

Information Dynamics and Open Systems: Tensor networks for quantum transport

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with
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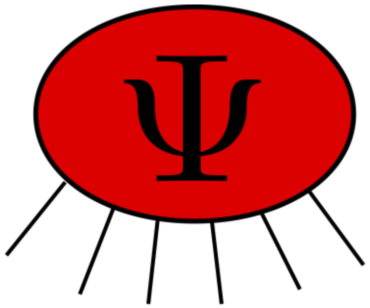
Based on:
MMR, MZ, Phys. Rev. Lett. 124, 137701 (2020);
GW, JE, MMR, MZ, Phys. Rev. A 101, 050301(R) (2020).

Tensor networks:

Curse of dimensionality $\xrightarrow{\text{representability}}$ Curse of entanglement (entanglement barrier)

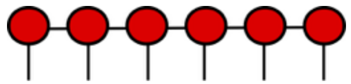
$$|\Psi\rangle = \sum_{\{i_n\}} \Psi_{i_1,\ldots,i_N} |i_1,\ldots,i_N\rangle$$

$$\|$$

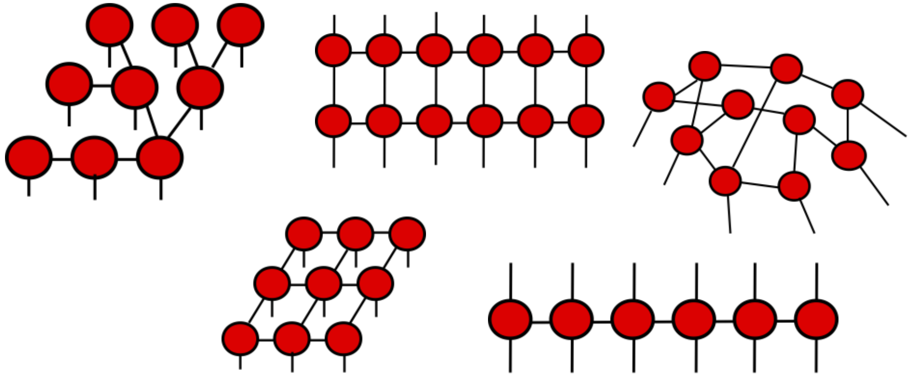


Area law for entanglement entropy $\longrightarrow$

Tensor network states:



$\longleftrightarrow$ Matrix product state (MPS)



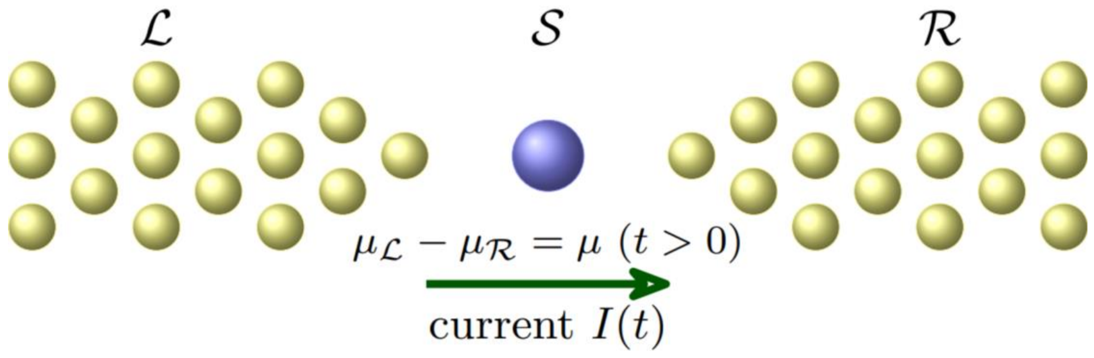
Building a complicated many-body wave function from small managable pieces.

Physically-relevant corner of the Hilbert space:

- ground and thermal states of local Hamiltonians
- … including dynamics after local perturbations
- dynamics in systems exhibiting localization
- ??? ~~generic quantum many-body dynamics~~ ???

F. Verstraete, et al., Adv. Phys. (2008);
U. Schöllwock, Ann. Phys. (2011);
R. Orús, Ann. Phys (2014);
…

Electron transport through quantum point contact:



Potential, occupation or temperature imbalance drives a current though the impurity region

$$H = H_{\mathcal{S}} + H_{\mathcal{I}} + H_{\mathcal{L}} + H_{\mathcal{R}}$$

$H_{\mathcal{S}}$ = interacting many-body impurity

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

$$H_{\mathcal{I}} = \sum_{i \in \mathcal{S}, k \in \mathcal{LR}} \hbar v_{ik} \left(c_i^\dagger a_k + a_k^\dagger c_i \right)$$

A.-P. Jauho, N. S. Wingreen, Y. Meir, PRB (1994)

Structure of Hamiltonian matters:

1D position basis (or a Wilson chain):

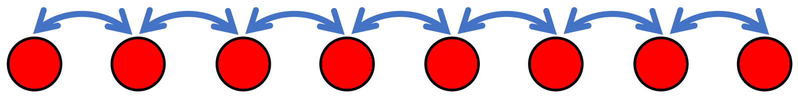
$$H_{\mathcal{L}} = \hbar\omega_0 \sum_{i\in\mathcal{L}} \left(b_j^\dagger b_{j+1} + b_{j+1}^\dagger b_j \right) + \hbar\mu_{\mathcal{L}} \sum_{j\in\mathcal{L}} b_j^\dagger b_j$$

$$H_{\mathcal{I}} = \hbar v \sum_{\sigma, l=1_{\mathcal{L}}, 1_{\mathcal{R}}} \left(c_\sigma^\dagger b_{l\sigma} + b_{l\sigma}^\dagger c_\sigma \right)$$

Time evolution of Matrix Product States

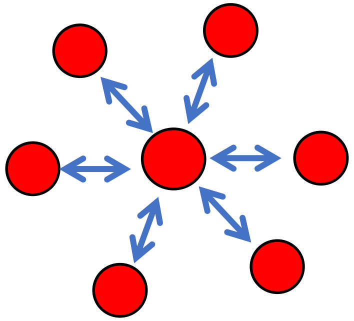
→ Nearest-neighbour interactions;

TEBD, G. Vidal, PRL (2003)
tDMRG, S. White, A. Feiguin PRL (2004)



