Classical simulation of short time many-body dynamics

Alvaro M. Alhambra

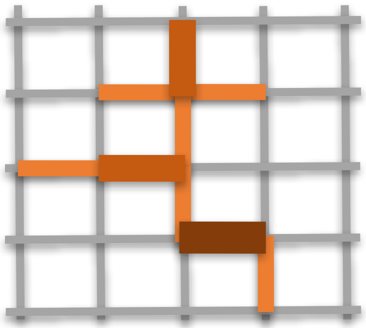
(Instituto de Fisica Teorica CSIC -Madrid)

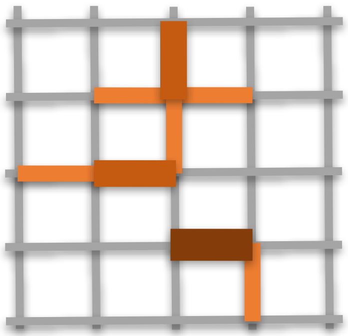
w/ Dominik Wild

(Max Planck Institute for Quantum Optics)

(arXiv:2210:11490)

PRX Quantum 4, 020340

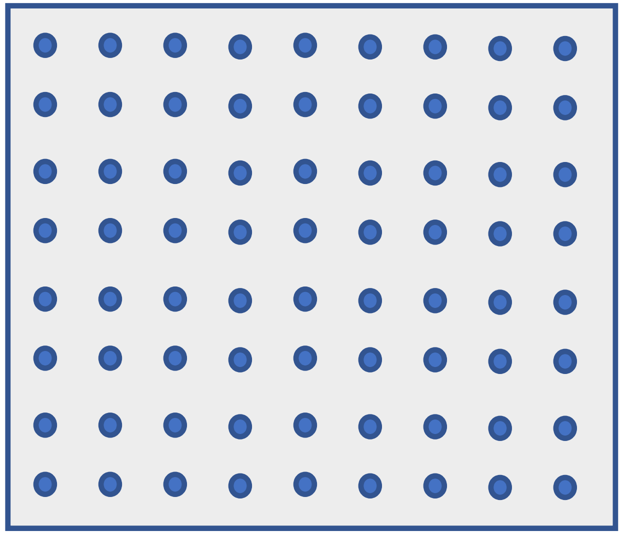




Quantum many body systems (on the lattice)

$$H = \sum_i h_i$$

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



"The quantum many-body problem"

IMPORTANT:

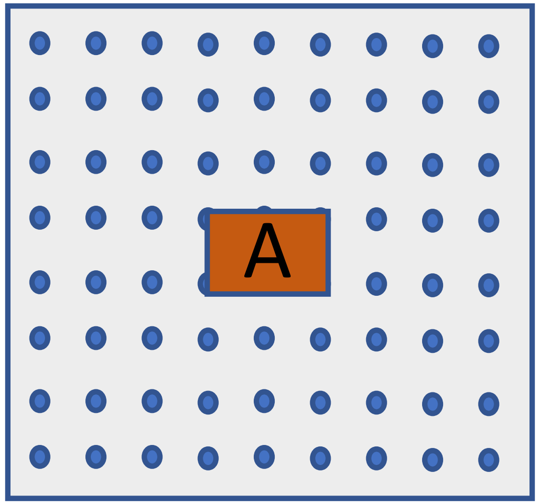
- Quantum information
- Q Computation and complexity theory
- Condensed matter
- High energy physics
- Quantum chemistry
- ….

…but HARD:

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

Simulating many-body dynamics

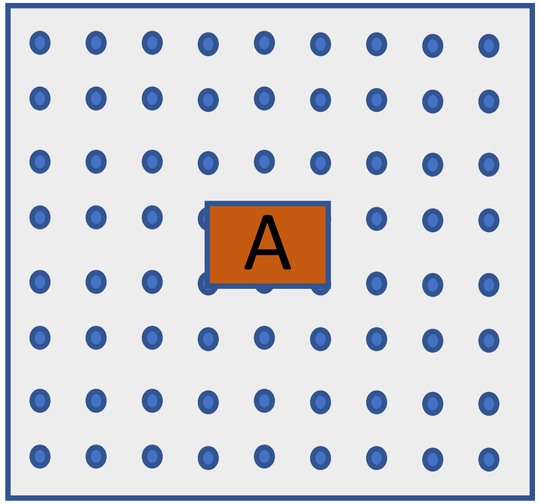
$$U = e^{-itH} \qquad H = \sum_i h_i$$



$$A(t) = e^{-iHt} A e^{iHt}$$

Simulating many-body dynamics

- Time evolution operator: $$U = e^{-itH} \qquad H = \sum_i h_i$$
- Observable: $$A(t) = e^{-iHt} A e^{iHt}$$



