[GW *et al.*, arXiv:1911.09108]

Tensor Networks for Quantum Transport

Gabriela Wójtowicz

with

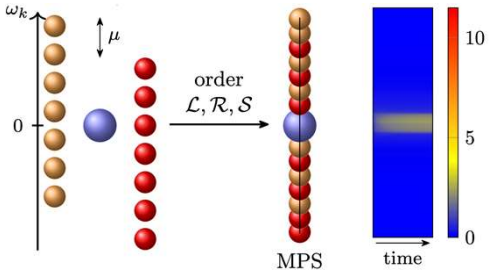
Marek M. Rams, Justin E. Elenewski and Michael Zwolak

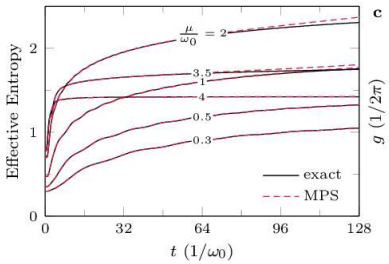
UNIWERSYTET JAGIELLOŃSKI
W KRAKOWIE

NIST
National Institute of
Standards and Technology
U.S. Department of Commerce

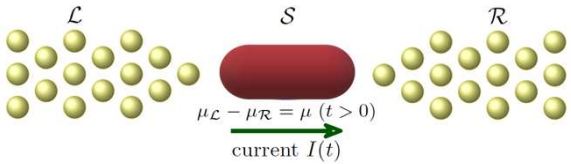
Outline

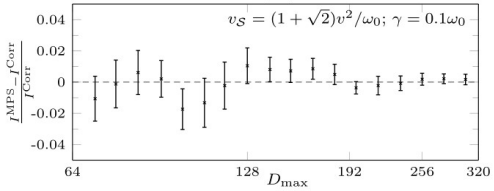
- Introduction:
  - impurity transport,
  - closed system approach.



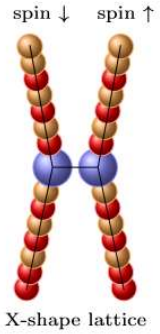


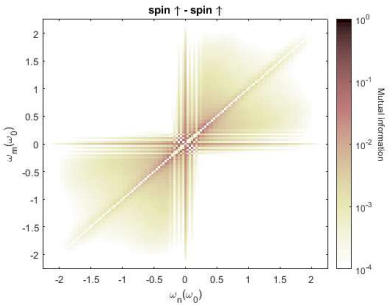
- Transport:
  - open system,
  - Kramers' crossover.





- Structure of correlations:
  - Anderson impurity,
  - spinfull model.



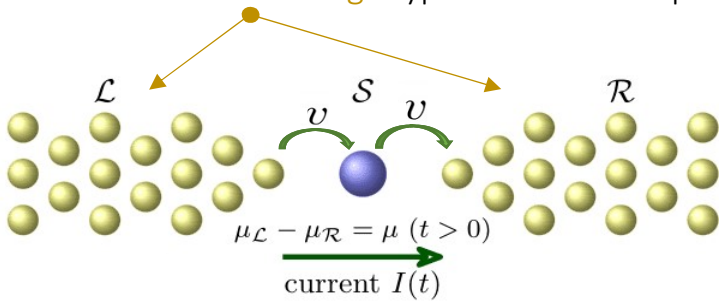


Aim: Accurate and efficient method.

Introduction: closed system

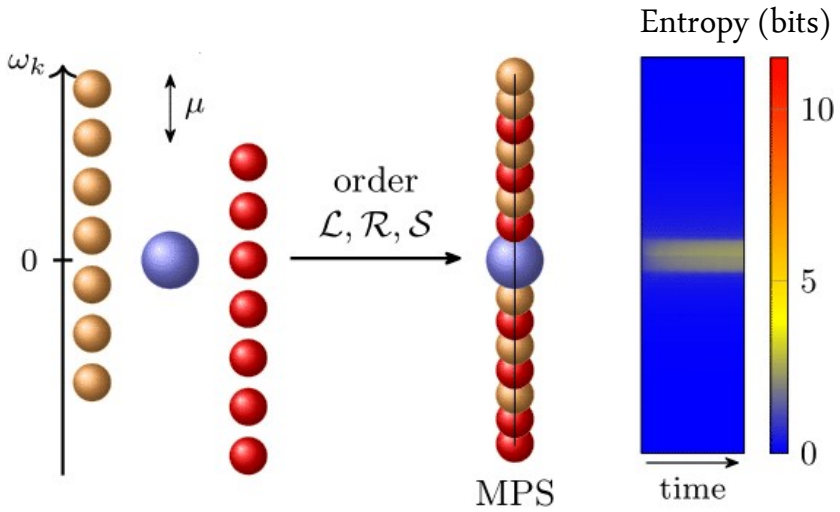
Impurity transport can be experimentally realized by e.g. single molecule, quantum dot, quantum point contact.