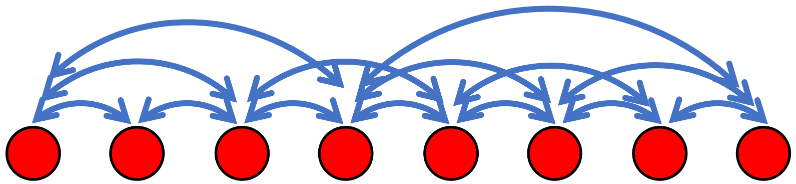
→ Star geometry (for DMFT impurity solvers)

F. A. Wolf, et. al., PRB (2014)
D. Bauernfeind, et. al. PRX (2017)



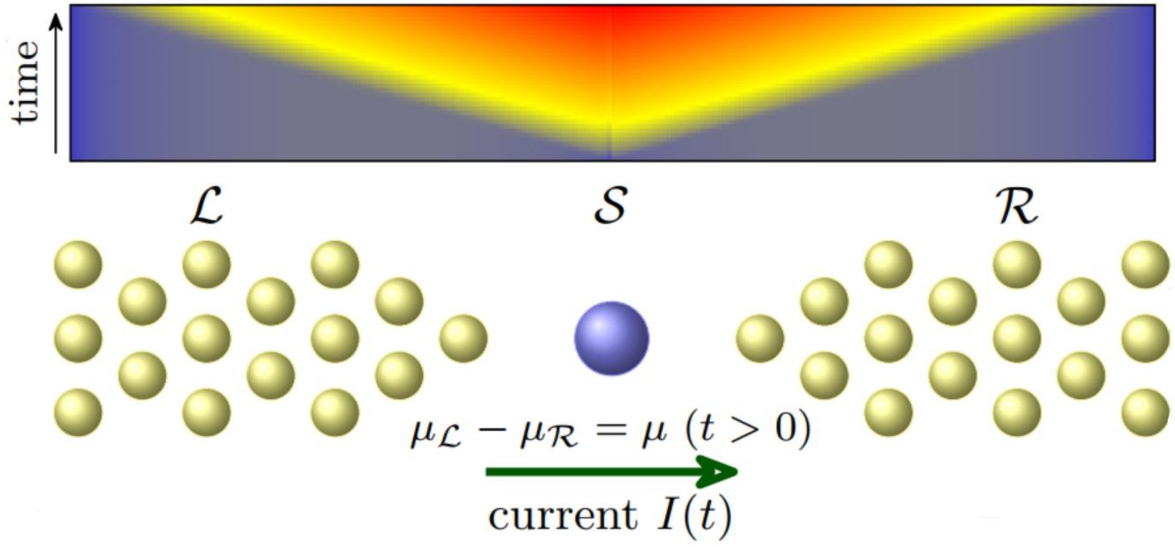
→ Long-range Hamiltonians:

TDVP, J. Haegeman et. al, PRB (2016)
Krylov based, P. Zatel et. al., PRB (2015)



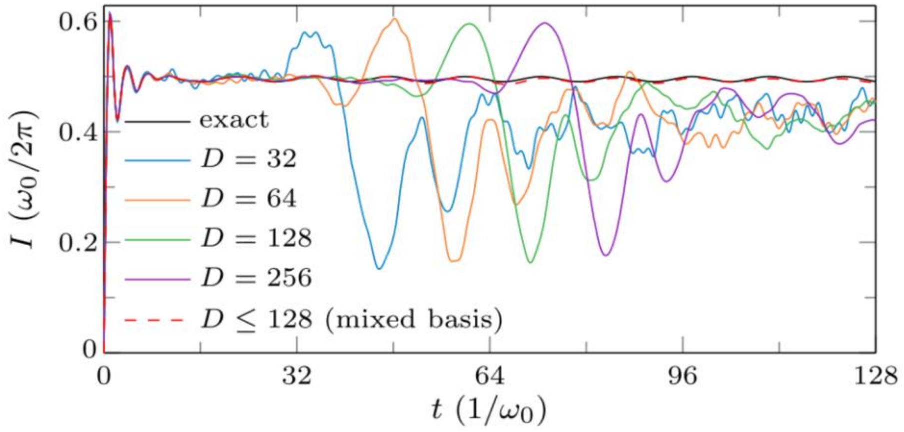
Entanglement barrier:

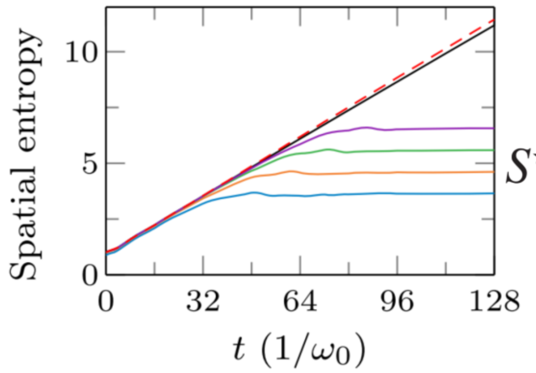
Bipartite von Neuman entanglement entropy in position basis



