Nonequilibrium Dynamical Mean Field Theory:

impurity solver by an auxiliary Master Equation approach

Enrico Arrigoni, Michael Knap, Wolfgang von der Linden

Institute of Theoretical Physics - Computational Physics

TU Graz

CCQS, Evora, Oct. 2012

Outline of the talk

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Nonequilibrium Strongly Correlated Systems

Systems and materials

- Ultracold atoms
- Transport through heterostructures / quantum dots / spintronics
- Quantum information

Issues

- Nonequilibrium quantum phase transitions
- Decoherence / dissipation
- Thermalisation

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for nonequilibrium strongly correlated systems

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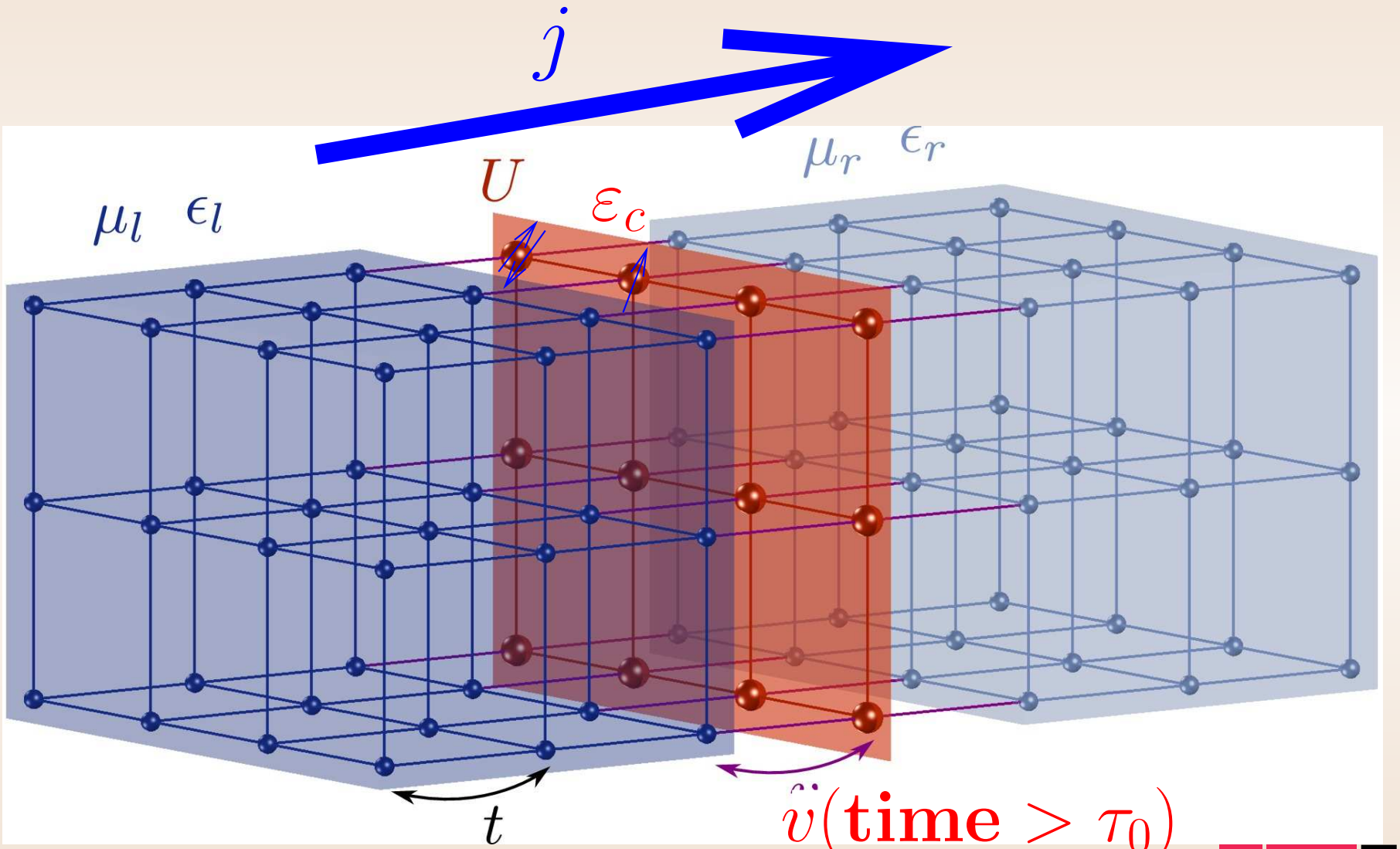
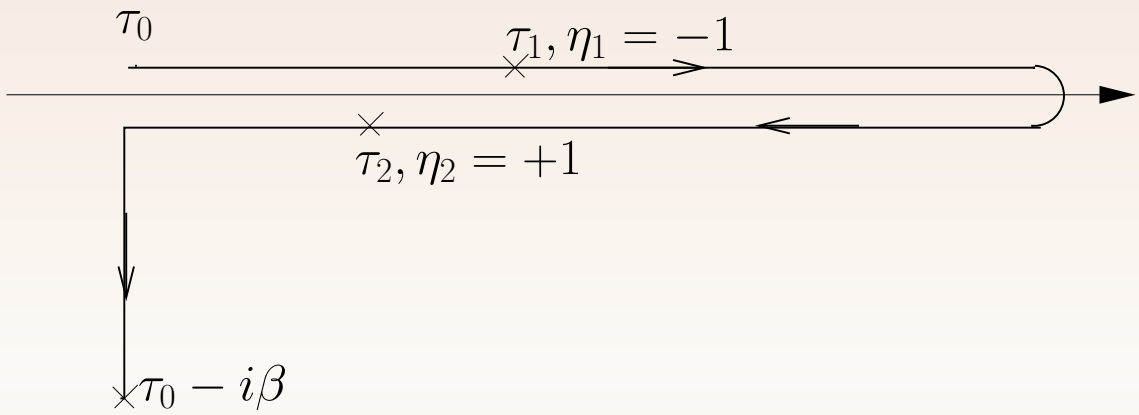
Model



Voltage $\phi = \mu_l - \mu_r$

Nonequilibrium Green's functions

(Kadanoff+Baym,Keldysh,Schwinger)



$$G(\tau_1\eta_1, \tau_2\eta_2) \Rightarrow \underline{G}(\tau_1, \tau_2) \Rightarrow \begin{pmatrix} G^R(\tau_1, \tau_2) & G^K(\tau_1, \tau_2) \\ 0 & G^A(\tau_1, \tau_2) \end{pmatrix}$$

After decay of transient: steady state $\underline{G}(\tau_1 - \tau_2) \Rightarrow \underline{G}(\omega)$

Needs dissipation, i.e. infinite system

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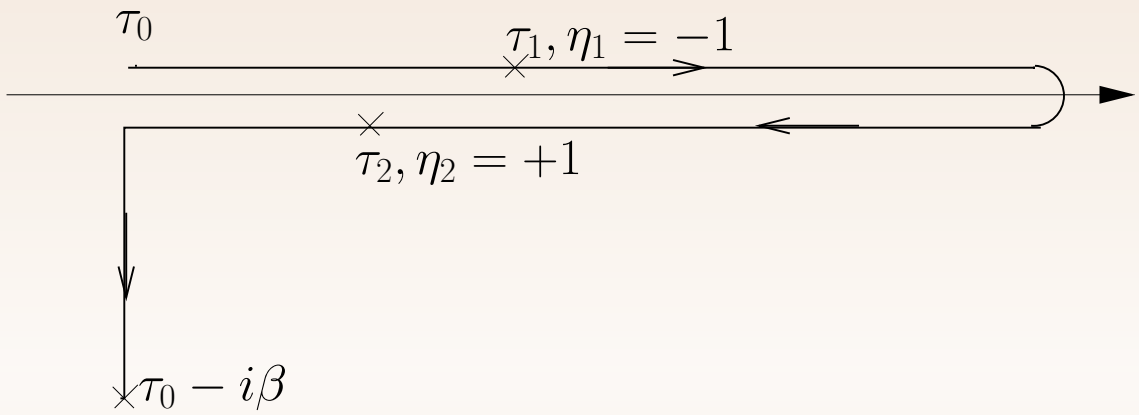

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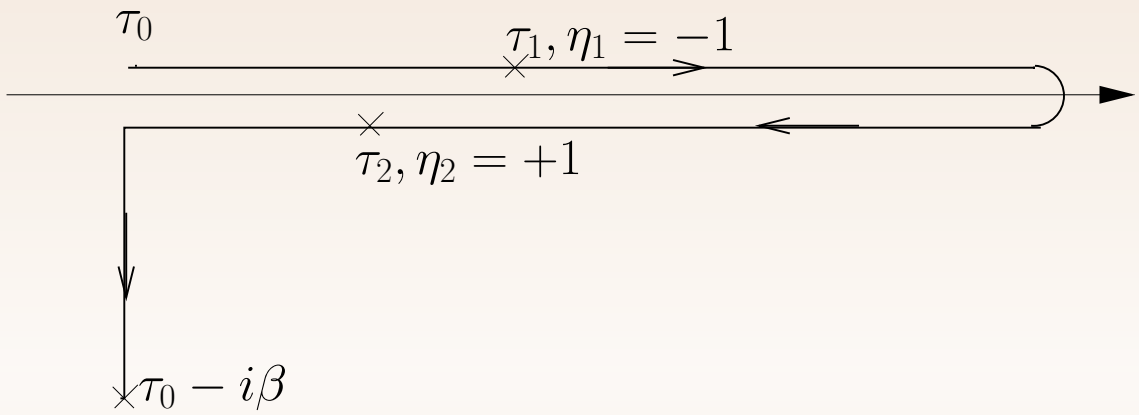