- Initial state: $$|\Phi\rangle = \bigotimes_i |\phi_i\rangle$$
- Goal:

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

Computational problem

- Local Hamiltonian on N particles + few-body observable

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

<u>Classically easy (P)</u>

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

$\cdots$

<u>Classically hard + quantum easy (BQP)</u>

$t = \mathrm{poly}(N)$

$\cdots$

time →

Computational problem

- Local Hamiltonian on N particles + few-body observable

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

Classically easy (P)

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

$\cdots$

Classically hard + quantum easy (BQP)

$$t = \mathrm{poly}(N)$$

$\cdots$

time

How do we study this problem classically?

- Exact diagonalization (small systems)
- Tensor networks (short times, one dimension)
- Many other methods….(model-specific?)
- ……..
- This talk: cluster expansion ← short times, but very accurate and analytically tractable

$$A(t) = e^{-iHt} A e^{iHt}$$

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

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

$$H = \sum_i h_i$$

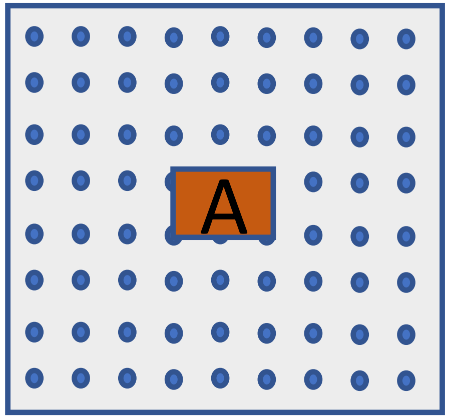
Summary of results

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

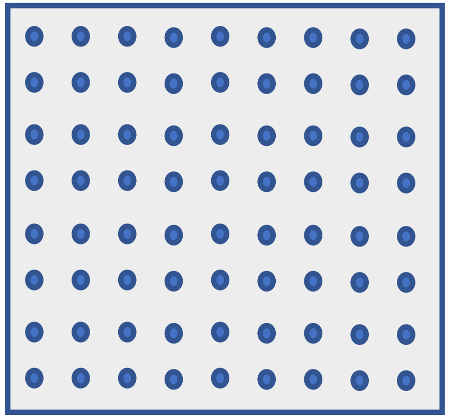
$$|F(t) - F_m(t)| \leq e^{-\mathcal{O}(m)}$$

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

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

<u>Ingredients:</u>

- 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.

$$\log Z \equiv \log \mathrm{Tr}[e^{-\beta H}] = \sum_m^{\infty} \frac{K_m^{(\beta)}}{m!}\beta^m$$

$$e^{-\beta H} = \mathbb{I} - \beta H + \frac{\beta^2}{2}H^2 + \ldots$$

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

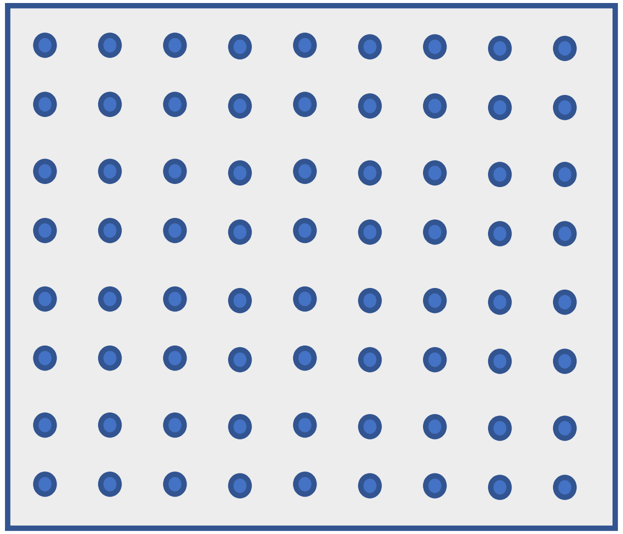
$$H = \sum_X h_X$$

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

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

- *CLUSTER*: A multiset of Hamiltonian terms

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



Cluster expansion: main idea

- Taylor series expansions for quantities defined on lattices.

