real-time dynamics of non-equilibrium transport in large open quantum spin systems driven by dissipation

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S. Caspar, FH, U.-J. Wiese, In preparation

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dynamics of closed quantum system

- expectation value of observables in equilibrium
  \[ \langle O \rangle_{eq} = \text{tr}[\rho_{eq}O] \sim \text{tr}[Oe^{-\beta H}] \]

- time-dependent expectation value of observables
  \[ \langle O \rangle(t) = \text{tr}[\rho(t)O] = \text{tr}[\rho(t_0)e^{-iH(t_0-t)}OE^{-iH(t-t_0)}] \]

severe sign problem prevents quantum Monte Carlo

\[\rightarrow\] exact Hilbert space methods (small systems)
\[\rightarrow\] DMRG/tensor network states (1-dimensional systems)
\[\rightarrow\] (quantum) kinetic theory (weakly coupled, dilute systems)
\[\rightarrow\] classical-statistical approximation (highly occupied bosons)
\[\rightarrow\] complex Langevin?! (\[\rightarrow\] D. Sexty)
\[\rightarrow\] Lefschetz thimble?! (\[\rightarrow\] L. Scorzato)
dissipative coupling to an environment

- coupling to an environment: decoherence
- unitary time-evolution $\rightarrow$ Lindblad evolution
- randomized nearest-neighbor spin interactions

quantum Monte Carlo possible (in certain cases)
outline

• dissipative dynamics
  → Lindblad equation

• hermitean Lindblad operators ('measurements')
  → equilibration dynamics
  → non-equilibrium transport of magnetization

• non-hermitean Lindblad operators
  → cooling of hardcore bosons

• summary
Lindblad equation (1)

- closed system (A+B): von-Neumann eq.
  \[ \frac{d}{dt} \rho_{AB}(t) = -i[H_{AB}, \rho_{AB}(t)] \]

- reduced density matrix (integrate out bath):
  \[ \rho_A(t) = \text{tr}_B [\rho_{AB}(t)] \]

- assumptions:
  - Born approximation (weak A-B coupling)
  - product initial state (no correlations): \[ \rho_{AB}(0) = \rho_A(0) \otimes \rho_B(0) \]
  - Markovian approximation (short memory)

  \[ \frac{d}{dt} \rho_A(t) = -i[H, \rho_A(t)] + \sum_i \gamma_i \left[ L_i \rho_A(t) L_i^\dagger - \frac{1}{2} L_i^\dagger L_i \rho_A(t) - \frac{1}{2} \rho_A(t) L_i^\dagger L_i \right] \]

Lindblad equation (2)

\[
\frac{d}{dt} \rho_A(t) = -i[H, \rho_A(t)] + \sum_i \gamma_i \left[ L_i \rho_A(t) L_i^\dagger - \frac{1}{2} L_i^\dagger L_i \rho_A(t) - \frac{1}{2} \rho_A(t) L_i^\dagger L_i \right]
\]

- most general non-unitary, Markovian time evolution equation:
  - preserves: hermiticity and positive semi-definiteness of \( \rho_A(t) \)
  - quantum jump (Lindblad) operators: \( L_i \)

- hermitean Lindblad operators: \( L_i^\dagger = L_i \)
  - projection operators ↔ measurement of observables
  - nearest-neighbor spin operators with different symmetry properties
  - generally describe 'heating' of the system

- non-hermitean Lindblad operators: \( L_i^\dagger \neq L_i \)
  - may result in 'cooling' of the system
solving the Lindblad equation

- **time-discretized** Lindblad equation

\[
\rho(t_0 + N\epsilon) = (1 - \epsilon\gamma)^N \rho(t_0) + \sum_{s=1}^{N} (1 - \epsilon\gamma)^{N-s} (\epsilon\gamma)^s \sum_{i_1 < \ldots < i_s} L_{i_s} \ldots L_{i_1} \rho(t_0) L_{i_1}^\dagger \ldots L_{i_s}^\dagger
\]