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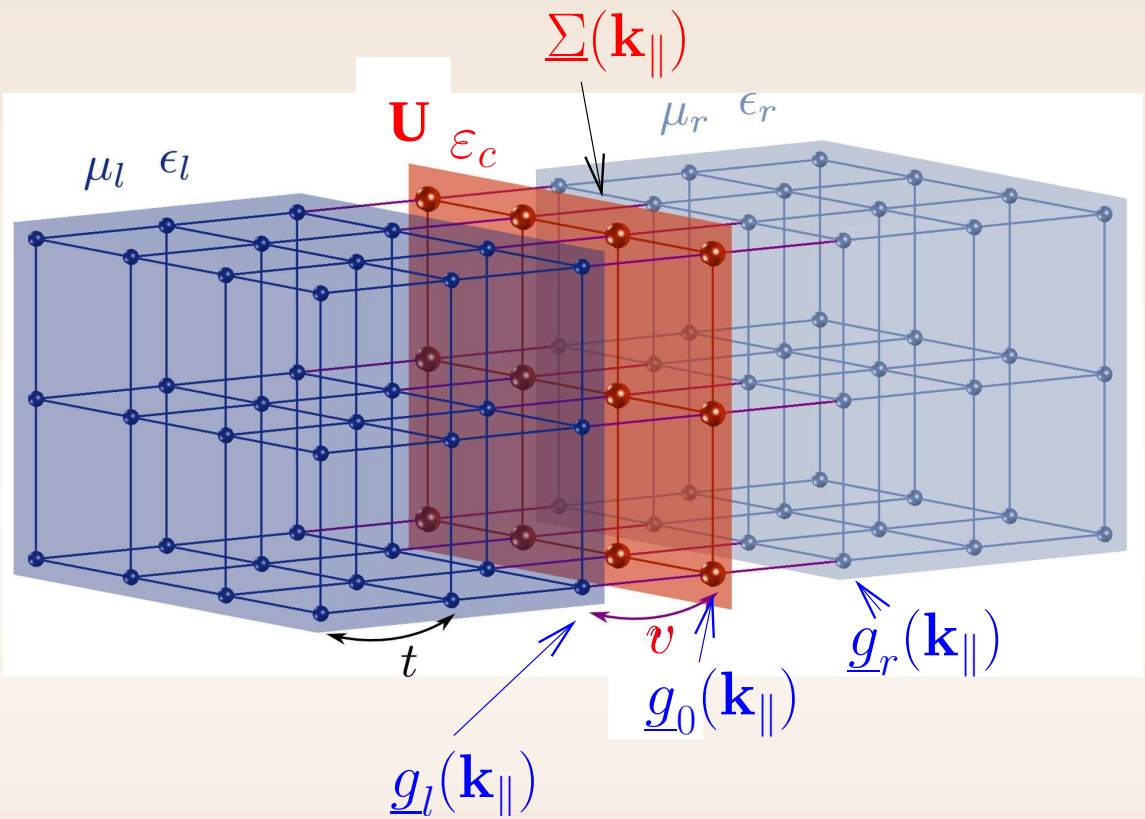
Dynamical Mean-Field Theory



$v = 0$ Green's functions:

$$(g_0(\mathbf{k}_\parallel)^{-1})^R = (\omega - \varepsilon_c - t(\mathbf{k}_\parallel))$$

$$(g_0(\mathbf{k}_\parallel)^{-1})^K = 0$$

$$g^R_\alpha(\mathbf{k}_\parallel) = g_{\frac{1}{2}chain}(\omega - \varepsilon_\alpha - t(\mathbf{k}_\parallel))$$

$$g^K_\alpha(\mathbf{k}_\parallel) = = 2i\mathrm{Im}\, g^R_\alpha(\mathbf{k}_\parallel)(1 - 2f_F(\omega - \mu_\alpha))$$

Dyson equation: (omit ω dependence)

$$\underline{G}(\mathbf{k}_\parallel)^{-1} = \underline{g}_0^{-1}(\mathbf{k}_\parallel) - \sum_{\alpha=l,r} v^2 \underline{g}_\alpha(\mathbf{k}_\parallel) - \underline{\Sigma}(\mathbf{k}_\parallel)$$

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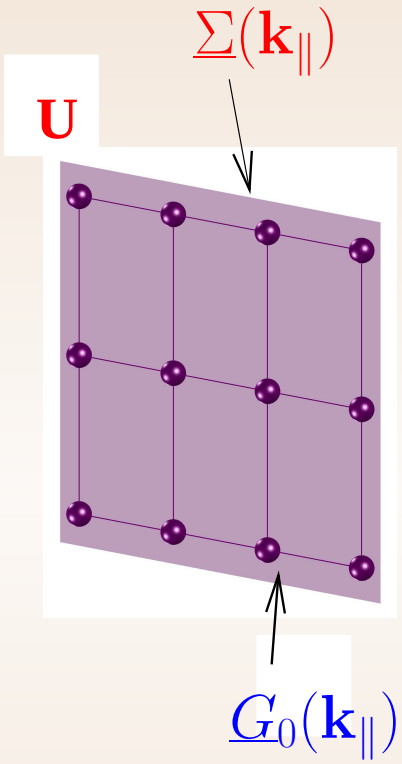

noninteracting leads can be eliminated

$$\underline{G}(\mathbf{k}_\parallel)^{-1} = \underline{G}_0(\mathbf{k}_\parallel)^{-1} - \underline{\Sigma}(\mathbf{k}_\parallel)$$

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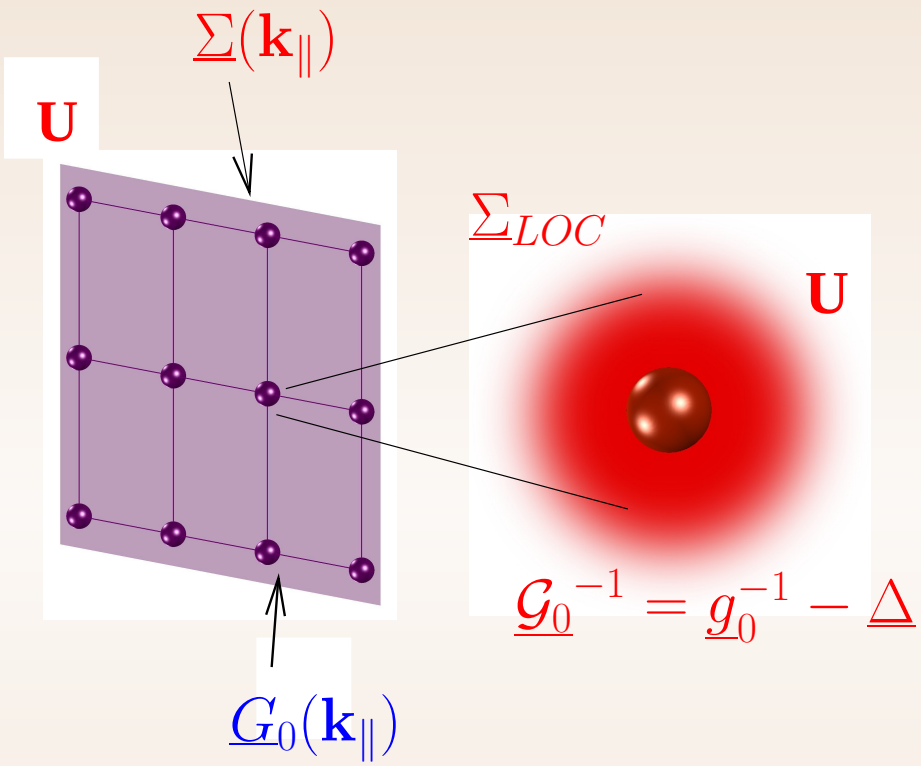

DMFT approximates $\underline{\Sigma}(\mathbf{k}_\parallel)$ by a local $\underline{\Sigma}_{LOC}$
obtained by solving an effective (nonequilibrium) impurity problem

$$\underline{G}^{-1}_{IMP} = \underline{\mathcal{G}_0}^{-1} - \underline{\Sigma}_{LOC} = \underline{g}_0^{-1} - \underline{\Delta} - \underline{\Sigma}_{LOC}$$

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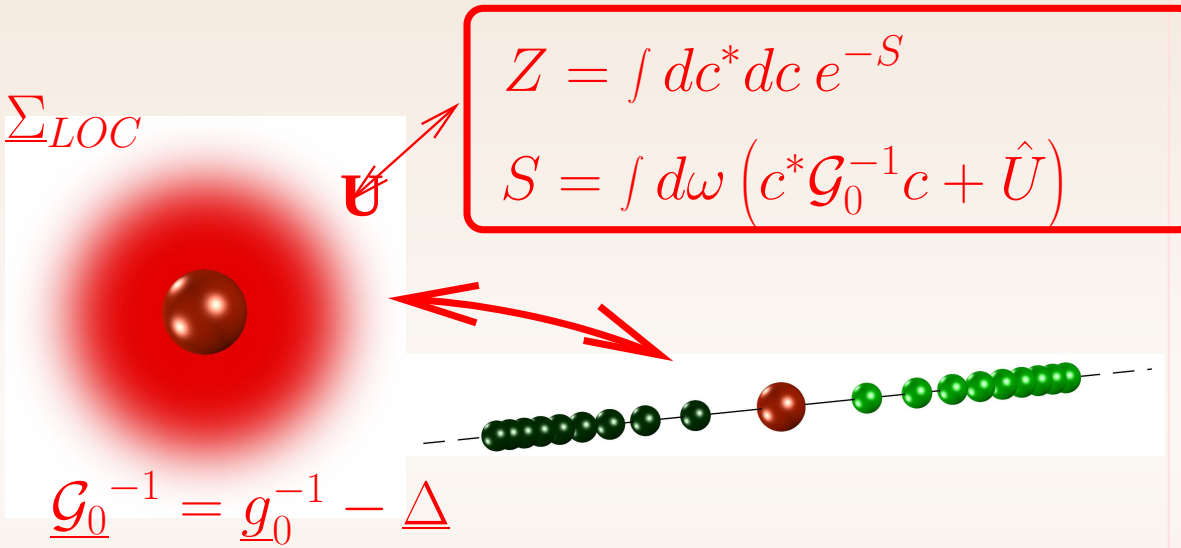

