Title: Classical simulation of short-time quantum dynamics

Speakers: Alvaro Martin Alhambra

Series: Perimeter Institute Quantum Discussions

Date: March 01, 2023 - 11:00 AM

URL: https://pirsa.org/23030000

Abstract: Recent progress in the development of quantum technologies has enabled the direct investigation of dynamics of increasingly complex quantum many-body systems. This motivates the study of the complexity of classical algorithms for this problem in order to benchmark quantum simulators and to delineate the regime of quantum advantage. Here we present classical algorithms for approximating the dynamics of local observables and nonlocal quantities such as the Loschmidt echo, where the evolution is governed by a local Hamiltonian. For short times, their computational cost scales polynomially with the system size and the inverse of the approximation error. In the case of local observables, the proposed algorithm has a better dependence on the approximation error than algorithms based on the Lieb-Robinson bound. Our results use cluster expansion techniques adapted to the dynamical setting, for which we give a novel proof of their convergence. This has important physical consequences besides our efficient algorithms. In particular, we establish a novel quantum speed limit, a bound on dynamical phase transitions, and a concentration bound for product states evolved for short times.

Joint work with Dominik S. Wild (arXiv:2210.11490)

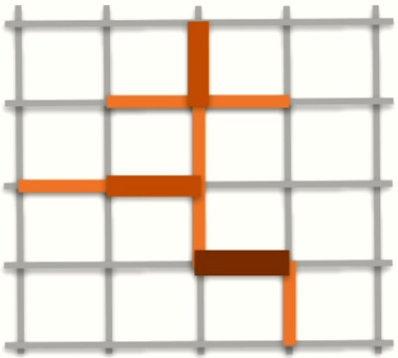
Zoom link: https://pitp.zoom.us/j/97166113711?pwd=UEg4NnJlQkkxQXFnN2xXYTBxS001Zz09

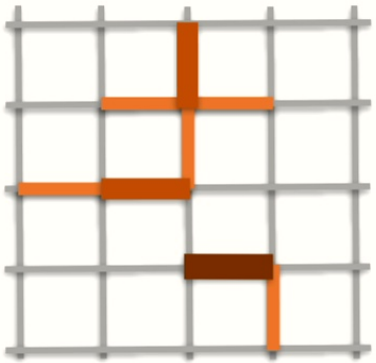
Classical simulation of short time many-body dynamics

Alvaro M. Alhambra (Instituto de Fisica Teorica UAM/CSIC - Madrid)

w/ Dominik Wild (MPQ)

(arXiv:2210:11490)

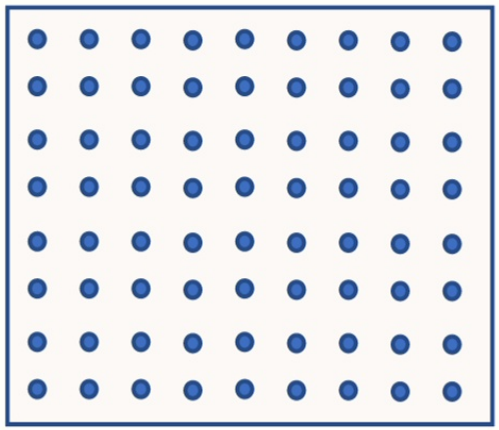




Quantum many body systems (on the lattice)

$$H = \sum_i h_i$$

Q: When and how can we compute physically relevant phenomena/features/quantities…for these models?



"The quantum many-body problem"

IMPORTANT:

- Quantum information
- Q Computation and complexity theory
- Condensed matter
- High energy physics
- Quantum chemistry
- ….

…but HARD:

- Hilbert space dimension exponential!
- Direct computational approaches are doomed to fail.
- Solution: understand the physics, and find smart workarounds.

Which states do we care about?

