Real-time simulation of dissipation driven quantum systems

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Outline

Introduction

Set-up of the problem

Real-time evolution in a large quantum system

Outlook

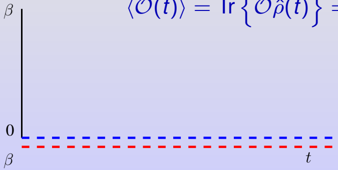
The Schwinger-Keldysh (closed-time) contour

- Quantum many-body system governed by $\hat{H}(t)$
- Initial state at $t = 0$ specified by density-matrix $\hat{\rho}(0)$.
- Evolution of the density matrix: $\frac{d\hat{\rho}(t)}{dt} = -i[\hat{H}(t), \hat{\rho}(t)]$
- Formal solution: $\hat{\rho}(t) = \hat{U}(t,0)\hat{\rho}(0)[\hat{U}(t,0)]^{\dagger}$

$$\begin{aligned} \hat{U}(t,t') &= \mathcal{T} \exp\left[-i \int_t^{t'} \hat{H}(\tau) d\tau\right] \\ &= \lim_{\epsilon \to 0} e^{-i\epsilon \hat{H}(t'-\epsilon)} \cdots e^{-i\epsilon \hat{H}(t+\epsilon)} e^{-i\epsilon \hat{H}(t)} \end{aligned}$$

- Calculations with normalized density matrix:

$$\langle \hat{\mathcal{O}}(t) \rangle = \mathrm{Tr}\left\{\hat{\mathcal{O}}\hat{\rho}(t)\right\} = \mathrm{Tr}\left\{\hat{U}(0,t)\hat{\mathcal{O}}\hat{U}(t,0)\hat{\rho}(0)\right\}$$



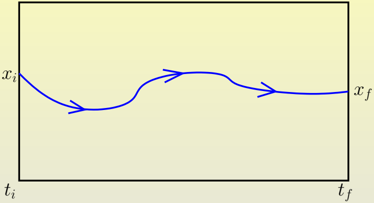
- "forward-backward" evolution along the real-time contour.
- Entanglement makes numerics hard.

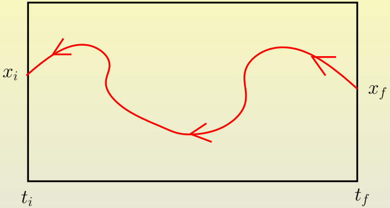
Measurements and Lindblads

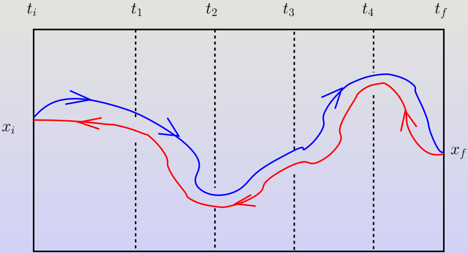
- Idea 1: repeated measurements on the system to reduce entanglement.
- Measurements of an observable $\hat{O}_k$ at time t_k can be represented by projection operator $\hat{P}_{O_k}$.
- Projects on to the sub-space of the Hilbert space spanned by eigenvectors of $\hat{O}_k$ with eigenvalue O_k.
- $\hat{P}^{\dagger}_{O_k} = \hat{P}_{O_k}$; $\hat{P}^{2}_{O_k} = \hat{P}_{O_k}$; $\sum_{O_k} \hat{P}_{O_k} = 1$
- Idea 2: stochastic measurements represent the Markovian, non-unitary dynamics of a quantum system interacting with an environment to a good approximation.
- The effect of the environment on the system is represented by the so-called Lindblad operators, which are related to the projection operators.
- They represent the quantum jumps the system makes while interacting with the environment, and given by $\hat{L}_{O_k} = \sqrt{\epsilon\gamma}\hat{P}_{O_k}$.
- $\gamma \rightarrow$ strength of the coupling to environment and $\epsilon \rightarrow$ discrete time.
- Schrödinger eqn $\longrightarrow$ Lindblad eqn:

$$
\begin{aligned}
\frac{d\rho(t)}{dt} &= -i\,[H,\rho] + \frac{1}{\epsilon}\sum_{o_k}\left[L_{o_k}\rho(t)L^{\dagger}_{o_k} - \frac{1}{2}\left\{L^{\dagger}_{o_k}L_{o_k},\rho(t)\right\}\right] \\
&= \gamma\sum_{o_k}\left[P_{o_k}\rho(t)P_{o_k} - \rho(t)\right] \ \text{(without H)}
\end{aligned}
$$

Why is the problem with measurements easier?