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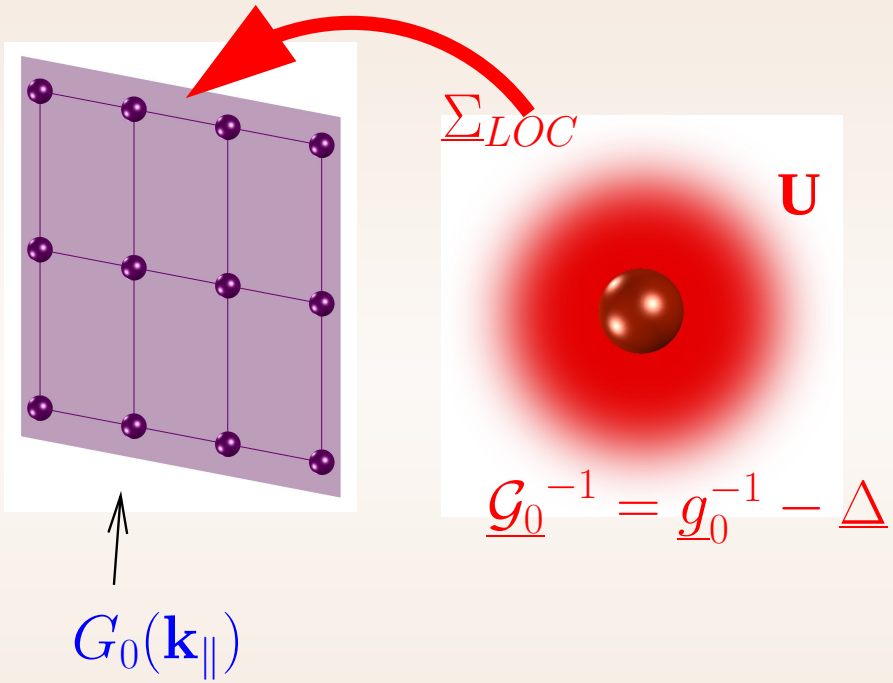
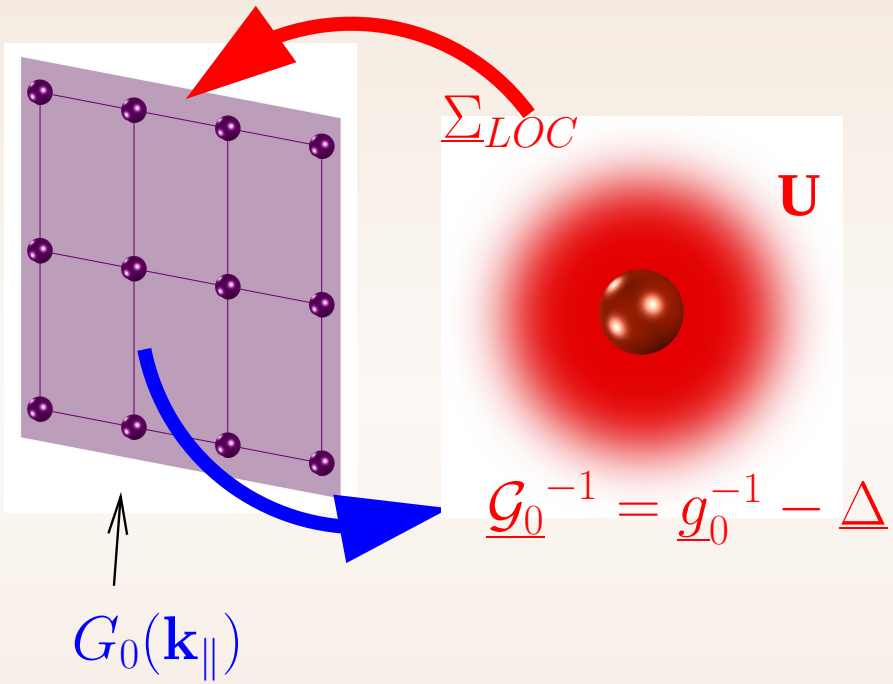


Σ_{LOC} is used in the Dyson equation

$$\underline{G}(\mathbf{k}_\parallel) = \left(\underline{G}_0(\mathbf{k}_\parallel)^{-1} - \underline{\Sigma}_{LOC}\right)^{-1}$$

Dynamical Mean-Field Theory



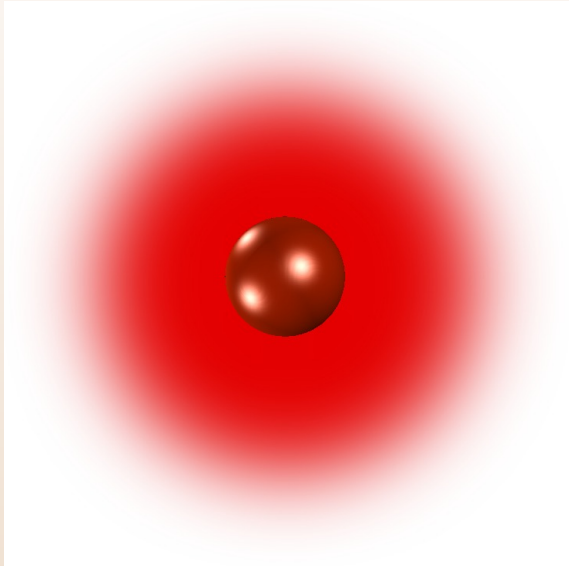
to obtain the self-consistent equation for bath hybridisation function $\underline{\Delta}$

$$\int_{BZ} \frac{d\mathbf{k}_\parallel}{(2\pi)^2}\, \underline{G}(\mathbf{k}_\parallel) \equiv \underline{G}_{LOC} = \underline{G}_{IMP} \equiv \left(\underline{g}_0^{-1} - \underline{\Delta} - \underline{\Sigma}_{LOC}\right)^{-1}$$

DMFT Impurity solvers

Bottleneck

- Iterated perturbation theory (Schmidt+Monien)
- (Continuous time) Quantum Monte Carlo (Eckstein+Werner)
- Noncrossing Approximation (Eckstein+Werner)
- Numerical RG (Anders et al.)
- Exact diagonalisation: $\underline{\Delta}(\omega)$
  is fitted by a small number of baths sites



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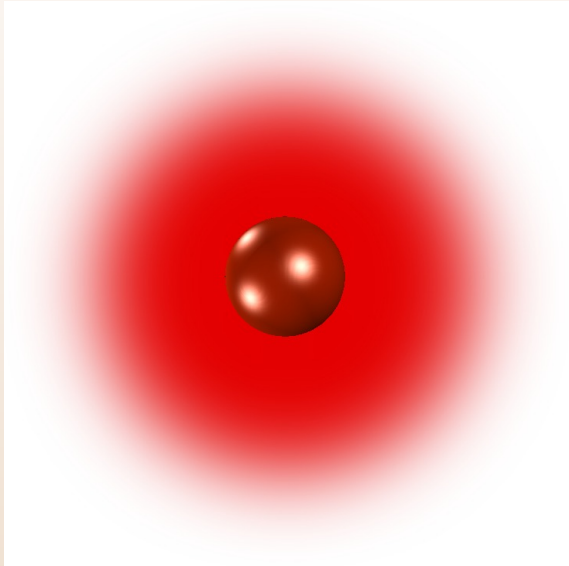

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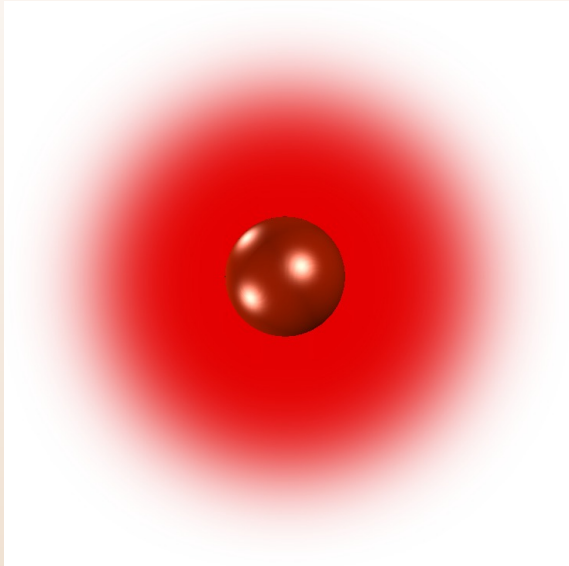

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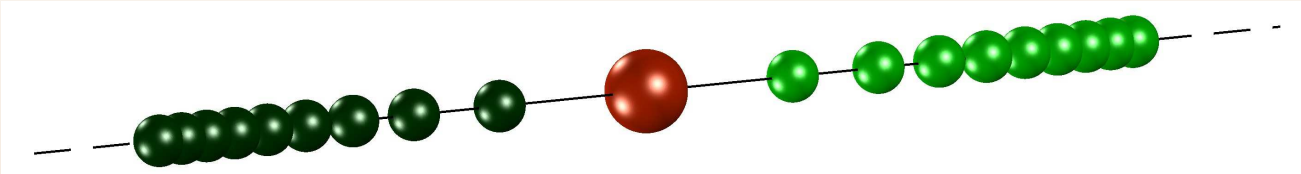

