Strongly correlated quantum systems out of equilibrium: A variational cluster approach

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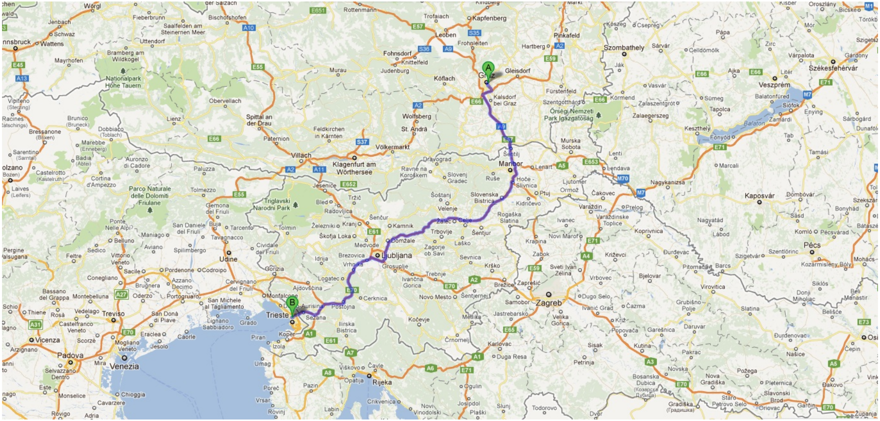

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Balatonfüred

Non-equilibrium Group at Technical University Graz

Outline

1. Manybody Cluster Methods
   - Introduction
   - Cluster Perturbation Theory
   - Variational Cluster Approach
2. Non-equilibrium extension
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3. Results for a single quantum dot
   - Model
   - Results in equilibrium
   - Results out of equilibrium

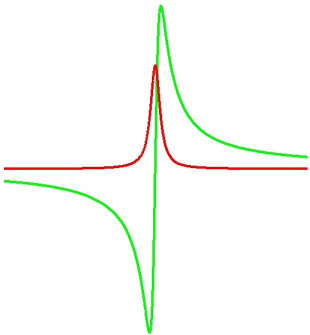
Generic lattice model

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

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

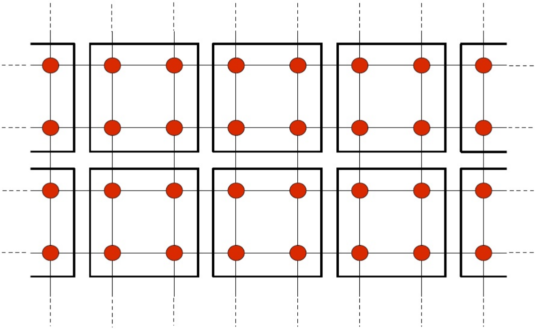
Atomic limit

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



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

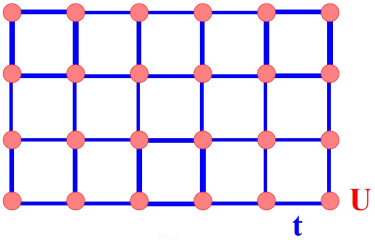
Manybody Cluster Methods



Extrapolate cluster to thermodynamic limit:

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

Correlated lattice model

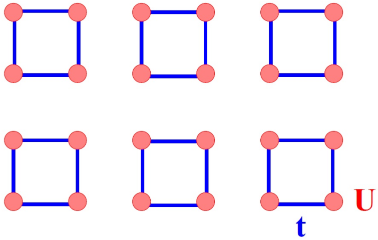


given: Hamiltonian e.g.
Hubbard model
$\hat{\mathcal{H}}$

ask for: Green's function
G = ?

in general intractable ... :(

Cluster Tiling



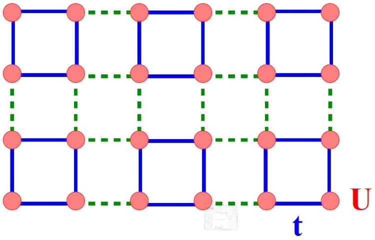
$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_{\text{cluster}}$$

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

(numerically) exactly solvable ... :)

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

Cluster Perturbation Theory[2] [3]



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

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

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)

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[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)

Cluster Perturbation Theory - Motivation

Heuristic derivation using **Dyson's equation**:

$$\mathsf{G}^{-1} = \mathsf{G}_0^{-1} - \Sigma$$
$$\mathsf{G}_{\text{cluster}}^{-1} = \mathsf{G}_{\text{cluster},0}^{-1} - \Sigma_{\text{cluster}}$$

- $_0$ = non-interacting Green's functions

$$\mathsf{G}_0^{-1} = \omega + \mu - V$$

  - V = hopping matrix
- Σ = self-energy

Cluster Perturbation Theory - Motivation

$$\begin{aligned}
\mathsf{G}^{-1} &= \mathsf{G}_0^{-1} - \Sigma \\
&\approx \mathsf{G}_0^{-1} - \Sigma_{\text{cluster}} \\
&= \mathsf{G}_0^{-1} - \left(\mathsf{G}_{\text{cluster},0}^{-1} - \mathsf{G}_{\text{cluster}}^{-1}\right) \\
&= \mathsf{G}_{\text{cluster}}^{-1} - \left(\mathsf{G}_{\text{cluster},0}^{-1} - \mathsf{G}_0^{-1}\right) \\
&= \mathsf{G}_{\text{cluster}}^{-1} - \mathsf{T}
\end{aligned}$$

- Approximation: take **self-energy of the cluster**
- T = inter-cluster hopping:

$$\begin{aligned}
\left(\mathsf{G}_{\text{cluster},0}^{-1} - \mathsf{G}_0^{-1}\right) &= (\omega + \mu - V_{\text{cluster}}) - (\omega + \mu - V) \\
&= V - V_{\text{cluster}} = \mathsf{T}
\end{aligned}$$

Cluster Perturbation Theory - Limits

CPT is exact for

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

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.