- **time-dependent** expectation value of observables

\[
\langle O \rangle(t) = \text{tr}[\rho(t)O] \quad \text{with} \quad \rho(t_0) \sim \sum p_E |E\rangle\langle E| \sim \sum p_{ij} |i\rangle\langle j|
\]

numerical toolbox:

- loop-cluster algorithm (hermitean Lindblads)
- directed-loop algorithm (non-hermitean Lindblads)
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• summary
hermitean Lindblads: measurement

- nearest-neighbor spin interaction with different symmetry properties
  \[
  \mathcal{O}^{(1)} = (\vec{S}_x + \vec{S}_y)^2, \quad \left[ \mathcal{O}^{(1)}, S_x^3 + S_y^3 \right] = 0
  \]
  \[
  \mathcal{O}^{(2)} = S_x^1 S_y^1
  \]
  \[
  \mathcal{O}^{(3)} = S_x^1 S_y^1 - S_x^2 S_y^2, \quad \left[ \mathcal{O}^{(3)}, S_x^3 - S_y^3 \right] = 0
  \]
  2 Lindblad operators
  2 Lindblad operators
  3 Lindblad operators

- example \( \mathcal{O}^{(1)} \): total spin measurement

  \[ |SS^3\rangle : \quad |00\rangle \quad \{ |11\rangle, |10\rangle, |1 - 1\rangle \} \]
  singlet
  triplet

  \[ L_0 = \begin{pmatrix}
  0 & 0 & 0 & 0 \\
  0 & 1/2 & -1/2 & 0 \\
  0 & -1/2 & 1/2 & 0 \\
  0 & 0 & 0 & 0
  \end{pmatrix} \]
  \[ L_1 = \begin{pmatrix}
  1 & 0 & 0 & 0 \\
  0 & 1/2 & 1/2 & 0 \\
  0 & 1/2 & 1/2 & 0 \\
  0 & 0 & 0 & 1
  \end{pmatrix}
  \]

  identify exact cancellations in real-time path integral
Heisenberg AFM initial state

- initial state Hamiltonian: anti-ferromagnetic Heisenberg model

\[ H = J \sum_{\langle xy \rangle} \vec{S}_x \cdot \vec{S}_y, \quad J > 0 \]

- ground state (2D, bipartite square lattice): anti-ferromagnetic order

  \[ \rightarrow \text{ spontaneous symmetry breaking: } SU(2) \rightarrow U(1) \]

  \[ \rightarrow \text{ transition temperature: } T = 0 \text{ (Mermin-Wagner theorem)} \]

  \[ \rightarrow \text{ staggered magnetization: } M_s = \sum_x (-1)^{x_1+x_2} S_x^3 \]

- chiral perturbation theory + quantum Monte Carlo simulations

\[ \langle M_s^2 \rangle = \frac{M_s^2 L^4}{3} \sum_n a_n \left( \frac{c}{\rho_s L} \right)^n \]

[Goëckeler & Leutwyler, PLB 253 (1991)]
**equilibration dynamics**

- magnetization Fourier modes

\[ S(p) = \sum_x e^{i(p_1 x_1 + p_2 x_2)} S_x^3 \]

  ➞ uniform magnet.: \((0, 0)\)-mode

  ➞ staggered magnet.: \((\pi, \pi)\)-mode

\[
\mathcal{O}^{(1)} = (\tilde{S}_x + \tilde{S}_y)^2, \quad \left[ \mathcal{O}^{(1)}, S_x^3 + S_y^3 \right] = 0
\]

\[
\mathcal{O}^{(2)} = S_x S_y
\]

\[
\mathcal{O}^{(3)} = S_x^1 S_y^1 - S_x^2 S_y^2, \quad \left[ \mathcal{O}^{(3)}, S_x^3 - S_y^3 \right] = 0
\]

- final equilibrium values calculable

  ➞ unit density matrix (mod. symm.)

- non-trivial attractor (if conservation)

Equilibration is drastically slowed down if any of the Fourier modes is conserved.

[Banerjee et al., PRB 90 (2014)]
[FH et al., PRB 92 (2015)]
phase transition?!