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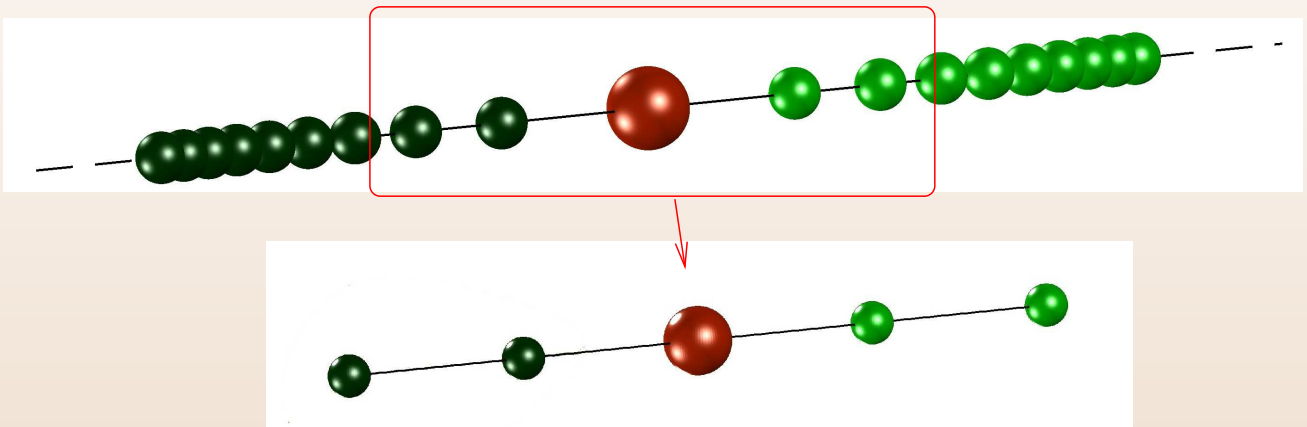
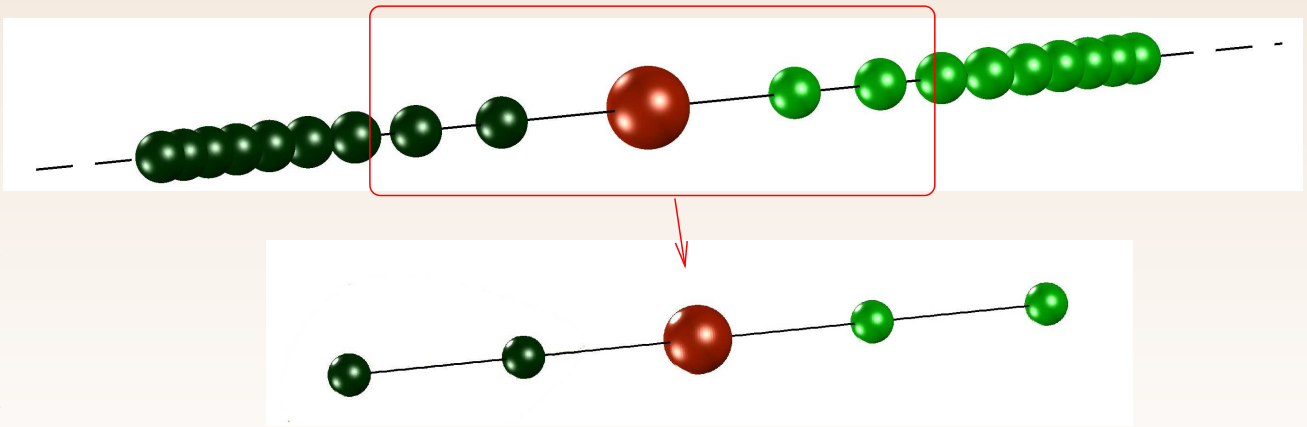


Exact diagonalisation of a finite cluster

Does it work for a nonequilibrium steady-state?



Problems in nonequilibrium:

- Time dependence: steady state is never reached (quasiperiodic behavior)
- Alternative: use equilibrium self energy: at what chemical potential? Temperature?
- $\Delta(\omega)$ must be fitted in real frequency (Matsubara frequencies do not exist) problem:peak structure

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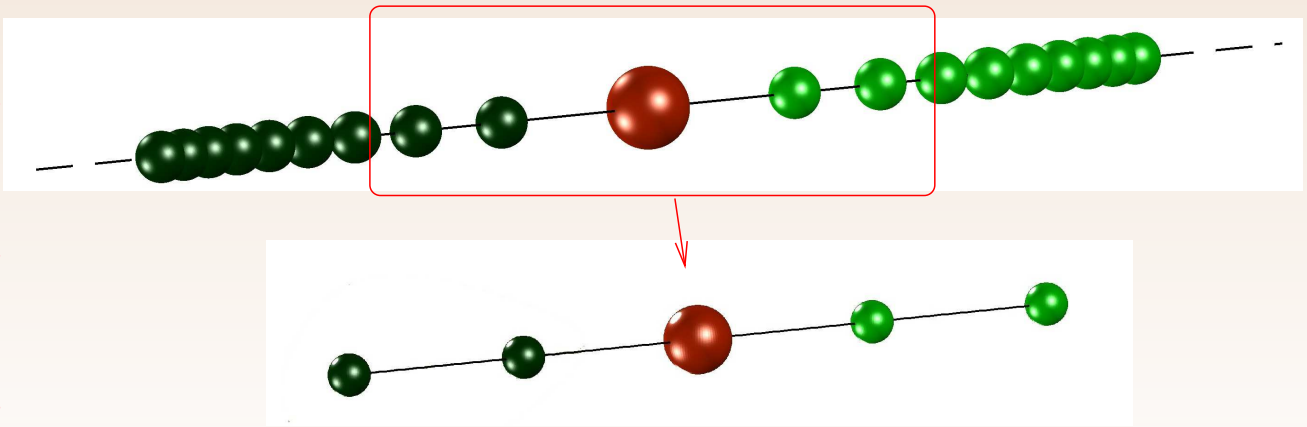

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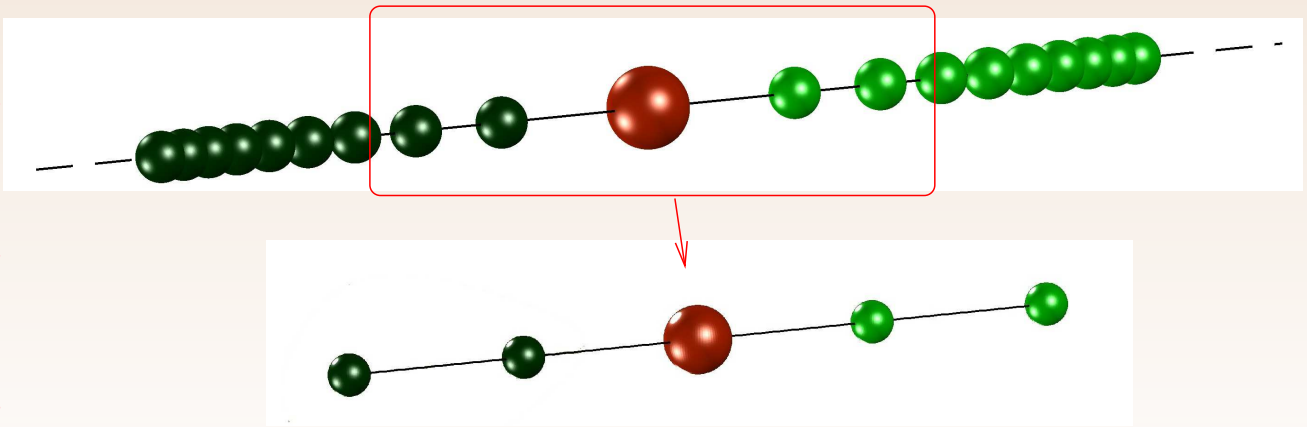

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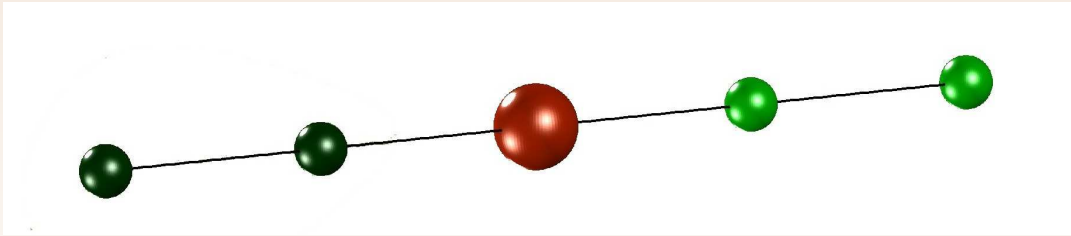
Effective quantum Master equation approach



Dynamics described by Markovian Master equation for density matrix ρ of "chain" (Lindblad 76):

$$\frac{d}{d\tau}\rho = \mathcal{L}\,\rho\,, \qquad \mathcal{L} = \mathcal{L}_H + \mathcal{L}_b \qquad \mathcal{L}_H\,\rho = -i[H,\rho].$$

$$\mathcal{L}_b\,\rho \equiv 2\sum_{n,m}\left(\Gamma^{(1)}_{n,m}\left(c_{n\sigma}\rho c^\dagger_{m\sigma} - \frac{1}{2}\{\rho, c^\dagger_{m\sigma}c_{n\sigma}\}\right) + \right.$$

