# Dephasing, relaxation and thermalization in one-dimensional quantum systems

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OPTIMAS

MATERIALS IN MAINZ SCIENCE

# Outline

1. Introduction
2. Dephasing, relaxation and thermalization
3. Particle injection into a chain
4. The lightcone renormalization group
5. Doublon decay in (extended) Hubbard models
6. Conclusions

# Collaborations

- Tilman Enss (TU München)
- Nick Sedlmayr (TU KL)
- Jie Ren (TU KL)
- Florian Gebhard (U Marburg)
- Benedikt Ziebarth (U Marburg)
- Kevin zu Münster (U Marburg)

# Classical dynamics

Newton's equations describe the time evolution of a given initial state of classical particles.
Deterministic: Velocities and positions are known at all times

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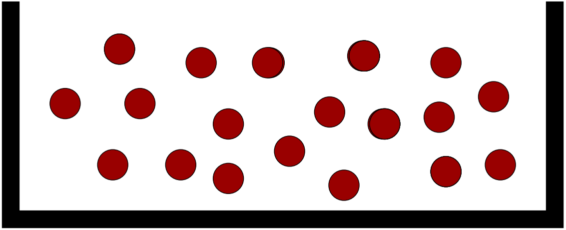
Thermalization:

- Expectation values of generic observables, for long times, should become time independent.
- Values depend only on few parameters, e.g. energy, not the initial state itself.
- They can be equally well described by a statistical average.
  Ergodicity: Time average $\leftrightarrow$ statistical average

# Classical dynamics



Ideal gas: Thermalization by

a) Minimal energy exchange with reservoir (dynamic walls)
b) Minimal interaction between the particles

Ideal gas law:

$$pV = Nk_B T$$

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$$i\hbar \frac{d}{dt}|\Psi\rangle = H|\Psi\rangle$$

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Thermalization of closed quantum system; $\hat{O}$ observable:

- $\bar{O} = \lim_{\tau\to\infty} \frac{1}{\tau}\int_0^\tau dt \langle\Psi(t)|\hat{O}|\Psi(t)\rangle$
  $\left[= \lim_{t\to\infty} \langle\Psi(t)|\hat{O}|\Psi(t)\rangle \equiv O_\infty \text{ (time independent)} \right]$
- Time $\leftrightarrow$ statistical average: $\bar{O} = \mathrm{Tr}\{\hat{O}\rho\}$

# Obvious questions

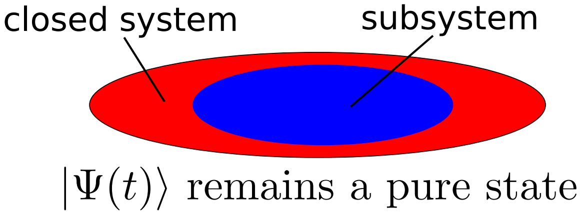
- Which density matrix $\rho$ (ensemble)?
- Which observables $O$ do we want to consider?
- Do we require only $\bar{O} = \mathrm{Tr}\{\hat{O}\rho\}$

  or in addition $\bar{O} = O_\infty$ time independent?

  - Thermodynamic limit; otherwise recurrence
  - True relaxation $\leftrightarrow$ interacting vs. non-int. system

# Thermalization of a closed quantum system

- Only a subsystem can be in a mixed state described e.g. by a canonical ensemble $\rho = \exp(-\beta H)/Z$
- rest might act as an effective bath



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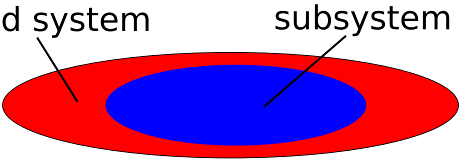


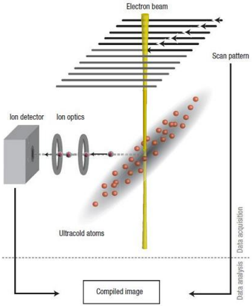

$$|\Psi(t)\rangle \text{ remains a pure state}$$

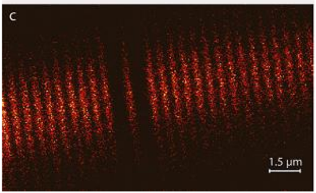
- However, coupling is not small, “bath” can have memory, ...