Path-Integral with measurements

- Time-evolution $t_k \to t_{k+1}$ described by $\hat{U}(t_{k+1}, t_k) = \hat{U}(t_k, t_{k+1})^\dagger$.
- At time t_k $(k \in \{1, 2, \cdots, N\})$ observable $\hat{O}_k$ measured with eigenvalue O_k.
- Consider an initial state, specified by a normalized density matrix $\rho = \sum_i p_i |i\rangle\langle i|$; with $0 \leq p_i \leq 1$ and $\sum_i p_i = 1$.
- Probability of making a single measurement of $\hat{O}_k$ at time t_k while evolving from t_i to t_f:
  $p_{\rho f}(O_k) = \sum_i \langle i|\hat{U}(t_i, t_k)\hat{P}_{O_k}\hat{U}(t_k, t_f)|f\rangle \langle f|\hat{U}(t_f, t_k)\hat{P}_{O_k}\hat{U}(t_k, t_i)|i\rangle \; p_i$
- With many measurements,
  $$p_{\rho f}(O_1, O_2, \cdots, O_N) = \sum_i \langle i|\hat{U}(t_i, t_1)\hat{P}_{O_1}\hat{U}(t_1, t_2)\hat{P}_{O_2} \cdots \hat{P}_{O_N}\hat{U}(t_N, t_f)|f\rangle \langle f|\hat{U}(t_f, t_N)\hat{P}_{O_N} \cdots \hat{P}_{O_2}\hat{U}(t_2, t_1)\hat{P}_{O_1}\hat{U}(t_1, t_i)|i\rangle \; p_i$$
- For PI, insert complete set of states $\sum_{n_k} |n_k\rangle\langle n_k| = \mathbb{I}$; $\sum_{n'_k} |n'_k\rangle\langle n'_k| = \mathbb{I}$ for the top and bottom contours respectively.
- Unavoidable sign problem for $\langle n_k|\hat{U}(t_k, t_{k+1})|n_{k+1}\rangle$ and/or $\langle n_{k+1}|\hat{U}(t_{k+1}, t_k)|n_k\rangle$.

Zeroth attempt: remove the Hamiltonian

- Take an extreme case: switch off the Hamiltonian completely for the real-time evolution.

$$\hat{U}(t_{k+1}, t_k) = \mathbb{I}.$$

Can the real-time evolution still be interesting?

- Time-evolution needs to be driven entirely by non-commuting measurements. Need to calculate the matrix elements of projection operators such as $\langle n_k|\hat{P}_{O_k}|n_{k+1}\rangle$.
- Use the re-writing:

$$\langle n_k|\hat{P}_{O_k}|n_{k+1}\rangle\langle n'_{k+1}|\hat{P}_{O_k}|n'_k\rangle = \langle n_k|\hat{P}_{O_k}|n_{k+1}\rangle\langle n'_k|\hat{P}^\dagger_{O_k}|n'_{k+1}\rangle$$
$$= \langle n_k n'_k|\left(\hat{P}_{O_k} \otimes \hat{P}^T_{O_K}\right)|n_k n'_{k+1}\rangle$$

- With only the measurements:

$$p_{\rho f}(o_1, o_2, \cdots, o_N) = \sum_i \langle i|P_{o_1}P_{o_2}\cdots P_{o_N}|f\rangle\langle f|P_{o_N}\cdots P_{o_2}P_{o_1}|i\rangle\, p_i$$
$$= \sum_i p_i\langle ii|(P_{o_1} \otimes P^T_{o_1})(P_{o_2} \otimes P^T_{o_2})\cdots(P_{o_N} \otimes P^T_{o_N})|ff\rangle$$

- In the doubled Hilbert space of states $|n_k n'_k\rangle$, for both pieces of the Keldysh contour (using $\langle n_0 n'_0| = \langle ii|$ & $|n_{N+1} n'_{N+1}\rangle = |ff\rangle$):

$$p_{\rho f}(o_1, o_2, \cdots, o_N) = \sum_i p_i \sum_{n_1 n'_1}\cdots\sum_{n_N n'_N}\prod_{k=0}^{N}\langle n_k n'_k|P_{o_k} \otimes P^T_{o_k}|n_{k+1} n'_{k+1}\rangle$$

