The Computational Complexity of Time Evolution of Quantum Systems

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Computing Properties of Time Evolution

The problem:

Start in quantum system in some state, evolve under some Hamiltonian, measure something at a later time.
Three problems:
1)Measuring different time correlations in the ground state:

$$\langle S_i^z(t) S_j^z(0) \rangle$$

$$O(t) \equiv \exp(i\mathcal{H}t) O \exp(-i\mathcal{H}t)$$

Common experimental problem.
2)Start a system in the ground state, change it locally (close a switch), measure something later. Similar to (1).
3)Start a system in the ground state of Hamiltonian $\mathcal{H}_0$, evolve under different $\mathcal{H}$. Very hard.

Brute force

Exact evolution of the state vector using sparse matrix techniques.

$$\begin{aligned} \psi(t) &= \exp(-i\mathcal{H}t)\psi(0) \\ &= \left(1 - i\mathcal{H}t - \mathcal{H}^2 t^2/2 + \ldots\right)\psi(0) \end{aligned}$$

Complexity scales as $D = 2^N$
Even using symmetries, limit around $30 - 40$ qubits.

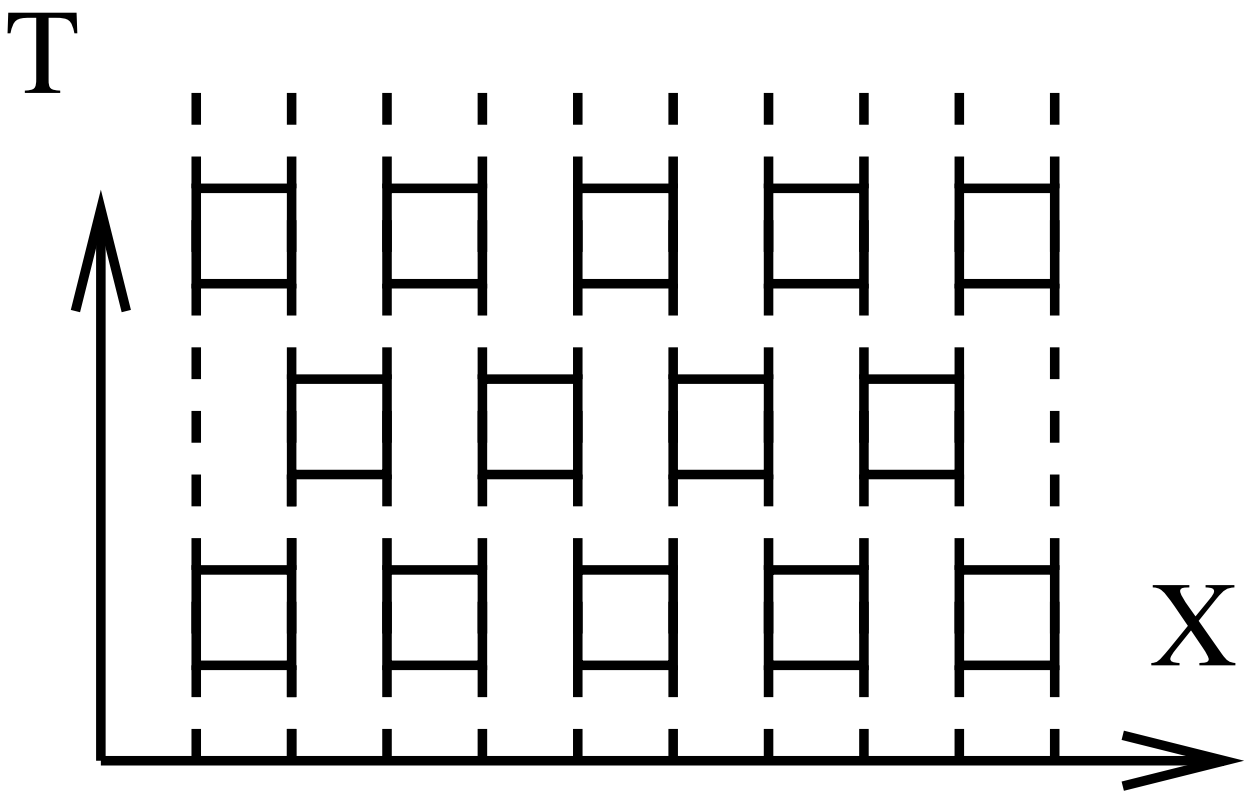
Matrix Product Methods

TEBD (Vidal, 2004)

Represent state as MPS.

Decompose evolution: $\mathcal{H} = \sum_{i=1}^{N-1} h_{i,i+1}$

$$\exp(-i\mathcal{H}\delta t) \approx \exp(-i\mathcal{H}_{odd}\delta t)\exp(-i\mathcal{H}_{even}\delta t)$$



Each time step increases bond dimension k. Truncate back to some k_{max}.

Matrix Product Methods

Success of these methods requires that state can be represented with small k.
Entropy:

$$k \sim \exp(S)$$

Case (1 and 2): Change system locally. Entropy typically grows logarithmically in time. Long time possible.
Case (3): Change system globally. Entropy typically grows linearly in time. Only short times possible.