Variational Cluster Approach[4]

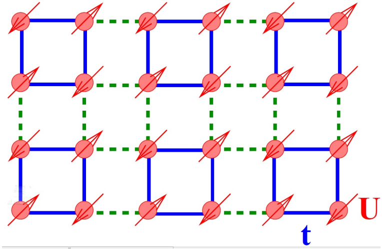
- VCA = variational extension to CPT - rigorously developed within the **Self-Energy Functional Approach** (SFA)[a,b],
- does **not** implement a variational principle in the sense of a Rayleigh-Ritz variational principle,
- is applicable to **broken-symmetry/ordered** phases.

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

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

Illustration of the Variational Cluster Approach

VCA = Variational CPT: **Optimize the initial state**



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

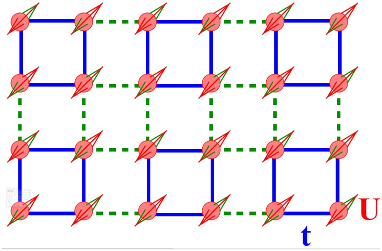
$$\mathbf{G}^{-1}_{\mathbf{CPT}}(\omega, \mathbf{k}) = \mathbf{G}'^{-1}_{\mathbf{cluster}}(\omega) - \mathbf{T}'(\mathbf{k})$$

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

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

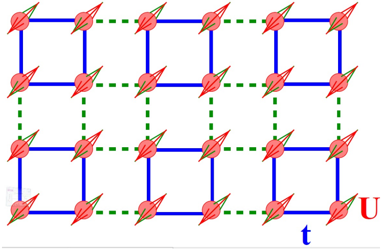
$$\hat{\mathcal{H}}'_{\text{cluster}} = \hat{\mathcal{H}}_{\text{cluster}} + \hat{h}_{\text{field}}$$

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

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



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

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

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

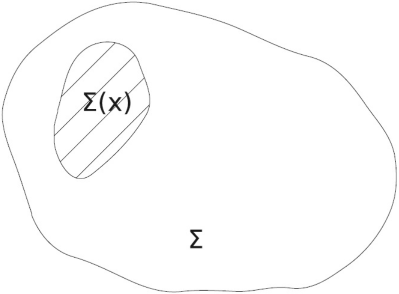
Stationary point of the grand potential:

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

VCA = CPT + variational principle

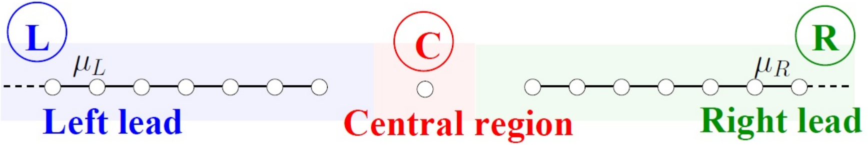
Restriction of self-energies

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



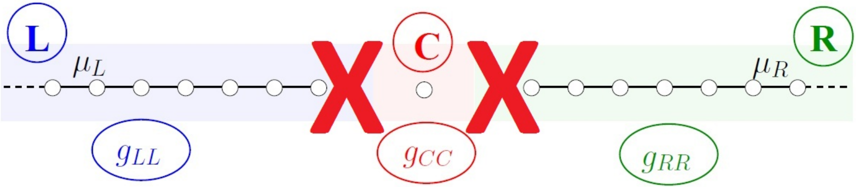
Outline

Illustration of a non-equilibrium system



simple model: non-interacting quantum dot

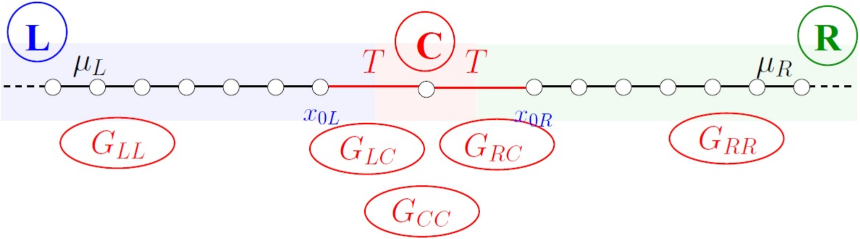
$t = t_0$: three decoupled systems



evaluate Green's function $\mathrm{g} = \mathrm{diag}(\mathrm{g}_{LL}, \mathrm{g}_{CC}, \mathrm{g}_{RR})$
of **decoupled** system