A concrete example

- For a model of dissipation, intermediate results are unimportant
  sum over all possible measurement results $\longrightarrow \widetilde{P_k} = \sum_{o_k} P_{o_k} \otimes P_{o_k}^T$,
- The probability $p_{\rho f}$ to reach the final state $|f\rangle$:

$$p_{\rho f} = \sum_{o_1} \sum_{o_2} \cdots \sum_{o_N} p_{\rho f}(o_1, o_2, \cdots, o_N) = \sum_i p_i \sum_{n_1, n_1'} \cdots \sum_{n_N, n_N'} \prod_{k=0}^{N} \langle n_k n_k' | \tilde{P}_k | n_{k+1} n_{k+1}' \rangle$$

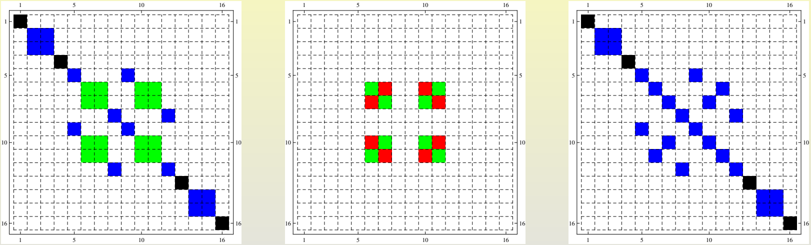
- Example: Two spins $\vec{S_x}$ and $\vec{S_y}$ forming total spin eigenstates:
  $|1,1\rangle = \uparrow\uparrow$, $|1,0\rangle = \frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow)$, $|1,-1\rangle = \downarrow\downarrow$; $|0,0\rangle = \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow)$
- Projection operator on spin-1: $P_1 = |1,1\rangle\langle 1,1| + |1,0\rangle\langle 1,0| + |1,-1\rangle\langle 1,-1|$
- Projection operator on spin-0: $P_0 = |0,0\rangle\langle 0,0|$

$$P_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & & 1 \end{pmatrix} \qquad P_0 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & & 0 \end{pmatrix}$$

- Negative entries in P_0 give rise to a sign problem.
- Measurements can also induce sign problems!

The sign-problem and it's solution

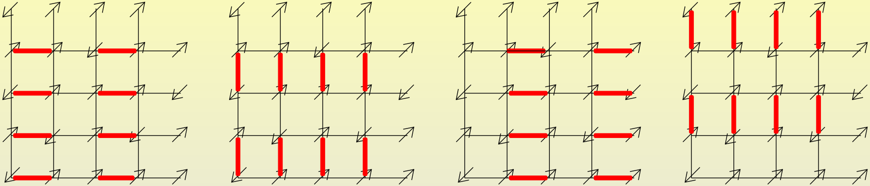
In the doubled Hilbert space, $P_1 \otimes P_1^T$, $P_0 \otimes P_0^T$ are 16×16 matrix with entries:



Legend: black $\rightarrow 1$; blue $\rightarrow \frac{1}{2}$; green $\rightarrow \frac{1}{4}$; red $\rightarrow -\frac{1}{4}$
Summing over all possible results eliminates the sign problem.

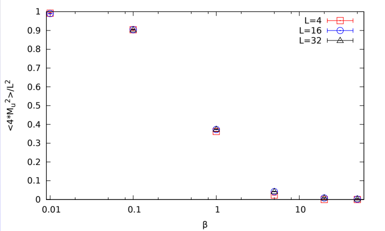
- Example of two-spin system easily extendable to large systems, where the environment couples to the total spin $(\vec{S}_x + \vec{S}_y)^2$ of the spin-pairs $\vec{S}_x$ and $\vec{S}_y$ in a spin system.
- System of quantum spins $\frac{1}{2}$ on a square lattice $L \times L$ with periodic boundary conditions.
- To define the initial density matrix $\hat{\rho} = \exp(-\beta \hat{H})$, use the Heisenberg anti-ferromagnet: $\hat{H} = J \sum_{<xy>} \vec{S}_x \cdot \vec{S}_y; \quad J > 0$.