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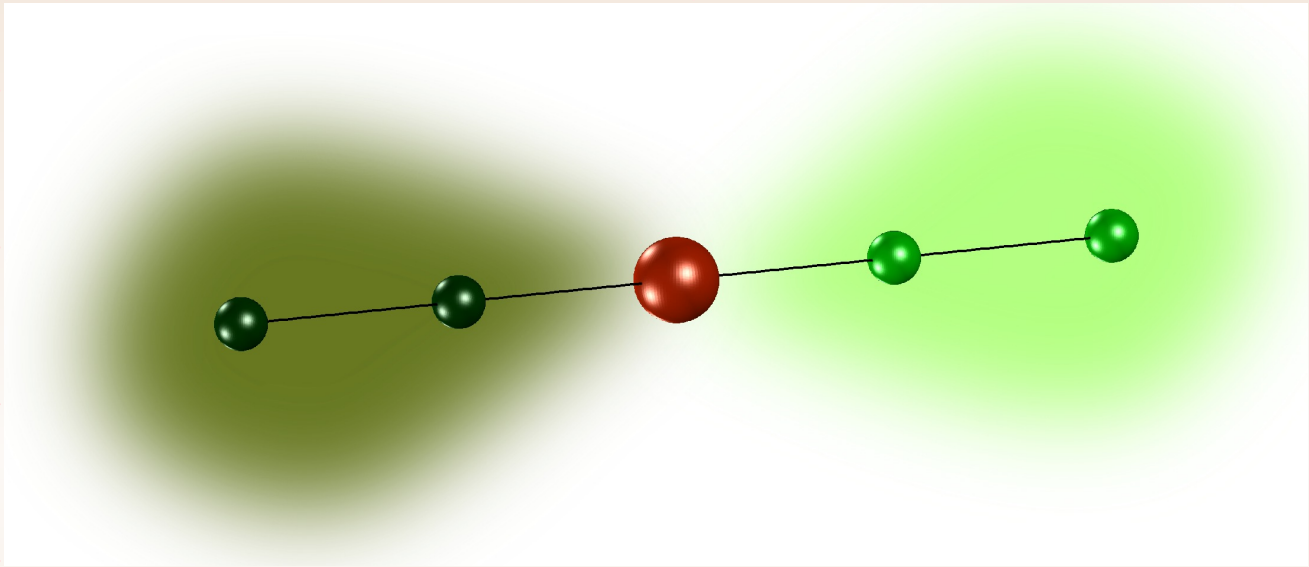
Effective quantum Master equation approach

Attach two Markovian baths near the end of the chain:



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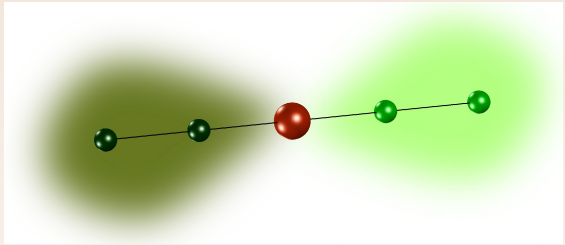

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$\Gamma_{n,m}$ as well as chain sites parameters (hoppings, energies) are used to fit $\Delta(\omega)$

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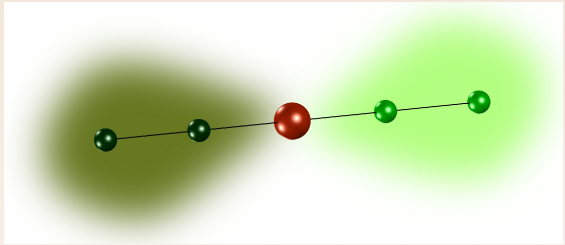

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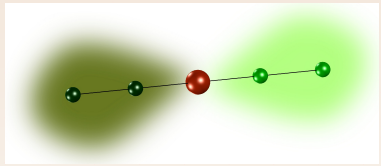

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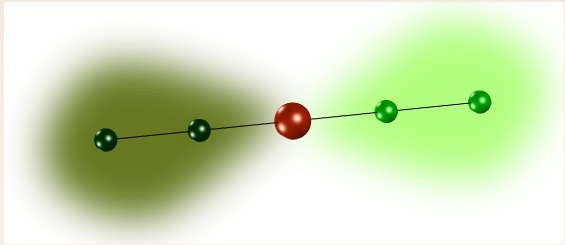

- Markovian Master equation: $\frac{d}{d\tau}\,\rho = \mathcal{L}\,\rho$
- Can be solved by exact diagonalisation:
  steady state, Green's function, and thus $\underline{\Sigma}_{LOC}$ can be determined
- Reproduces well the exact $\underline{\Delta}(\omega)$
  already with a few number of chain sites.
- $U = 0$ Green's function does not have "delta-peak" structure.
  Can be used to fit $\underline{\Delta}(\omega)$ for real ω.
- Markovian baths exactly describe a system with infinite bandwidth and $\mu = \pm\infty$.
  However, both are reduced effectively at the impurity site due to the chain sites in between.

Solution of the many-body Master equation

by exact diagonalisation (see e.g. Schmutz 78)

- Mapping onto a many-body problem with twice as many fermions

$$c_{r,\sigma} \Rightarrow \{c_{r,\sigma,A}, c_{r,\sigma,B}\}$$

"super" Hilbert space describe the space of density matrices

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- "Eigenvector" with zero eigenvalues is the steady-state density matrix ρ_{SS}
- Quantum regression theorem allows for evaluation of G_{IMP} and thus Σ_{LOC}

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by exact diagonalisation (see e.g. Schmutz 78)

- Mapping onto a many-body problem with twice as many fermions

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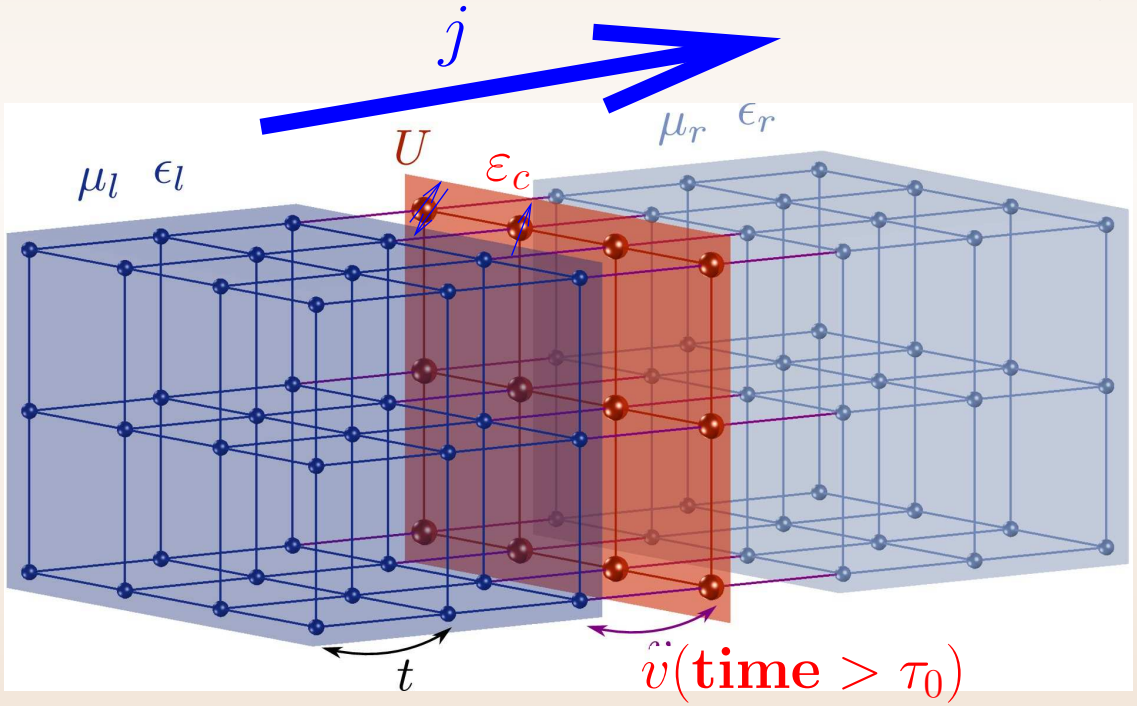
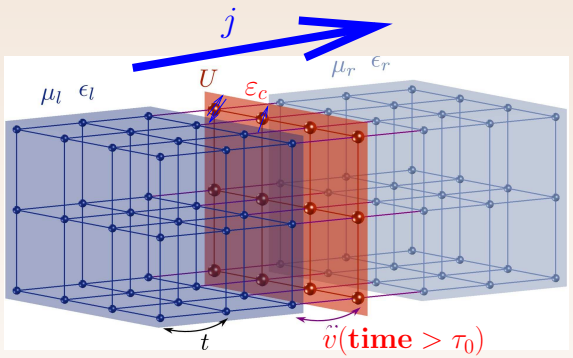
Model again

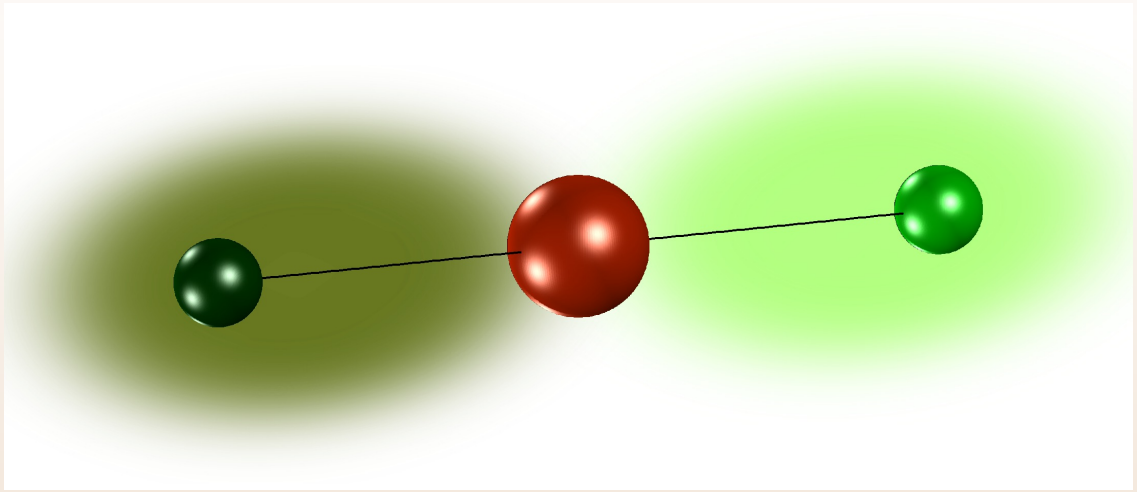
Parameters: Hopping $t = 1$, hopping to baths $v = \sqrt{0.1}$,
Voltage $\phi = \mu_l - \mu_r$.
Half-filling: $\varepsilon_l = \mu_l = -\mu_r = -\varepsilon_r$, $\varepsilon_c = -U/2$.