# Dynamics in quantum systems: Experiments

## Ultracold gases: Quenches

Closed quantum system, tunable → simple Hamiltonians

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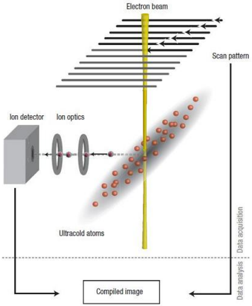


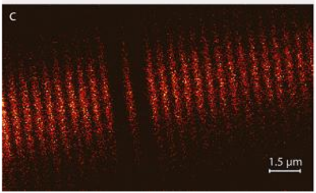


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Measurements: Position and time resolved measurements of observables and correlations are becoming possible

# Long-time mean: Diagonal ensemble and fluctuations

The long-time mean: $\bar{O} = \lim_{\tau\to\infty} \frac{1}{\tau} \int_0^\tau dt \langle \Psi(t)|\hat{O}|\Psi(t)\rangle$

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$$\bar{O} = \lim_{\tau\to\infty} \sum_{n,m} \frac{1}{\tau}\int_0^\tau dt\, \mathrm{e}^{i(E_m-E_n)t} c_n^* c_m \langle E_m|\hat{O}|E_n\rangle = \sum_n |c_n|^2 \hat{O}_{nn}$$

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Fluctuations around long-time mean can decay due to

- dephasing: already for non-interacting systems
- exponential relaxation: only in interacting systems

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Generalized Gibbs ensemble: Choose $\rho = \exp(\sum_n \lambda_n \hat{Q}_n)/Z$ with Lagrange multipliers $\lambda_n$ determined such that

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- Projectors onto eigenstates: $Q_n \equiv P_n = |n\rangle\langle n|$
- Free fermions, $H = \epsilon_k n_k$: $Q_k = n_k$

## $Q_n \equiv P_n = |n\rangle\langle n|$

- $H|n\rangle = E_n|n\rangle$, $[H,|n\rangle\langle n|] = 0$, $\rho_{GGE} = \exp(-\lambda_n P_n)/Z$

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Diagonal ensemble reproduced by fixing exponentially many Lagrange multipliers

M. Rigol *et al.*, Nature **852**, 454 (08)

# GGE for free fermion models

- $H = \sum_k \epsilon_k n_k$
- $\rho_{GGE} = \frac{1}{Z} \exp(-\sum_k \lambda_k n_k)$
- $\langle \Psi_0 | n_k | \Psi_0 \rangle = \mathrm{Tr}(\rho_{GGE} n_k)$ Rigol *et al.* PRA **74**, 053616 (2006) + many others

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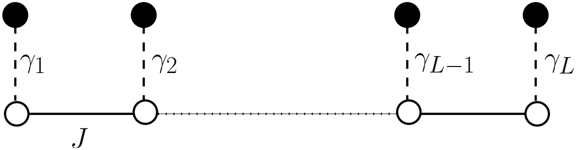
In general, no relaxation:

For non-conserved observables we have $\langle \Psi(t) | \mathcal{O} | \Psi(t) \rangle$ oscillating (undamped) or power law decay towards $\mathcal{O}_\infty$ (dephasing)

# An example: Particle injection into a chain

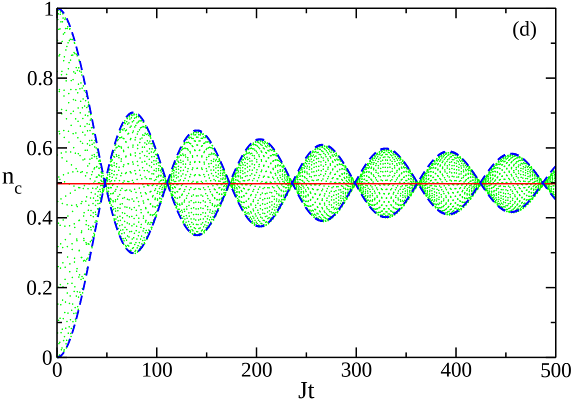



$$H = -J \sum_{l=1}^{L-1} \left( \hat{c}_{l+1}^\dagger \hat{c}_l + h.c. \right) + \gamma \sum_{l=1}^{L-1} \left( \hat{c}_l^\dagger \hat{s}_l + h.c. \right)$$

$$\text{initial state} : |\Psi(0)\rangle = \prod_{l=1}^{L} \hat{s}_l^\dagger |\text{vac}\rangle$$