Minimal example for benchmark:
Non-interacting single-site impurity

D = finite MPS bond dimension





$S^{\star} = \log_2 D$

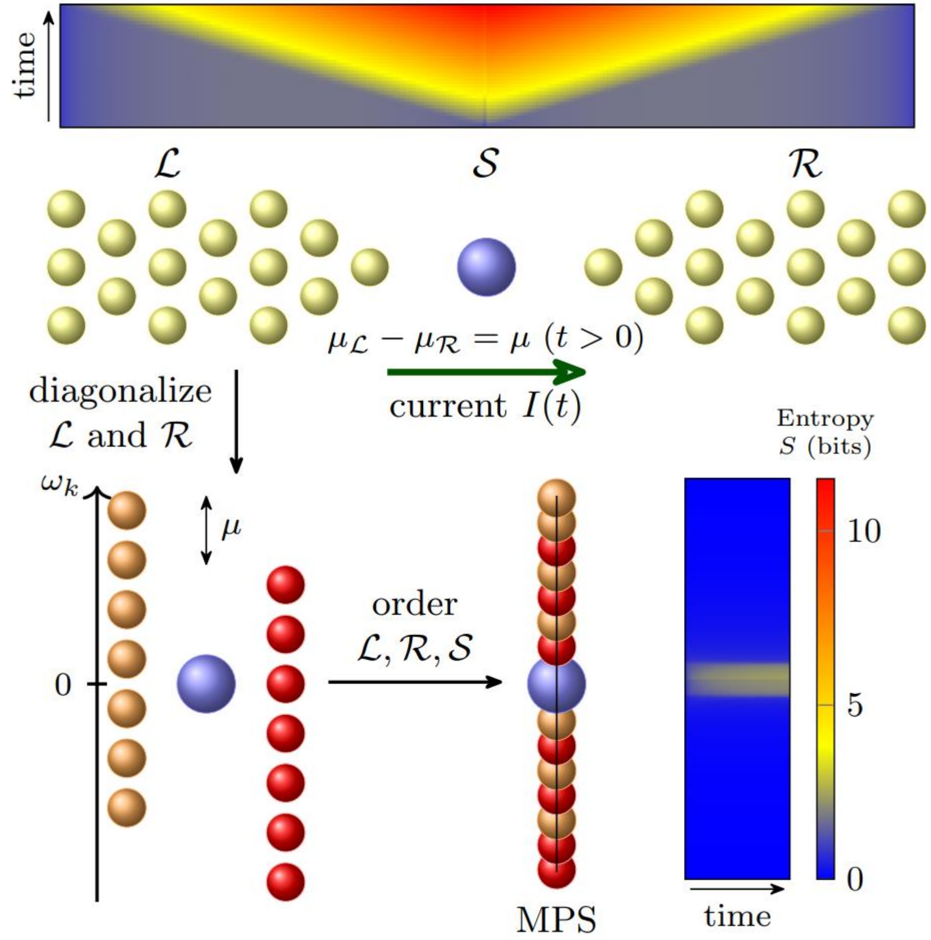
Entangled particle-hole pairs: $\sqrt{T(0)}|0_{\mathcal{L}}1_{\mathcal{R}}\rangle + \sqrt{1-T(0)}|1_{\mathcal{L}}0_{\mathcal{R}}\rangle$

Entanglement between left and right reservoirs: $S \approx H[T(0)]\,\dfrac{\mu t}{2\pi}$

C. W. J. Beenakker (2006); Klich, L. Levitov, PRL (2009);
L. Levitov, F. Lesovik, JETP (1993)

Breaking the entanglement barrier:

Spatial bipartite entropy

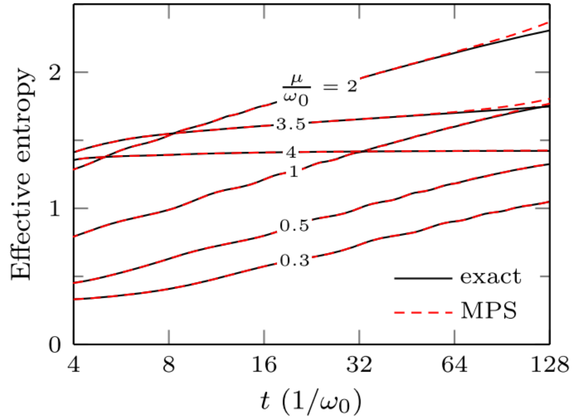


Mixed-basis bipartite entropy

Particles tend to flow from a state with given frequency to a state with similar frequency.

In the mixed basis, the entanglement remains localized with logarithmic growth in time/system size.

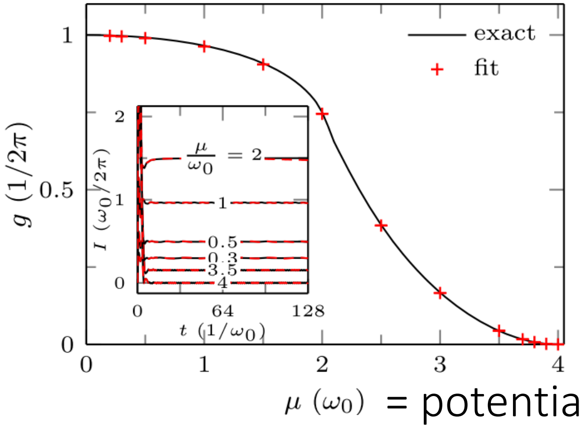
Bipartite entropy in mixed basis



μ = potential bias

Accurate simulations possible for large system sizes and long times → exponential speed-up.