$t > t_0$: coupled system

at time $t > t_0$: the **coupling is switched on**: $T \propto \Theta(t - t_0)$

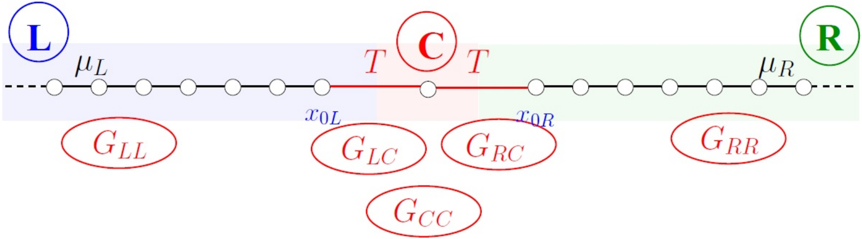


non equilibrium situation → **Keldysh Green's functions**

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

notation from Rammer+Smith '86

Dyson equation

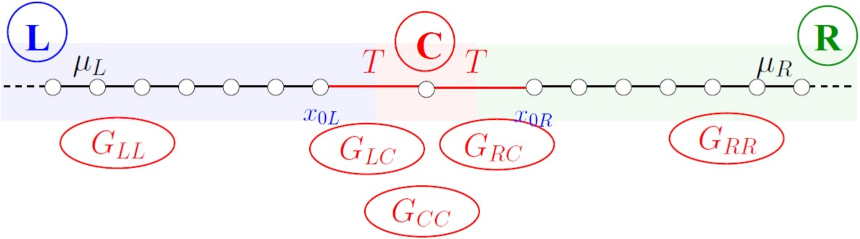


Dyson equation

$$G = g + g \circ T \circ G$$

exact for noninteracting system

Steady-state

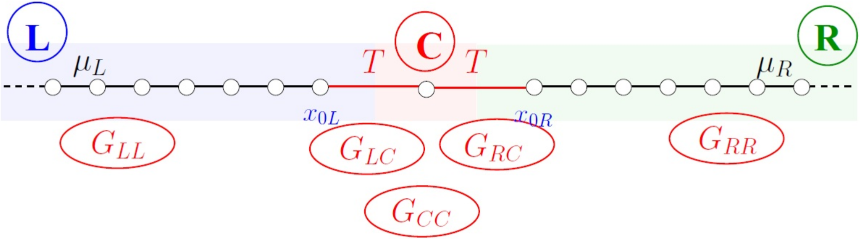


at $t \to \infty$ system reaches **steady state**

time translationally invariant

$\to$ Fourier transform to ω

Green's function of central region



Dyson equation **reduces** to

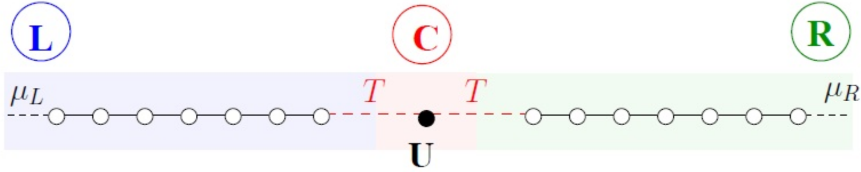
$$\mathsf{G}_{CC} = \mathsf{g}_{CC} + \mathsf{g}_{CC}\Sigma_{eff}\mathsf{G}_{CC}$$

2x2 Keldysh matrices

$$\Sigma_{eff} = \mathsf{T}\left(\mathsf{g}_{LL}(r_{0L}) + \mathsf{g}_{RR}(r_{0R})\right)\mathsf{T}$$

see e.g. Haug+Jauho

Interacting quantum dot

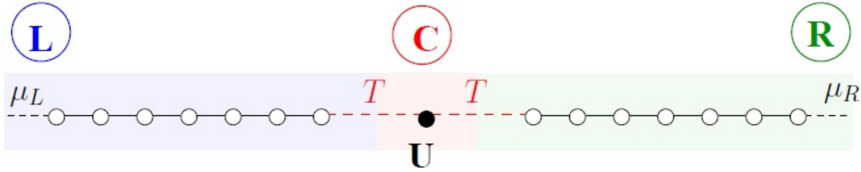


Interacting system: Dyson Equation

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

$\mathsf{g} = \mathrm{diag}(\mathsf{g}_{LL}, \mathsf{g}_{CC}, \mathsf{g}_{RR})$ of decoupled system evaluated exactly

CPT approximation

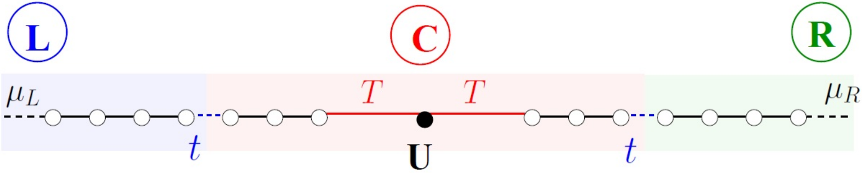


CPT interacting system: Dyson Equation

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

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

Applying CPT



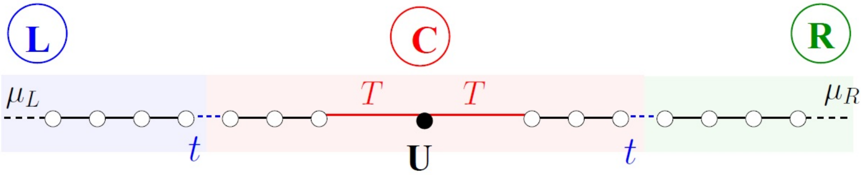
take **larger central region** and solve larger cluster exactly
treat inter-cluster hopping (t) perturbatively