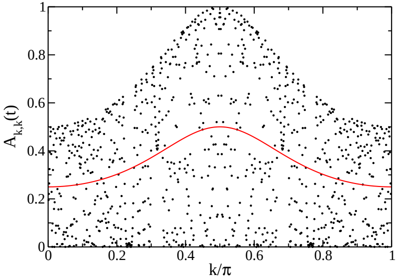
[F. Gebhard, JS *et al.* Ann. Phys. (2012)]

# Particle density in the chain in the TD limit for $\gamma/J = 10$



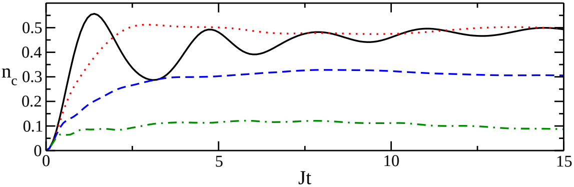

Non-interact.: Slow dephasing of two-level systems $\sim \sqrt{\frac{\gamma/J}{Jt}}$

# $A_{k,k}$ for $\gamma/J = 1$, $L = 1000$ at $Jt = 5000$




- $A_{k,k} = \langle \Psi(t) | c_k^\dagger c_k | \Psi(t) \rangle$ is collection of undamped oscillators.
- Size of fluctuations depends on initial state; can be as large as the long-time mean $\bar{A}_{k,k}$
- Determining mean by ensemble average seems fairly useless in this case

# Relaxation in the interacting case




- t-DMRG for $L = 50$ and $\gamma/J = 1$ with nearest neighbor interaction $V = 1, 2, 3, 4$
- Interaction leads to exponential relaxation

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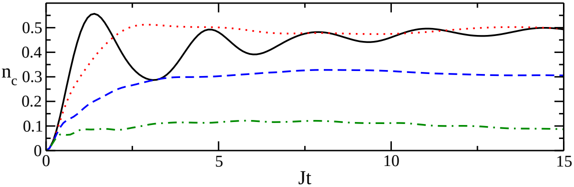


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- Interaction leads to exponential relaxation

GGE seems unobservable even in weakly interacting systems

- slow power-law versus fast exponential relaxation
- no separation of time scales

# One possibly interesting question

Can $O_\infty = \lim_{t\to\infty} O(t)$ in an interacting system in the TD limit with $O$ a local observable be described by a statistical average including only the local conservation laws $\mathcal{Q}_j$?

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If answer is yes this is potentially useful because calculating

$$O_\infty = \lim_{t\to\infty} \langle \Psi(t)|O|\Psi(t)\rangle$$

is hard (dynamical problem) whereas

$$\langle O\rangle_\rho = \frac{1}{Z}\mathrm{Tr}\{O\exp(-\sum_j \lambda_j \mathcal{Q}_j)\}$$

is usually much easier (static problem)

Universality: Independent of initial state

## Integrable versus non-integrable 1D models

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Generic quantum system with short-range interactions:

- Only $H$ is locally conserved
- canonical ensemble: $\rho = \mathrm{e}^{-\beta H}/Z$
- $T = 1/\beta$ fixes initial energy

# Dynamical density-matrix renormalization group

DMRG: Approximate $|\Psi(t)\rangle$ in a finite dimensional Hilbert space consisting of matrix product states

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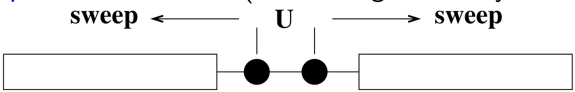


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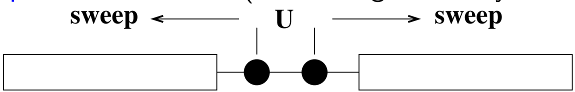


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  - Very versatile: Equ. dynamics, quenches, transport
  - finite systems; eigenstates are calculated explicitly
- TEBD and iTEBD (Vidal, 2004, 2007)
  - Direct matrix product state representation
  - Time evolution by Trotter-Suzuki decomposition
  - Thermodynamic limit if system is translationally invariant

# Specifications of an efficient algorithm

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We have developed the lightcone renormalization group (LCRG) algorithm which makes progress concerning many of the points listed above [T. Enss, JS, New J. Phys. **14**, 023008 (2012)]