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

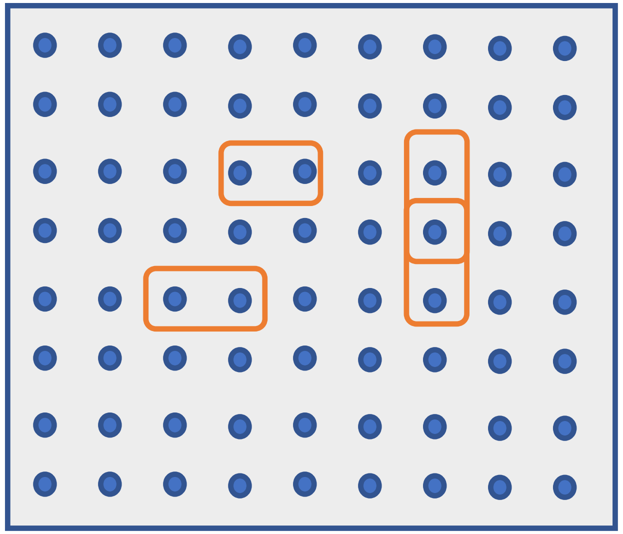
$$e^{-\beta H} = \mathbb{I} - \beta H + \frac{\beta^2}{2} H^2 + \dots$$

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

$$H = \sum_X h_X$$

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

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

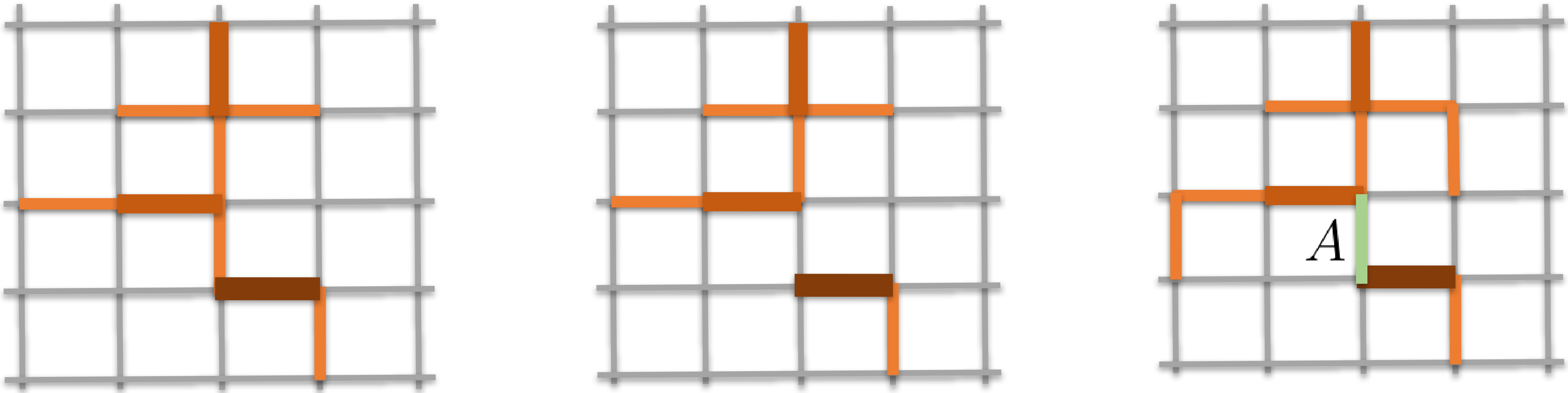


- *CLUSTER*: A multiset of Hamiltonian terms

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

Types of clusters

- Connected
- Disconnected
- Connected to A



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

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

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

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

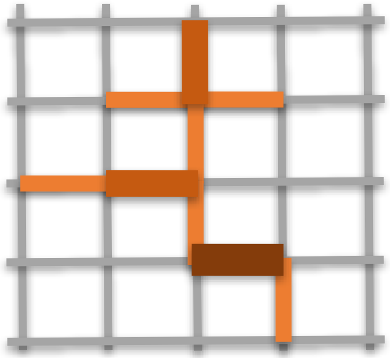
Cluster expansion:

- KEY: Only connected 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*: $\Phi(\mathbf{W})$