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

cf. short time dynamics by Balzer+Potthoff '11

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

Adding a single-particle field



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

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

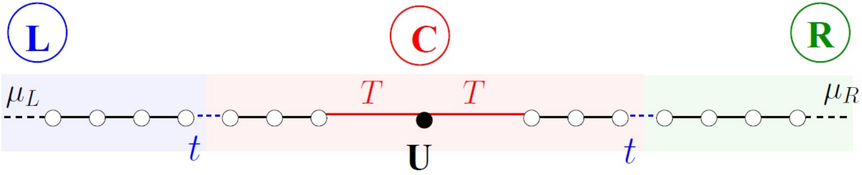
start from better initial state at $\tau < \tau_0$ → variational optimization:

minimize difference between initial and final state

by adding $\hat{h}_{\text{field}}$ (here ΔT) at $\tau < \tau_0$

and subtract it again for $\tau > \tau_0$

Subtracting a single-particle field



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

start from better initial state at $\tau < \tau_0$ → 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 $\hat{h}_{\text{field}}$

Self-consistency condition

New optimization criterion in non-equilibrium:

$$\langle \frac{\partial \mathcal{H}}{\partial \Delta T} \rangle_{\tau < \tau_0} \stackrel{!}{=} \langle \frac{\partial \mathcal{H}}{\partial \Delta T} \rangle_{\tau \to \infty}$$

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

for impurity systems there are more accurate methods
see e.g. Mehta+Andrei '06, Anders '08, ...

Evaluating physical quantities

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

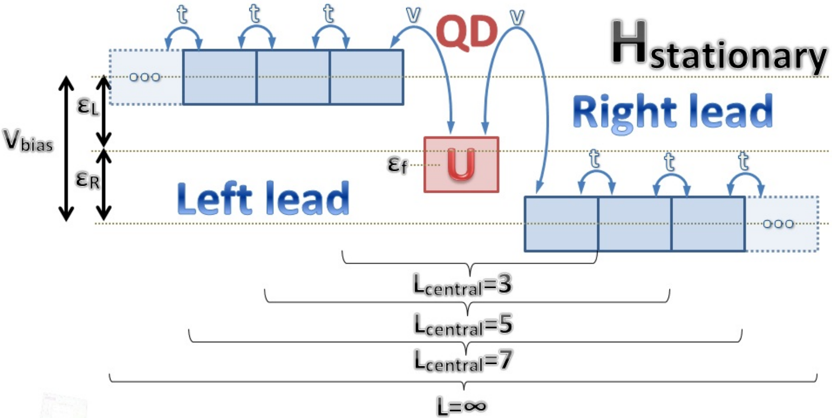
$$j_{ij} = \frac{t_{ij}}{2} \sum_{\sigma} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \Re\mathrm{e} \left(\mathsf{G}_{ij}^{K\sigma}(w) - \mathsf{G}_{ji}^{K\sigma}(w) \right) ,$$

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

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

Outline

model of a single quantum dot



- Initial state: **three decoupled systems in equilibrium**
- Apply a **symmetric bias** $\frac{V_{\text{bias}}}{2} = \epsilon_L = \mu_L = -\epsilon_R = -\mu_R$.
- At some time τ_0 the **coupling** (t **or** V) **is switched on**.
- We are interested in the long time **steady-state properties**.

VCA reference system

Two parts

- a cluster part and
- an infinite environment.

Green's functions

- Lanczos/Band-Lanczos method for the cluster part,
- analytically for the environment part.

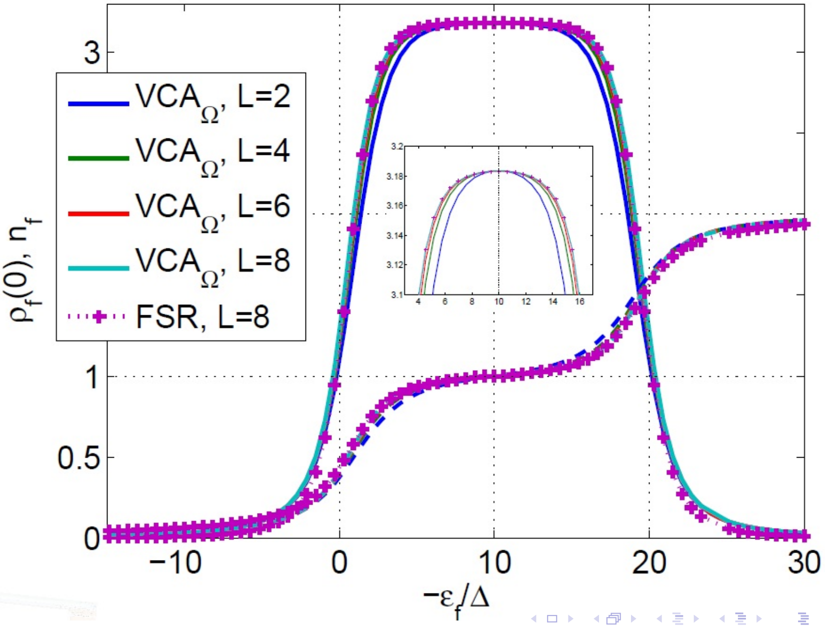
Summary of results for semi-infinite model