Ground states

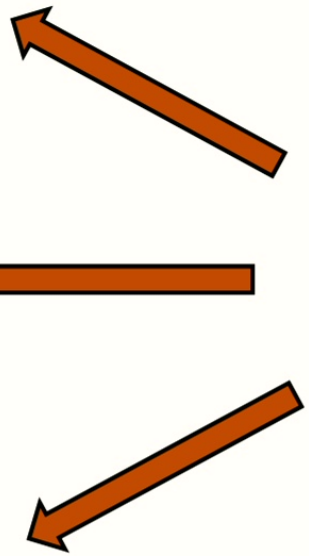
$$H = \sum_i h_i \qquad |0\rangle\langle 0|$$

Thermal states

$$\rho_\beta = \frac{e^{-\beta H}}{Z}$$

Dynamics

(this talk) $\qquad e^{-itH}|\Psi\rangle$



How can we study them?

- Quantum simulation?
- Efficient classical ways of approximating them, that allow us to extract physical information.
- Ideally, have a physical understanding of why they work.

Quantum dynamics: simple or not?

A HUGE matrix you cannot diagonalize

$$U \in (\mathbb{C}^d)^{\otimes N}$$

The exponential of a "simple" local operator

$$U = e^{-itH}$$

$$H = \sum_i h_i$$

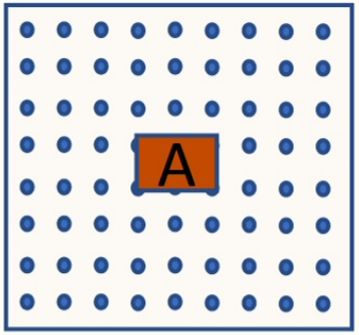
Summary of results

Approx. Heisenberg evolution:

$$|\langle\Phi|A(t)|\Phi\rangle - f(t)| \leq \epsilon$$

Runtime:

$$\left(\exp(\mathcal{O}(t))\frac{1}{\epsilon}\right)^{\exp(\mathcal{O}(t))}$$



Approx. Loschimidt echo:

$$|\log\langle\Phi|e^{-itH}|\Phi\rangle - g(t)| \leq \epsilon$$

Runtime:

$$\mathrm{poly}(N, \epsilon^{-1})$$

$$t \leq t^* = \mathcal{O}(1)$$

Taylor expansion and computation

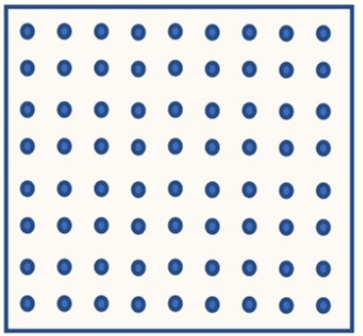
$$|F(t) - F_m(t)| \leq e^{-\mathcal{O}(m)}$$

$$F(t) = \sum_{m=0}^{\infty} \frac{K_m}{m!} t^m$$

$$F(t)_M = \sum_{m=0}^{M} \frac{K_m}{m!} t^m$$

Ingredients:

- Prove convergence of Taylor series for high enough degree (analyticity).
- Estimate cost of calculating Taylor coefficients.
- Taylor series gives approximation.



Cluster expansion: main idea

- Taylor series expansions for quantities defined on lattices.

$$\log Z \equiv \log \mathrm{Tr}[e^{-\beta H}] = \sum_{m}^{\infty} \frac{K_m^{(\beta)}}{m!} \beta^m \qquad e^{-\beta H} = \mathbb{I} - \beta H + \frac{\beta^2}{2} H^2 + ...$$

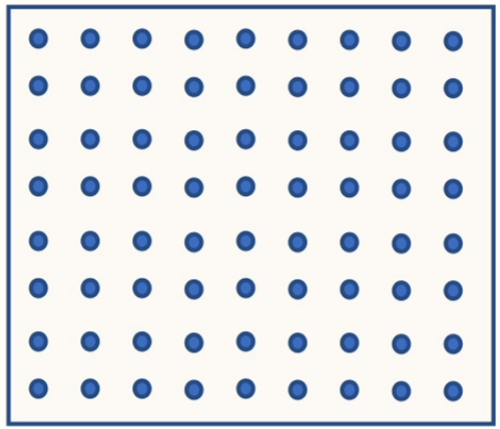
- Efficient way of writing the Taylor moments in terms of *clusters*

$$H = \sum_X h_X \qquad K_m^{(\beta)} = \sum_{\mathbf{W}} \prod (...) \mathrm{Tr}[h_1 .... h_n]$$

