mathbf{G} = ?$

in general intractable ... :(

Illustration of Cluster Perturbation Theory

Cluster Tiling



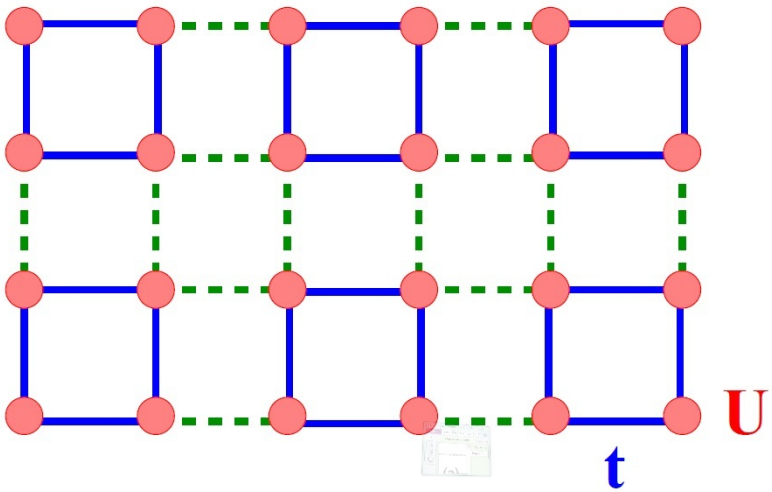
$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_{\text{cluster}}$$

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

(numerically) exactly solvable ... :)

... but isn't this quite different from original system ... :(

Cluster Perturbation Theory[2] [3]



$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_{\text{cluster}} + \hat{\mathcal{H}}_{\text{inter-cluster}}$$

$$\mathbf{G}^{-1}_{\mathbf{CPT}}(\omega, \mathbf{k}) = \mathbf{G}^{-1}_{\mathbf{cluster}}(\omega) - \mathbf{T}(\mathbf{k})$$

First order result for the lattice Green function G

- $G_{cluster}$ = exact Green's function of the **cluster**
- T = **inter**-cluster off diagonal one particle terms (i.e. hopping)

[2] C. Gros and R. Valenti, Phys. Rev. B 48, 418 (1993)

[3] D. Sénéchal, D. Perez, and M. Pioro-Ladriére, Phys. Rev. Lett. 84, 522 (2000)

Approximation - Limits

Approximation: take **self-energy of the cluster** $\Sigma = \Sigma_{cluster}$

CPT is exact for

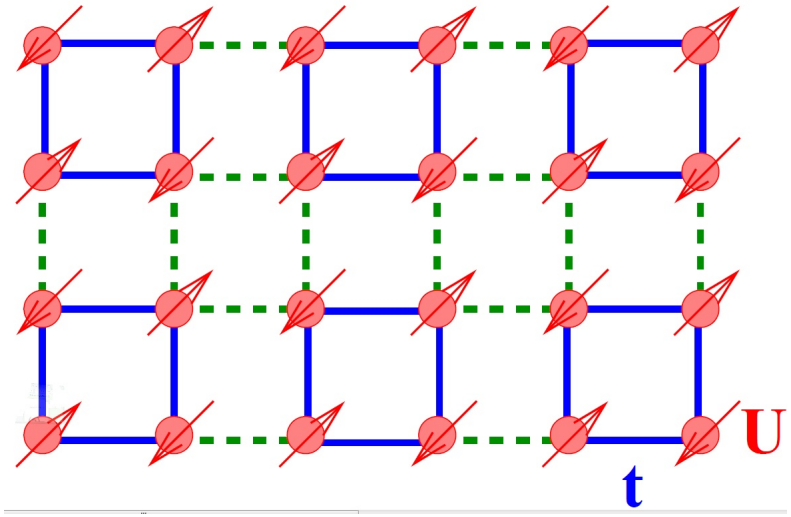
- $t \to 0$,
- $U \to 0$,
- $L \to \infty$.

CPT captures **short-range correlations** exactly, long-range correlations are neglected.

CPT is usually improved not by considering higher order expansions in the inter-cluster hopping but by **increasing the cluster** size.

Illustration of the Variational Cluster Approach

VCA[4] = Variational CPT: **Optimize the initial state**



$$\hat{\mathcal{H}} = \hat{\mathcal{H}}'_{\text{cluster}} + \hat{\mathcal{H}}'_{\text{inter-cluster}}$$

$$\mathbf{G}^{-1}_{\mathbf{CPT}}(\omega, \mathbf{k}) = \mathbf{G}'^{-1}_{\mathbf{cluster}}(\omega) - \mathbf{T}'(\mathbf{k})$$

Variational aspect: Add **virtual field** to cluster Hamiltonian

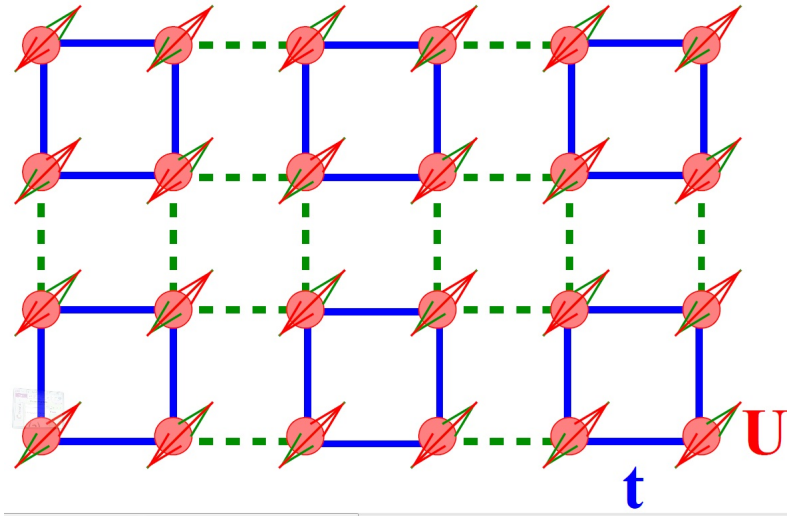
$$\hat{\mathcal{H}}'_{\text{cluster}} = \hat{\mathcal{H}}_{\text{cluster}} + \hat{h}_{\text{field}}$$

field: **any single particle terms** of original Hamiltonian + bath sites

[4] M. Potthoff, M. Aichhorn, and C. Dahnken, Phys. Rev. Lett. 91, 206402 (2003)

Illustration of the Variational Cluster Approach

Adding and subtracting single-particle terms



$$\hat{\mathcal{H}} = \hat{\mathcal{H}}'_{\text{cluster}} + \hat{\mathcal{H}}'_{\text{inter-cluster}}$$

$$\mathbf{G}^{-1}_{\mathbf{CPT}}(\omega, \mathbf{k}) = \mathbf{G}'^{-1}_{\mathbf{cluster}}(\omega) - \mathbf{T}'(\mathbf{k})$$

Variational aspect: Add **virtual field** to cluster Hamiltonian

$$\hat{\mathcal{H}}'_{\text{cluster}} = \hat{\mathcal{H}}_{\text{cluster}} + \hat{h}_{\text{field}}$$

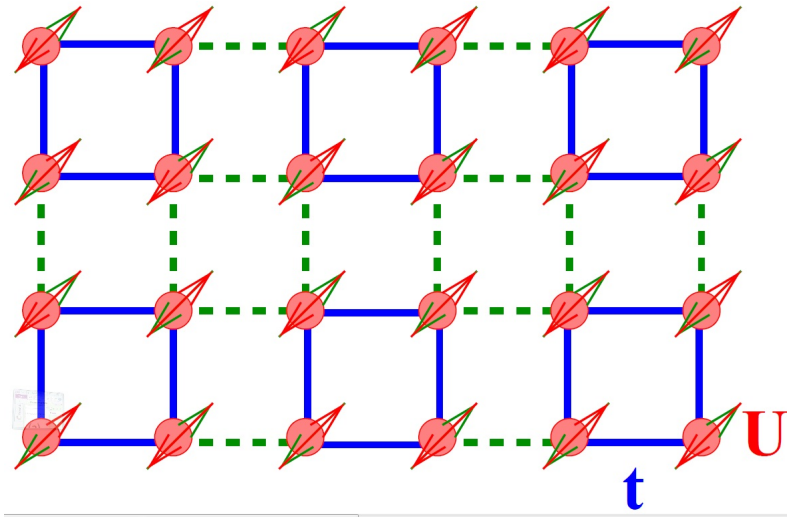
subtract field again via CPT

$$\hat{\mathcal{H}}'_{\text{inter-cluster}} = \hat{\mathcal{H}}_{\text{inter-cluster}} - \hat{h}_{\text{field}}$$

field: **any single particle terms** of original Hamiltonian + bath sites

Illustration of the Variational Cluster Approach

How is $\hat{h}_{\text{field}}$ determined?