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



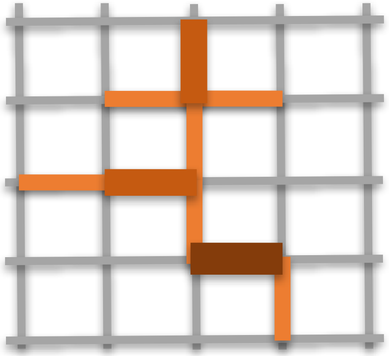
- We need to know:

  -How to count connected clusters are there

  -How do they contribute (Ursell function)

Cluster expansion: convergence

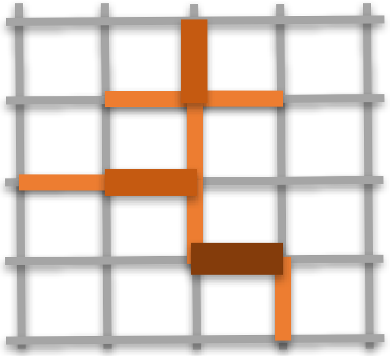
- Rough intuition: (Kuwahara & Saito 1906.10872* , Haah et al 2108.04842*)



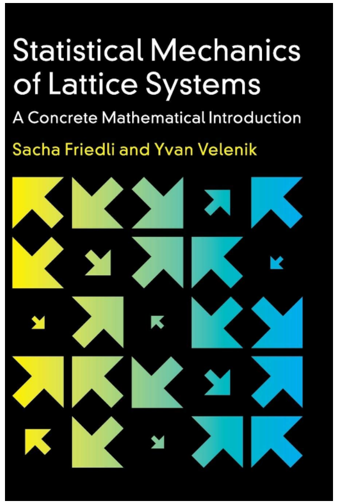
  - There are exponentially many connected clusters: $|\mathcal{G}_m| \leq N c_1^m$
  - Weight of each cluster term to the sum is : $(\ldots) \leq m! c_2^m$
  - Total Taylor term: $|K_m^{(\beta)}| \leq m! N (1/\beta^*)^m \quad \beta < \beta^*$
  - Series converges exponentially $| \log Z - \sum_{m=0}^{M}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

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: $|K_m^{(\beta)}| \leq m! N (1/\beta^*)^m \quad \beta < \beta^*$
  - Series converges exponentially $| \log Z - \sum_{m=0}^{M} \frac{\beta}{m!} K_m^{(\beta)} | \leq N \frac{(\beta/\beta^*)^M}{1-(\beta/\beta^*)}$



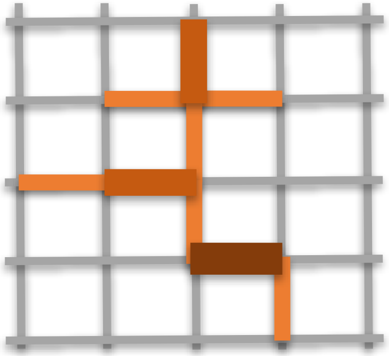
- General framework (polymer models) – (Kotecky&Preiss ´86 + others)

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

Cluster expansion: computation

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

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



- Cluster enumeration (Helmuth et al 1806.11548):

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

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

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

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

- Computing Taylor series:

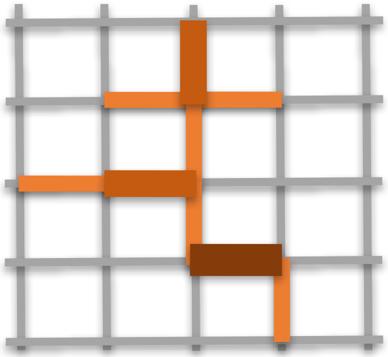
$$|\log Z - \sum_{m=0}^{M} \frac{\beta^m}{m!} K_m| \leq \epsilon \qquad M = \mathcal{O}(\log(N/\epsilon))$$

$$\boxed{\text{runtime} = \text{poly}(N/\epsilon)}$$

Cluster expansion: dynamics

- Loschmidt echo: $\log\langle\Phi|e^{-itH}|\Phi\rangle$ vs. $\log[\mathrm{Tr}e^{-\beta H}]$