$$||h_X|| \leq 1$$

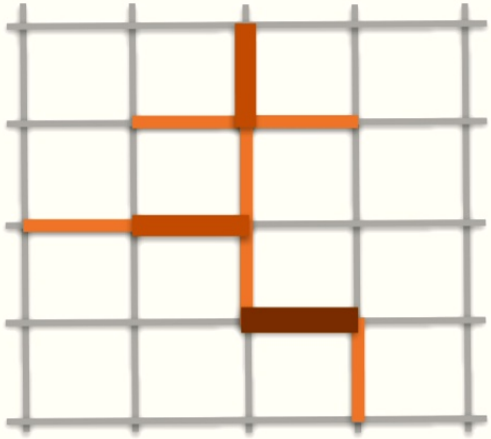
- *CLUSTER*: A multiset of Hamiltonian terms

$$\mathbf{W} = \{h_1, h_1, h_2, ..., h_l, h_l\}$$



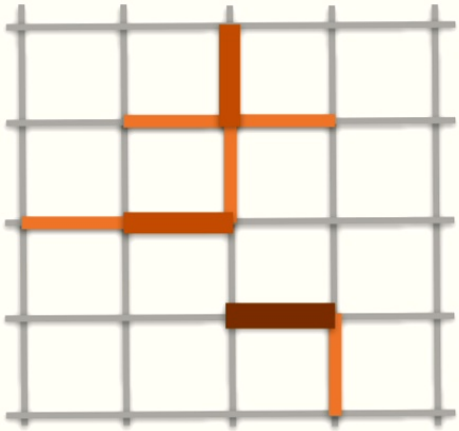
Types of clusters

- Connected



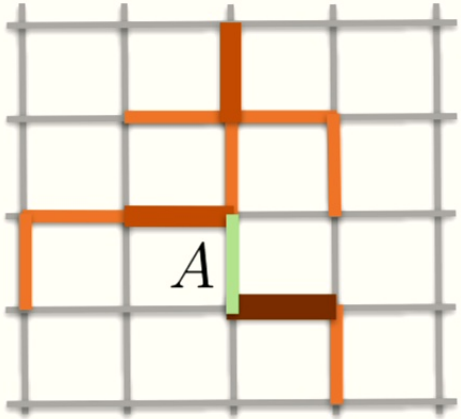
$\mathbf{W} \in \mathcal{G}_m$

- Disconnected



$\mathbf{W} \in \mathcal{C}_m \setminus \mathcal{G}_m$

- Connected to A



$\mathbf{W} \in \mathcal{G}_m^A$

$$\mathbf{W} = \{h_1, h_1, h_2, ..., h_l, h_l\}$$

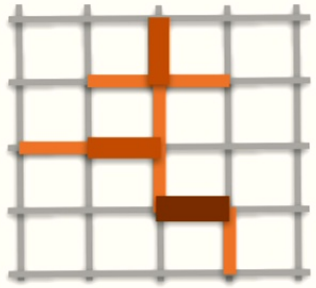
Cluster expansion:

- KEY: Only <u>connected</u> contribute to the log-partition function:

$$\log Z \equiv \log \mathrm{Tr}[e^{-\beta H}] = \sum_m^{\infty} \frac{K_m^{(\beta)}}{m!} \beta^m \qquad K_m^{(\beta)} = \sum_{\mathbf{W} \in \mathcal{G}_m} \prod (...) \mathrm{Tr}[h_1 .... h_n]$$

- How to calculate the contributions? *Ursell function*: $\Phi(\mathbf{W})$

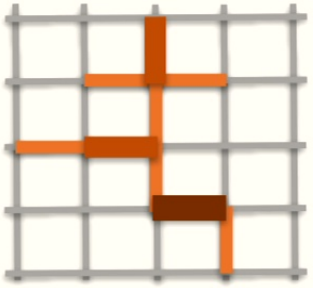
$$\Phi(\{h_1, h_2\}) = \mathrm{Tr}[h_1 h_2] - \mathrm{Tr}[h_1]\mathrm{Tr}[h_2]$$