$$\hat{\mathcal{H}} = \hat{\mathcal{H}}'_{\text{cluster}} + \hat{\mathcal{H}}'_{\text{inter-cluster}}$$

$$\mathbf{G}^{-1}_{\mathbf{CPT}}(\omega, \mathbf{k}) = \mathbf{G}'^{-1}_{\text{cluster}}(\omega) - \mathbf{T}'(\mathbf{k})$$

The self energy functional approach (SFA)[5] provides a variational principle:

Stationary point of the grand potential:

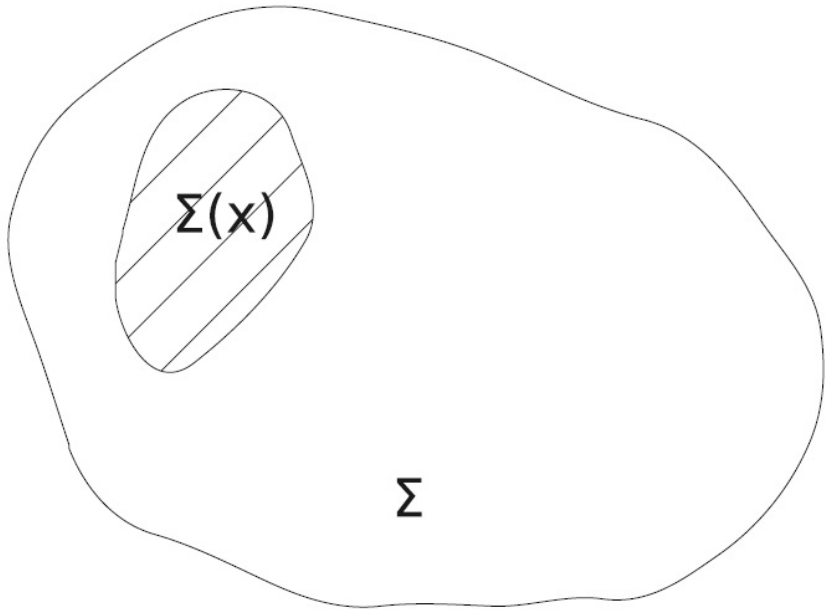
$$\frac{\delta \Omega}{\delta h_{\text{field}}} \stackrel{!}{=} 0$$

VCA = CPT + variational principle

[5] M. Potthoff, Eur. Phys. J. B 32, 429 (2003), M. Potthoff, Eur. Phys. J. B 36, 335 (2003)

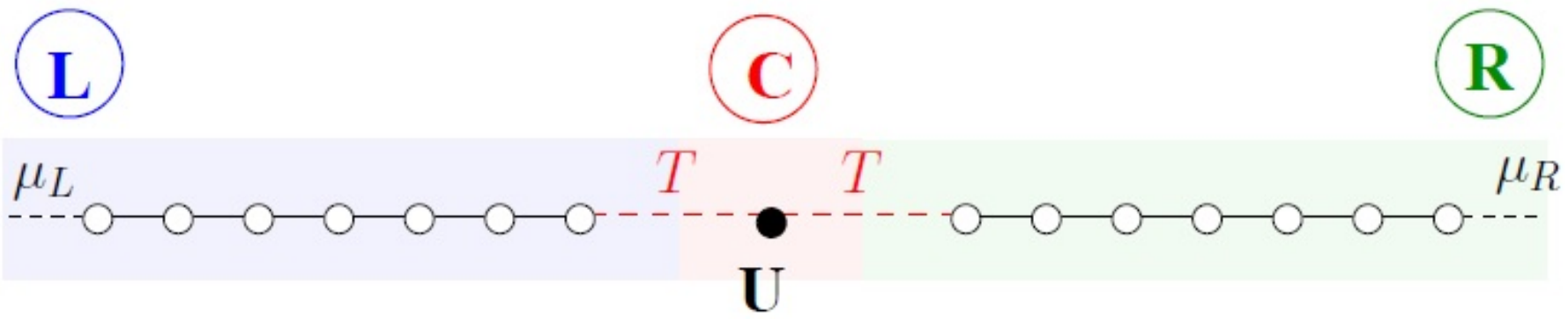
Restriction of self-energies

Self-energy $\Sigma(x)$ = self-energy of the reference system $\Sigma(x')$
x = single particle parameters, **restricting the space of available self-energies**.



Outline

Interacting quantum dot

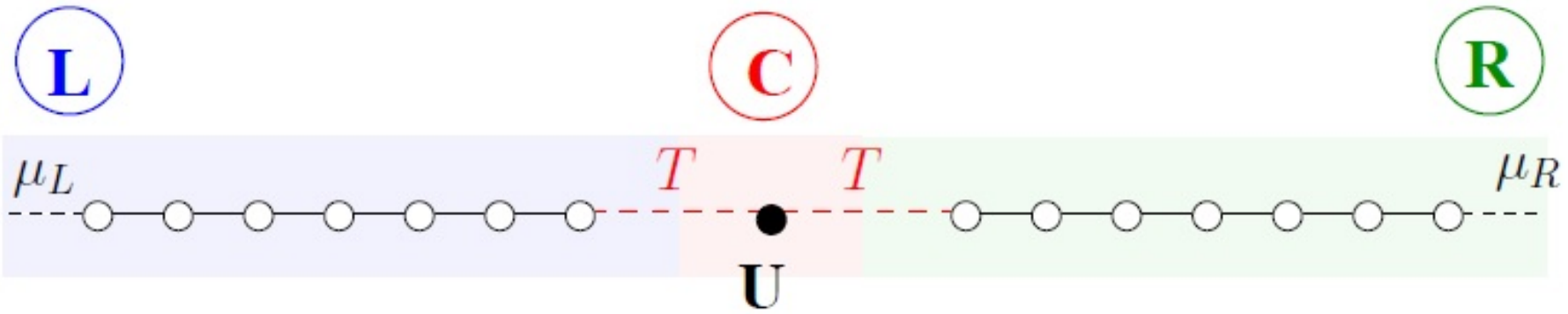


- g = diag(g_{LL}, g_{CC}, g_{RR}) of decoupled system evaluated exactly
- at time t_0 coupling T is switched on
- non equilibrium situation $\longrightarrow$ **Keldysh Green's functions**

$$\tilde{\mathrm{g}}(r, r'; t, t') = \begin{pmatrix} \mathrm{g}^R & \mathrm{g}^K \\ 0 & \mathrm{g}^A \end{pmatrix}$$

notation from Rammer+Smith '86

Interacting quantum dot

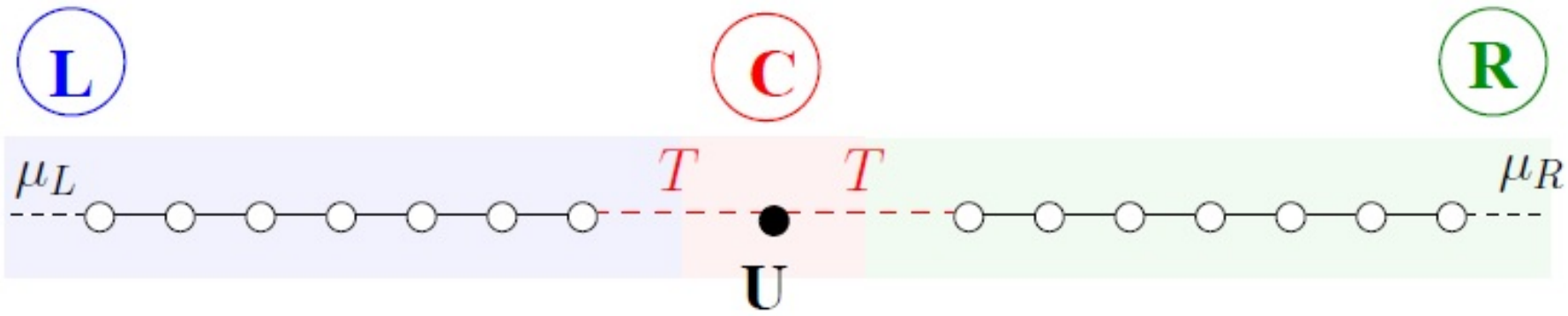


- at $t \to \infty$ system reaches **steady state**
  time translationally invariant
  $\to$ Fourier transform to ω
- **Interacting** system: Dyson Equation

$$\mathsf{G} = \mathsf{g} + \mathsf{g} \circ (\mathsf{T} + \Delta\Sigma) \circ \mathsf{G}$$