- Heisenberg AFM initial state: $\langle M_s^2 \rangle / L^2 \sim L^2$
- Dissipation-driven final state: $\langle M_s^2 \rangle / L^2 \sim$ volume independent

non-equilibrium phase transition

$B_4 = \langle M_s^4 \rangle(t) / [\langle M_s^2 \rangle(t)]^2$

$\mathcal{M}_s(t) / \mathcal{M}_s(0)$

phase transition takes an infinite amount of time!

[Banerjee et al., PRB 90 (2014)]
[FH et al., PRB 92 (2015)]
equilibration as diffusion

- if any of the Fourier modes conserved → non-trivial attractor
- two time scales:
  → attraction: momentum-dependent \( \sim \exp(-t/T(p)) \)
  → equilibration: determined by slowest mode
- quadratic momentum dependence of attraction time

equilibration as diffusion of the conserved quantity

[Banerjee et al., PRB 90 (2014)]
[FH et al., PRB 92 (2015)]
transport of magnetization

- study the **diffusion** of the conserved quantity directly in **real-space**

![Image of diffusion patterns](image)

**Initial state (AFM / FM)**

**Destruction of AFM order**

**Long-time relaxation**
transport as diffusion

• loop-cluster algorithm ↔ diffusion equation for expectation value

\[
\frac{d}{dt} \langle \rho_x \rangle(t) = \frac{\gamma}{2} \sum_i \left[ \langle \rho_{x+\hat{a}_i} \rangle(t) - 2\langle \rho_x \rangle(t) + \langle \rho_{x-\hat{a}_i} \rangle(t) \right]
\]

• dependence on opening size:

• is the problem classical?!

\textbf{NO!}

\[ \langle \rho_x \rangle(t) \] probes only \textbf{diagonal elements} of density matrix (classical)

\[ \rightarrow \text{in principle: off-diagonal elements accessible (not classical)} \]

problem is \textbf{genuine QM}, certain aspects behave \textbf{classical}

[Banerjee et al., PRB 92 (2015)]
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- summary
cooling of hardcore bosons  
[Caspar et al., In preparation]

- Bose-Hubbard with infinite on-site repulsion = hardcore bosons
  - exact mapping to quantum-XY model
  - superfluid phase transition (2D: BKT, 3D: 2nd order)
  - experimental relevance for ultracold atoms

- $t_0$: quantum-XY model initial state

$$H = J \sum_{\langle xy \rangle} \left[ S_x^{(1)} S_y^{(1)} + S_x^{(2)} S_y^{(2)} \right]$$

- $t > t_0$: purely dissipative dynamics (Lindblad)

$$L_0 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1/2 & -1/2 & 0 \\ 0 & 1/2 & -1/2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \neq L_0^\dagger$$
$$L_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1/2 & 1/2 & 0 \\ 0 & 1/2 & 1/2 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = L_1^\dagger$$

$L_0 |00\rangle \rightarrow |10\rangle$
$L_0 |1x\rangle \rightarrow 0$

complete symmetrization!

$[Diehl et al., PRL 105 (2010)]$

$L_1 |00\rangle \rightarrow 0$
$L_1 |1x\rangle \rightarrow |1x\rangle$
cooling of hardcore bosons [Caspar et al., In preparation]

- Observable: 2-point correlation function
  \[ C(x, y) = \langle S_x^+ S_y^- + S_x^- S_y^+ \rangle \]

- Fourier space: finite momentum modes & condensate fraction

**Preliminary**

Time-scales of finite momentum modes: \( \tau(p \neq 0) \sim p^{-2} \)
cooling of hardcore bosons  [Caspar et al., In preparation]

- observable: 2-point correlation function

\[ C(x, y) = \langle S_x^+ S_y^- + S_x^- S_y^+ \rangle \]

- Fourier space: finite momentum modes & condensate fraction

Preliminary

time-scale of condensate fraction: \[ \tau(p = 0) \sim V = L^3 \]
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summary

- hermitean Lindblad operators:
  - symmetry determines the equilibration time scale
  - equilibration as diffusion of the conserved quantity

- non-hermitean Lindblad operators:
  - detailed understanding on how cooling of hardcore bosons proceeds

Thank you!