Equilibrium results

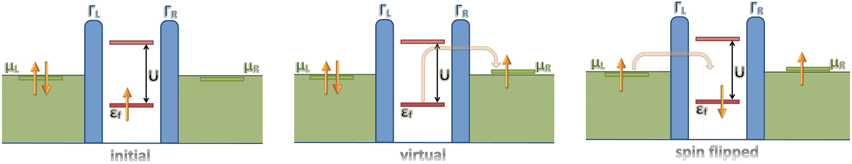
- **VCA** » CPT
- **Hubbard bands** (position + width)
- **all parameter regions** (pinning of Kondo resonance)
- Σ exact for high Matsubara frequency
- **Kondo peak** + exponential scale in U (although wrong prefactor)
- **fast**

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

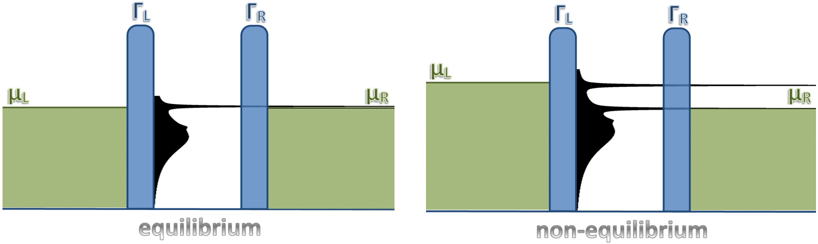
Impurity Occupation



Quantum dot <-> Kondo physics



Non-equilibrium physics

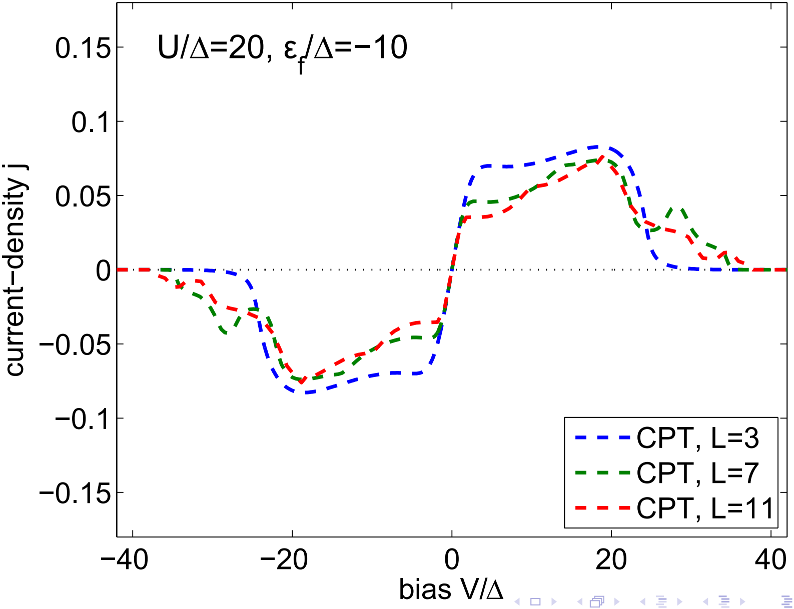


Steady-state current density

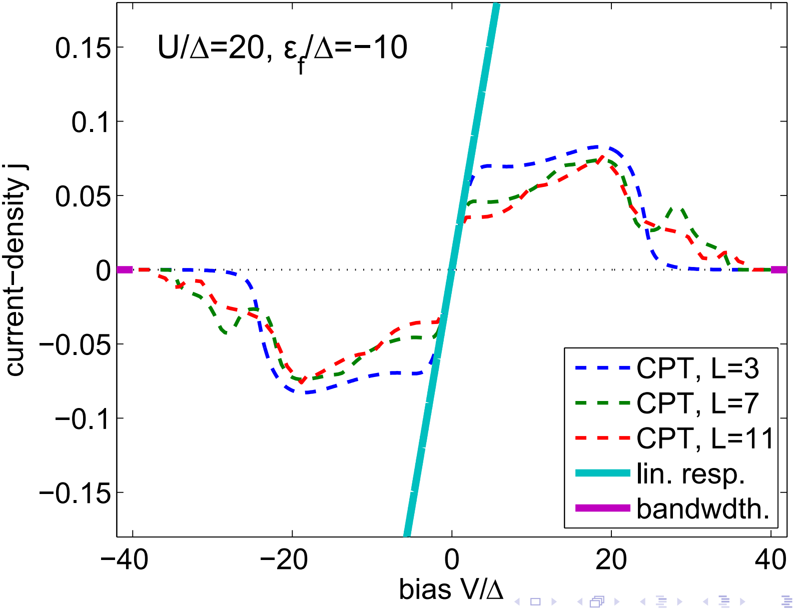
- **steady-state current density**: j fulfills continuity equation
- **particle-hole symmetric** model at relatively high interaction strength
- **bias voltage** is applied in an **asymmetric fashion**
- **symmetric** dot-lead **couplings**