2x2 Keldysh matrices

CPT approximation

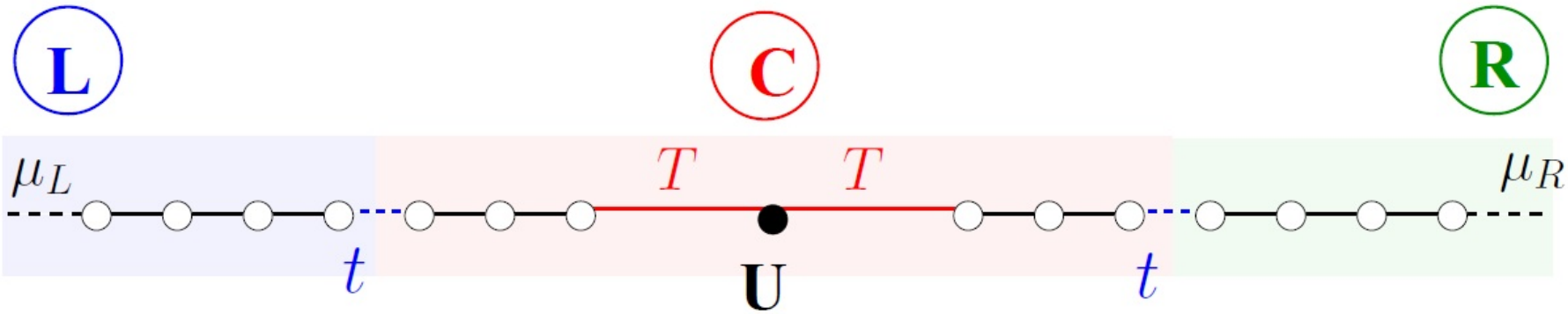


CPT interacting system: Dyson Equation

$$\mathsf{G} = \mathsf{g} + \mathsf{g} \circ (\mathsf{T} + \Delta\Sigma) \circ \mathsf{G}$$

Lowest-order strong-coupling expansion (in T) consists in neglecting $\Delta\Sigma$ (Hubbard I approximation)

Applying CPT



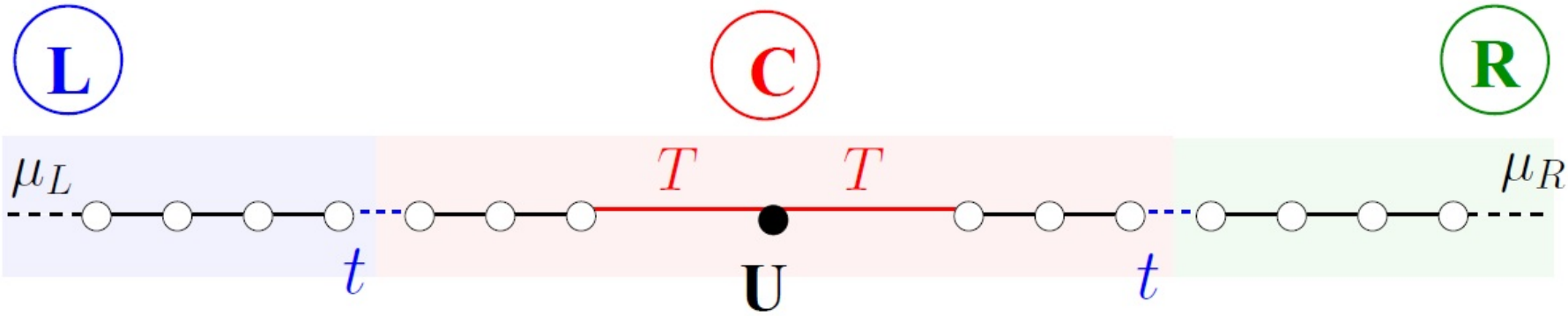
take **larger central region** and solve larger cluster exactly
treat inter-cluster hopping (t) perturbatively

$$\mathsf{G} = \mathsf{g} + \mathsf{g} \circ \left(\hat{t}\right) \circ \mathsf{G}$$

cf. short time dynamics by Balzer+Potthoff '11

short times Δt: perturbation due to coupling to leads $\propto \Delta t.T$,
accounted for in first order perturbation theory, but long time behavior ???

Adding a single-particle field

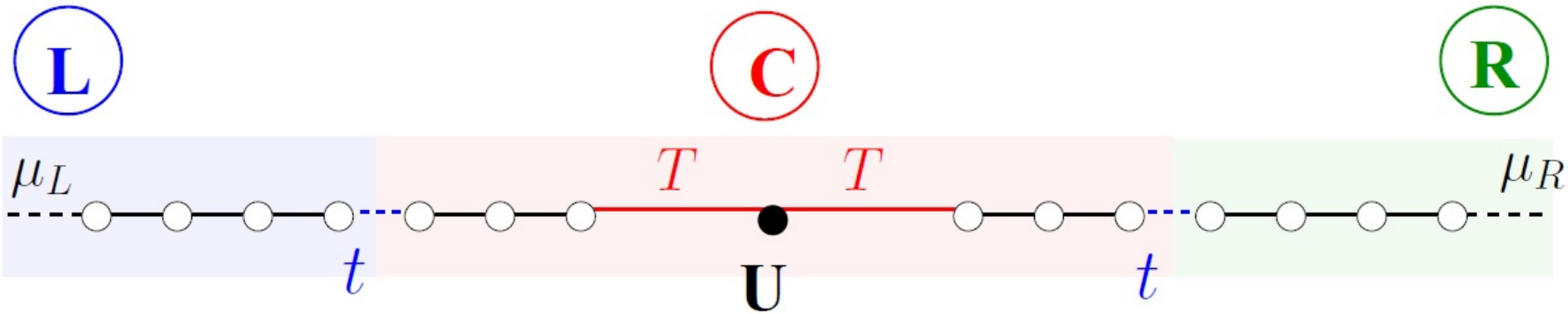


non equilibrium **Variational Cluster Approach (VCA)**

$$\mathsf{G} = \mathsf{g} + \mathsf{g} \circ \left(\hat{t} - \Delta\hat{T} \right) \circ \mathsf{G}$$

start from better initial state at $t < t_0 \rightarrow$ variational optimization:
minimize difference between initial and final state
by adding $\hat{h}_{\text{field}}$ (here ΔT) at $t < t_0$
and subtract it again for $t > t_0$

Subtracting a single-particle field



$$\mathsf{G} = \mathsf{g} + \mathsf{g} \circ \left(\hat{t} - \Delta\hat{T} \right) \circ \mathsf{G}$$

start from better initial state at $t < t_0 \rightarrow$ variational optimization:
minimize difference between initial and final state
(Exact) steady state should not depend on $\hat{h}_{\text{field}}$
due to the CPT approximation, results do depend on $\hat{h}_{\text{field}}$

Non-equilibrium self-consistency condition

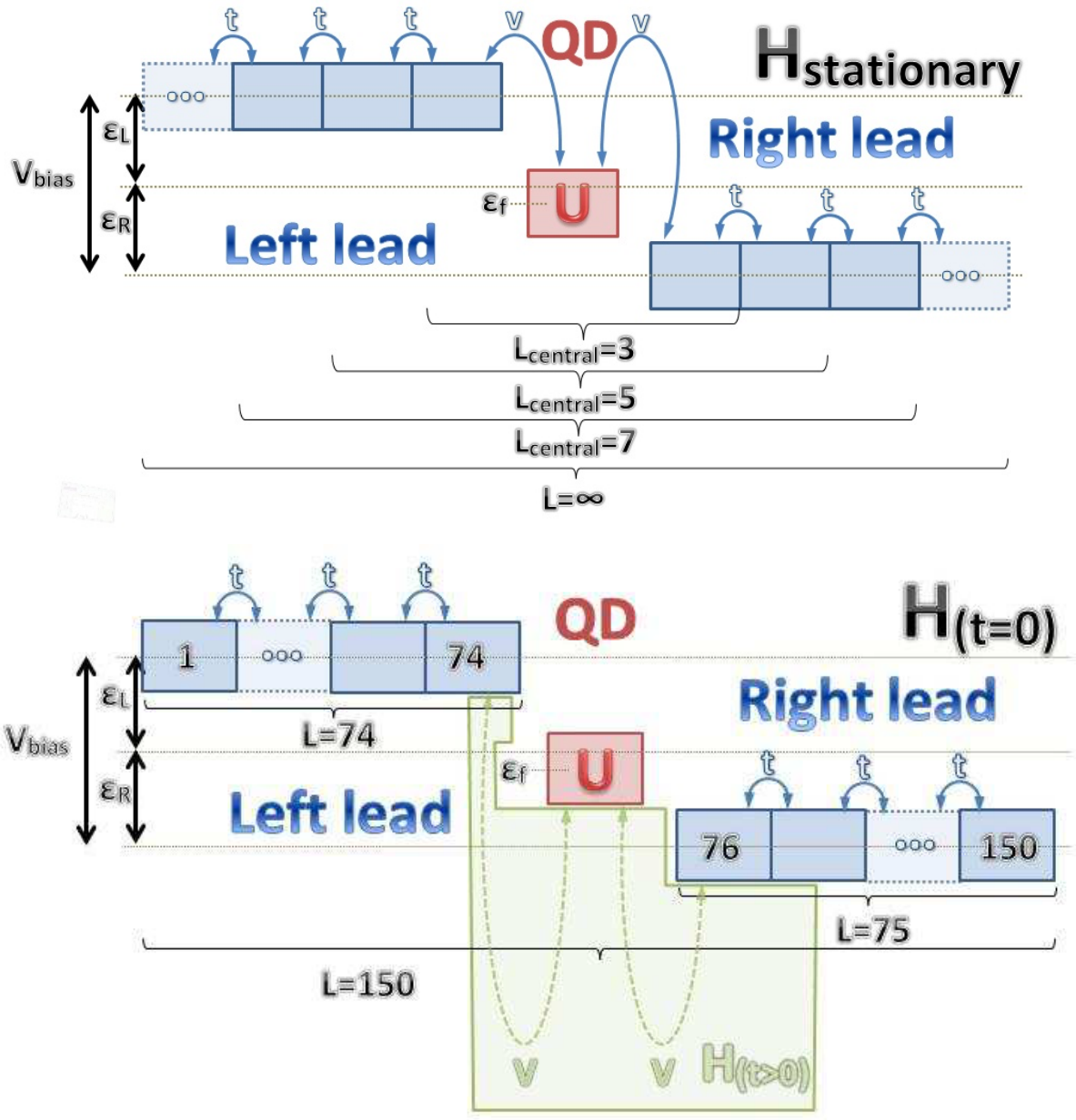
New optimization criterion in non-equilibrium:

$$\langle \frac{\partial \mathcal{H}}{\partial \Delta T} \rangle_{t<t_0} \stackrel{!}{=} \langle \frac{\partial \mathcal{H}}{\partial \Delta T} \rangle_{t\to\infty}$$

achieved by requiring **single-particle expectations** values in initial state to match those in final state