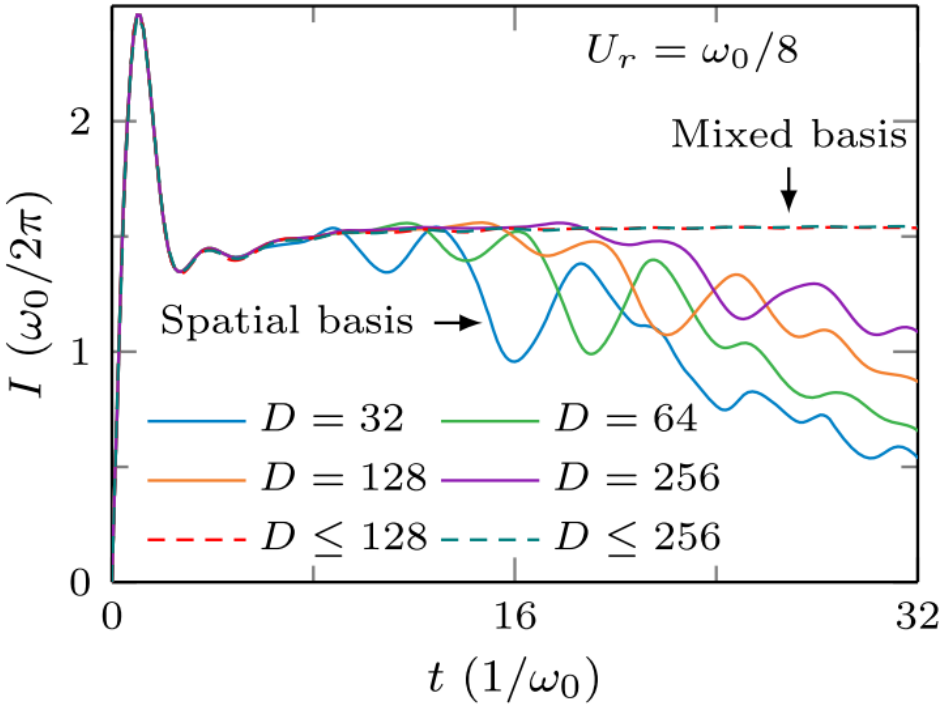
Conductance

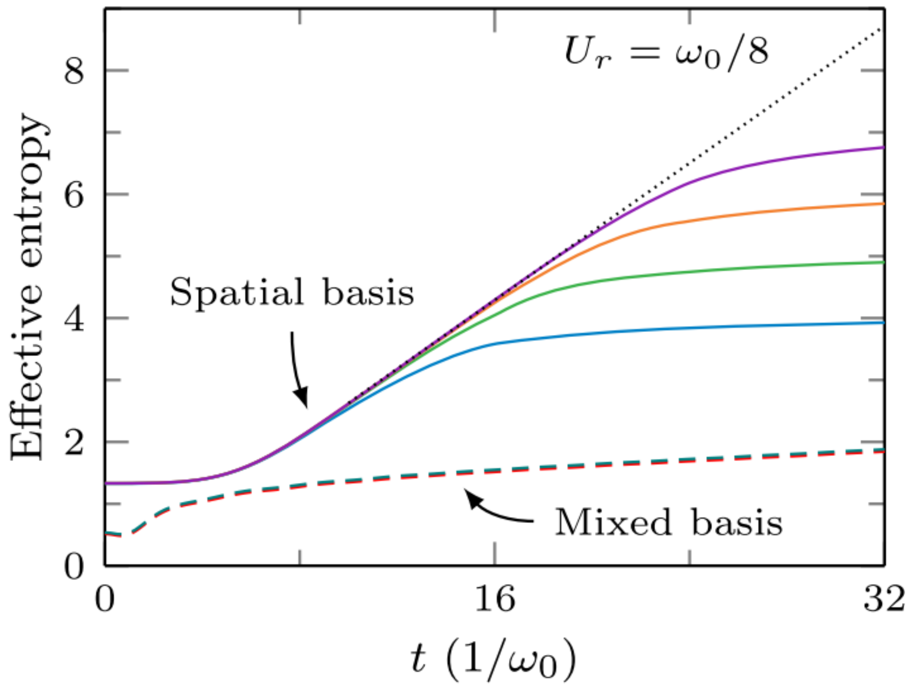


= potential bias

… even for interacting reservoirs:

$$H_{\mathcal{L}} = \hbar\omega_0 \sum_{j\in\mathcal{L}} \left(b_j^\dagger b_{j+1} + b_{j+1}^\dagger b_j\right) + \hbar\mu_{\mathcal{L}} \sum_{j\in\mathcal{L}} b_j^\dagger b_j \quad + \quad \hbar U_r \sum\nolimits_{j\in\mathcal{LR}} (n_j - 1/2)(n_{j+1} - 1/2)$$

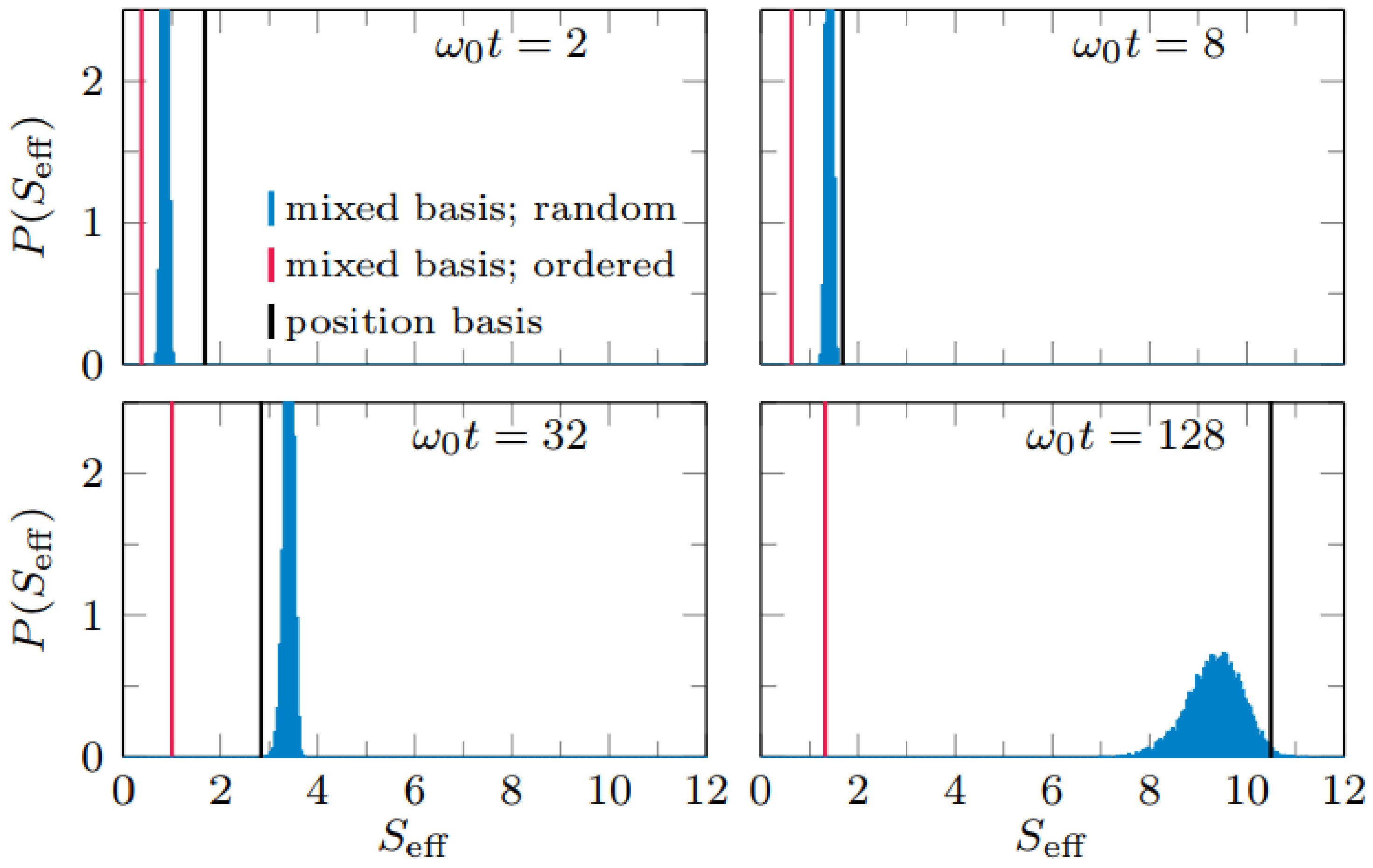




Similar in spirit to: *C. Krumnow, J. Eisert, Ö. Legeza, ArXiv (2019),*
who try to find local disentanglers via local basis transformations.