Fit of bath hybridisation function $\underline{\Delta}(\omega)$



Fit of $\mathrm{Im}\,\Delta^R$ and $\mathrm{Im}\,\Delta^K$ with three chain sites $\Rightarrow 8$ fitting parameters.



$\underline{\Delta}_{fit} = v^2 \sum_{\alpha=l,r} \underline{g}_{\alpha,eff}$ vs. $\underline{\Delta}_{DMFT} = \underline{g}_0^{-1} - \underline{G}_{LOC}^{-1} - \underline{\Sigma}_{LOC}$

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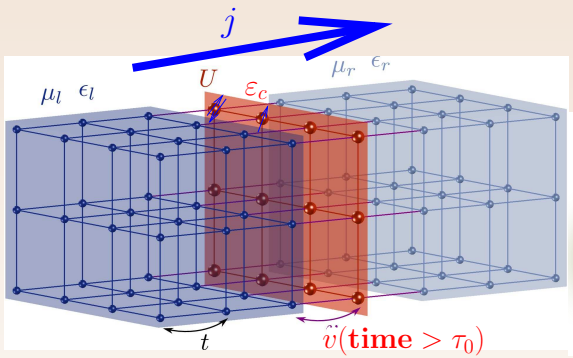

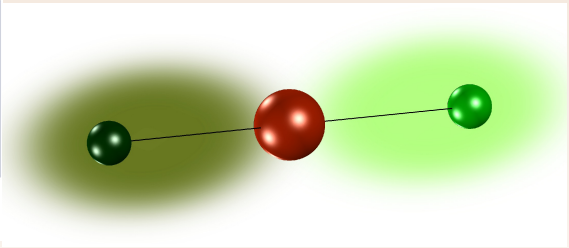

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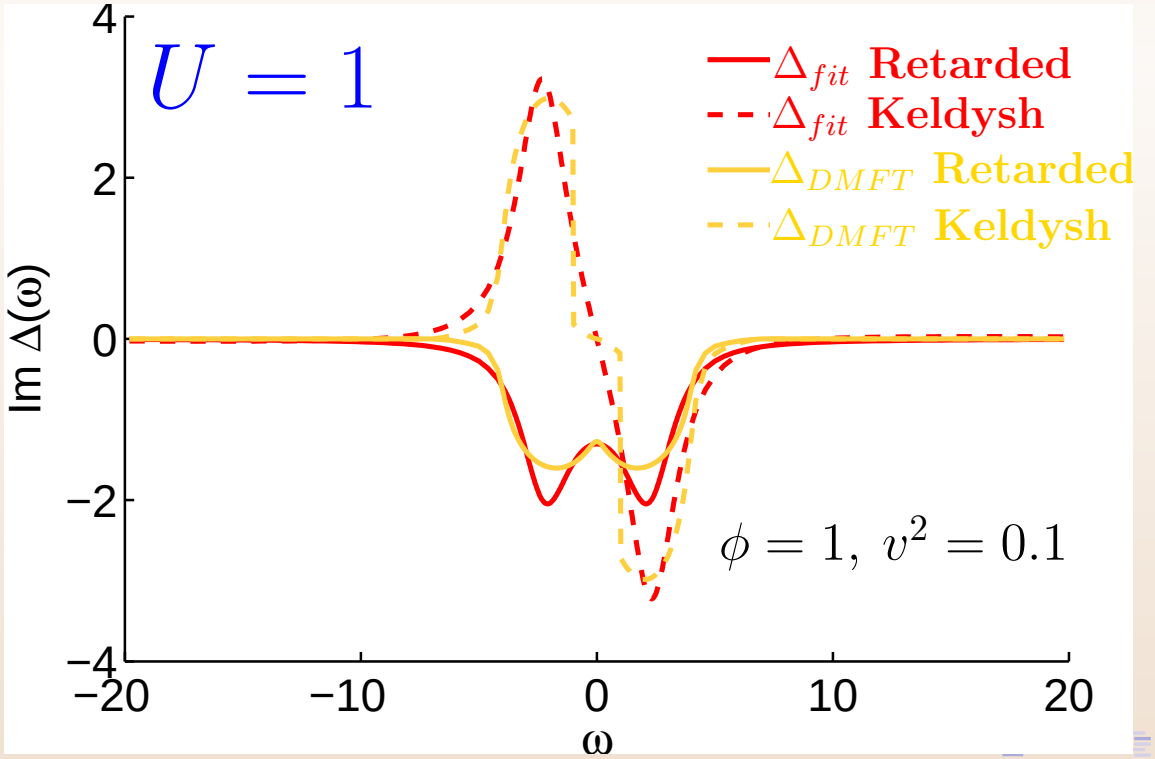

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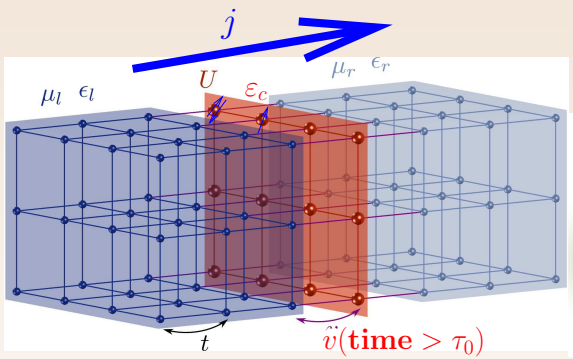

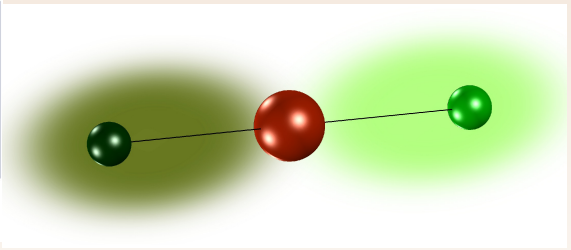

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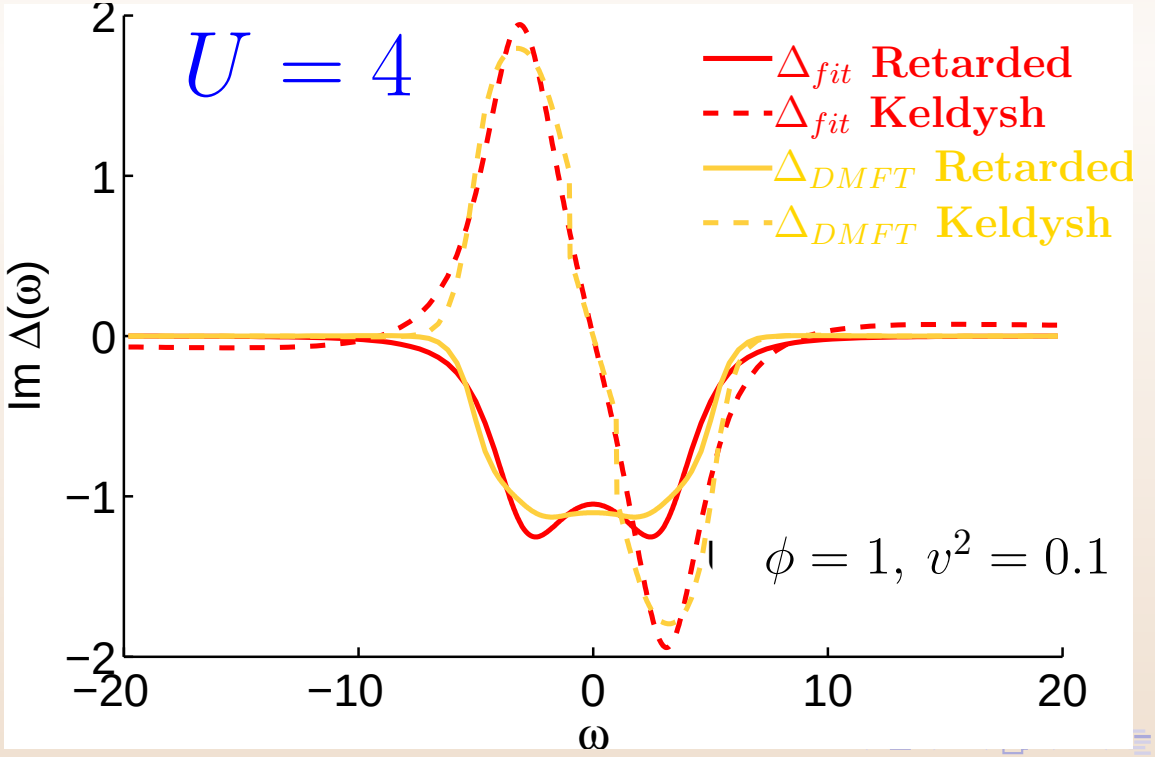
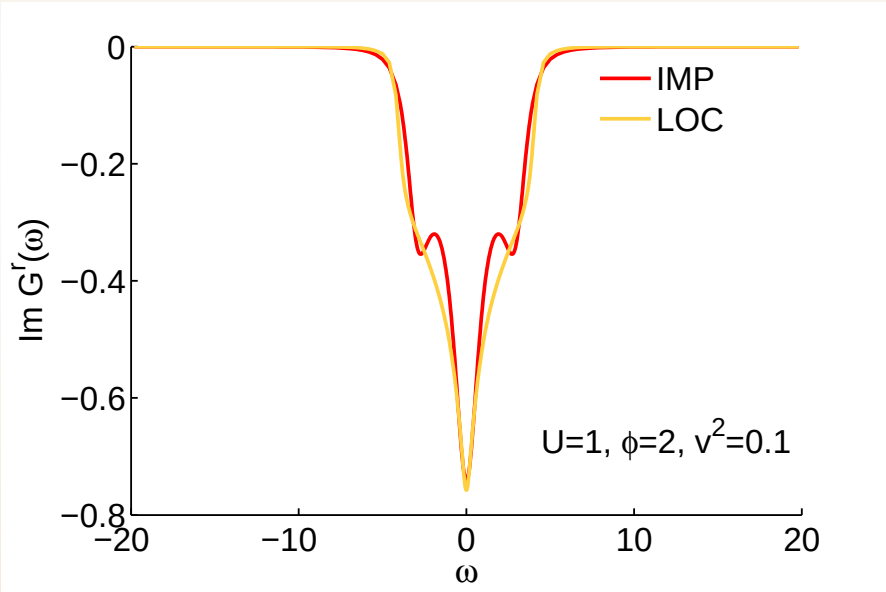