Outline

Model within nCPT/nVCA and DMRG/TEBD



Tests for quasi steady state behavior of TEBD

- checked convergence in: system **size** L, **trotter** time step δt, TEBD matrix size χ (**truncated weight**), ...
- investigated **various quenches** all leading to the same results in the steady state
- checked vs. **analytically** available $U = 0$ results

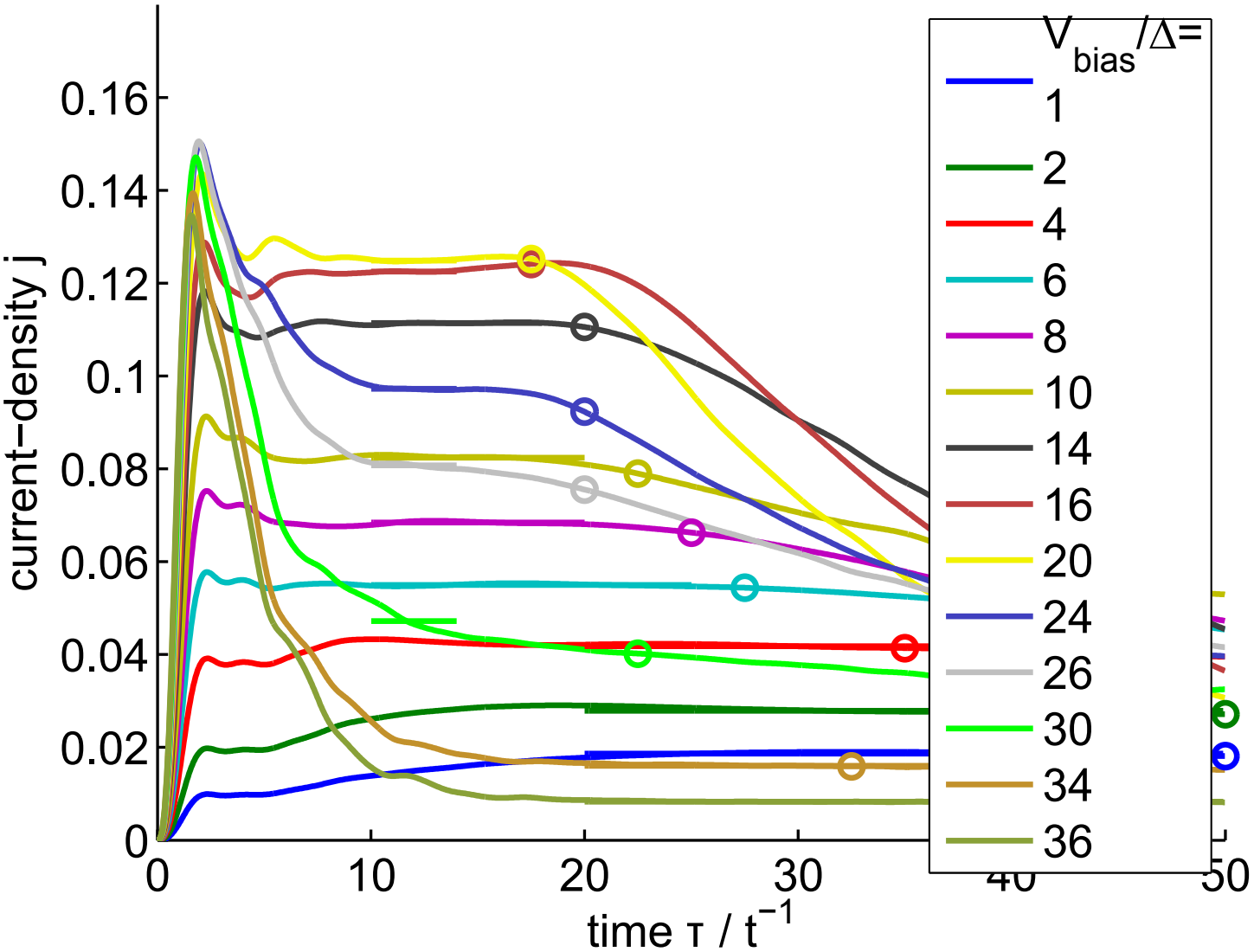
Results in equilibrium by CPT/VCA

- **VCA** » CPT
- **Hubbard bands** (position + width)
- **all parameter regions** (pinning of Kondo resonance)
- **Kondo peak** + exponential scale in U (although wrong prefactor)

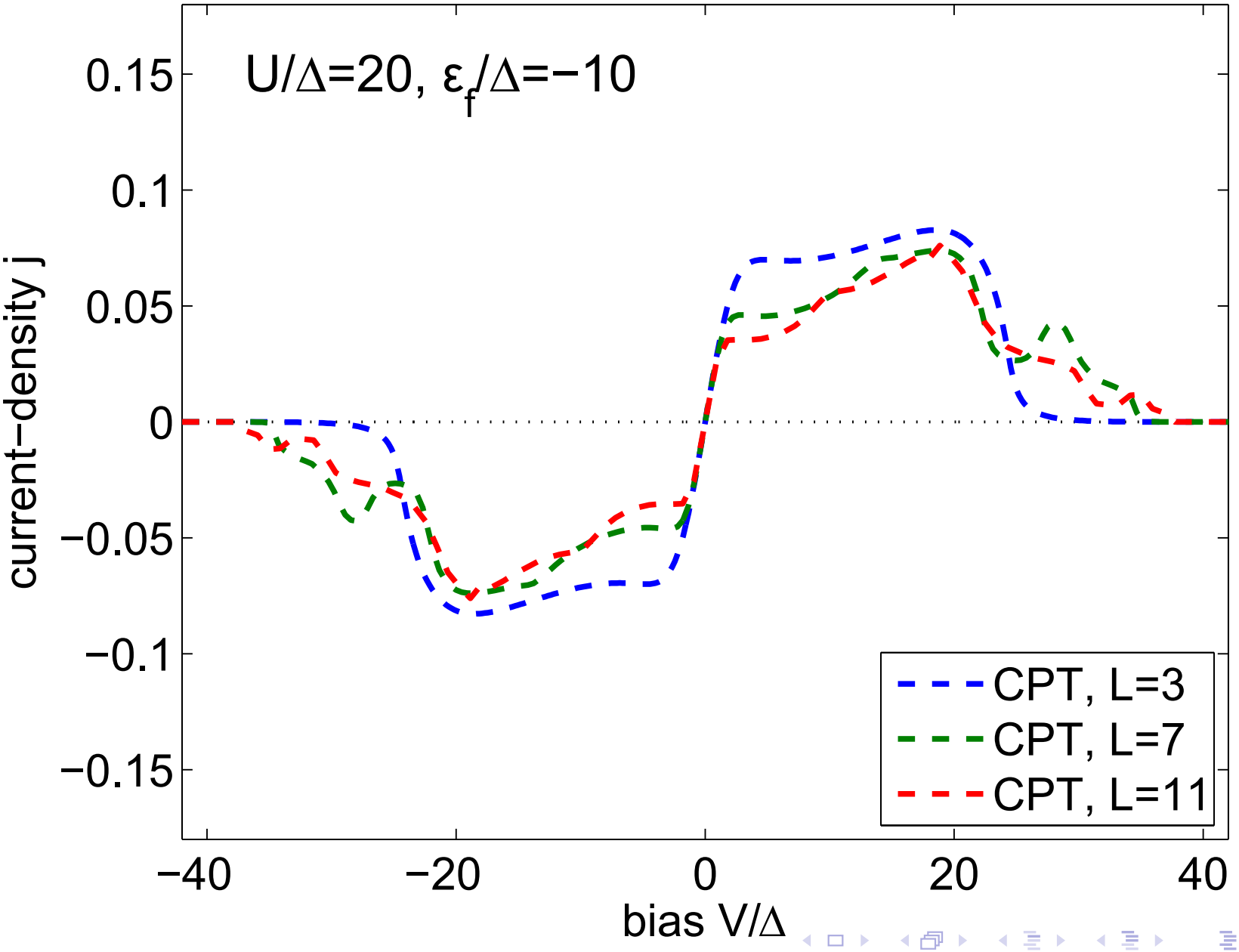
M. Nuss, E. Arrigoni, M. Aichhorn and W. von der Linden, arXiv:1110.4533 (2011)