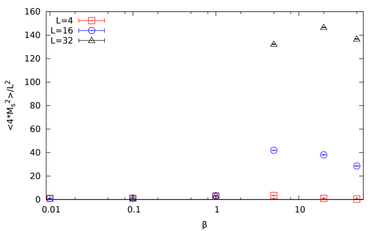
Extension to large systems



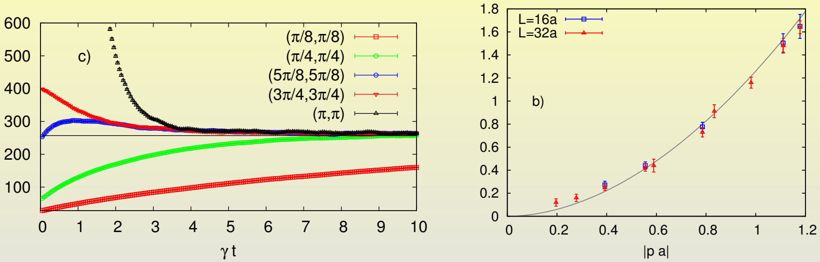
- Sporadic non-commuting measurements drive dynamics from initial state.
- Initial state $\longrightarrow$ low-T (large β) of antiferromagnet, Néel state.
- Order parameters: uniform and staggered magnetizations

$$M_u = \frac{1}{2}\sum_x S_x^3; \quad M_{stag} = \frac{1}{2}\sum_x (-1)^{x_1+x_2} S_i^3$$



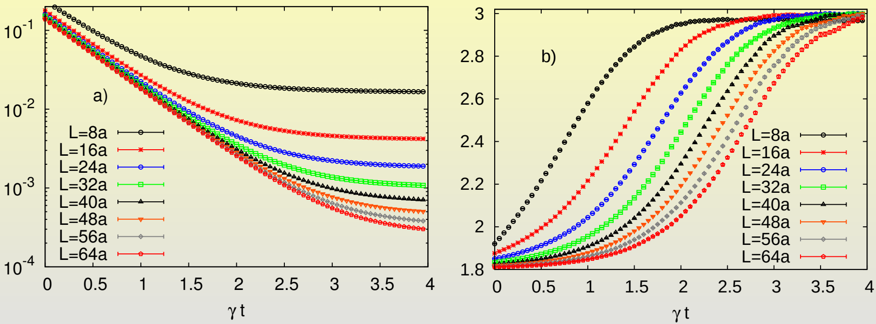


Lindblad evolution: Structure factors



- Evolution of the Fourier-modes can be parametrized by $\langle|\widetilde{S(p)}|^2\rangle \rightarrow A(p) + B(p)\exp(-t/\tau(p))$
- For small momenta, $1/[\gamma\tau(p)] = C|pa|^r$ with $r = 1.9(2)$
- Clearly identifiable two different time scales.
- Final state at $t \rightarrow \infty$ is a paramagnet with short range correlations.
- More extensive investigations PRB 92 (2015), 3, 035116 by Hebenstreit et. al. suggest that this exponent might be unique for all 2-spin observables, and evolution about a conserved quantity for various quantum-spin Hamiltonians in (2+1)-d.
- Dynamic universality classes.

Phase Transitions in real-time?



- Staggered susceptibility $\langle M_s^2 \rangle / L^2 \propto L^2$ for small-t.
- For large-t, this becomes independent of volume.
- Breaking of SU(2) symmetry restored at late (real) times.
- Does a phase transition to the symmetry-restored phase take place at finite time t_c?
- Left plot: $\chi_s / L^2 = \langle M_s^2 \rangle / L^4$.
- Right plot: Binder cumulant $\langle M_s^4 \rangle / \langle M_s^2 \rangle^2$.
- Curves do not cross, indicating the transtion is complete only for infinite real-times.

Chi PT for low energy anti-ferromagnets

- SU(2) Heisenberg antiferromagnets in (2+1)-d share many features with QCD.
- For both the systems, the low-energy effective theory can be captured by an effective field theory, which describes the magnon-magnon interaction in anti-ferromagnets, similar to the pion interactions in QCD.

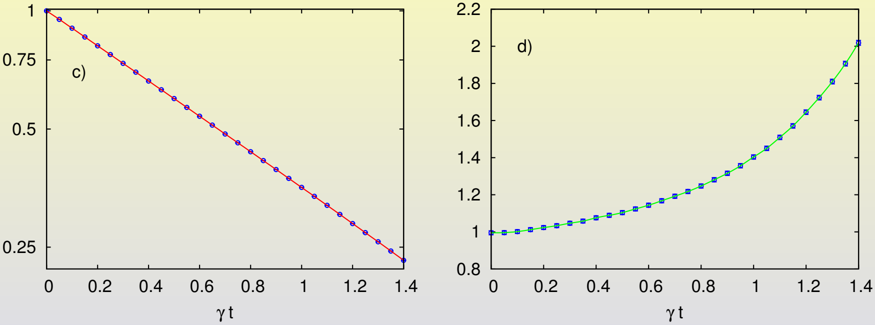
$$S[\vec{e}] = \int d^2x dt \frac{\rho_s}{2} \left(\partial_i \vec{e}.\partial_i \vec{e} + \frac{1}{c^2} \partial_t \vec{e}.\partial_t \vec{e} \right)$$