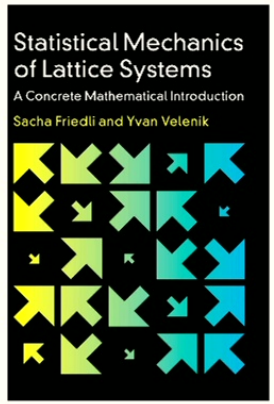
- We need to know:
  - -<u>How to count</u> connected clusters are there
  - -How do they contribute (Ursell function)

Cluster expansion: convergence

- Rough intuition: (Kuwahara & Saito 1906.10872* , Haah et al 2108.04842*)



  - There are exponentially many connected clusters: $|\mathcal{G}_m| \leq N c_1^m$
  - Weight of each cluster term to the sum is : $(\ldots) \leq m! c_2^m$
  - Total Taylor term: $K_m^{(\beta)} \leq m!(1/\beta^*)^m \qquad \beta < \beta^*$
  - Taylor series converges exponentially $|\log Z - \sum_{m=0}^{M} \frac{\beta^m}{m!} K_m^{(\beta)}| \leq \frac{(\beta/\beta^*)^M}{1-\frac{\beta}{\beta^*}}$



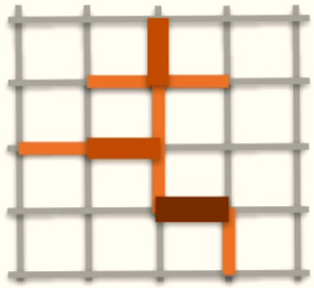
- General framework (polymer models) – (Kotecky&Preiss ´86 + others)

- Related to phase diagram: expansion converges away from phase transitions.

Cluster expansion: computation

- Ursell function can be computed efficiently: (Bjorklund et al 0711.2585)

$$\Phi(\mathbf{W}) \qquad t \sim e^{\mathcal{O}(m)}$$



- Cluster enumeration (Helmuth et al 1806.11548):

  (remember $|\mathcal{G}_m| \leq N c_1^m$)

$$t \sim N e^{\mathcal{O}(m)}$$

- Cluster contributions: (operator on region of size m)

$$t \sim e^{\mathcal{O}(m)} \qquad \beta < \beta^*$$

- Computing Taylor series:

$$|\log Z - \sum_{m=0}^{M} \frac{\beta^m}{m!} K_m| \leq \epsilon \qquad M = \mathcal{O}(\log(N/\epsilon))$$

$$\boxed{t = \mathrm{poly}(N/\epsilon)}$$

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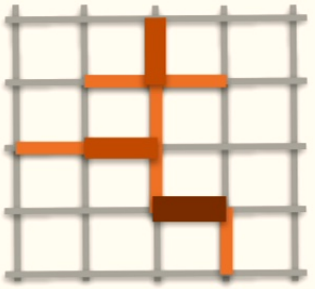

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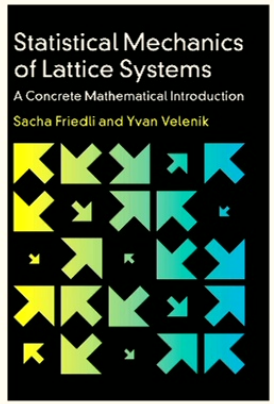

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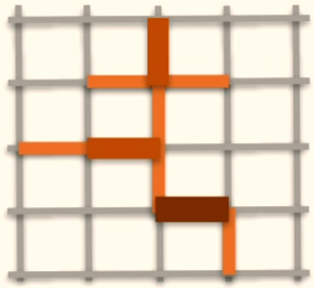

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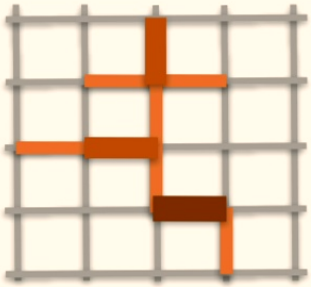
Cluster expansion in QI (so far)

Different ideas proven this way:

- Approximations of partition functions (Harrow et al. 1910.09071, Mann & Helmuth 2004.11568)
- Concentration bounds for Gibbs states: (Kuwahara & Saito 1906.10872)*
- Optimal learning of Gibbs states (Haah et al 2108.04842)*