M. Nuss, E. Arrigoni and W. von der Linden, to appear in: AIP Conf. Proc. XVI TCPSCS (2012)

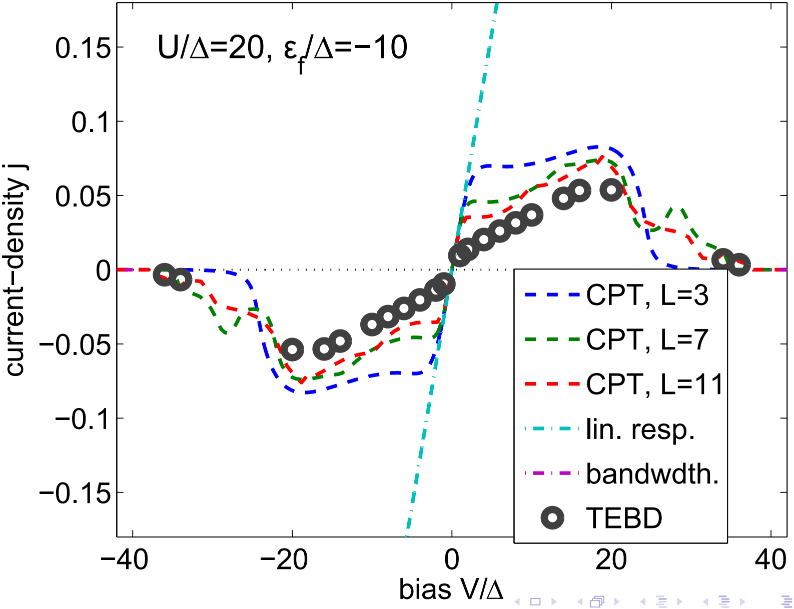
Non equilibrium cluster perturbation theory