Optimal basis ordering:

Bipartite entanglement entropy in different basis and orderings of the modes.

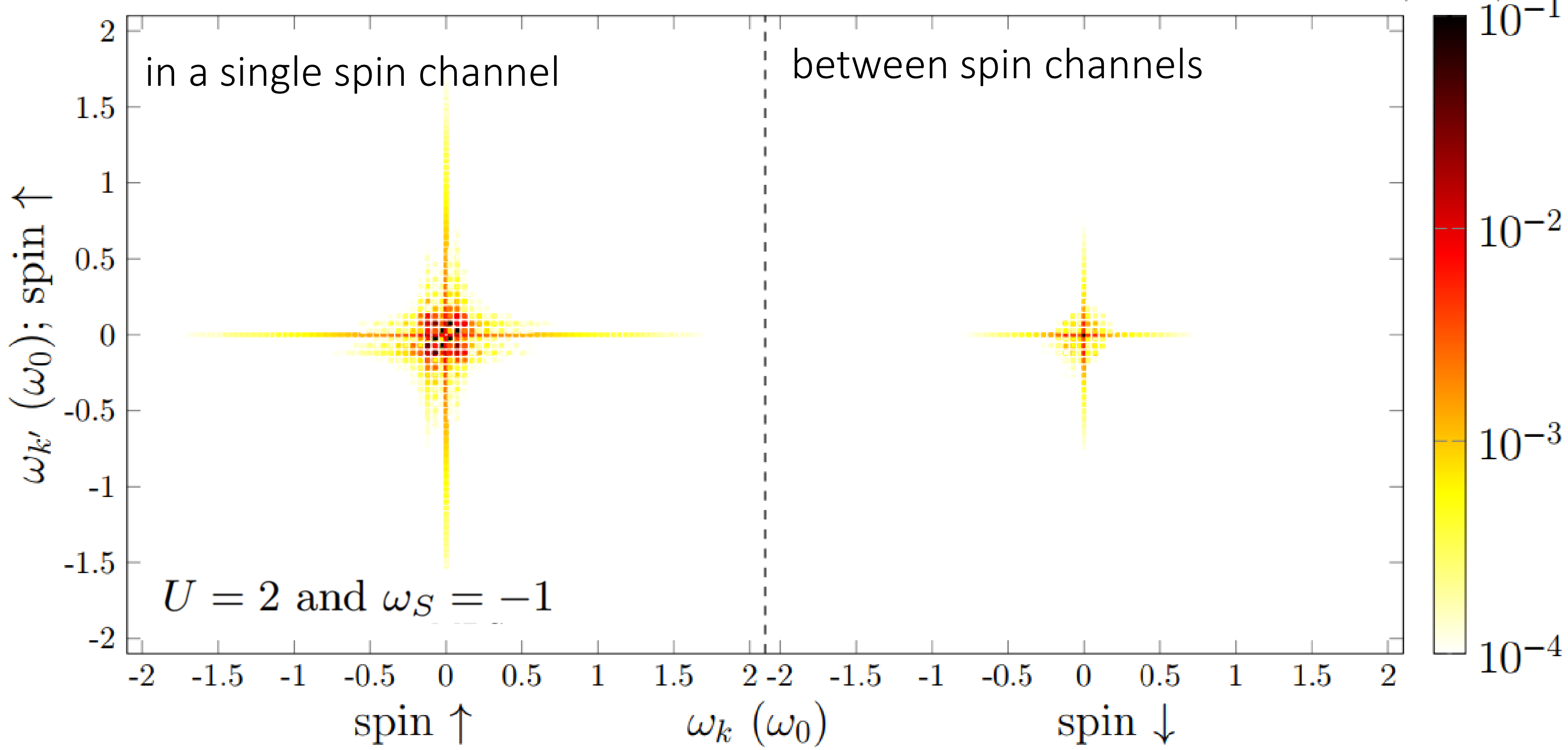


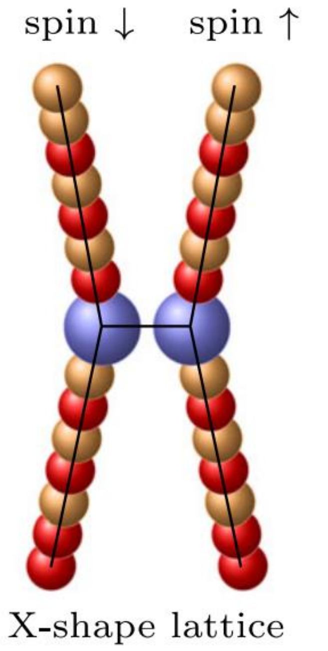
Single-impurity Anderson model:

$$H_S = \hbar\omega_S \sum_\sigma n_\sigma + U n_\uparrow n_\downarrow$$ two spin channels

$$C_{kk'} = \langle n_k n_{k'} \rangle - \langle n_k \rangle \langle n_{k'} \rangle$$

Density-density correlations at long times
(mutual information has the same structure)





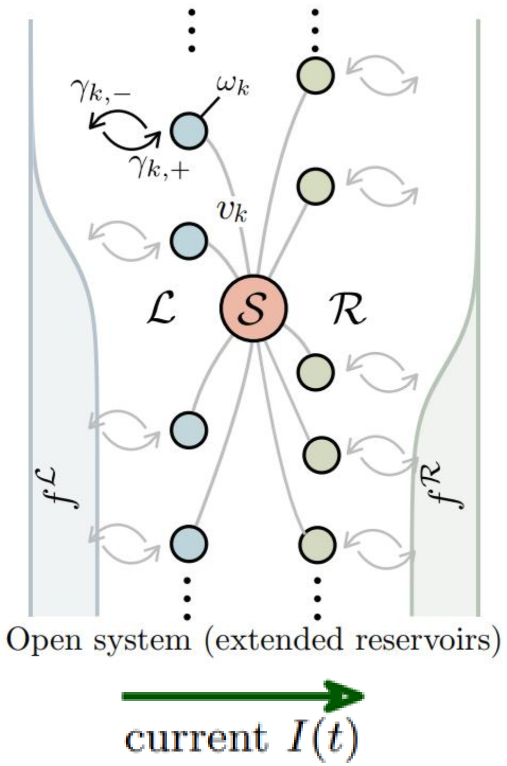
Motivates using
tree tensor networks

Open-systems approach (extended reservoir)