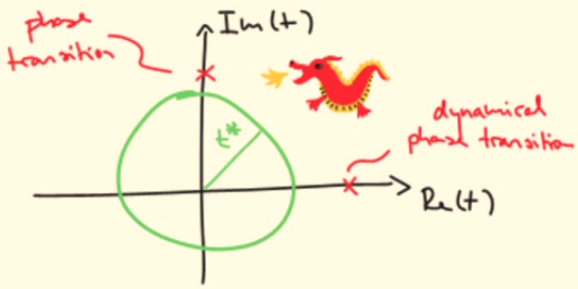
$$\frac{e^{-\beta H}}{Z} \qquad \beta < \beta^*$$

- Connected to Barvinok's interpolation method and Lovasz's local lemma (e.g. estimation of expectation values of shallow circuits Bravyi et al. 1909.11485)
- + likely many others….

No large improvement possible

- Result: analyticity and efficient algorithm for

$$\log\langle\Phi|e^{-itH}|\Phi\rangle \qquad t \leq t^*$$



- For longer times: log becomes non-analytic.

-State may become orthogonal to the initial one

-Dynamical phase transitions (Heyl 1709.07461)

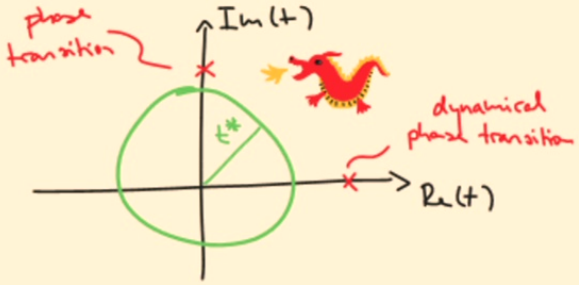
$$t = \mathcal{O}(1)$$

- Computation: computing complex Ising partition function at O(1) times (even approximately) is **#P hard**. (Galanis et al 2005.01076)

Some physical consequences:

- Result: analyticity and efficient algorithm for

$$\log\langle\Phi|e^{-itH}|\Phi\rangle \qquad t \leq t^*$$



- So it takes at least t^* to become orthogonal to initial state
- Strengthening over previous Quantum Speed Limits (Mandeltam-Tamm, Margolus-Levitin)

$$t_{QSL} \geq t^* = \mathcal{O}(1) \qquad \text{Vs.} \qquad t_{QSL} \geq \mathcal{O}(1/\sqrt{N})$$

- Dynamical phase transitions (Heyl 1709.07461): t^* is a lower bound to how fast they occur. (in analogy with thermal phase transitions)
- **BONUS**: concentration bounds (Chernoff) for short-time evolved states.

Heisenberg time evolution

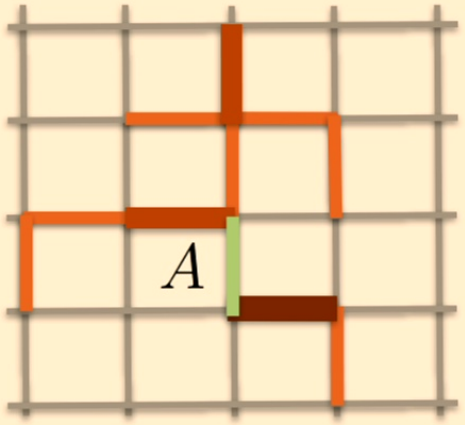
- Classical simulation of

$$\langle\Phi|e^{-itH}Ae^{itH}|\Phi\rangle = \sum_{m=0}^{\infty}\frac{(it)^m}{m!}\langle\Phi|[H,[H,...[H,A]]|\Phi\rangle$$

$$= \sum_{m=0}^{\infty}\frac{(it)^m}{m!}\sum_{\mathcal{G}_m^A}\langle\Phi|[h_{X_1},[h_{X_2},...[h_{X_m},A]]|\Phi\rangle$$