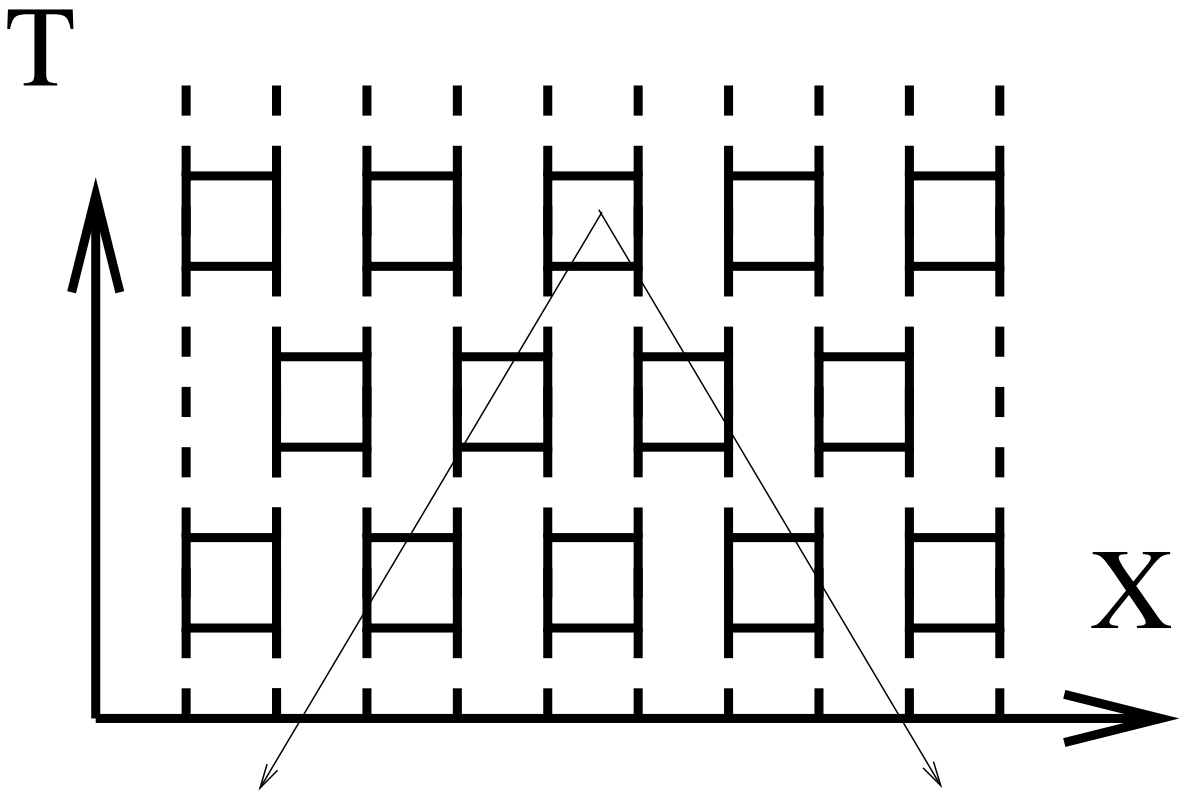
Computing Properties of Time Evolution

General problem is BQP complete

Evolving a state under a local Hamiltonian can mimic a set of local gates. If we could compute this classically, even for 1D systems, we could do anything a quantum computer could. So, probably not possible!

Computing Properties of Time Evolution

Light-cone in unitary circuit:



No influence outside the light-cone.

Note: unitary circuit is an approximation. We need to take time step $\delta t \to 0$ to make it accurate.

$$\exp(-i\mathcal{H}\delta t) \approx \exp(-i\mathcal{H}_{odd}\delta t)\exp(-i\mathcal{H}_{even}\delta t)$$

Velocity is:

$$v \propto 1/\delta t$$

Can we do better?

Lieb-Robinson bound (finite velocity of propagation):

The following can be proven for a wide class of local Hamiltonians: there is a constant v_{LR} such that for

$$|t| \leq l/v_{LR}$$

the commutator bound holds:

$$\|[A(t), B]\| \leq \exp(-\mathcal{O}(l))$$

$$A(t) = \exp(i\mathcal{H}t)A\exp(-i\mathcal{H}t)$$

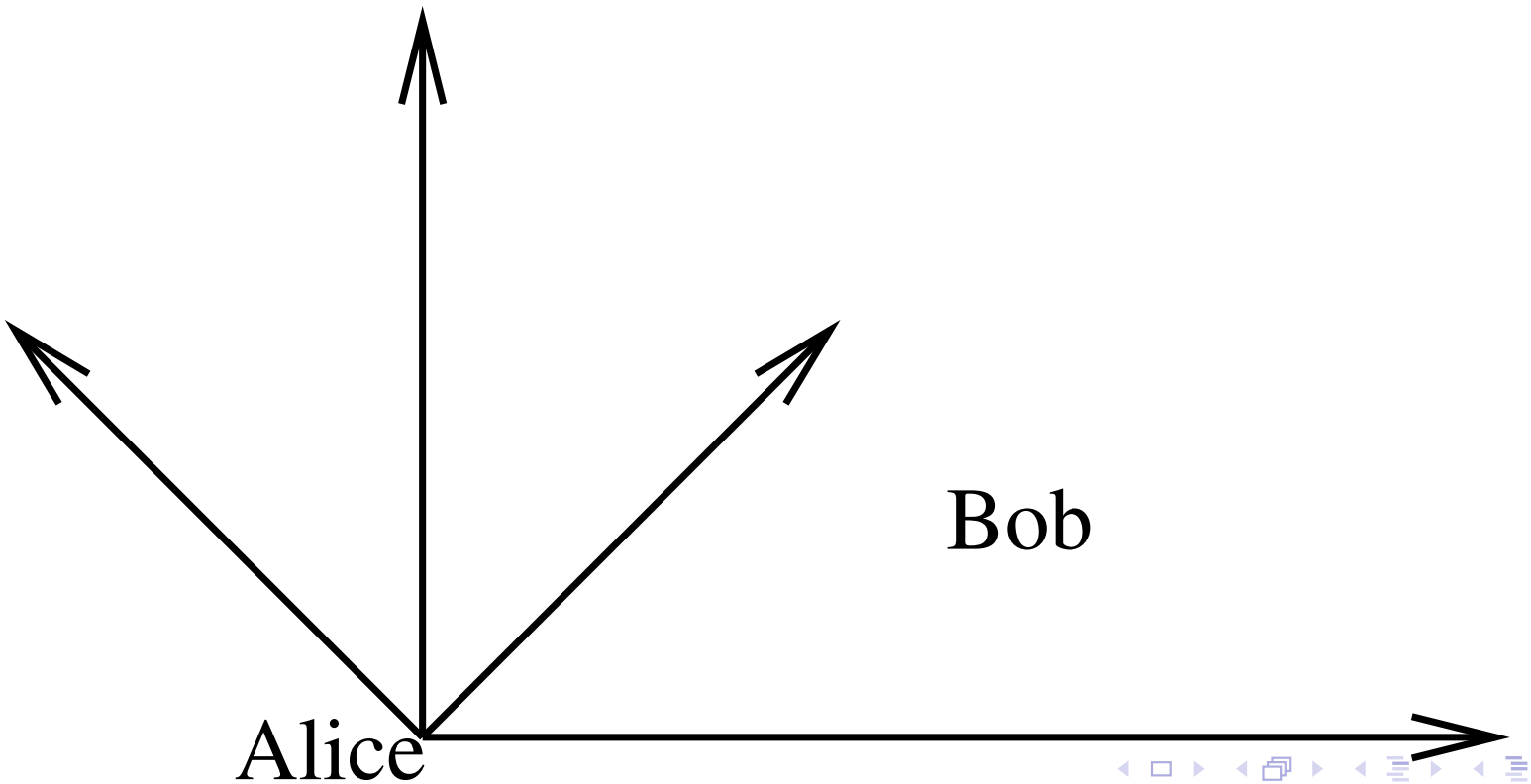
$$l = \mathrm{dist}(\mathrm{supp}A, \mathrm{supp}B)$$

Lieb-Robinson bounds for bounded range Hamiltonians and Hamiltonians with exponentially decaying interactions on general graphs. (Lieb and Robinson, Hastings, Koma, Nachtergaele, Sims, Ogata,...)

Lieb-Robinson bound application: finite velocity of propagation

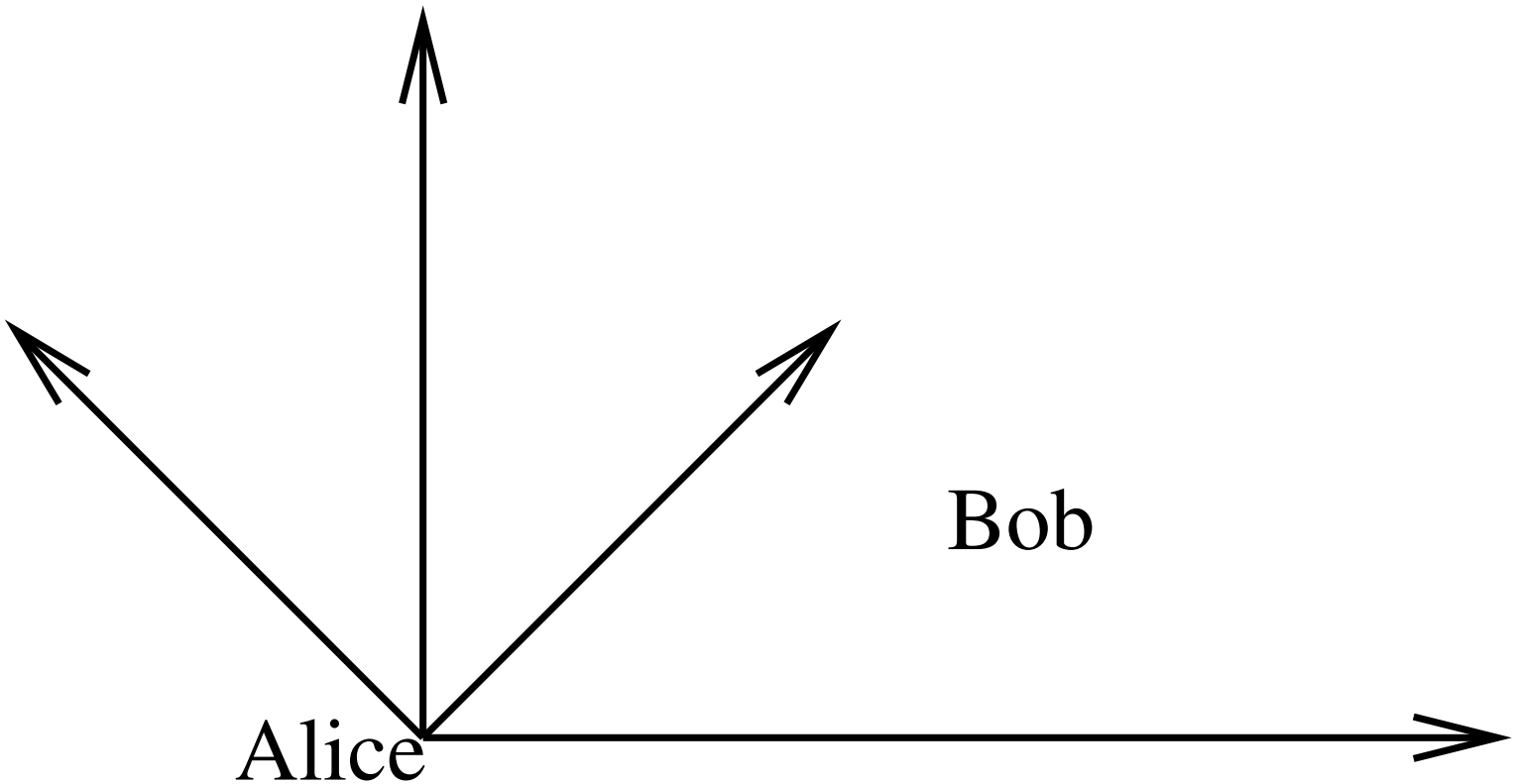
Alice applies unitary U_A at time 0.
Bob measures O_B at time t