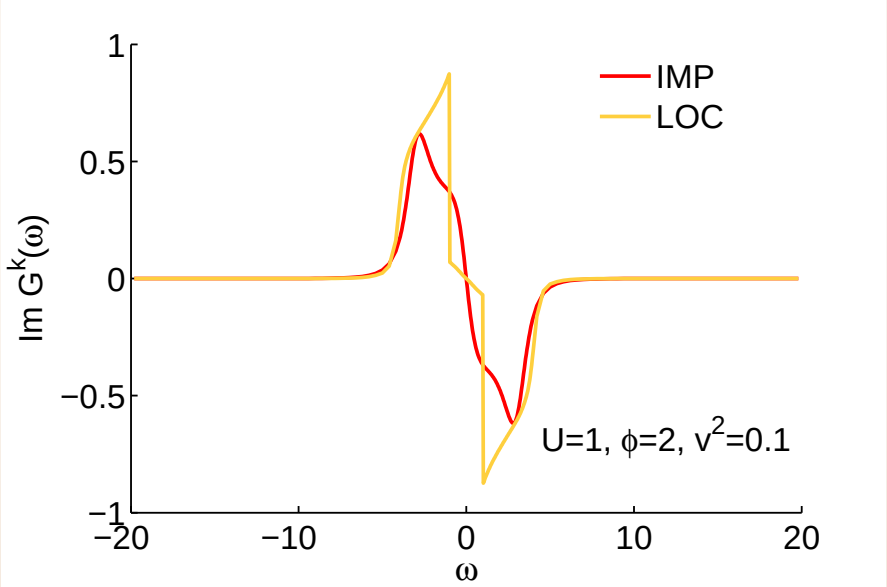
Local Green's function

$U = 1$, Voltage $\phi = 2$

Im G Retarded



Im G Keldysh



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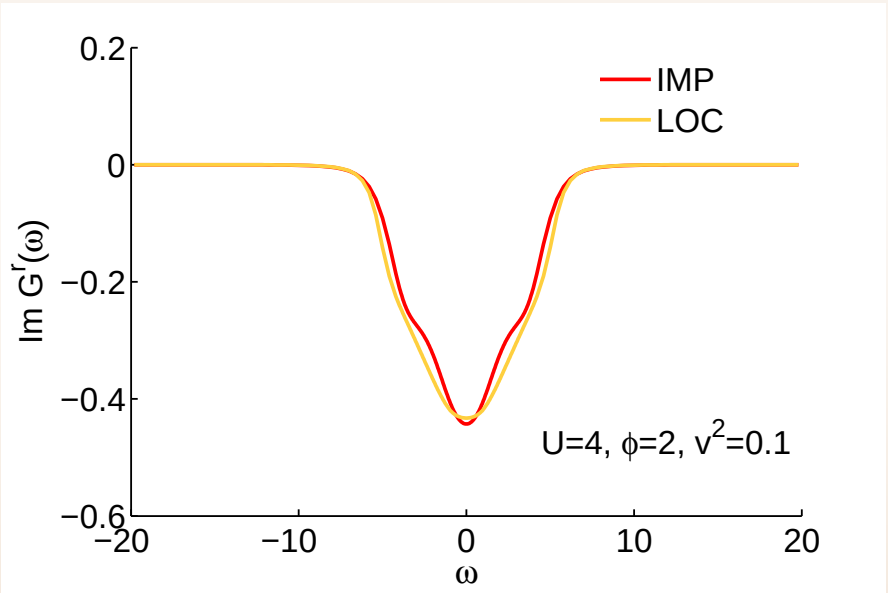
Im G Retarded



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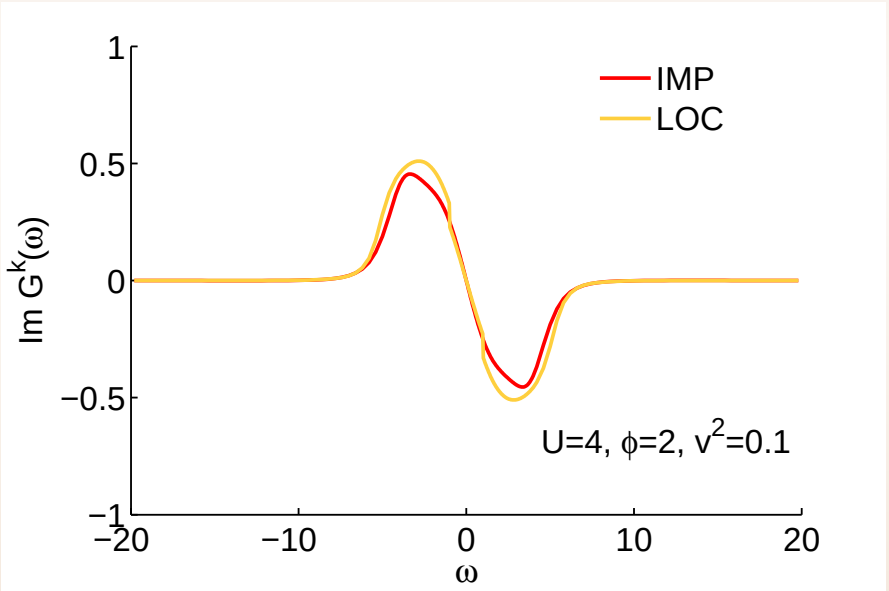
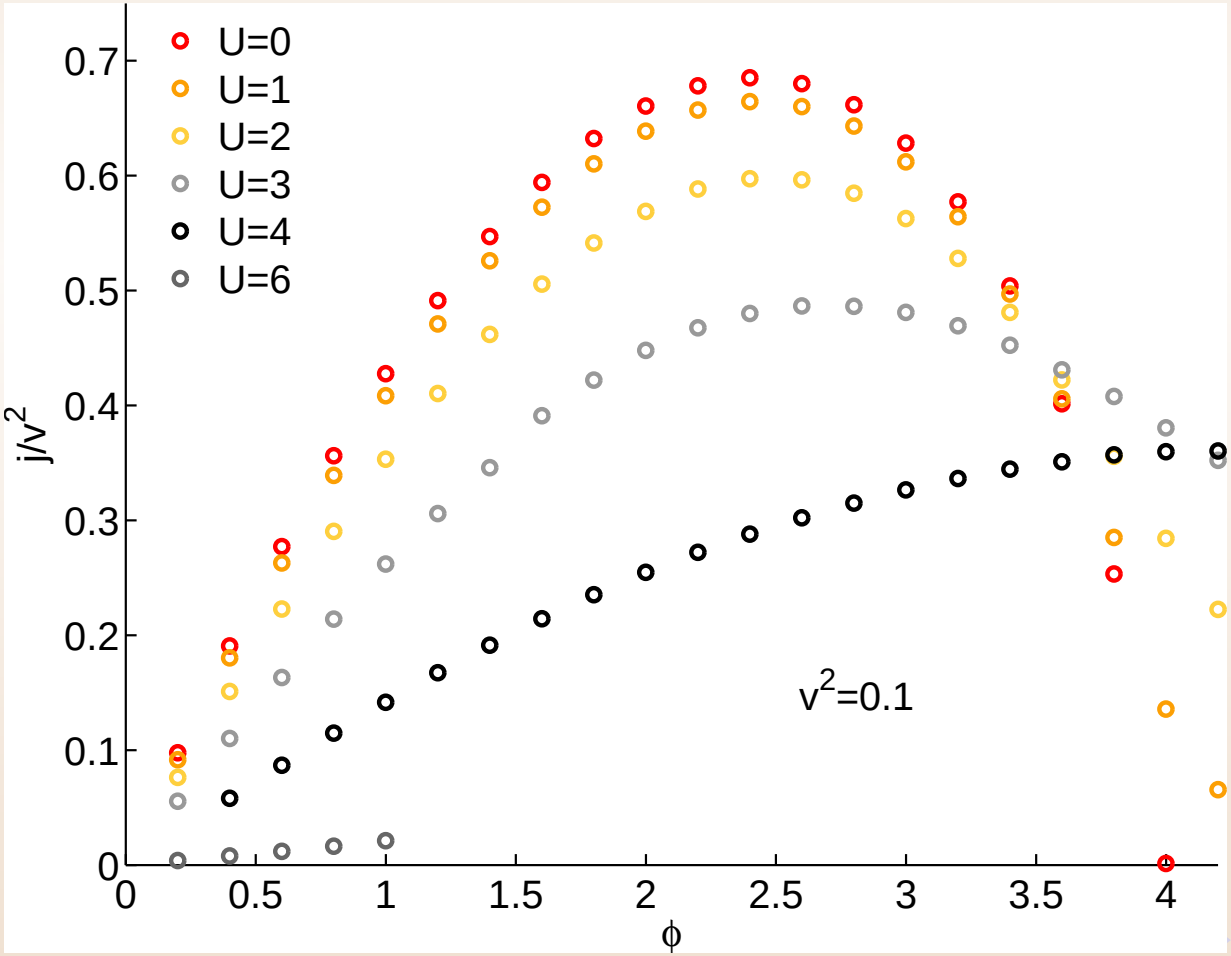