Non-interacting - typical for Fermi liquid picture



Diagonalize

L and R



$$H = H_S + H_L + H_R + H_I$$

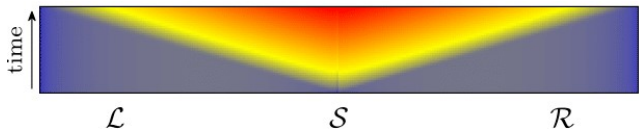
System Hamiltonian

- many-body interaction

Reservoir-system coupling

$$H_{L/R} = \sum_{k \in L/R} \hbar \omega_k a_k^\dagger a_k$$

$$H_I = \sum_{k \in L/R} \sum_{i \in S} \hbar v_{ki} (c_i^\dagger a_k + a_k^\dagger c_i)$$



Spatial basis: scattering on the impurity

Mixed basis:

- star geometry [as in impurity solver for DMFT, Wolf et al., PRB (2014)]
  + global energy-mode ordering

[M. M. Rams and M. Zwolak, arXiv:1904.12793]

Introduction: closed system

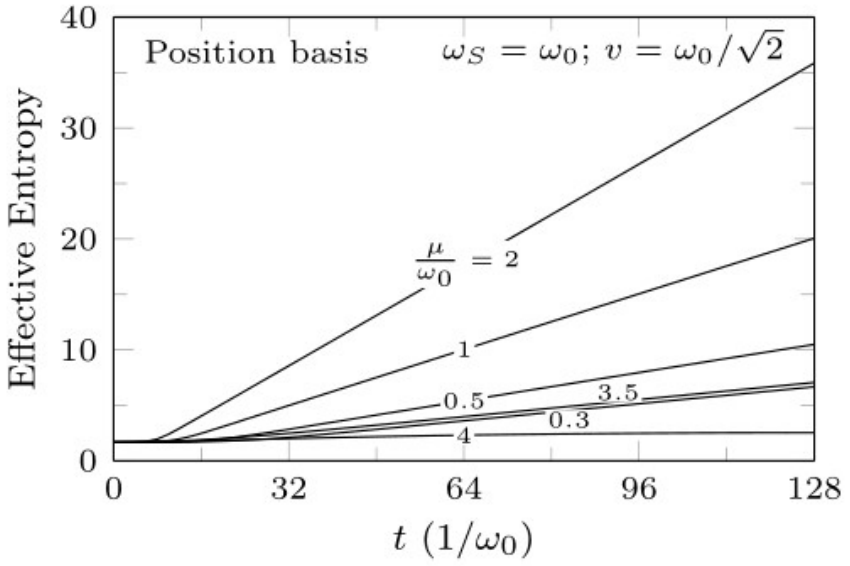
Spatial basis:

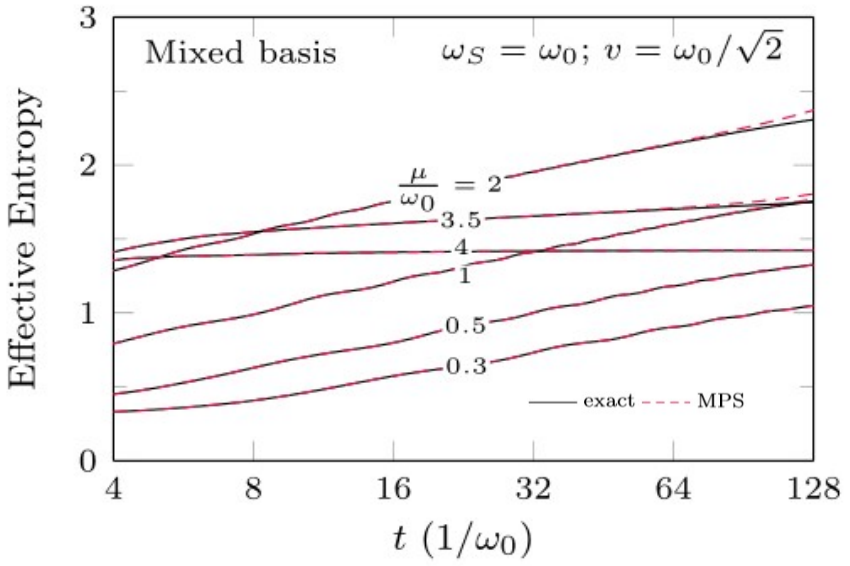
- entropy growth **linear** in time: $S \sim time$
- entanglement barrier: $D \sim e^S$

Mixed basis:

- entropy growth reduced to **logarithmic** in time
- entanglement reduced to eqienergetic modes