- KEY INSIGHT: with product states also only connected clusters contribute



$$|\Phi\rangle = |\phi\rangle^{\otimes N}$$

- The previous results follow (mostly straightforward), resulting in

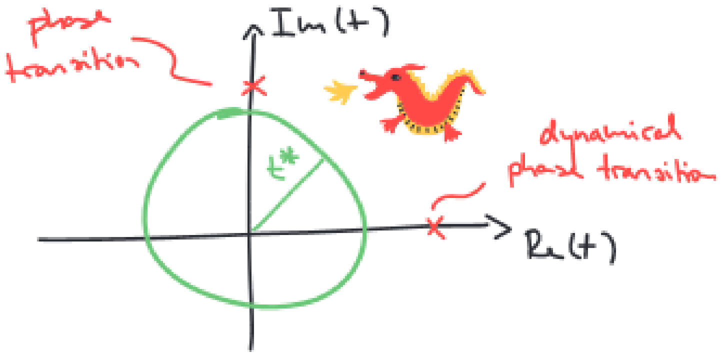
$$|\log\langle\Phi|e^{iHt}|\Phi\rangle - \sum_{m=0}^{M}\frac{t^m}{m!}K_m| \leq \epsilon \qquad t \leq t^*$$

$$M = \mathcal{O}(\log(N/\epsilon)) \quad \rightarrow \quad \boxed{\mathrm{runtime} = \mathrm{poly}(N/\epsilon)}$$

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.

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

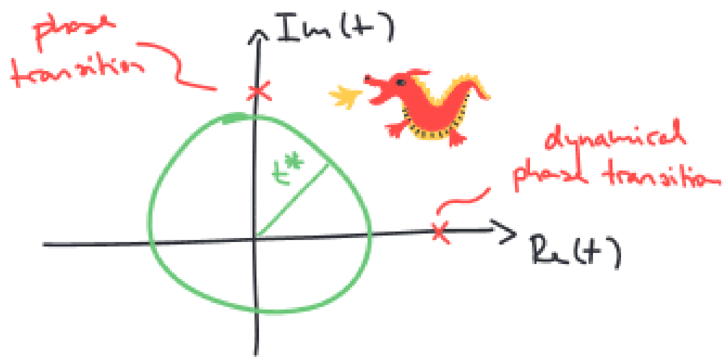
-State may become orthogonal to the initial one

-Dynamical phase transitions (Heyl 1709.07461)

- 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)
- **Probability theory**: concentration bounds (Chernoff) for short-time evolved states + Berry-Esseen theorem (Rae, AMA, Cirac, see arXiv next week).

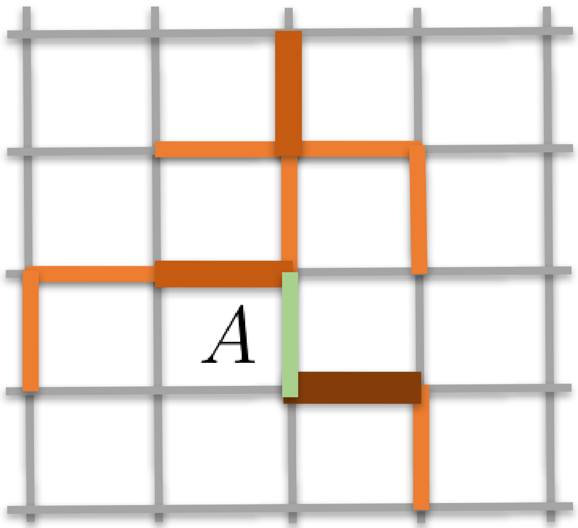
Heisenberg time evolution

- 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

Heisenberg time evolution

- Classical simulation of

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

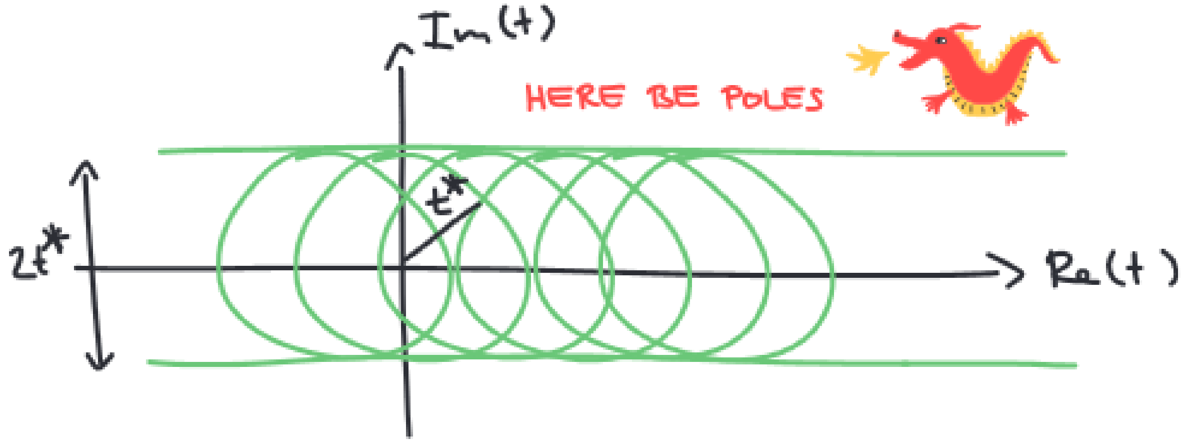
$$= \sum_{m=0}^{\infty}\frac{(it)^m}{m!}\sum_{\mathcal{G}_m^A}\langle\Phi|[h_{X_1},[h_{X_2},...[h_{X_m},A]]|\Phi\rangle$$