$$\begin{aligned}\langle\Psi|U_A^\dagger O_B U_A|\Psi\rangle &= \langle\Psi|U_A^\dagger U_A O_B|\Psi\rangle + \langle\Psi|U_A^\dagger[O_B, U_A]|\Psi\rangle \\ &= \langle\Psi|O_B|\Psi\rangle + \mathcal{O}(\|[O_B, U_A]\|)\end{aligned}$$



No signalling outside the light-cone in relativistic theory.
Exponentially small leakage outside the light-cone even non-relativistically!

$$\begin{aligned}\langle\Psi|U_A^\dagger O_B U_A|\Psi\rangle &= \langle\Psi|U_A^\dagger U_A O_B|\Psi\rangle + \langle\Psi|U_A^\dagger[O_B, U_A]|\Psi\rangle \\ &= \langle\Psi|O_B|\Psi\rangle + \mathcal{O}(\|[O_B, U_A]\|)\end{aligned}$$



Lieb-Robinson bound application: exponential decay of correlations. Connecting dynamics and ground state

Theorem

Suppose there is a spectral gap ΔE. Then correlations decay exponentially in space:

$$\left|\langle AB\rangle - \langle A\rangle\langle B\rangle\right| \leq \exp(-l/\xi) \tag{1}$$

(Hastings, 2004)

$$\left|\langle AB\rangle - \langle A\rangle\langle B\rangle\right| \leq \exp(-l/\xi) \tag{2}$$

Proof:

- Without loss of generality, assume $\langle A\rangle = \langle B\rangle = 0$.
- Define B^+ to be the positive energy part of B. i.e., in a basis of eigenstates of $\mathcal{H}$, ψ_i with energy E_i, $B^+_{ij} = B_{ij}\theta(E_i - E_j)$. Then,
$$\langle AB\rangle = \langle AB^+\rangle = \langle [A, B^+]\rangle$$
- Define $\tilde{B}^+$ to be an approximation to B^+ as follows:
$$\tilde{B}^+ = \lim_{\epsilon\to 0^+} \frac{1}{2\pi}\int \mathrm{d}t \frac{1}{it+\epsilon} B(t)\exp[-(t\Delta E)^2/2q]$$
- Using the spectral gap
$$\langle [A, B^+]\rangle = \langle [A, \tilde{B}^+]\rangle + \mathcal{O}(\exp(-q/2))$$
- Using the Lieb-Robinson bounds, $\|[A, \tilde{B}^+]\|$ is small for q sufficiently small.
- Optimize in q to get desired bound