Single Anderson impurity: $H_S = \hbar\omega_S(n_\uparrow + n_\downarrow) + Un_\uparrow n_\downarrow,$





$$S_{eff} = ln \sqrt[3]{\sum_i e^{3S_i}/N} \qquad S_i \text{ - entropy on } i^{th} \text{ bond}$$

[M. M. Rams and M. Zwolak, arXiv:1904.12793]

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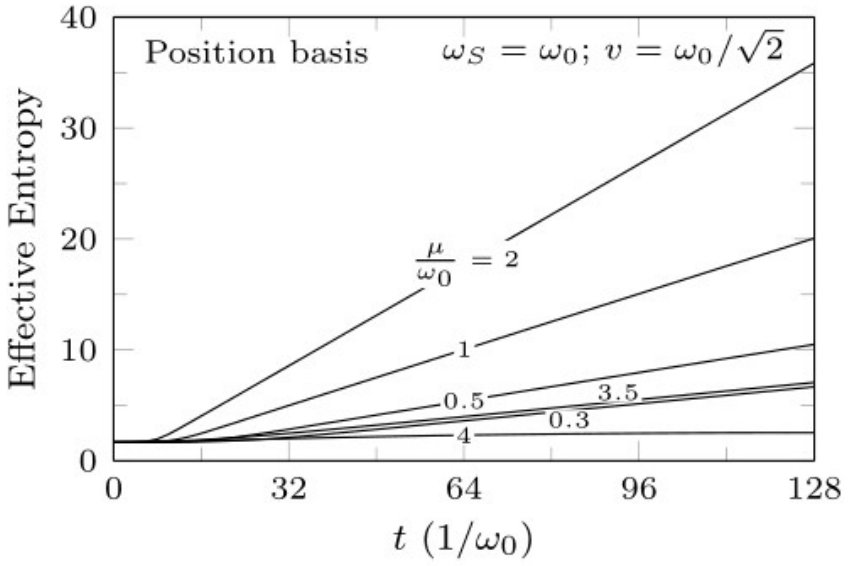
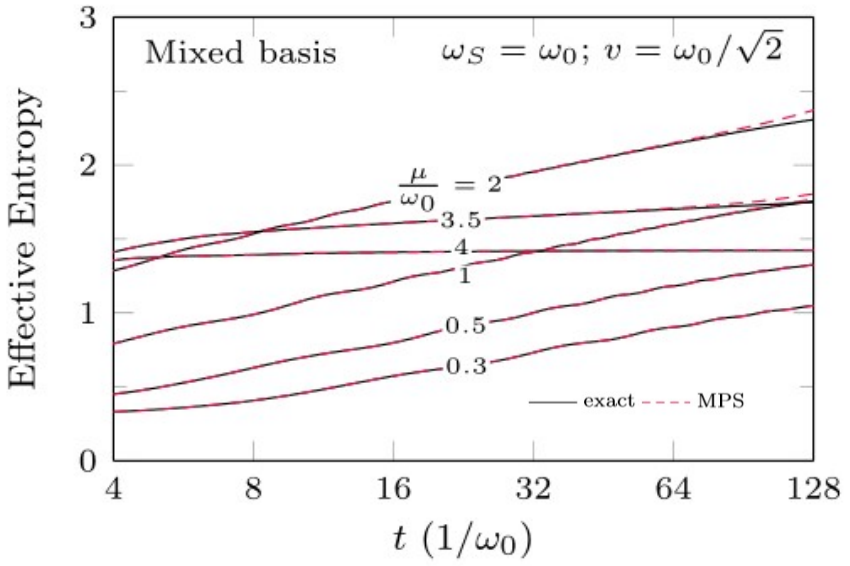




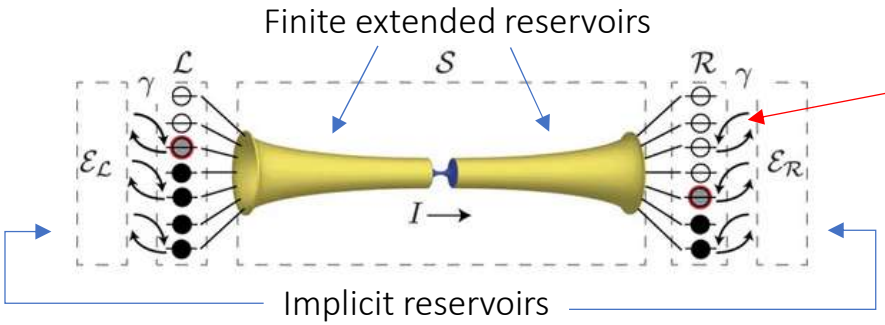
LIMITATIONS of the CLOSED SYSTEM:

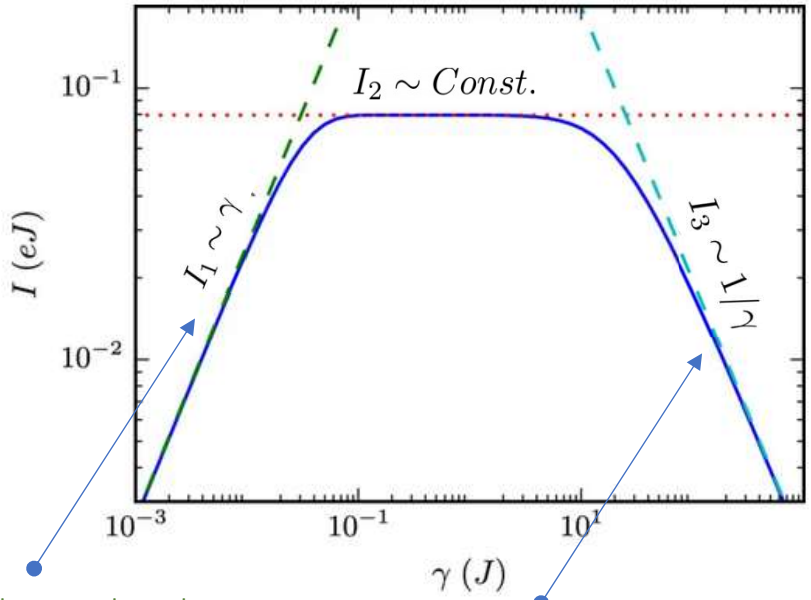
- no true steady state
- limited simulation time

$$S_{eff} = ln \sqrt[3]{\sum_i e^{3S_i}/N}$$ S_i - entropy on i^{th} bond

[Gruss, Velizhanin and Zwolak Sci Rep 6, 24514, (2016)]

Open system: Kramers' crossover



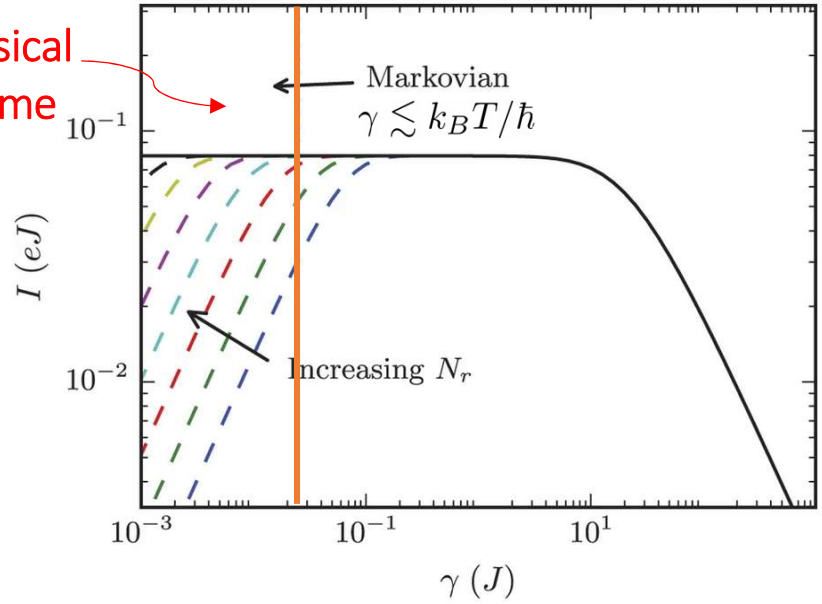


Slow replenishing of modes in L/R

Lack of coherence between L/R and S

Plateau expansion in reservoir size:

Physical regime



[GW et al., arXiv:1911.09108]

Open system approach

Markovian master equation - valid for $\gamma <$ thermal relaxation:

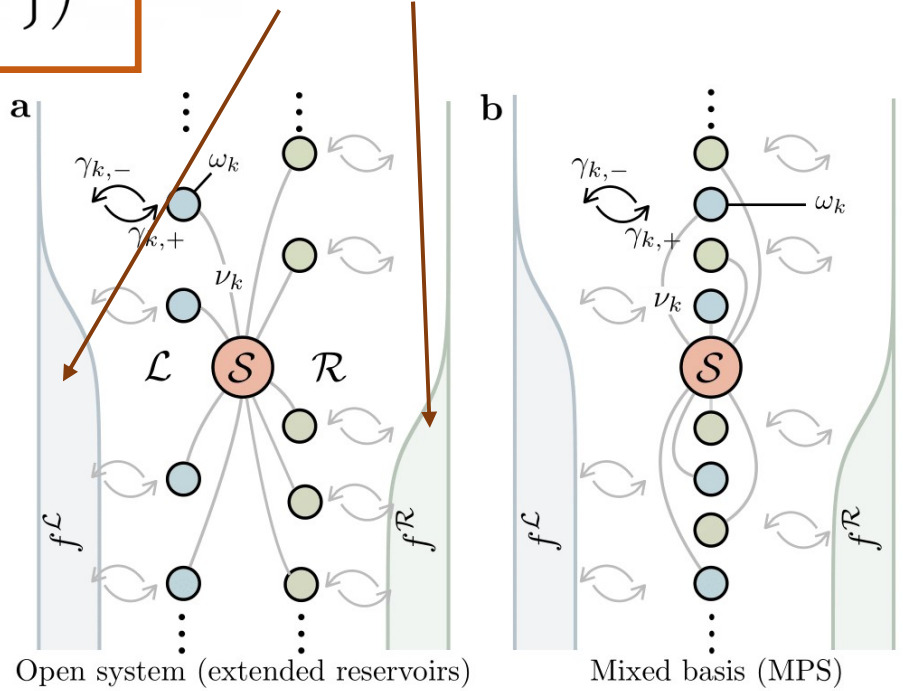
$$\dot{\rho} = -\frac{i}{\hbar}[H,\rho] + \sum_k \gamma_{k+}\left(a_k^\dagger \rho a_k - \frac{1}{2}\left\{a_k a_k^\dagger, \rho\right\}\right) + \gamma_{k-}\left(a_k \rho a_k^\dagger - \frac{1}{2}\left\{a_k^\dagger a_k, \rho\right\}\right)$$

$$\gamma_+, \gamma_- \sim \gamma \text{ (relaxation rate)}$$

Exchange with implicit reservoirs

↕

Relaxation to Fermi-Dirac distribution



- Permits long-time simulation at finite temperature,
- Compact MPO for the Lindblad super-operator,
- MPS + ordering according the scattering nature of current-carrying states.

While other approaches exists we use TDVP with vectorized density matrix.

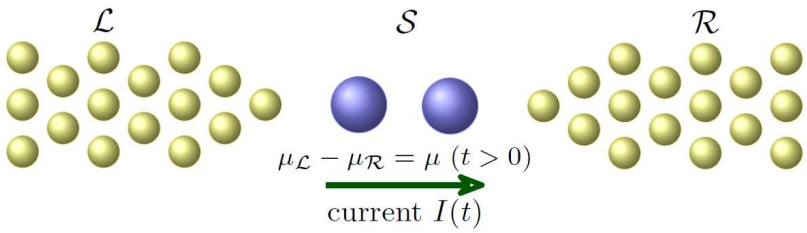
[Haegeman *et. al.*, PRB(2016)]

[Zwolak and Vidal, PRL(2004), Verstraete *et al.*, PRL(2004)]

Aim: Accurate and efficient method.

[GW et al., arXiv:1911.09108]

Two-site impurity model



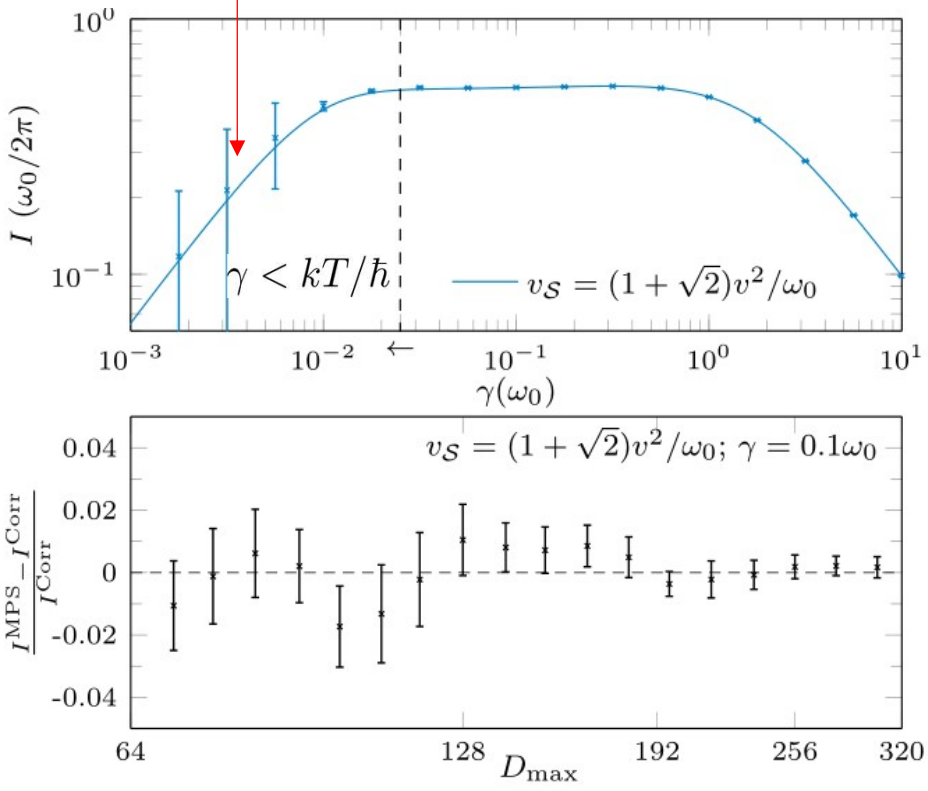
$$H_S = \hbar v_S (c_1^\dagger c_2 + \text{h.c.}) + \hbar\omega_S (n_1 + n_2) + U n_1 n_2,$$

The accuracy of the arises from:

- finite size of extended reservoir ~N,
- MPS truncation:
  → slow convergence with non-monotonic behaviour
- interactions in the system:
  → the plateau development depends on the nature of the interaction

Hard to capture with MPS.