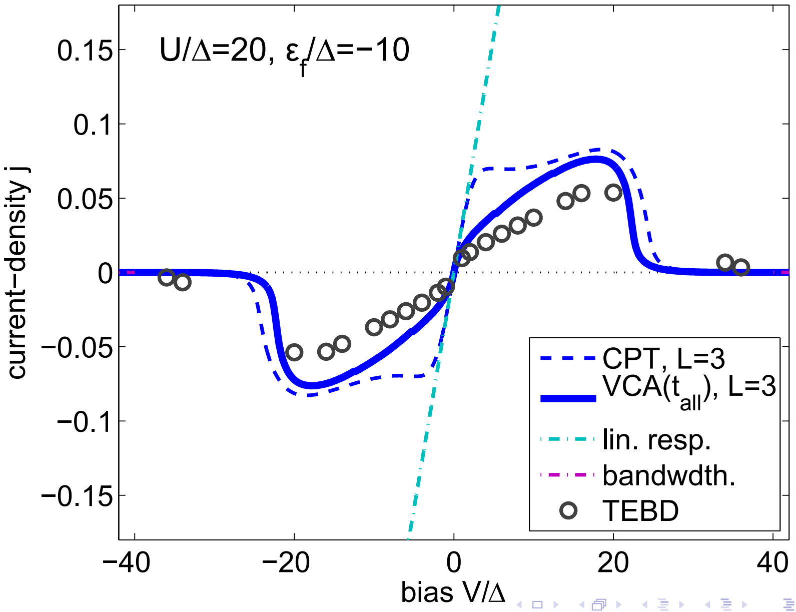


Exact limits

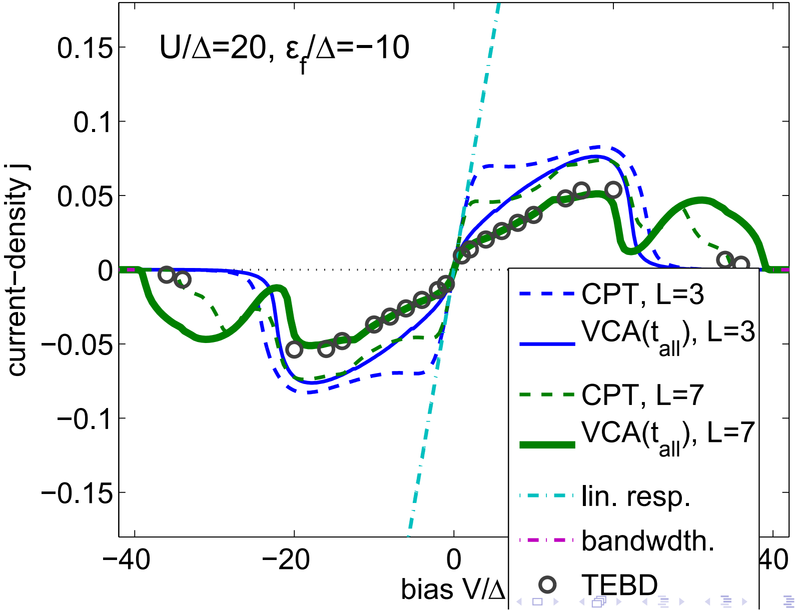


Quasi stationary state of exact time evolution

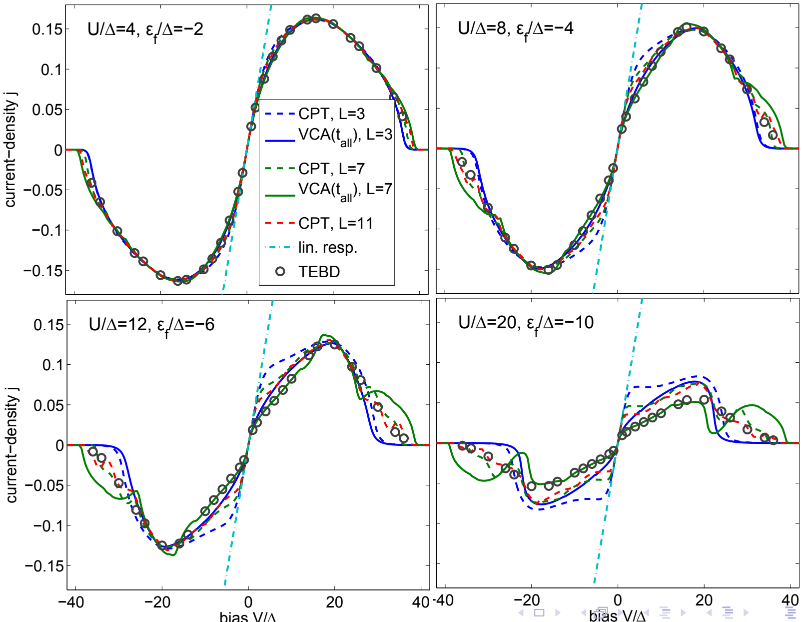



U/Δ=20, ε_f/Δ=−10
0.15
0.1
0.05
0
−0.05
−0.1
−0.15
current−density j
−40
−20
0
20
40
bias V/Δ
CPT, L=3
VCA(t_all), L=3
lin. resp.
bandwdth.
TEBD