Gorini-Kossakowski-Sudarshan-Lindblad master equation:

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

$$\gamma_{k+} \equiv \gamma f^\alpha(\omega_k) \text{ and } \gamma_{k-} \equiv \gamma[1 - f^\alpha(\omega_k)]$$



- Injection and deplition rates relaxing reservoirs (in isolation) toward Fermi-Dirac distributions.
- They fix the bias that is driving the current though impurity.

Widely-used approach for transport in non-interacting systems:

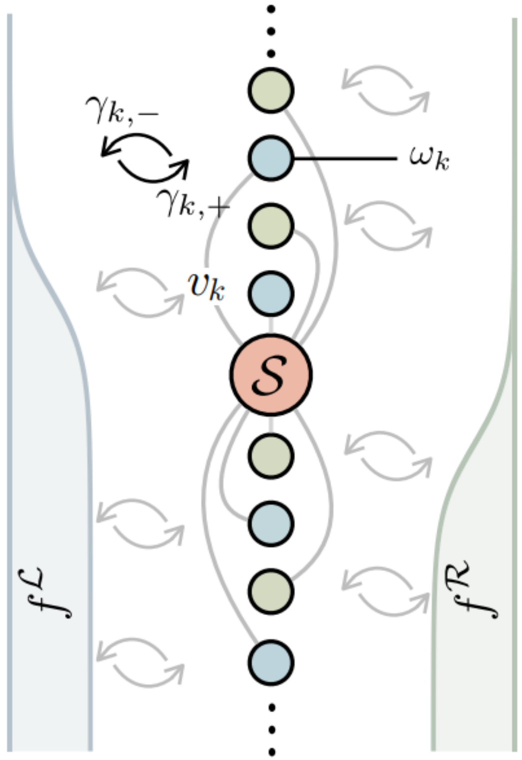
Y. Dubi, M. Di Ventra, Nano Lett. (2009);
A. Dzhioev, D. Kosov, J. Chem. Phys. (2011);
T. Zelovich, L. Kronik, O. Hod, J. Chem. Theory Comput. (2014);
D. Gruss, K. A. Velizhanin, M. Zwolak, Sci. Rep. (2016).

Related approaches to represent non-Markovian dynamics:

A. Imamoglu, PRA (1994);
B. M. Garraway, PRB (1997);
E. Arrigoni, M. Knap, W. v. d. Linden, PRL (2013);
D. Tamascelli, A. Smirne, S. F. Huelga, M. B. Plenio, PRL (2018).

Extended reservoir for interacting impurities using MPS:

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



Mixed basis (MPS)

- We vectorize density matrix to represent it as MPS

M. Zwolak, G. Vidal, PRL (2004); F. Verstraete, et. al. PRL (2004)

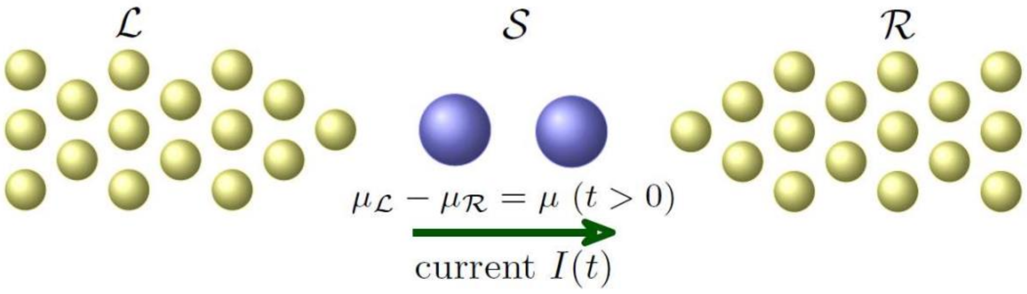
- We employ mixed basis to ordered MPS sites according to the scattering structure of the current-carrying states

- TDVP for MPS to solve GKSL equation with long-range interactions.

J. Haegeman et. al., PRB (2016)

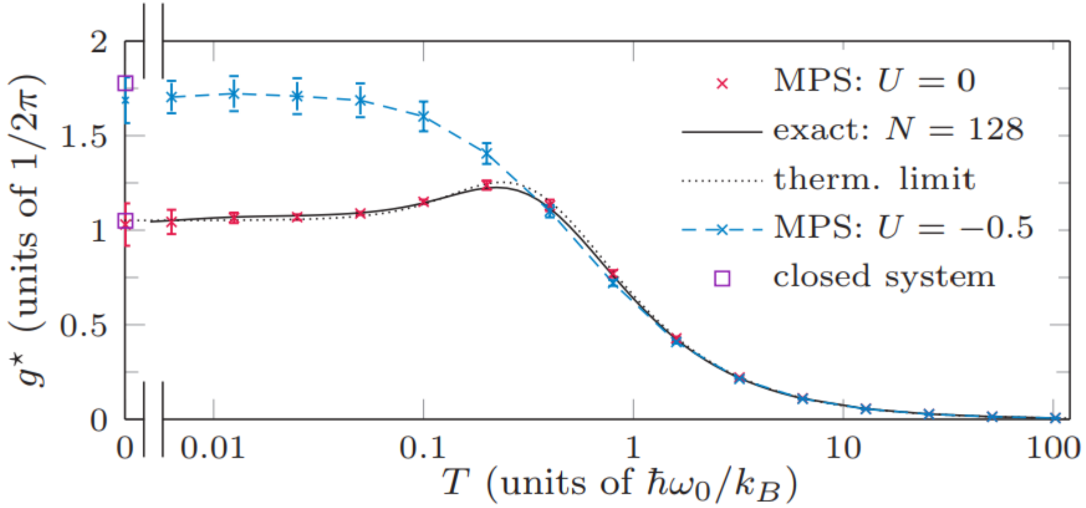
G. Wójtowicz., J. Elenewski., MMR., M. Zwolak., PRA (2020).
Closely related: M. Brenes, J. J. Mendoza-Arenas, A. Purkayastha, M. T. Mitchison, S. R. Clark, and J. Goold, PRX (2020).