Nature of corelations and optimal TN structure
[J.E. Elenewski *et al., in prep.*]

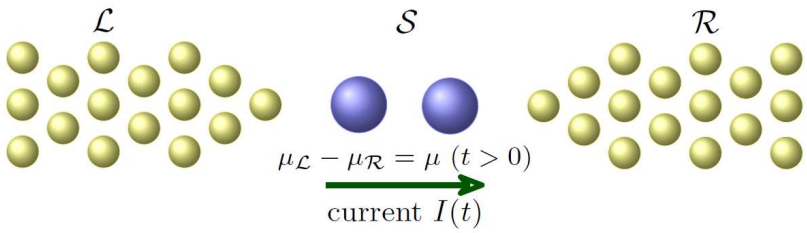


MSP of N=128, D<256, compared to exact soluton via correlation matrix.

Aim: Accurate and efficient method.

[GW et al., arXiv:1911.09108]

Two-site impurity model



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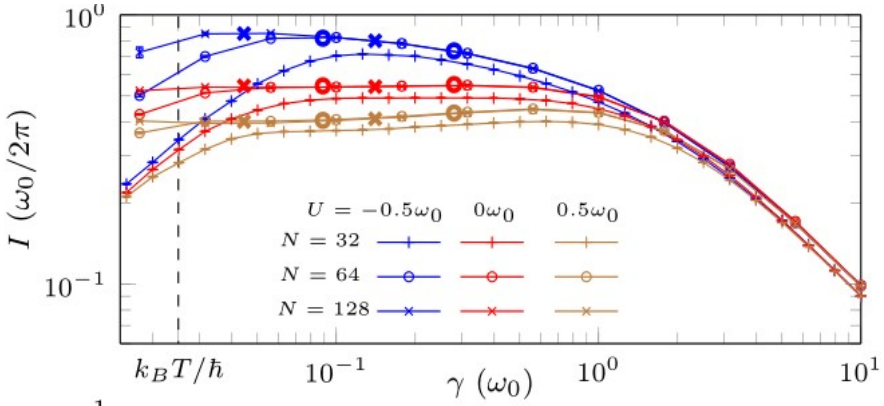
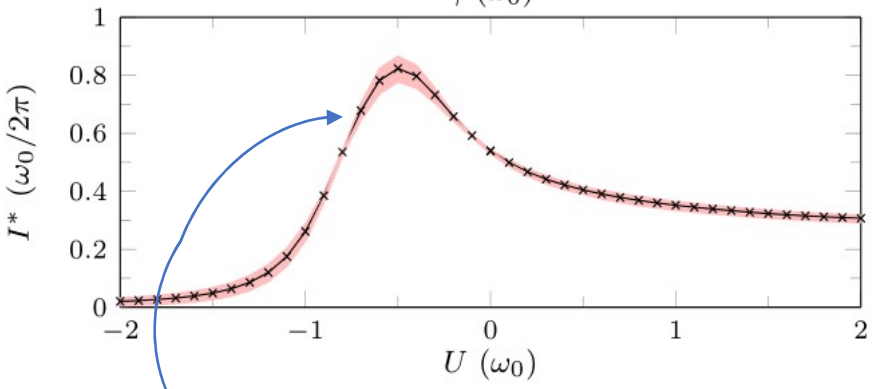