Current vs voltage ϕ

at different U

Current density

$$J \propto v \int_{BZ} \frac{d\mathbf{k}_\parallel}{(2\pi)^2} \int d\omega \, \mathrm{Re} \left(G^R_{layer}(\omega, \mathbf{k}_\parallel) g^K_l(\omega, \mathbf{k}_\parallel) + G^K_{layer}(\omega, \mathbf{k}_\parallel) g^A_l(\omega, \mathbf{k}_\parallel) \right)$$



Current vs. U

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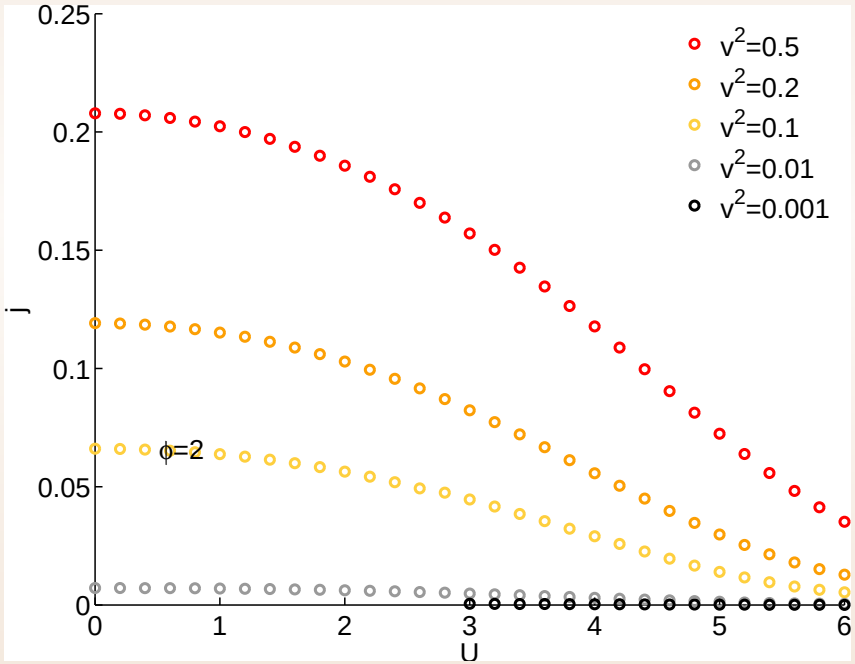

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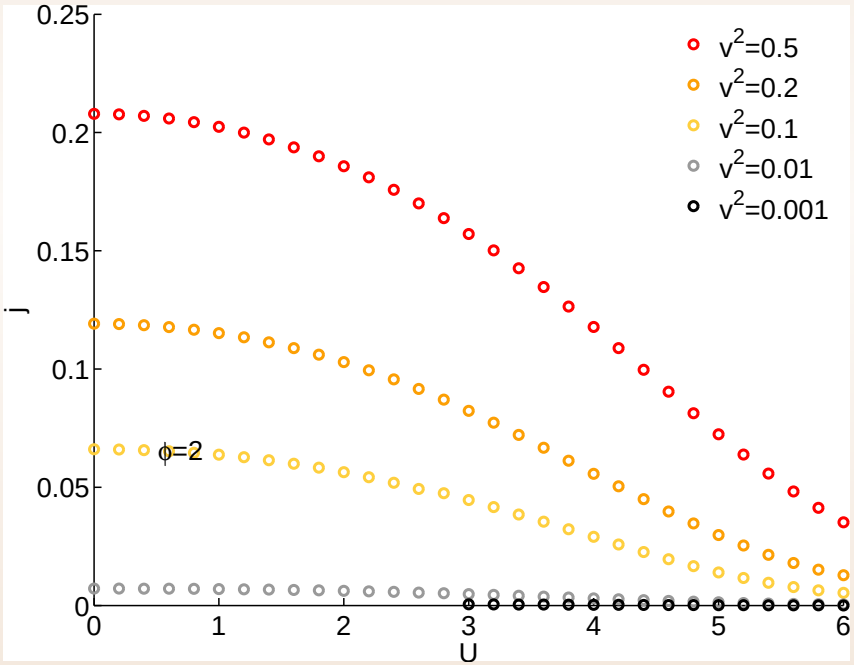

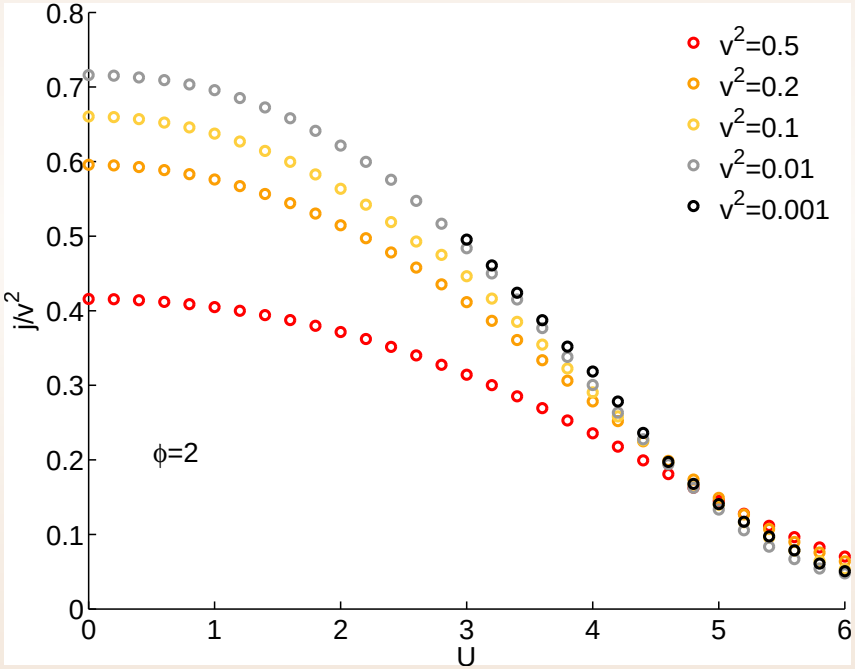

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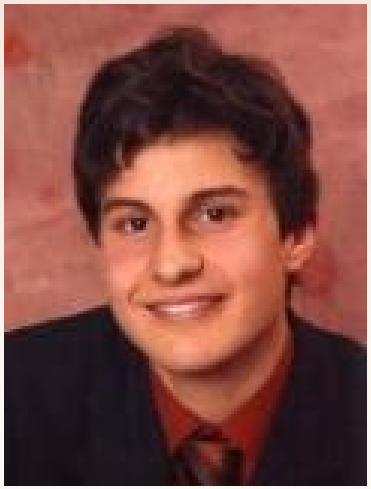

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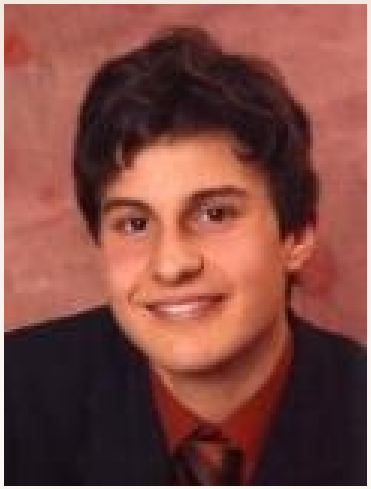

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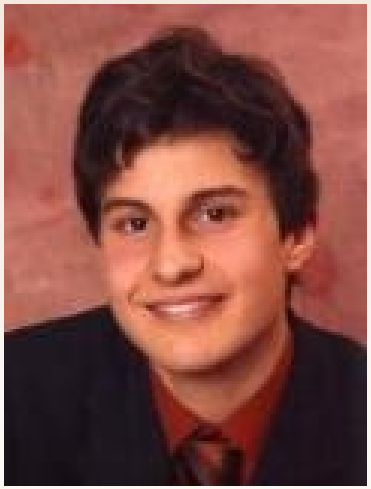

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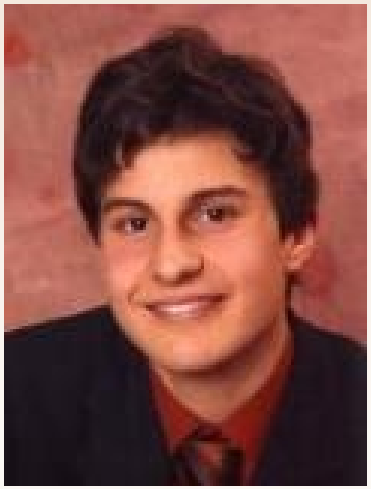

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FWF

Project P24081-N16

TU Graz

Summary and Outlook

- Approach to solve the DMFT impurity problem based on Exact diagonalisation of an effective Lindblad quantum Master equation
- Problem: "Super"-Hilbert space is much larger
  However: Number of fit parameters also increases faster.

Outlook:

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  Periodic driving (Bloch oscillations)
  Floquet treatment
- Cluster extensions: variational cluster approach, cluster dinamical mean-field theory
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