# The Lieb-Robinson bound

Consider a (Spin-)Hamiltonian with finite range interactions and two strictly local operators $A$, $B$: (Lieb,Robinson, Comm. Math. Phys **28**, 251 (72))

$$||[A(L,t),B(0,0)]|| \leq C \exp\left(-\frac{L - v_{LR}|t|}{\xi}\right)$$

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Define $S$ as the set of sites having distance of at least $l$ from the local operator $A$: (Bravyi *et al* PRL **97**, 050401 (06))

$$A^l(t) \propto \mathrm{Tr}_S[A(t)] \otimes 1_S$$

# The Lieb-Robinson bound (II)

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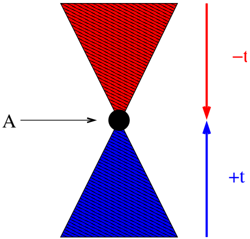
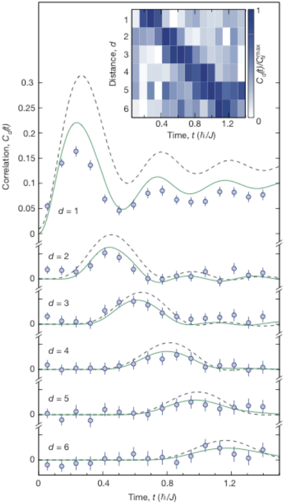


# Recent experimental test

- Bose-Hubbard model, filling $\bar{n} = 1$
- Quench: $U/J = 40 \;\rightarrow\; U/J = 9$
- Parity correlation: $C_d(t) = \langle e^{i\pi[n_j(t)-\bar{n}]} e^{i\pi[n_{j+d}(t)-\bar{n}]} \rangle_{\mathrm{conn.}}$
- Lightcone for doublon/holon propagation

[Cheneau *et al.* Nature **481**, 484 (2012)]



# Light cone renormalization group algorithm

We want to calculate:

$$\langle o_{[j,j+n]}\rangle^{I}(t) \equiv \langle \Psi_I | \mathrm{e}^{\mathrm{i}Ht} o_{[j,j+n]} \mathrm{e}^{-\mathrm{i}Ht} | \Psi_I \rangle$$

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- $H = \sum h_{j,j+1}$ local Hamiltonian
- $|\Psi_I\rangle$ initial product state (thermal state also possible)
- $o_{[j,j+n]}$ local observable

# Light cone renormalization group algorithm

We want to calculate:

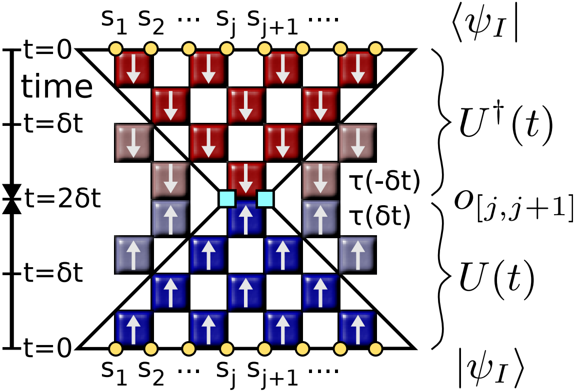
$$\langle o_{[j,j+n]}\rangle^I(t) \equiv \langle\Psi_I|e^{iHt}o_{[j,j+n]}e^{-iHt}|\Psi_I\rangle$$

- $H = \sum h_{j,j+1}$ local Hamiltonian
- $|\Psi_I\rangle$ initial product state (thermal state also possible)
- $o_{[j,j+n]}$ local observable

Use Trotter-Suzuki decomposition of time evolution operator:

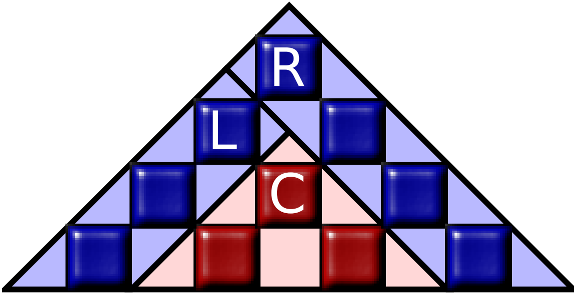
$$\begin{aligned} e^{itH} &= \lim_{N\to\infty}\left(e^{i\delta tH}\right)^N = \lim_{N\to\infty}\left(e^{i\delta tH_{\text{even}}}e^{i\delta tH_{\text{odd}}}\right)^N \\ &= \left(\prod_{j\,\text{even}} \underbrace{e^{i\delta t h_{j,j+1}}}_{\tau_{j,j+1}(\delta t)} \prod_{j\,\text{odd}} e^{i\delta t h_{j,j+1}}\right)^N \end{aligned}$$