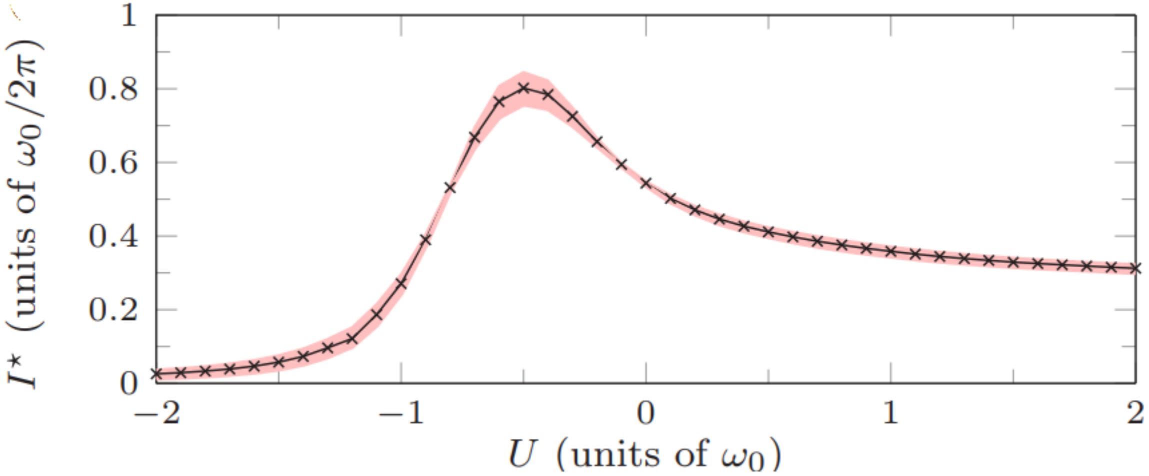
Example: 2-sites spinless impurity:



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

Conductance/current characteristics vs temperature and interaction.





Promising platform to consider more complicated interacting impurities and transport scenarios, time-dependet processes, Floquet states, etc. etc.

Relevance of relaxation rate: Kramers crossover

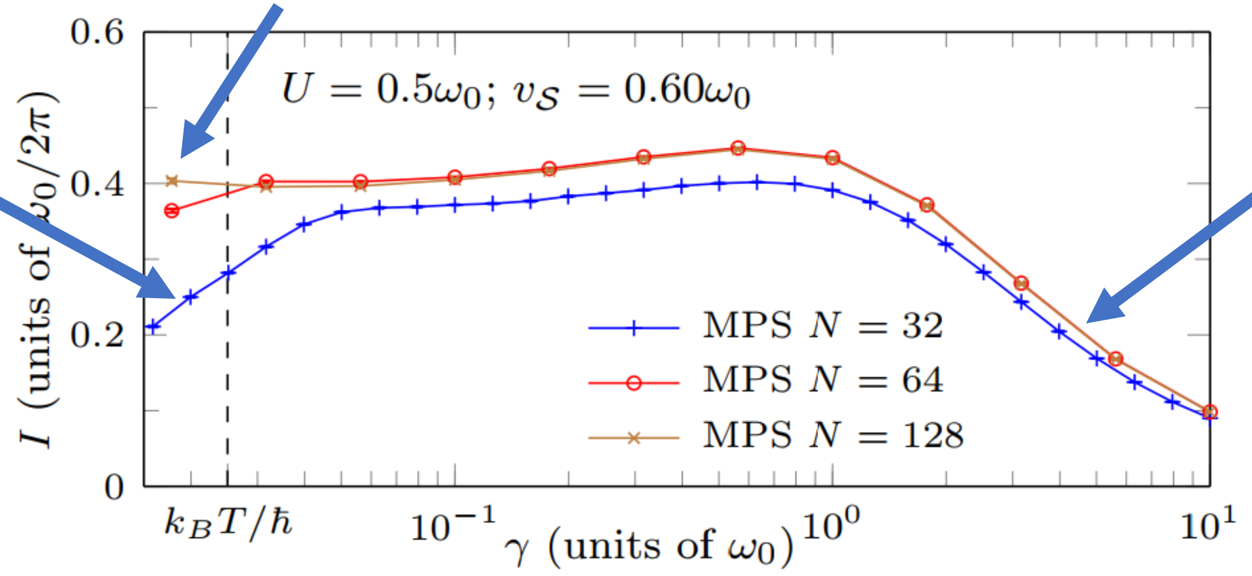
$$\dot{\rho} = -\frac{\imath}{\hbar}[H,\rho] + \sum_k \gamma_{k+}\left(a_k^\dagger \rho a_k - \frac{1}{2}\{a_k a_k^\dagger, \rho\}\right) + \sum_k \gamma_{k-}\left(a_k \rho a_k^\dagger - \frac{1}{2}\{a_k^\dagger a_k, \rho\}\right)$$

$$\gamma_{k+} \equiv \gamma f^\alpha(\omega_k) \text{ and } \gamma_{k-} \equiv \gamma[1 - f^\alpha(\omega_k)]$$

Three regimes of transport (five regimes, if you look closely: GW, JE, MMR, MZ in prep.)

Physical plateau (recovering thermodynamic limit)

Slow replenishing of current carriers (i.e. contact limited)



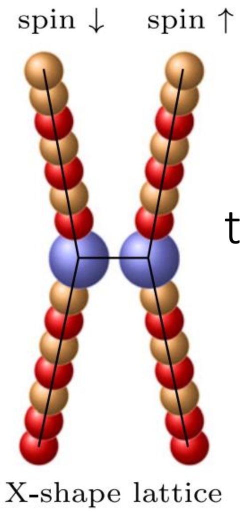
Strong relaxation destroys coherence (i.e. diffusive behavior)

The approach limits to Meir-Wingreen result (for many-body systems) and Landauer result (for non-interacting systems).