Non equilibrium Variational cluster approach

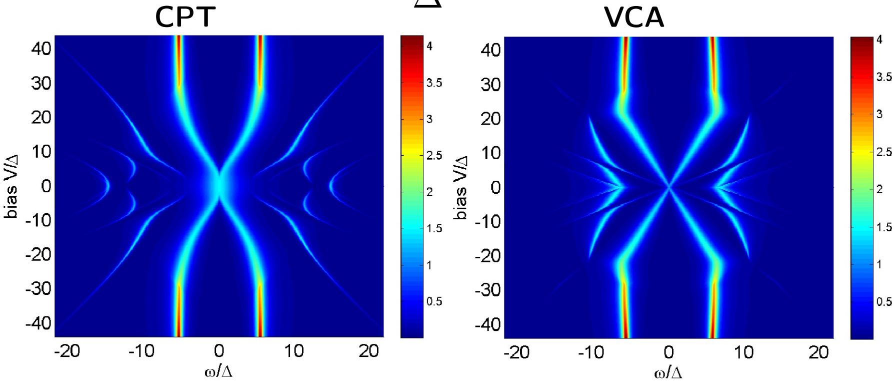


Results for various interaction strength



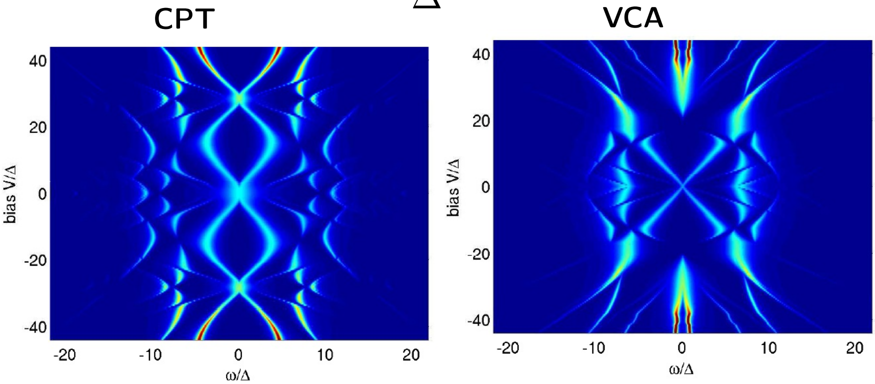
Non-equilibrium density of states

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

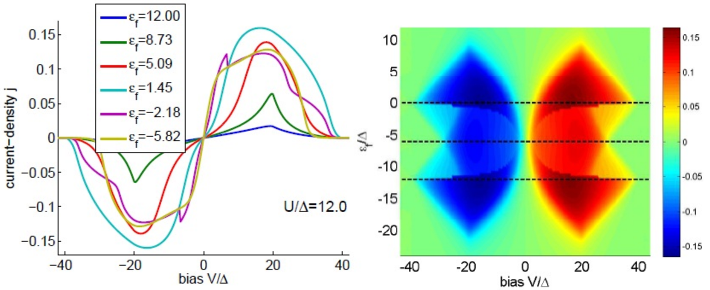


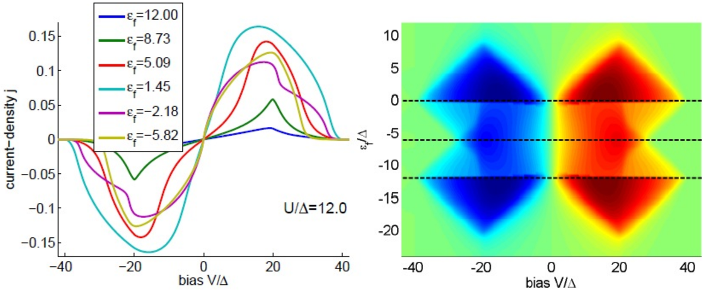
Non-equilibrium density of states

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



Results away from particle hole symmetry





Conclusion

- non-linear steady-state current available in **all parameter regions**
- nCPT and nVCA **exact** for $U = 0$
- nCPT and nVCA respect the **low bias** lin. resp. result and the **high bias** band cutoff
- VCA results agree reasonably well with (exact) data from **DMRG** time evolution
- low U: **CPT and VCA** perform excellently
- high U: **VCA » CPT** (self-consistent feedback critical!)
- current differs with increasing U sooner from lin. resp. due to **thinning** of Kondo resonance
- VCA: linear (U) dependent **splitting of Kondo resonance** in LDOS
- Kondo resonance **joins** with Hubbard bands at certain bias voltage
- calculation **outside** Kondo region performs extremely well
- in Kondo region at high U and high bias calculations become **challenging**

Open issues and future challenges

- Finding the most suitable, best performing **optimization condition**.
- Identifying most suitable **variational parameters**.
- **Application** to multi-impurity systems.
- **high bias/U**
- **Comparison** to other methods

Thank You!

Thank you for your attention!

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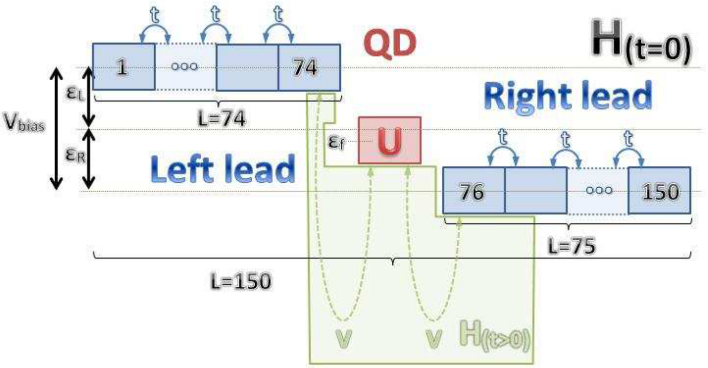
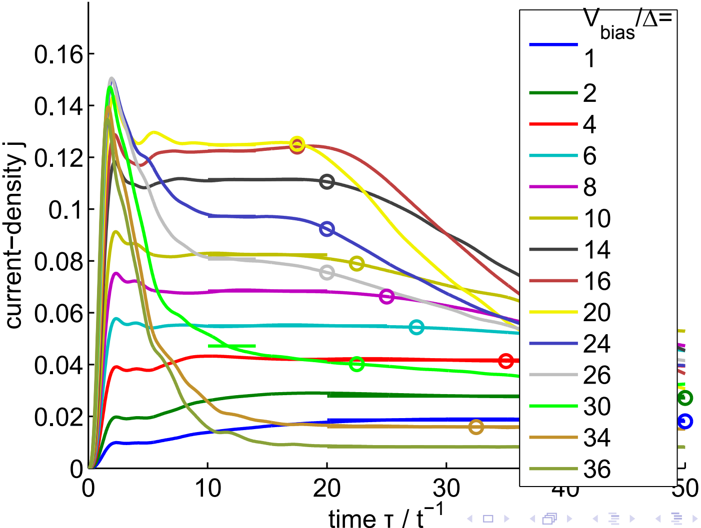
Short time TEBD dynamics: quench



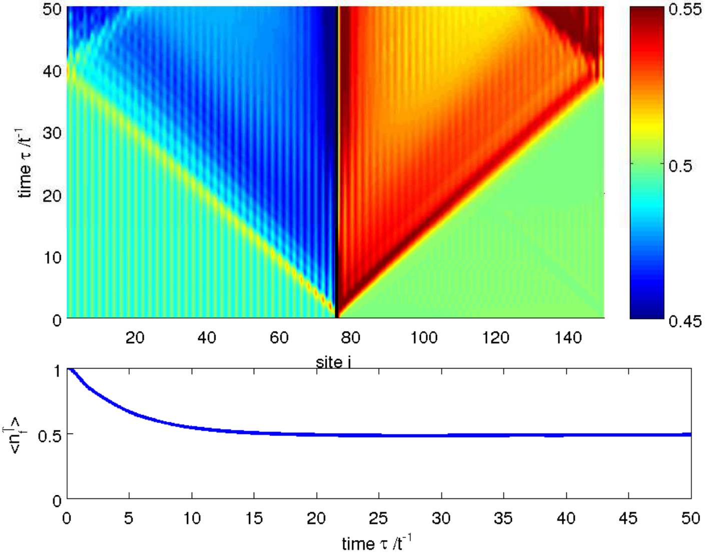
Short time TEBD dynamics: quasi-stationary-state current density

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



Short time TEBD dynamics: particle number

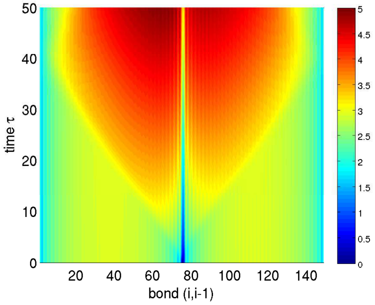
$$L = 150, U = 12\Delta, V_{\text{bias}} = 14\Delta$$



Short time TEBD dynamics: entanglement

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

entanglement entropy



truncated weight