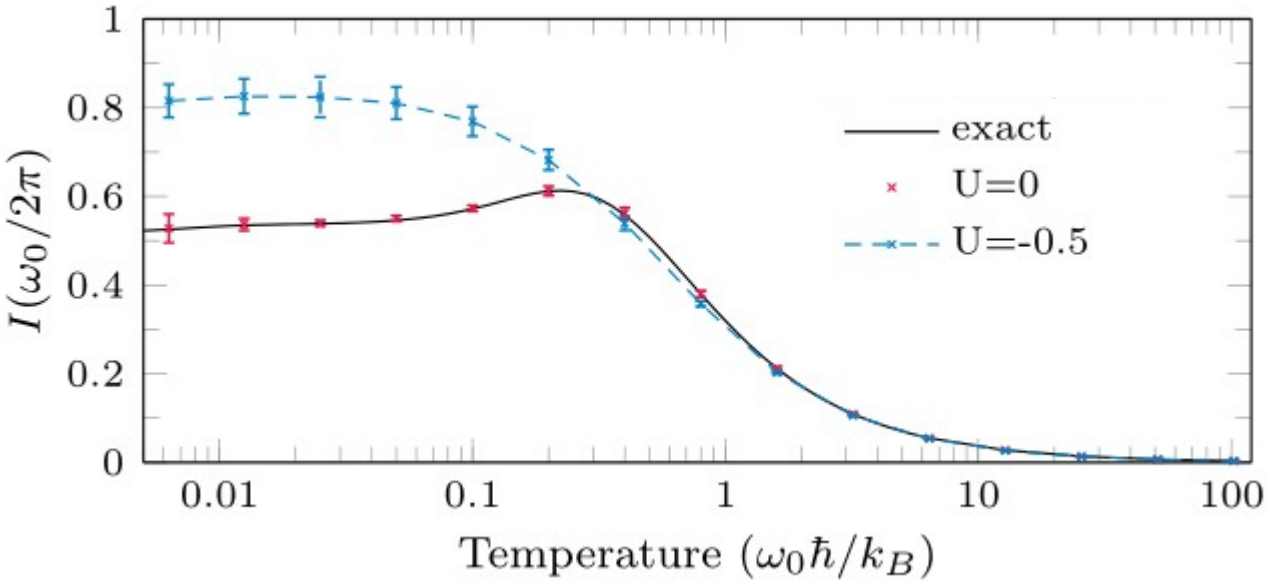


- plateau deformation
- truncation error

[GW et al., arXiv:1911.09108]

Temperature-dependent transport

MPS result for reservoir of N=128 modes and bond dimension D≤256



Markovian master equation is valid for $\gamma \lesssim k_B T/\hbar$

↕

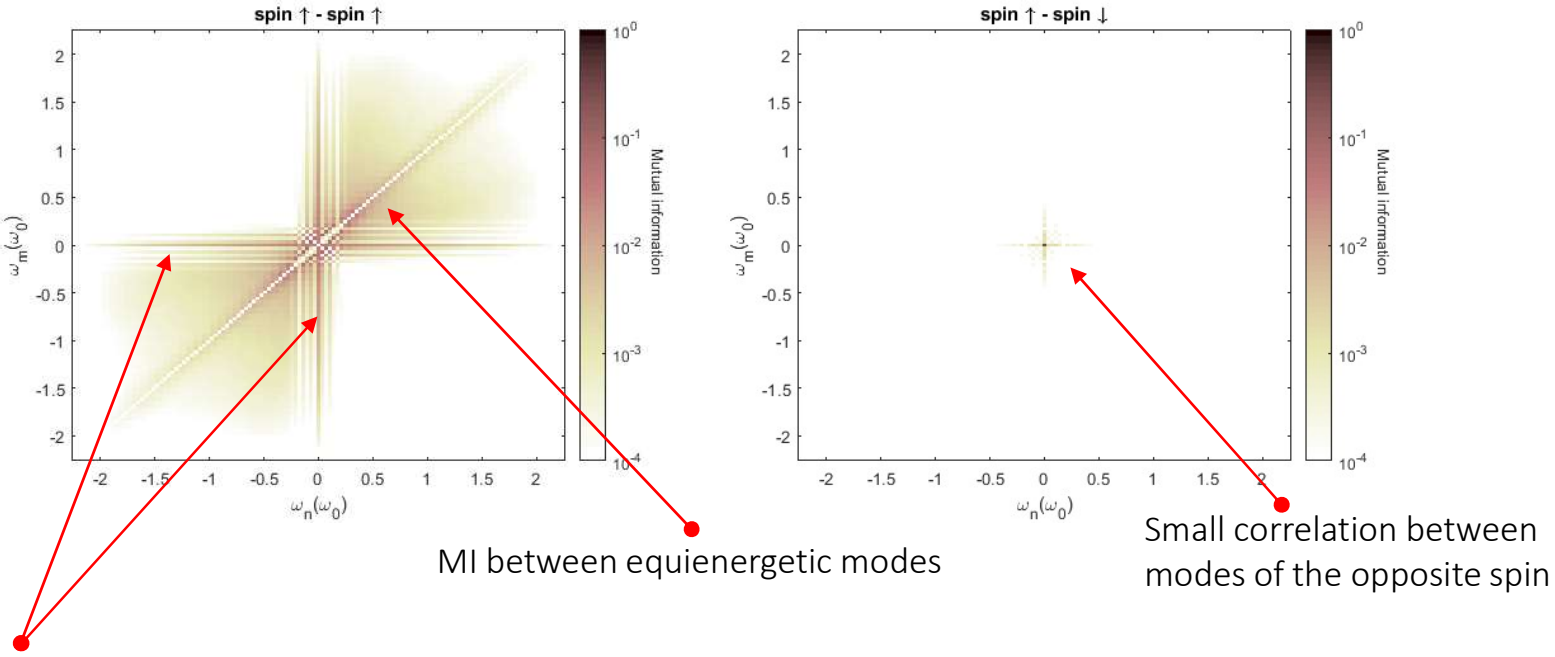
Low temperatures = bigger extended reservoirs