  where is a Goldstone boson (magnon) field in
  $SU(2)/U(1) = S^2; \ \ \vec{e}(x) = (e_1(x), e_2(x), e_3(x)), \ \ \vec{e}(x)^2 = 1$
- The low-energy constants of the theorys are the staggered magnetization $\mathcal{M}_s$, the spin stiffness ρ_s, the speed of sound c.
- check the applicability of Eulidean time methods in real-time.
- For example, take the expression for χ_s

$$\chi_s = \frac{\mathcal{M}_s^2 L^2 \beta}{3} \left\{ 1 + 2 \frac{c}{\rho_s L l} \beta_1(l) + \left(\frac{c}{\rho_s L l} \right)^2 [\beta_1(l)^2 + 3\beta_2(l)] + \mathcal{O}(\frac{1}{L^3}) \right\}$$

- Make the LEC's time dependent and see real-time behaviour.

Chiral PT to study the real-time evolution



- Exponential decay of the staggered magnetization: $\mathcal{M}_s(t) = \mathcal{M}_s(0)\,\exp(-t/\tau)$
- The lengthscale $\xi = c/(2\pi\rho_s)$ diverges as the spin stiffness ρ_s vanishes.
- Destruction of order takes place very rapidly $t = 1/\gamma$ in contrast to the diffusion process, which is a power law.

In progress: 1,2,3, $\cdots$, ∞

- Ref. PRB 92 (2015), 3, 035116 by Hebenstreit et. al. studied all possible measurement processes using two-spin observables for a variety of models (ferro, anti-ferro Heisenberg model, XY) in $(2+1)$-d. Besides confirming the general picture in this study, we find similar behaviour of the diffusion of the momentum modes around the conserved quantity.

- A real-time transport (spin diffusion) process was studied in Ref: arXiv: 1505.00135 by present authors. Diffusion of ferromagnetic order into an anti-ferromagnet when the systems are kept in contact under the influence of this measurement process.

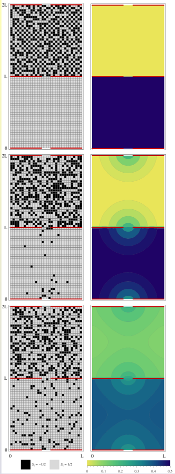
- Cooling into dark states, instead of heating up.

- Different initial states in different phases in a model with richer phase structure.

- Bring back the Hamiltonian.

- Progess seems possible with fermions in the game as well.

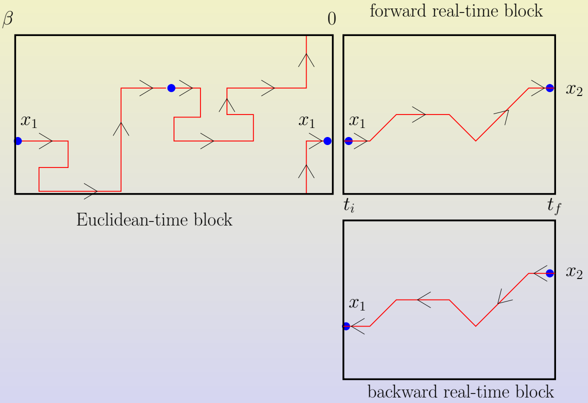
Thank you for your attention



Diffusion of M_u from a ferromagnetic initial state to an anti-ferromagnetic one at different times $t = 0$, $t = 50/\gamma$ and $t = 500/\gamma$.

Backup 1: Models and Algorithms

- The existing highly efficient loop-cluster algorithm for anti-ferromagnets can be naturally extended to this particular case of real-time evolution.
- Resulting clusters are closed loops extending in both Euclidean and real-time, which are updated together.



Identical clusters in the forward and backward real-time evolution. Summed over "all intermediate measurements", and all spins are measured in the final state. Cluster bonds are decided with the matrix elements in the matrix $\widetilde{P} = P_1 \otimes P_1^T + P_0 \otimes P_0^T$.