- Taylor expansion in terms of clusters $\mathbf{W} \in \mathcal{G}_m^A$

- Difference: Function analytic for all times



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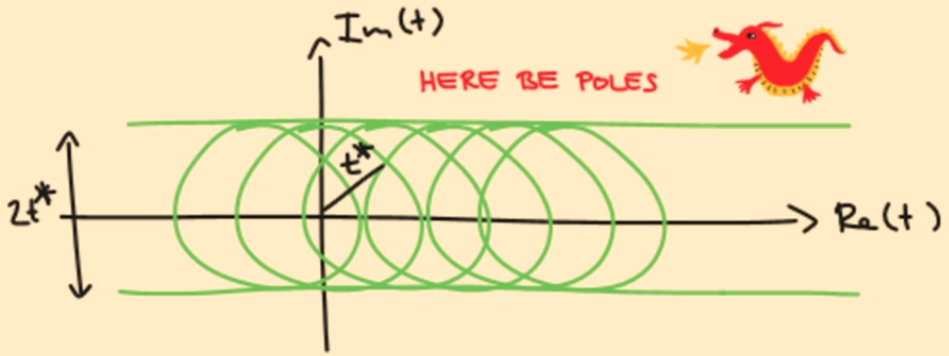
$$= \sum_{m=0}^{\infty}\frac{(it)^m}{m!}\sum_{\mathcal{G}_m^A}\langle\Phi|[h_{X_1},[h_{X_2},...[h_{X_m},A]]|\Phi\rangle$$

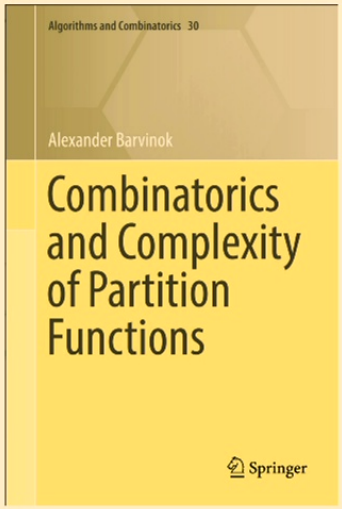
- Count connected clusters: $|\mathcal{G}_m^A| \leq c_1^m$
- Weight of each cluster: $m!2^m||A||$
- Similar convergence of Taylor series (and algorithm) for short times $t \leq t^*$

$$|\langle\Phi|A(t)|\Phi\rangle - \sum_{m=0}^{M}\frac{t^m}{m!}K_m| \leq \frac{(t/t^*)^M}{1-(t/t^*)}||A||$$

Arbitrary times: analytic continuation

- Function is analytic on a strip, not just a disk. $|\langle e^{-itH} A e^{itH} \rangle| \leq ||A||$
- Analytic continuation (Barvinok '16, Harrow et al. 1910.09071).
- We can use Taylor series at the origin to calculate any later point, with overhead.
- Idea: use series of a function that maps disk to rectangle.





Arbitrary times: result

- Series converges for all times, but degree grows fast.

$$|\langle\Phi|e^{-iHt}Ae^{iHt}|\Phi\rangle - \sum_{m=0}^{M}\frac{t^m}{m!}K_m| \leq \left(1-e^{-\pi t/t^*}\right)^M\left(e^{\pi t/t^*}-1\right)||A||$$

- RESULT: There is an algorithm outputting $f(t)$ such that:

$$|\langle\Phi|e^{-itH}Ae^{itH}|\Phi\rangle - f(t)| \leq \epsilon$$

With runtime:

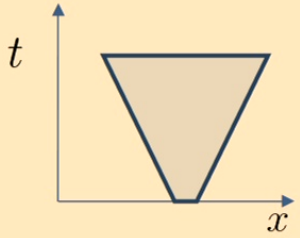
$$\left(\exp(\mathcal{O}(t))\frac{1}{\epsilon}\right)^{\exp(\mathcal{O}(t))}$$

- Remark: if $t = \mathcal{O}(1)$, runtime is $\mathrm{poly}(\epsilon^{-1})$

Alternative: Lieb-Robinson bounds

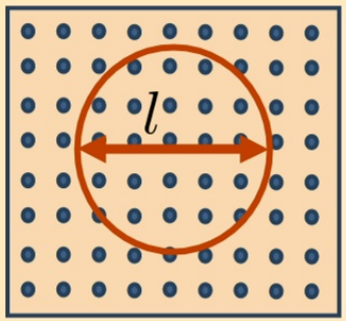
- Simple strategy: simulate Lieb-Robinson light-cone exactly.

$$\epsilon \sim e^{\mathcal{O}(vt-l)} \qquad l \sim vt + \mathcal{O}(\log(1/\epsilon))$$



- <u>COST</u>: $e^{\mathcal{O}(l^D)} \sim e^{\mathcal{O}((vt+\log(1/\epsilon))^D)}$

- Super-poly in higher dimensions for ϵ^{-1}



- <u>OUR RESULT</u>: With clusters: polynomial in ϵ^{-1}, for all dimensions! (even expander graphs).