[J.E. Elenewski *et al., in prep.*]

Correlation structure

Spinfull Anderson impurity model: $H_S = \hbar\omega_S(n_\uparrow + n_\downarrow) + Un_\uparrow n_\downarrow,$

$N = 64, D < 100, \omega_S = -\omega_0, U = 4$



MI between equienergetic modes

Small correlation between modes of the opposite spin

MI between system and reservoirs' modes

- decay for modes further on energy scale

[J.E. Elenewski *et al., in prep.*]

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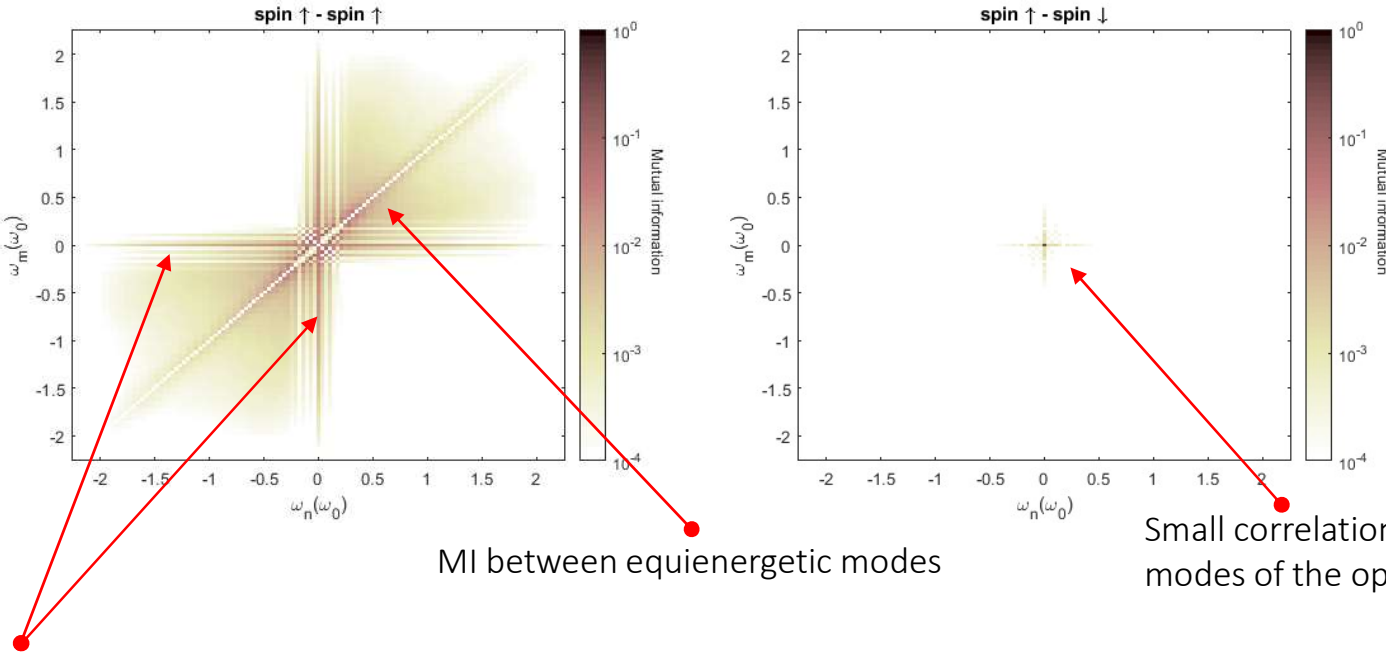

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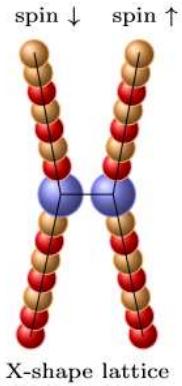
Best to use

TTN



X-shape lattice

Summary

- Quantum transport can be efficiently simulated using TN by considering evolution of the density matrix
- The accuracy of the approach depends on the relaxation rate, extended reservoir size and complexity of the interactions
- The mixed-basis with proper ordering eliminated constraints on accessible time
- Open system approach allows to directly target steady-state currents using procedure similar to ground state search
- The approach is useful for studying long time simulation for complex systems and non-zero temperature and periodic driving
- The structure of correlations suggest the most optimal geometry of TN

THANK YOU FOR YOUR ATTENTION !