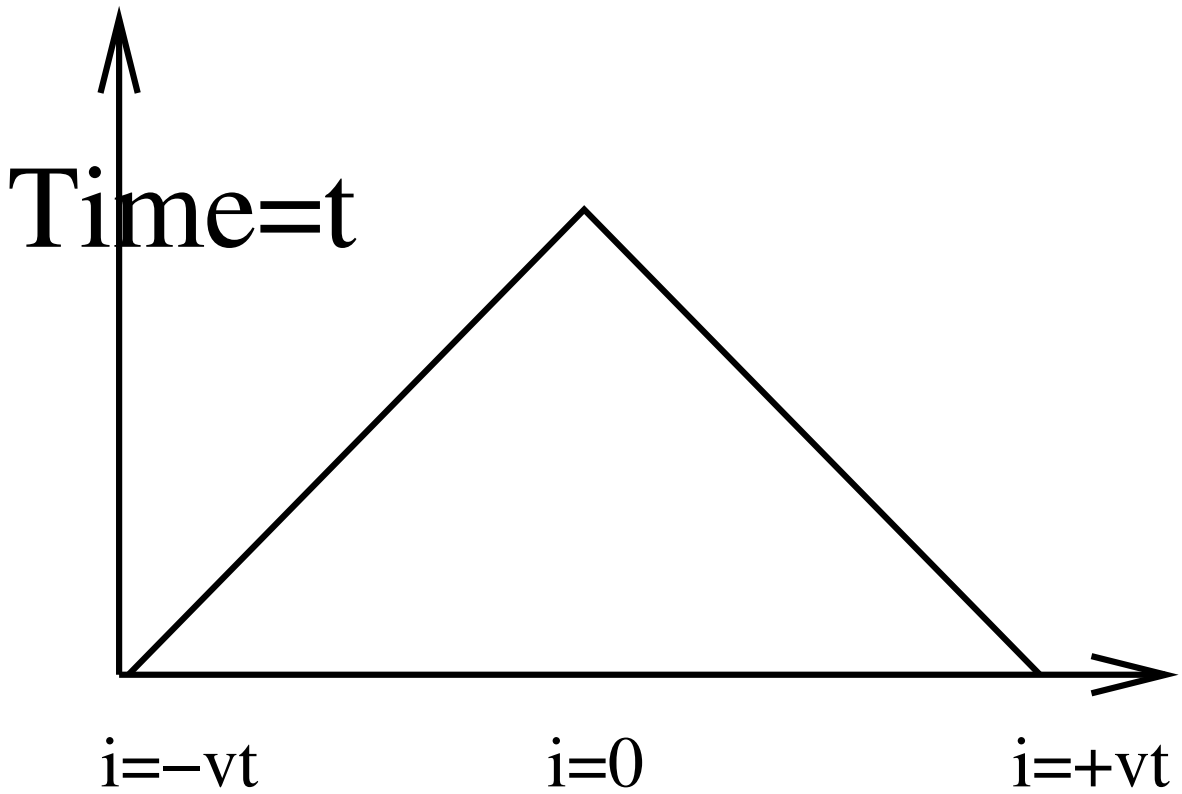
Computing Properties of Time Evolution

Light-cone for quantum simulation

Problem: given an initial product state $\psi(0)$, and a Hamiltonian $\mathcal{H}$, determine

$$\langle\psi(0)|S_0^z(t)|\psi(0)\rangle \equiv \langle\psi(0)|\exp(i\mathcal{H}t)S_0^z\exp(-i\mathcal{H}t)|\psi(0)\rangle.$$

Using the light-cone, we only need to simulate spins within distance v_{LR} of 0

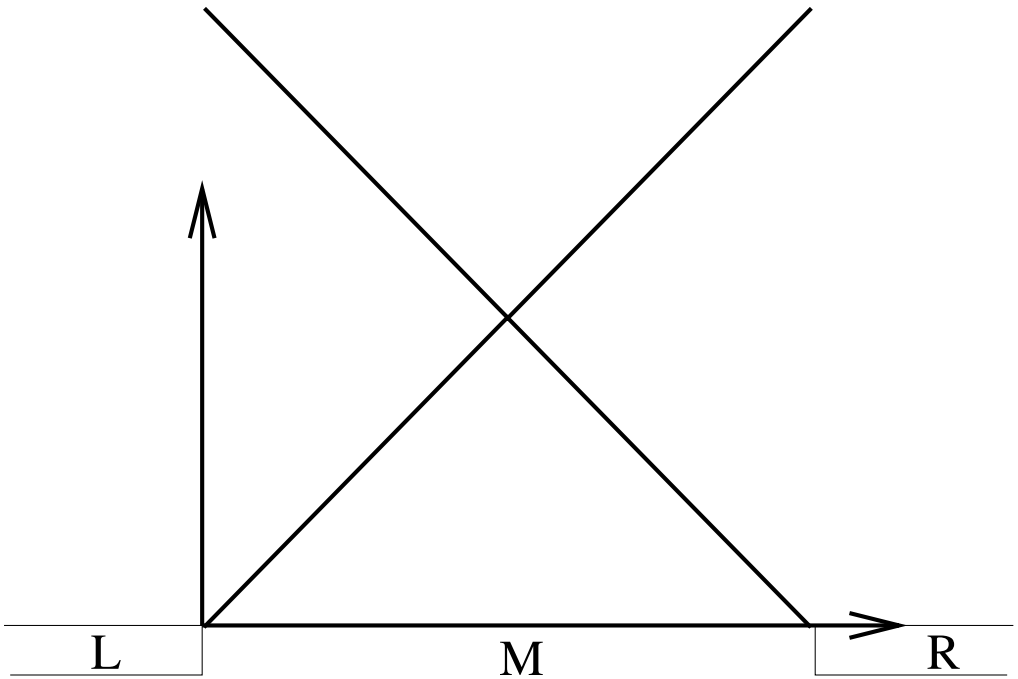


Reduce complexity from 2^N to $2^{2v_{LR}t}$

Light-cone for quantum simulation

Problem: given an initial arbitrary state $\psi(0)$, and a Hamiltonian $\mathcal{H}$, determine

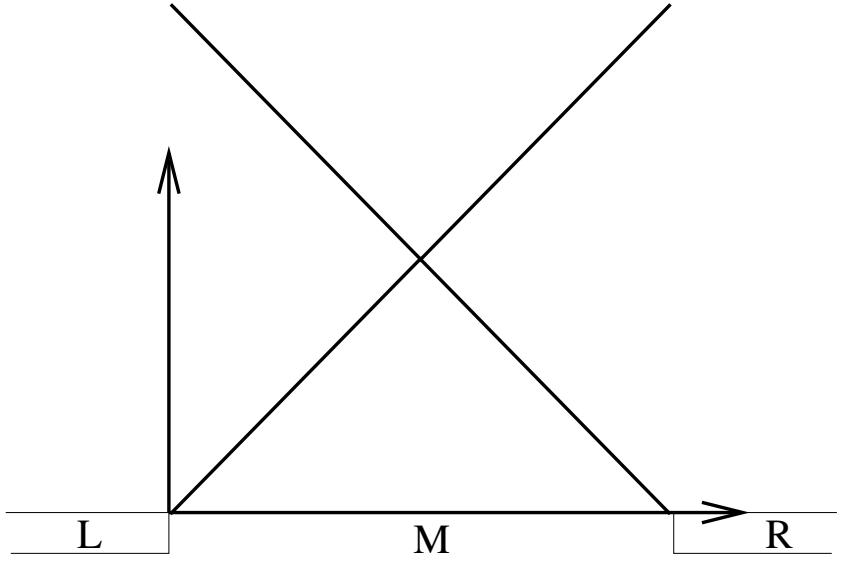
$$\langle\psi(0)|S_0^z(t)|\psi(0)\rangle \equiv \langle\psi(0)|\exp(i\mathcal{H}t)S_0^z\exp(-i\mathcal{H}t)|\psi(0)\rangle.$$