TEBD quasi-stationary-state current density

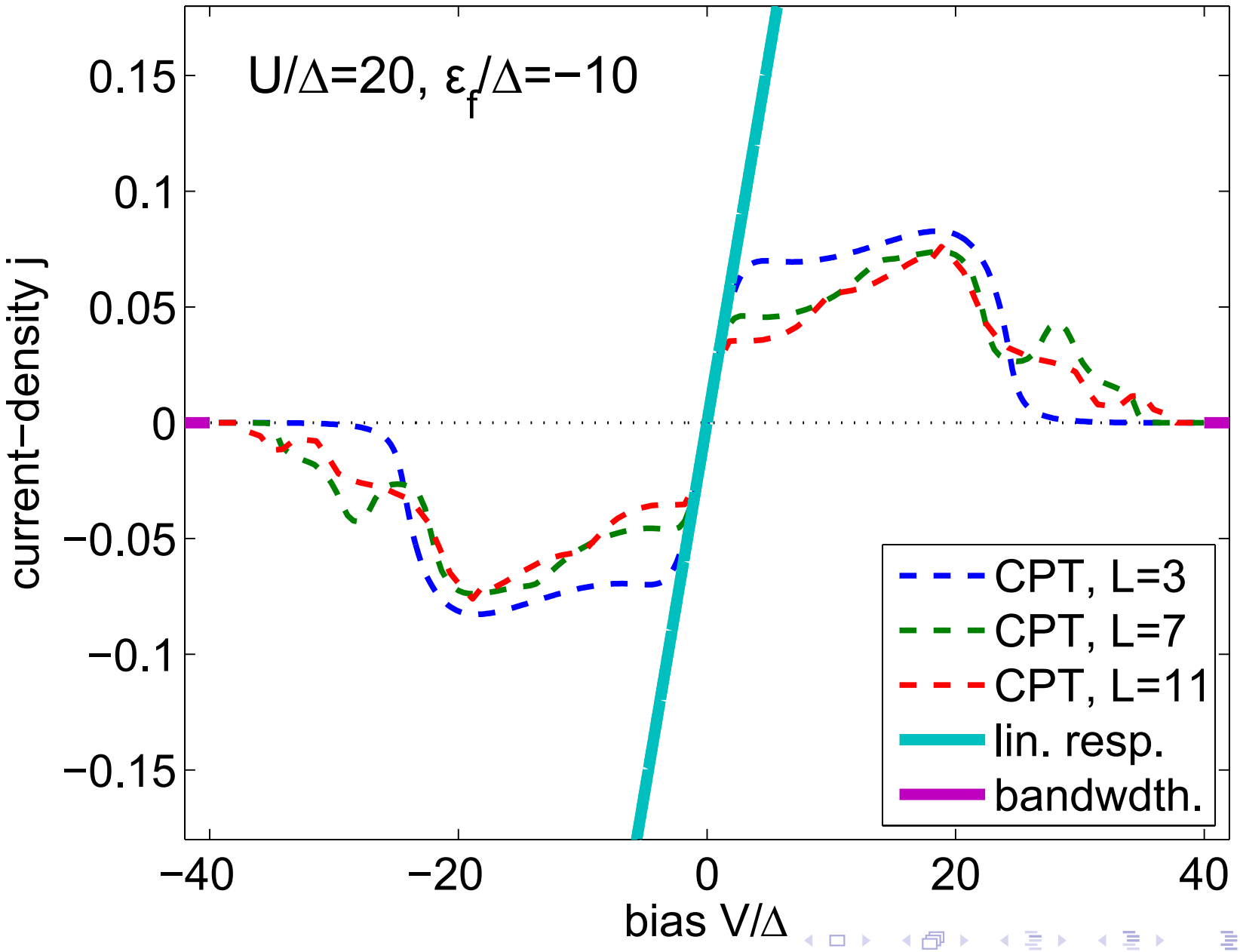
$$L = 150, U = 12\Delta$$



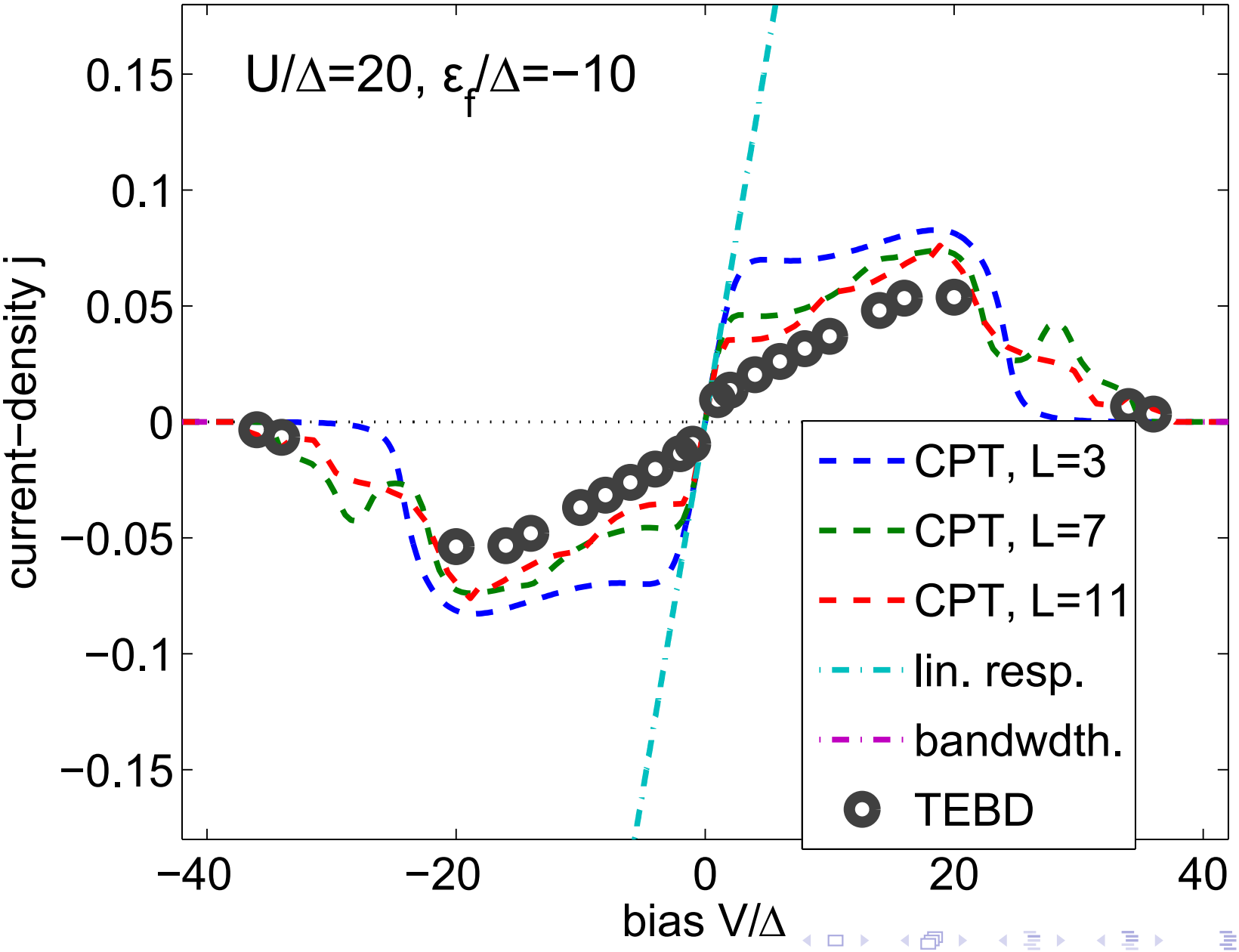
Non equilibrium cluster perturbation theory