# Light cone renormalization group algorithm




- $\tau_{j,j+1}(\delta t)\tau_{j,j+1}(-\delta t) = \text{id}$
- "Speed" in T-S decomposition $\gg v_{LR} \rightarrow$ Thermodyn. limit

# Light cone renormalization group algorithm

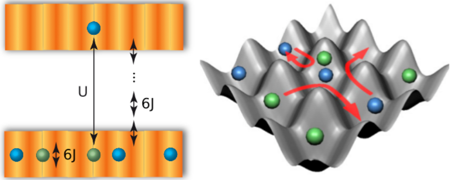


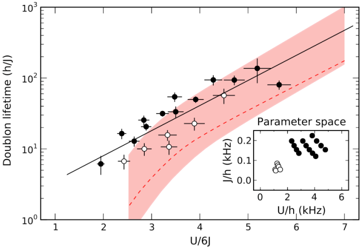

- Light cone grows by adding diagonal transfer matrices
- Optimal Hilbert space chosen by appropriate reduced density matrix (Density-matrix renormalization group)

# Decay of double occupancies in fermionic Hubbard models

Experiments on ultracold fermions in 3D optical lattices

[Strohmaier *et al.* PRL **104**, 080401 (10)]



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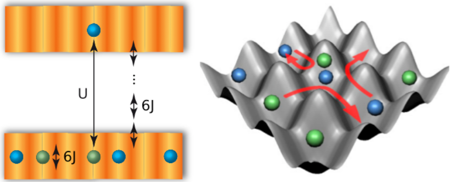


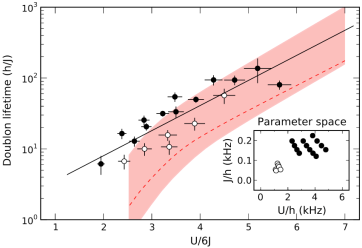


Metastability: If $U \gg 6J$ (bandwidth) then several scattering processes are necessary to dissipate large energy $U$
$\rightarrow$ lifetime of double occupancies $\sim \exp(U/6J)$

# Model, initial state and symmetries

We consider the (extended) Hubbard model:

$$\begin{aligned} H_{U,V} &= -J \sum_{j,\sigma=\uparrow,\downarrow} (c^\dagger_{j,\sigma} c_{j+1,\sigma} + h.c.) + U \sum_j (n_{j\uparrow} - 1/2)(n_{j\downarrow} - 1/2) \\ &+ V \sum_j (n_j - 1)(n_{j+1} - 1) \end{aligned}$$

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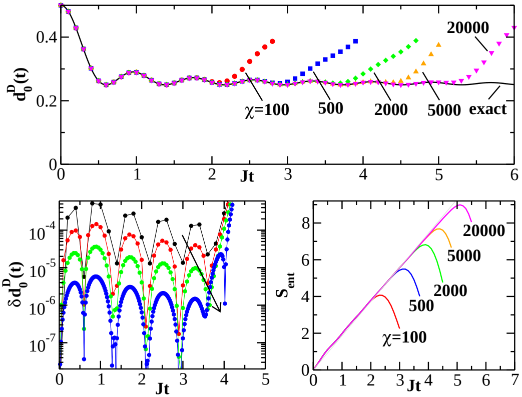
$$+ \; V \sum_j (n_j - 1)(n_{j+1} - 1)$$

We want to study the following initial state and observable:

- Doublon lattice: $|\Psi_D\rangle = \prod_j c^\dagger_{2j\uparrow} c^\dagger_{2j\downarrow} |0\rangle$
- Double occupancy: $d^D_{U,V}(t) = \frac{1}{L} \sum_j \langle \Psi_D(t) | n_{j\uparrow} n_{j\downarrow} | \Psi_D(t) \rangle$
- Symmetries: $d^D_{U,V}(t) = d^D_{-U,-V}(t)$

# Free fermions: A test case




- Error up to the point where simulation breaks down is controlled by the Trotter error
- The entanglement entropy grows linearly in time

# Limitations of DMRG-type algorithms

The eigenvalues of a reduced density matrix $\rho_s = \text{Tr}_E \rho$ are used to determine the states which are kept to approximate $|\Psi(t)\rangle$