Write:

$$|\psi(0)\rangle = \sum_{\alpha\beta} |\psi_L^\alpha\rangle \otimes |\psi_M^{\alpha\beta}\rangle \otimes |\psi_R^\beta\rangle$$

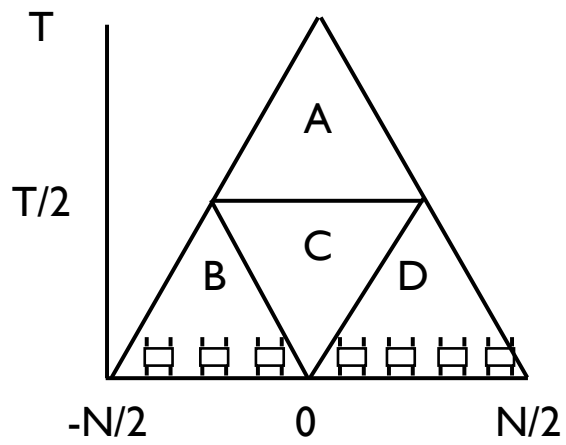
for orthonormal bases $\psi_L^\alpha, \psi_R^\beta$.



$$
\begin{aligned}
& \langle \psi(0)|S_0^z(t)|\psi(0)\rangle \\
= & \sum_{\alpha,\beta,\overline{\alpha},\overline{\beta}} \langle \psi_L^{\overline{\alpha}} \otimes \psi_M^{\overline{\alpha}\overline{\beta}} \otimes \psi_R^{\overline{\beta}}|S_0^z(t)|\psi_L^{\alpha} \otimes \psi_M^{\alpha\beta} \otimes \psi_R^{\beta}\rangle \\
\approx & \sum_{\alpha,\beta,\overline{\alpha},\overline{\beta}} \langle \psi_L^{\overline{\alpha}}|\psi_L^{\alpha}\rangle\langle \psi_R^{\overline{\beta}}|\psi_R^{\beta}\rangle\langle \psi_M^{\overline{\alpha}\overline{\beta}}|S_0^z(t)|\psi_M^{\alpha\beta}\rangle \\
= & \sum_{\alpha,\beta} \langle \psi_M^{\alpha\beta}|S_0^z(t)|\psi_M^{\alpha\beta}\rangle
\end{aligned}
$$

Statistically sample sum over α, β. Still reduce complexity from 2^N to $2^{2v_{LR}t}$.

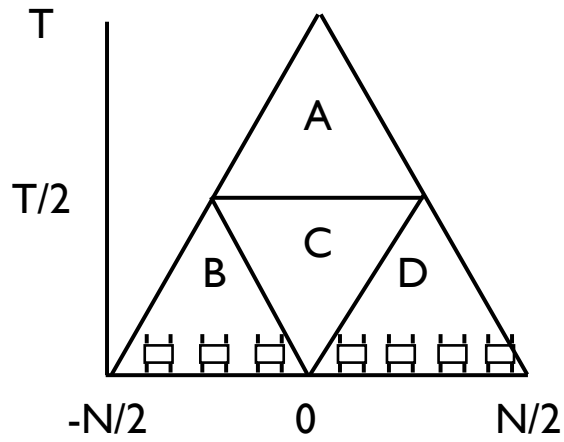
Light-cone for quantum simulation: can do even better!



- Evolve in region B and D (effort 2^N) for time $T/2$
- Statistically sample outside the light-cone to create pure state on sites $-N/4...N/4$
- Evolve regions A and C

Allows simulation of time T for effort $2^{v_{LR}t}$ rather than $2^{2v_{LR}t}$. Can be a large speedup!
Certifiable

Light-cone for quantum simulation



$$
\begin{aligned}
& \langle \Psi_L \otimes \Psi_R | U_B^\dagger U_D^\dagger U_C^\dagger U_A^\dagger S_0^z U_A U_C U_D U_B | \Psi_L \otimes \Psi_R \rangle \\
= \quad & \langle U_B \Psi_L \otimes U_D \Psi_R | U_C^\dagger U_A^\dagger S_0^z U_A U_C | U_B \Psi_L \otimes U_D \Psi_R \rangle \\
= \quad & \sum_{\alpha,\beta} \langle U_B \Psi_L \otimes U_D \Psi_R | \Pi_\alpha^L \Pi_\beta^R U_C^\dagger U_A^\dagger S_0^z U_A U_C \Pi_\alpha^L \Pi_\beta^R | U_B \Psi_L \otimes U_D \Psi_R \rangle
\end{aligned}
$$