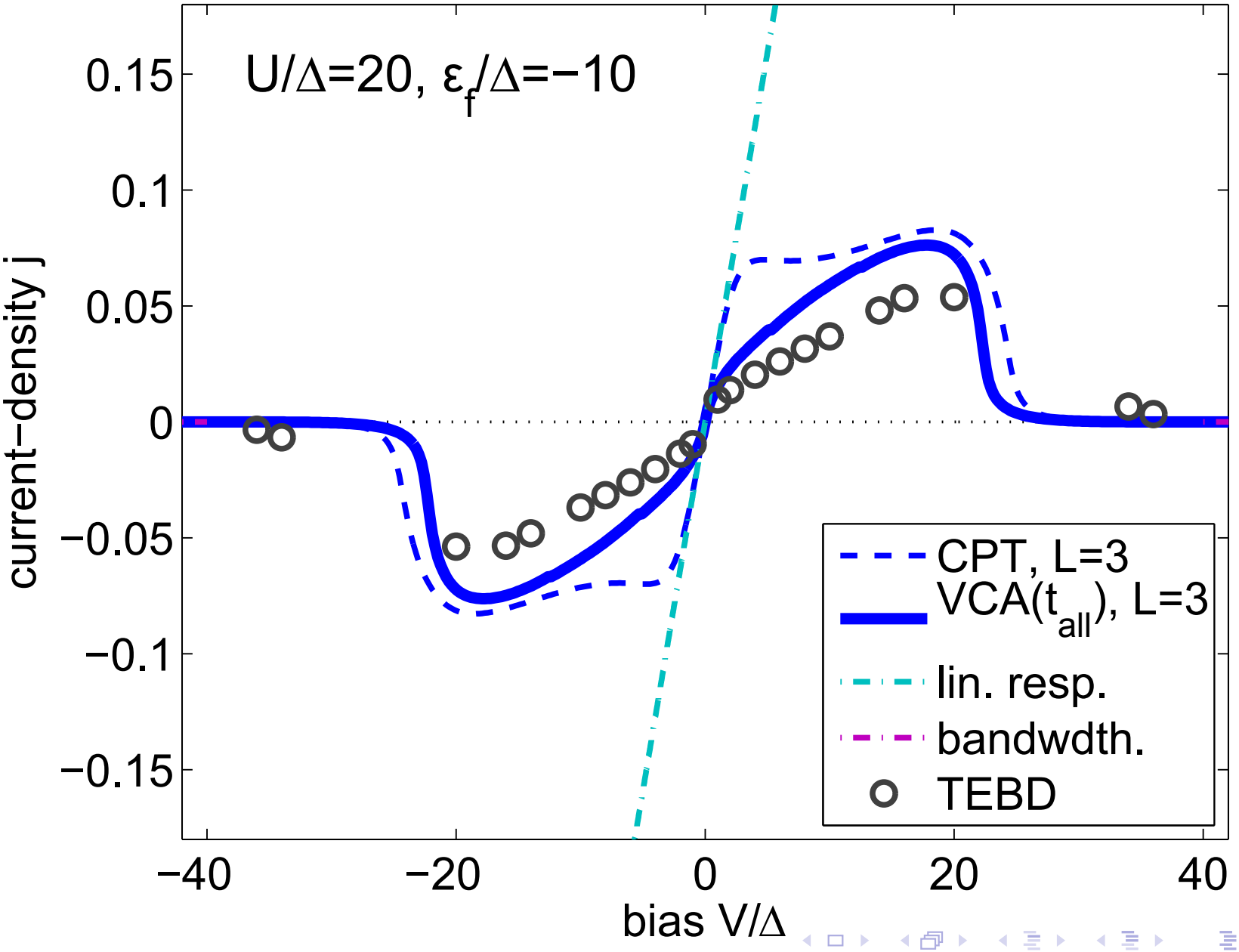
Exact limits



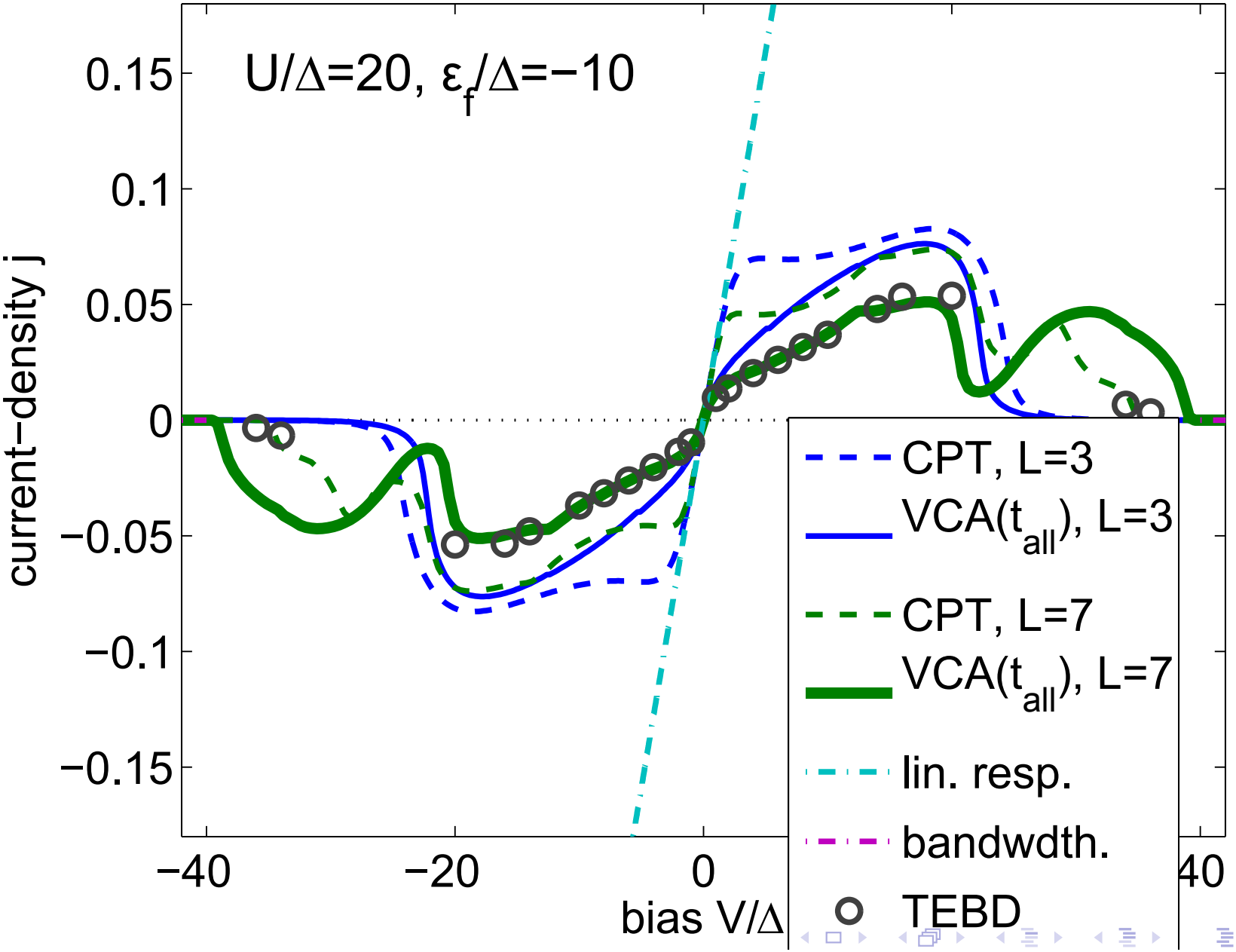
Quasi stationary state of exact time evolution



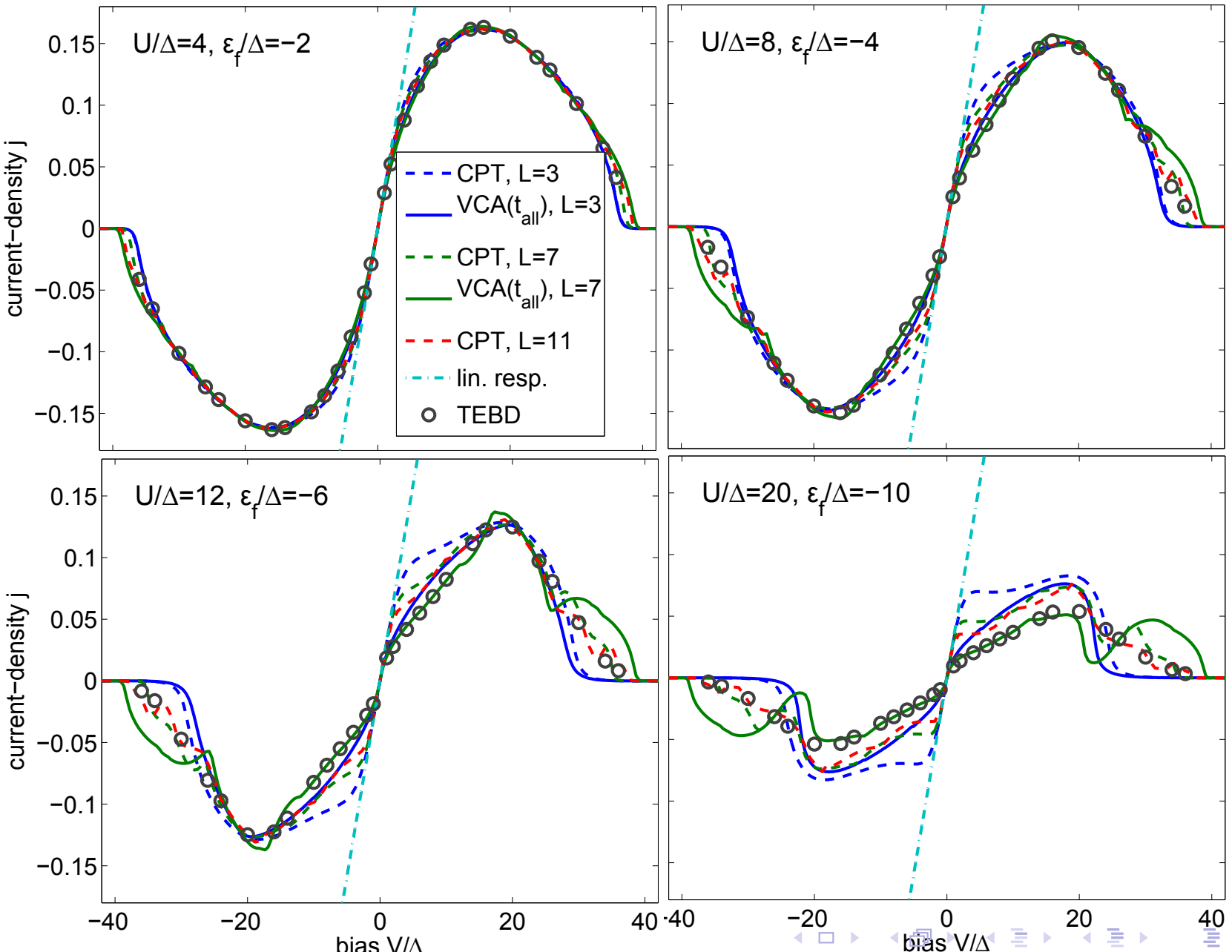
Non equilibrium Variational cluster approach