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**Entanglement entropy**

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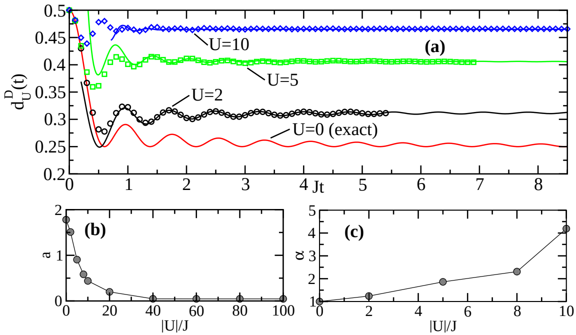
von Neumann entropy of reduced density matrix

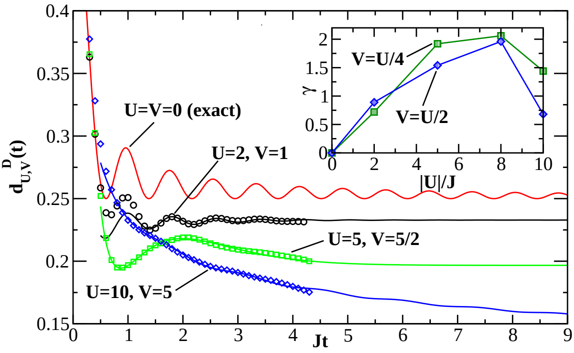
The entanglement entropy which can be faithfully represented is limited for finite matrix dimension

# Doublon decay in the Hubbard model




- Fit: $d^d_{\pm U}(t) = d^D_{\pm U}(\infty) + e^{-\gamma t}[\mathcal{A} + \mathcal{B}\cos(\Omega t - \phi)]/t^\alpha$
- $\gamma \approx 0$: Pure power law decay (?)
- $S_{\mathrm{ent}} = aJt$: large $U \to$ longer simulation times

# Doublon decay in the extended Hubbard model




- Exponential relaxation in the extended Hubbard model
- Extrapolation problematic for large $U$

# Thermalization in the extended Hubbard model

- We use canonical ensemble, ignore other local conservation laws in integrable case, $V = 0$
- Energy is fixed by: $\langle H \rangle_I = \langle \Psi_D | H | \Psi_D \rangle / L = U/4 - V$
- Temperature determined by $\langle H \rangle_I = \langle H \rangle_{\mathrm{th}} = \mathrm{Tr}\{H e^{-H/T}\}/LZ$

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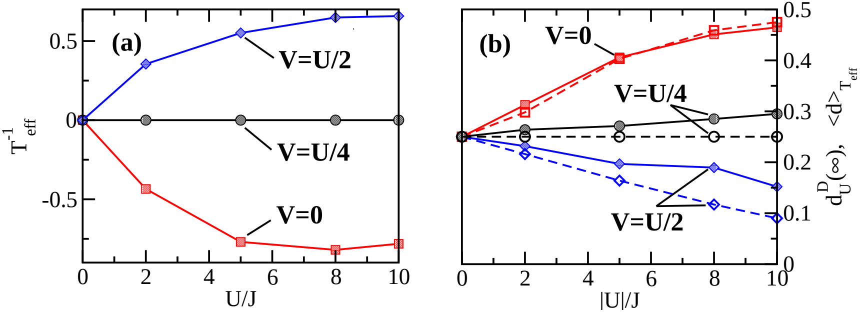
**Repulsive case**

- $T > 0$ for $V > U/4$
- $T < 0$ for $V < U/4$
- Vice versa in attractive case

# Thermalization in the extended Hubbard model




- Excellent agreement for Hubbard model ($V = 0$)
- Deviations larger the larger $V/U$ and $U$ are
- Additional relaxation for $Jt \gg \exp(U/J)$ not covered by fit?

# Conclusions

- Thermalization in closed interacting quantum systems:
  - Time average ↔ statistical average
  - Including all projection op. $P_n$ reproduces time average
  - Free-model GGE seems not very useful: no damping or only slow power law decay versus exp. decay in interacting case

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Can long-time mean of local observables for int. systems in the TD limit be described by including only local conserved quantities?

- Doublon decay in 1D extended Hubbard models
  - Analysis of data: pure power-law relaxation of double occ. in the integrable case; exp. relaxation in the non-integrable case
  - Thermalization: Eff. temperatures can be positive/negative
  - Additional relaxation at $Jt \gg \exp(U/J)$? Influence of other conservation laws in integrable case?