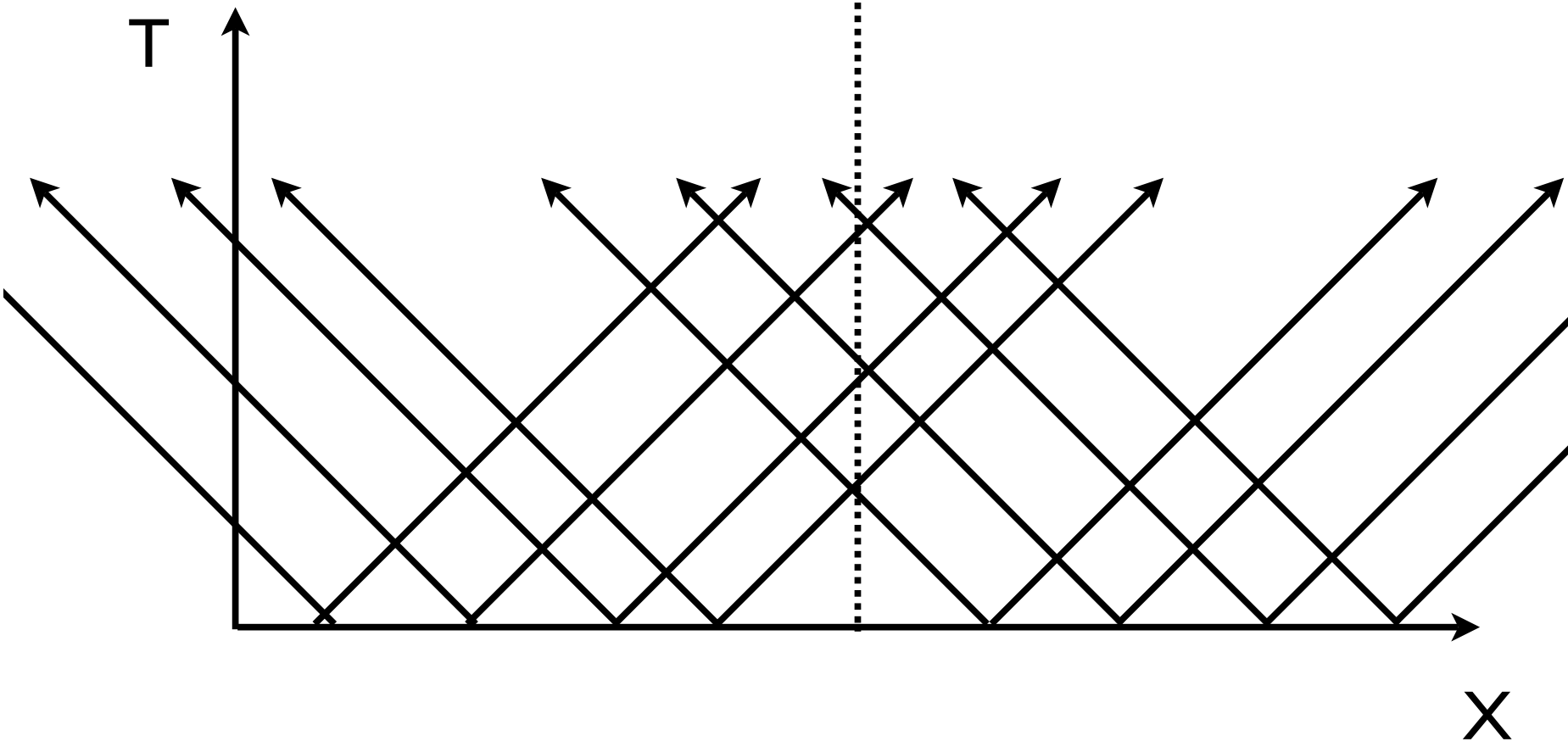
Computing Properties of Time Evolution

Example problem

XXZ Hamiltonian

$$\mathcal{H} = \sum_i S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z$$

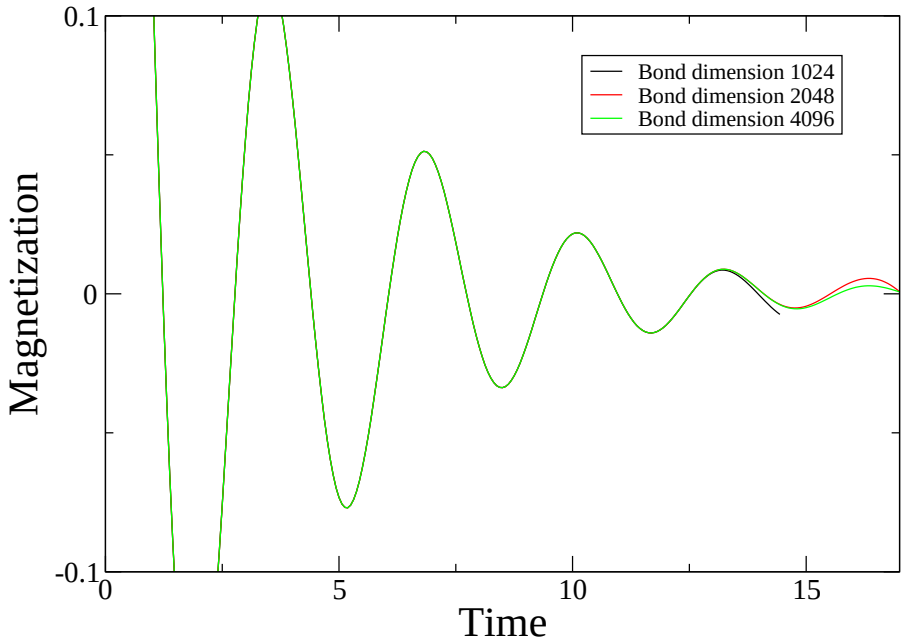
Δ is parameter. Start at $\Delta = \infty$. Alternating $\uparrow\downarrow\uparrow\downarrow$ ...
Suddenly change to finite Δ. Compute $S_0^z(t)$