Non equilibrium Variational cluster approach

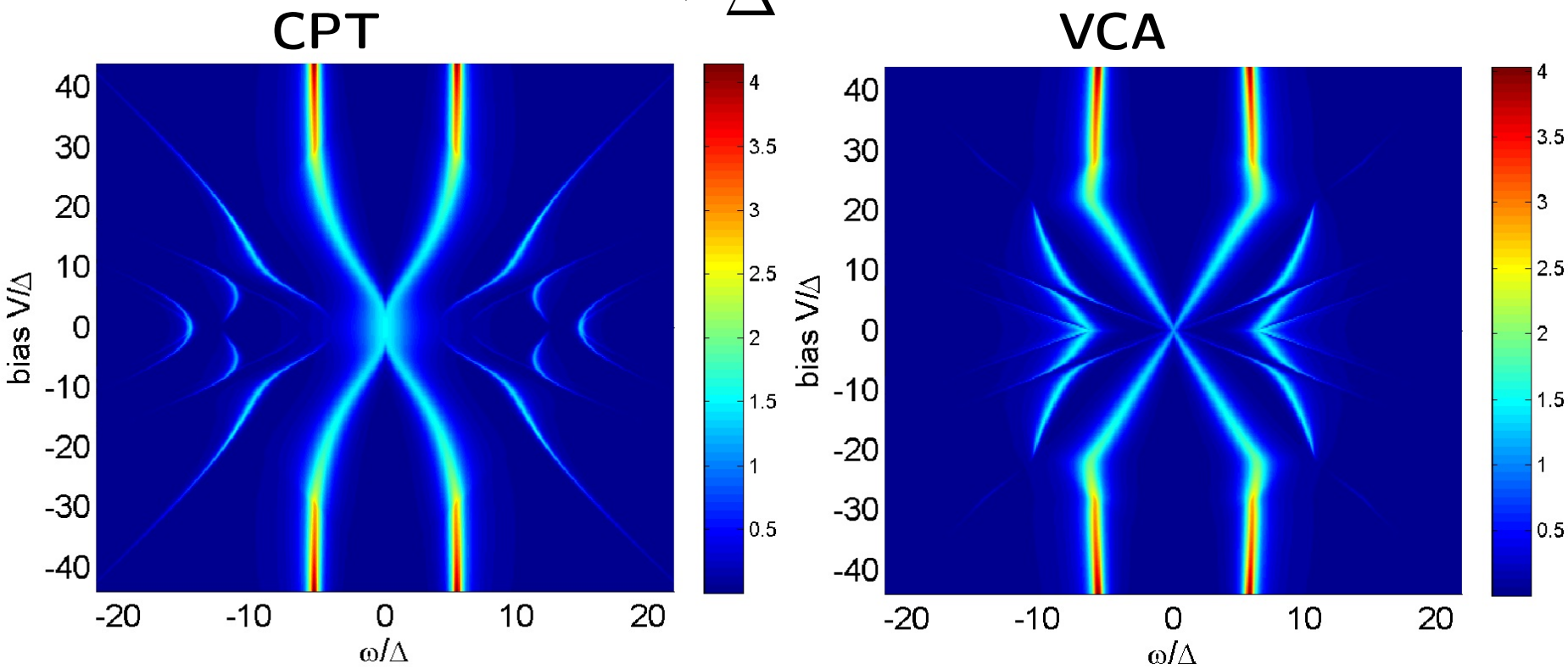


Results for various interaction strength



Non-equilibrium density of states

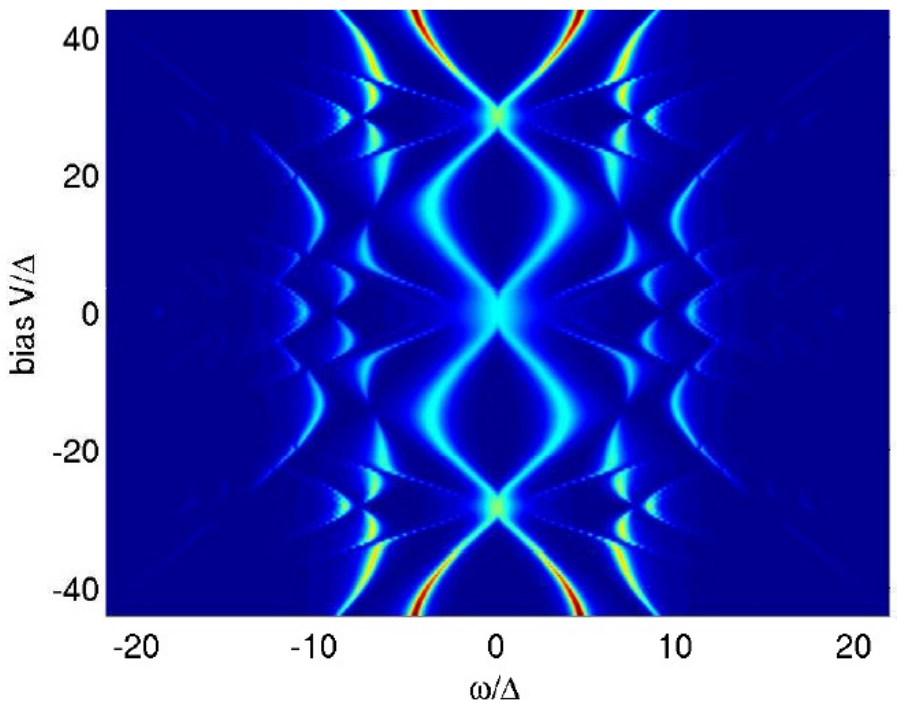
$$L = 3, \frac{U}{\Delta} = 12$$



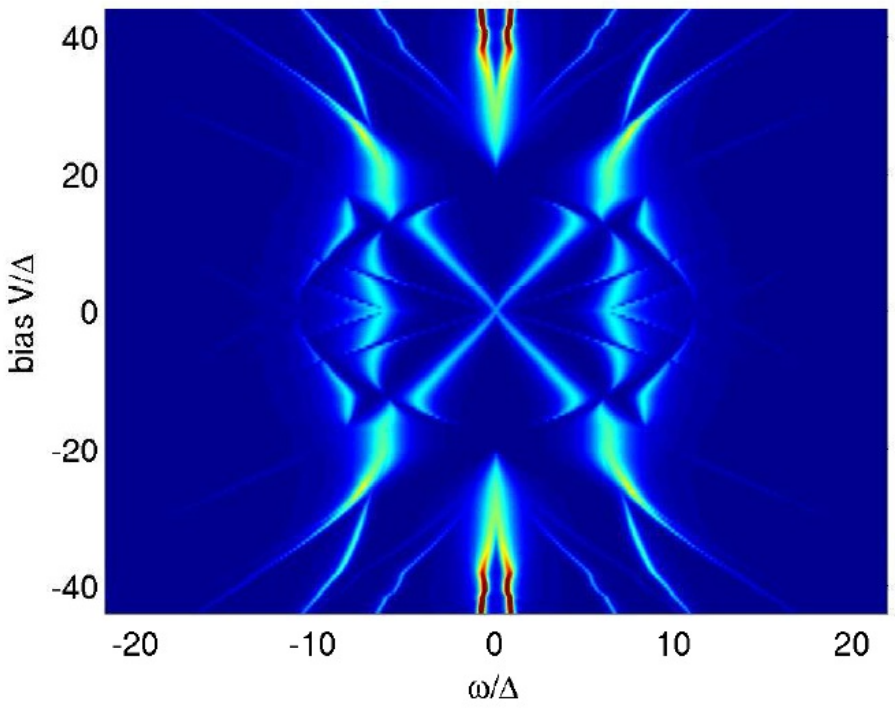
Non-equilibrium density of states

$$L = 7, \frac{U}{\Delta} = 12$$

CPT



VCA



Conclusion

- non-linear steady state current available in **all parameter regions**
- nCPT and nVCA as well as DMRG/TEBD respect the **low bias** lin. resp. result and the **high bias** band cutoff and the reproduce the non-interacting results
- low U: **nCPT and nVCA** perform excellently (benchmarked vs DMRG/TEBD)
- high U: **nVCA » nCPT** (self-consistent feedback critical!)
- VCA: linear (U) dependent **splitting of Kondo resonance** in LDOS

Open issues and future challenges

- Finding the most suitable, best performing **optimization condition** for nCPT/nVCA.
- **Application** to multi-impurity systems.
- Combination with ab-initio methods for real materials.
- **Regime of high bias/interaction strength**.
- **Comparison** to other methods.