D. Gruss, K. A. Velizhanin, M. Zwolak, Sci. Rep. (2016);
J. E. Elenewski, D. Gruss, M. Zwolak, J. Chem. Phys. (2017).

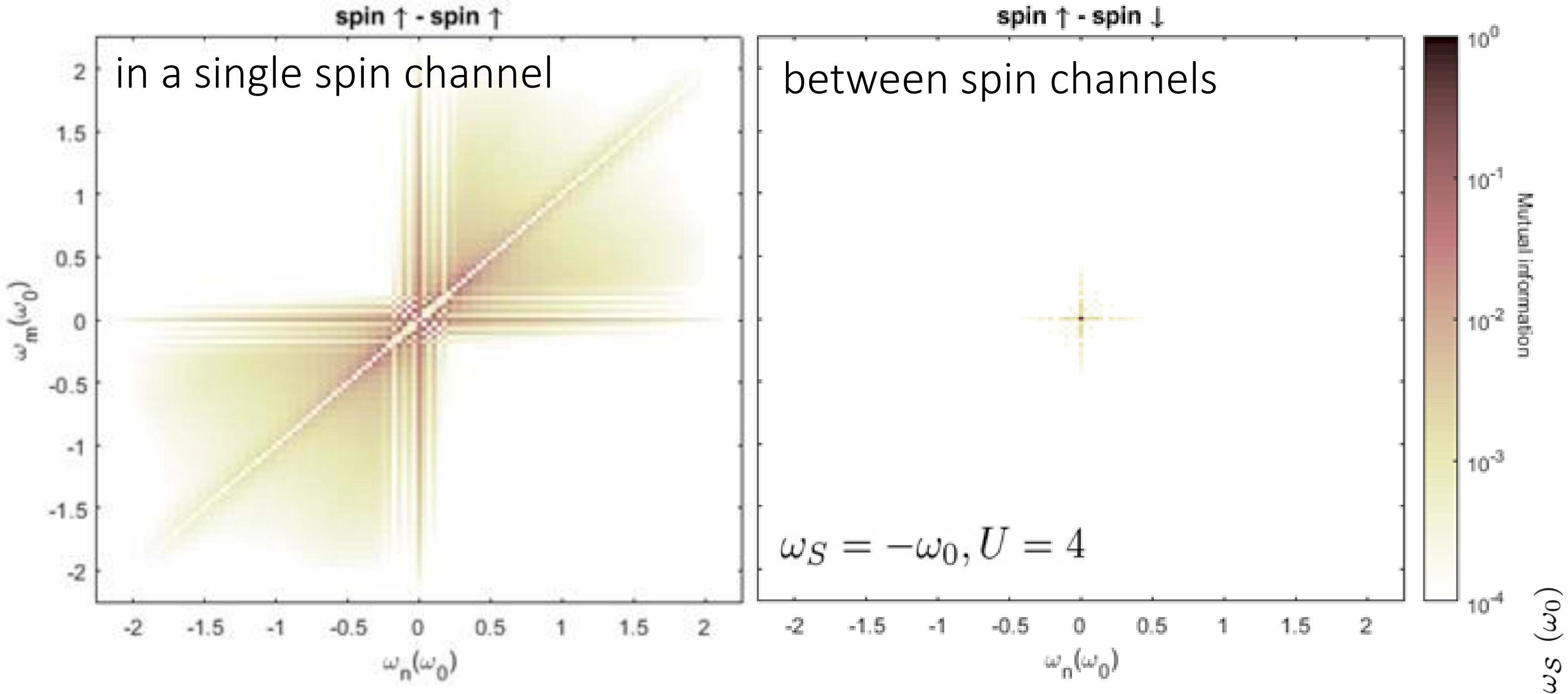
Structure of correlations: spinful Anderson impurity model

$$H_{\mathcal{S}} = \hbar\omega_{\mathcal{S}} \sum_{\sigma} n_{\sigma} + U n_{\uparrow} n_{\downarrow}$$ → two spin channels

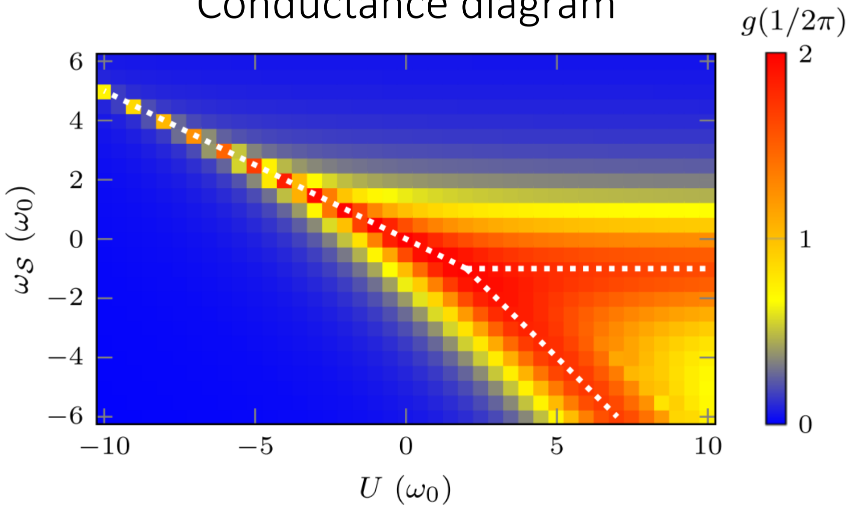


motivates using tree tensor networks as a correct ansatz

Mutual information across energy scales



Conductance diagram



Similar structure as in closed systems.

Summarizing:

Quantum information theory and the recognition of the correlation structure (resulting from dynamical processes) can lead to efficient and accurate simulations of complicated quantum many-body phenomena, pushing the boundaries of what can be described using classical resources (here, for quantum transport problems).

„In general, information is not invariant with respect to … transformations, and this is natural (since information is defined with respect to a given reference,…).„

R. S. Ingarden, A. Kossakowski, M. Ohya,
„Information dynamics and open systems"

Thank you!

M. M. Rams, M. Zwolak, Phys. Rev. Lett. 124, 137701 (2020);
G. Wójtowicz, J. Elenewski, M. M. Rams, M. Zwolak, Phys. Rev. A 101, 050301(R) (2020).