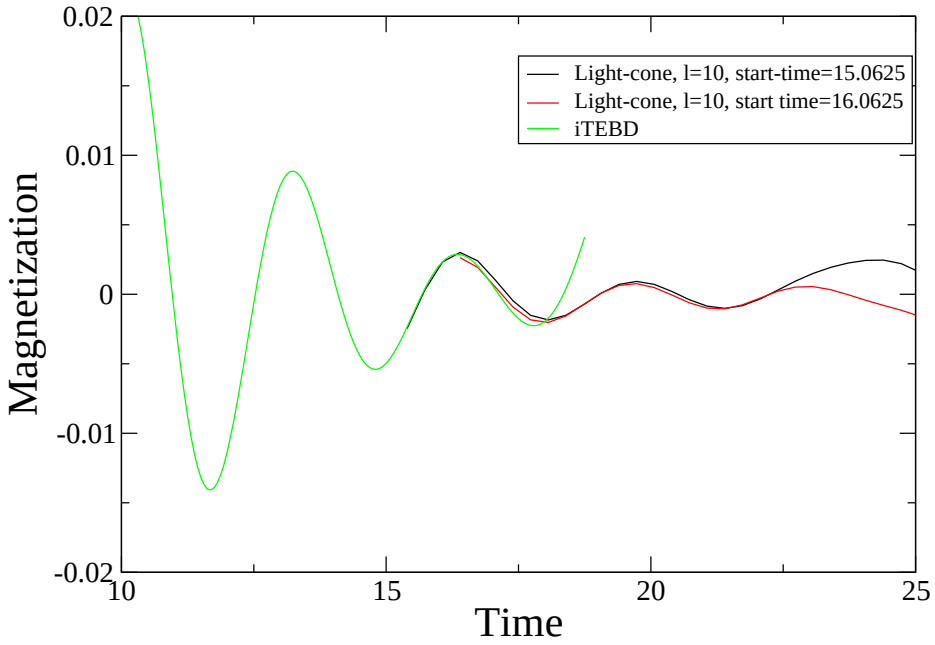
Excitations carry information across cut. Entropy grows linearly with time. This is wost case (Bravyi, Hastings, Verstraete, 2006 and Eisert and Osborne, 2006).

Physical interest in a global quench

Does the system thermalize? Does reduced density matrix approach a thermal density matrix?
What if the system is integrable or there are other conserved quantities?
How does the system thermalize? Studies of XXZ spin chain show interesting new dynamics before thermalization.



XXZ Chain after Quench



Measured magnetization using iTEBD and iTEBD followed by light-cone.

Computing Properties of Time Evolution

Adiabatic Evolution of Gapped Systems

$$\mathcal{H}_s, \quad s = 0 \to 1$$

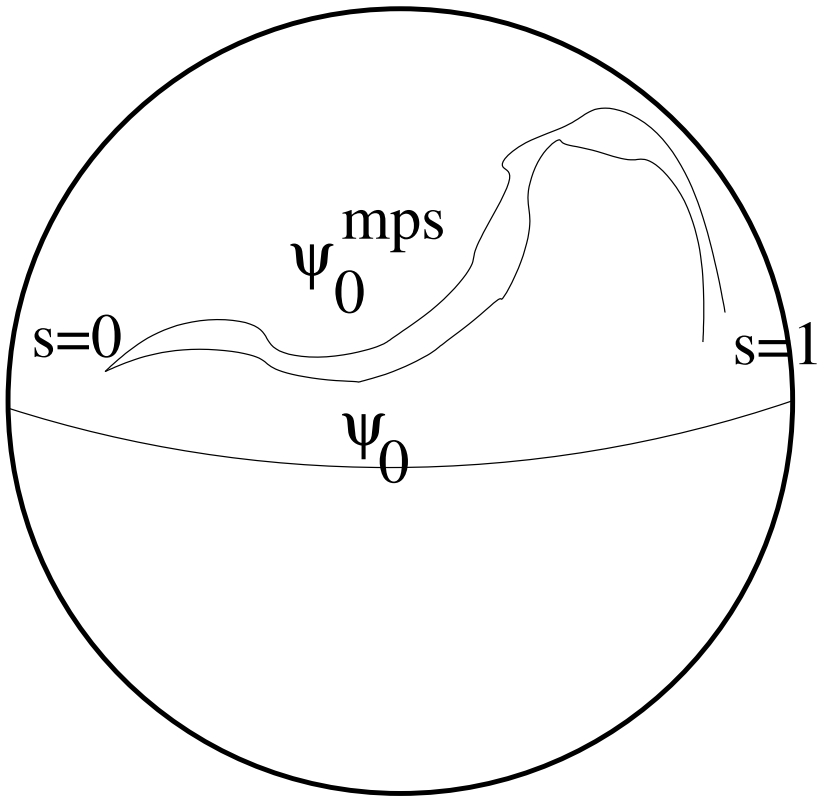
Seems hard. By definition, long time.
However (quasi-adiabatic evolution), one can show that

$$\partial_s \Psi_0(s) = \mathcal{D}_s \Psi_0(s)$$

for a new local operator $\mathcal{D}_s$
Evolve as before.
Can evolve logarithmically long paths with constant gap.

Adiabatic Evolution of Gapped Systems

Can evolve system, and truncate to matrix product state
Can approximate $\psi_0(s)$ by $\psi_0^{mps}(s)$ and follow approximation along path.



Can evolve polynomially long paths with constant gap.
Question: what can be done with constant gap in 2D? Constant gap gives error correction for adiabatic QC.

Computing Properties of Time Evolution

Conclusion:

- General time evolution is hard.
- Our current general algorithms take CPU time exponential in time simulated. Probably cannot be improved.
- Many physical cases can be done faster.
- Interesting physical problems in thermalization