Thank You!

Thank you for your attention!

contact: martin.nuss@student.tugraz.at

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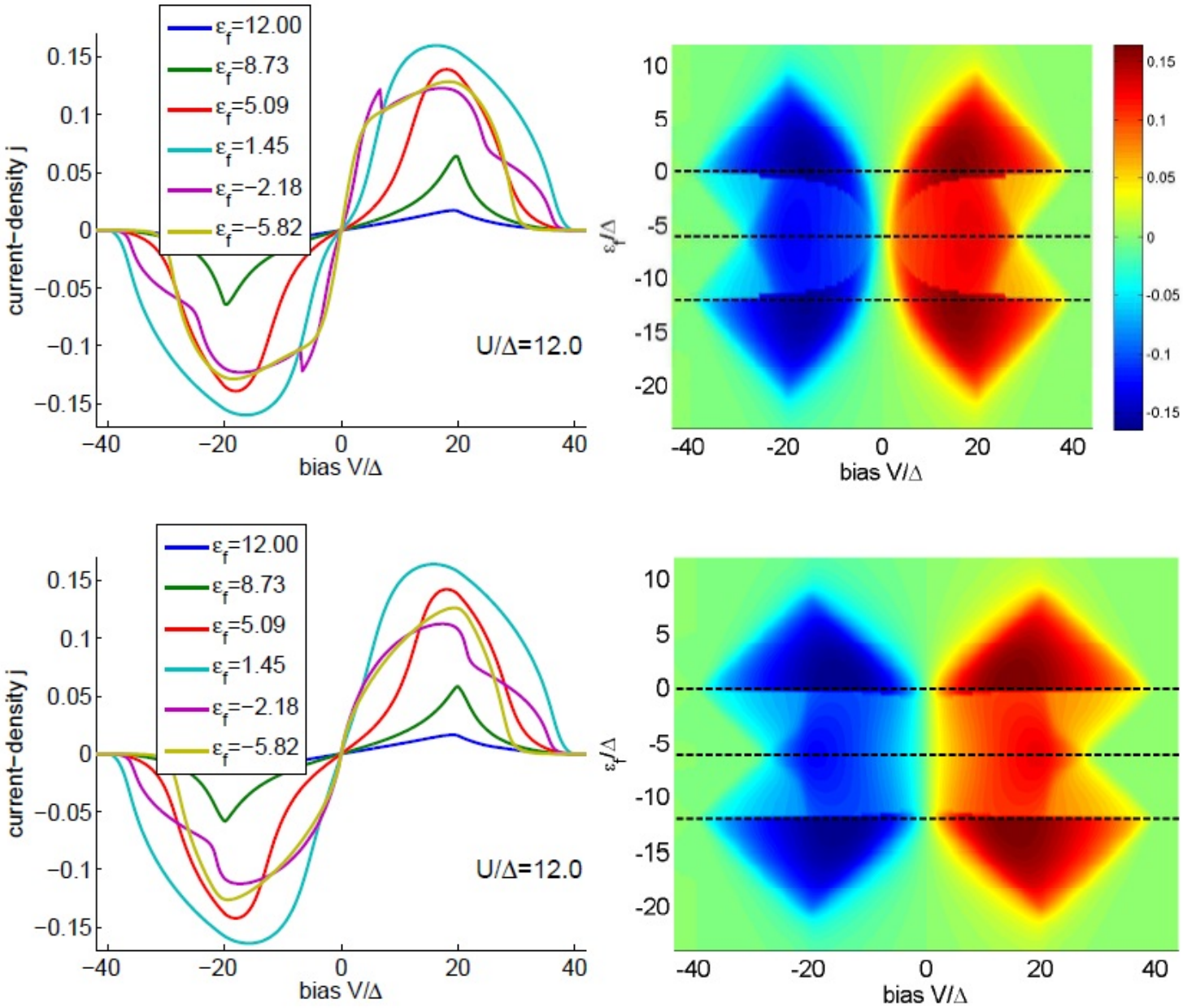
Part of the numerical work has been performed on the Vienna scientific cluster (VSC-I and VSC-II).

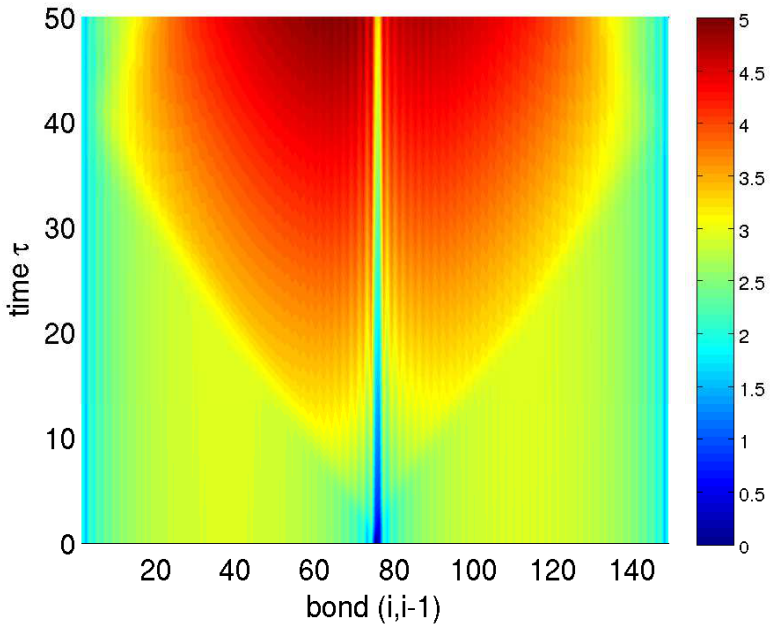
Results away from particle hole symmetry



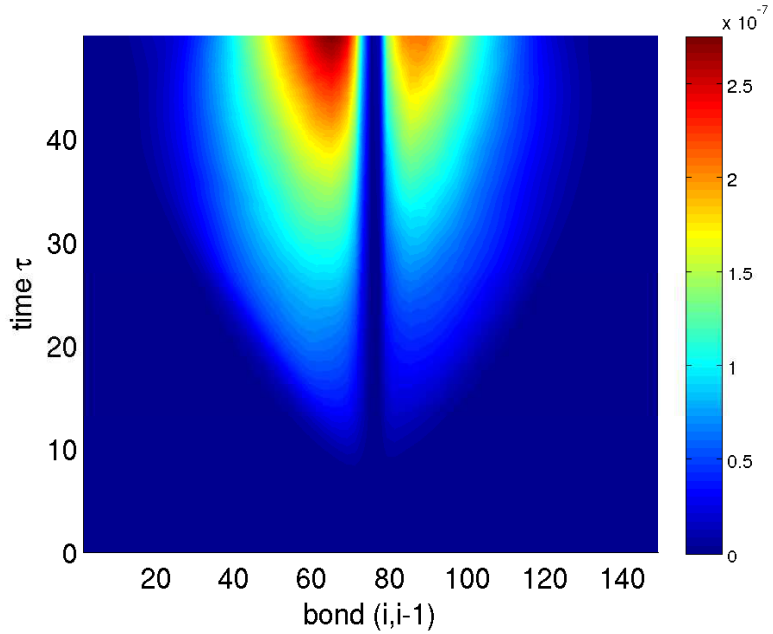
Short time TEBD dynamics: entanglement

$$L = 150, U = 20\Delta, V_{\text{bias}} = 2\Delta$$

entanglement entropy



truncated weight



Evaluating physical quantities

The steady-state current density is obtained via the Keldysh part of the Green's function

$$j_{ij} = \frac{t_{ij}}{2} \sum_{\sigma} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \Re\mathrm{e} \left(\mathsf{G}_{ij}^{K\sigma}(w) - \mathsf{G}_{ji}^{K\sigma}(w) \right) ,$$

non-equilibrium (local) density of states (nLDOS) of the dot:

$$\rho_f^{\sigma}(\omega) = -\frac{1}{\pi} \Im\mathrm{m} \left(\mathsf{G}_{ff}^{R\sigma}(\omega) \right)$$