Alternative: Lieb-Robinson bounds

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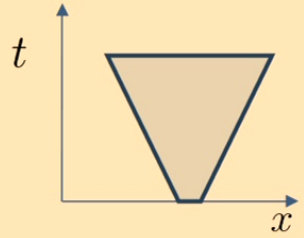

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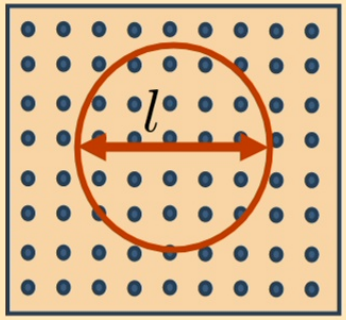

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Computational complexity of dynamics

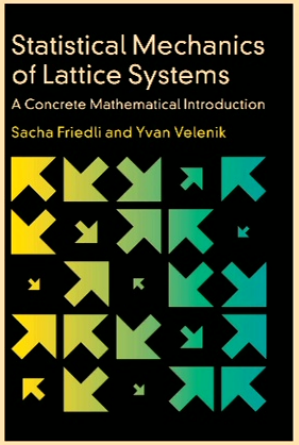
Evolution time	$\leq t^*$	$\mathcal{O}(1)$	$\mathcal{O}(\mathrm{polylog}(N))$	$\mathcal{O}(\mathrm{poly}(N))$
$\langle A(t)\rangle$	**P**	**P**	**??**	**BQP-complete**
$\log\langle e^{-itH}\rangle$	**P**	**#P-hard**	**#P-hard**	**#P-hard**
$\langle e^{-itH}\rangle$	**P**	**??**	**??**	**BQP-complete**

- Complexity of simulating to small additive error $\epsilon^{-1} = 1/\mathrm{poly(N)}$

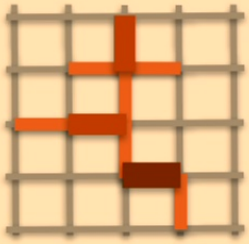
- #P hard -> Galanis et al 2005.01076
- BQP hardness: standard arguments + de las Cuevas (1104.2517)

Conclusions

- Cluster expansion: versatile and well-studied tool for partition functions + related problems.
  - -Shows convergence of Taylor approximation and yields efficient algorithms.
  - -Works for many different interaction graphs.



- Here: it also works for problems of **quantum dynamics**.
- Short time evolution of Loschmidt echo (below threshold) and Heisenberg time evolution (arbitrary times).



- Implications for: complexity of dynamics, dynamical phase transition, quantum speed limits,…

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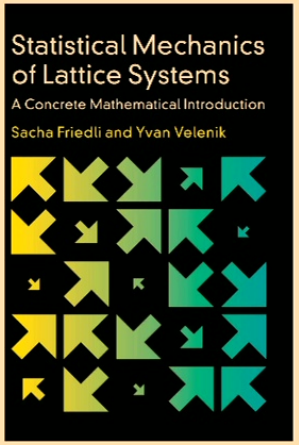
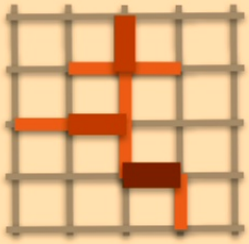
- Cluster expansion: versatile and well-studied tool for partition functions + related problems.
  - -Shows convergence of Taylor approximation and yields efficient algorithms.
  - -Works for many different interaction graphs.



- Here: it also works for problems of **quantum dynamics**.
- Short time evolution of Loschmidt echo (below threshold) and Heisenberg time evolution (arbitrary times).



- Implications for: complexity of dynamics, dynamical phase transition, quantum speed limits,…

arXiv:2210.11490

Thanks!!