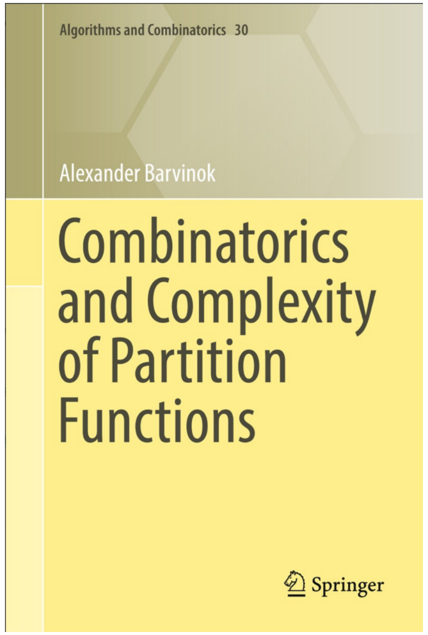
- Count connected clusters: $|\mathcal{G}_m^A| \leq c_1^m$
- Weight of each cluster: $m!2^m||A||$
- Similar convergence of Taylor series (and algorithm) for short times $t \leq t^*$

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

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.
- <u>Idea</u>: 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:

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

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:

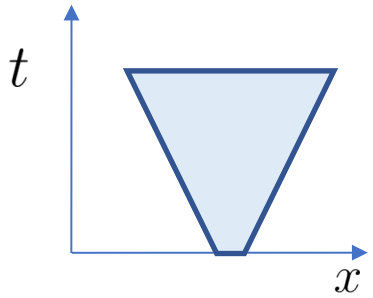
$$\left(\exp(\mathcal{O}(t))\frac{1}{\epsilon}\right)^{\exp(\mathcal{O}(t))}$$

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

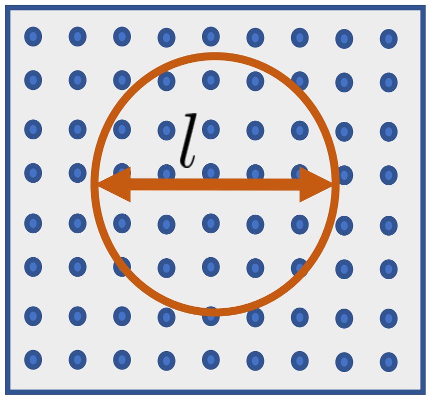
Alternative: Lieb-Robinson bounds

- 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>Runtime</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).

Computational complexity of dynamics

Evolution time	$\leq t^*$	$\mathcal{O}(1)$	$\mathcal{O}(\text{polylog}(N))$	$\mathcal{O}(\text{poly}(N))$
$\langle A(t) \rangle$	**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 $\epsilon = 1/\text{poly}(N)$

- #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.

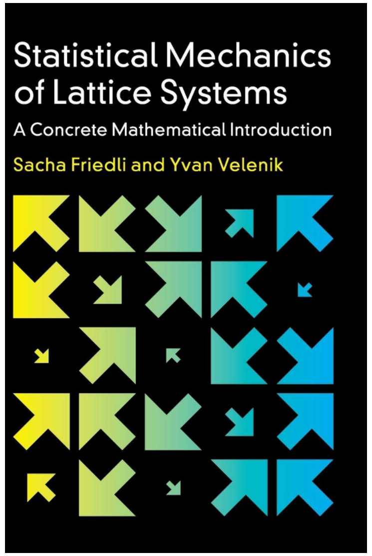
  -Shows convergence of Taylor approximation and yields efficient algorithms.

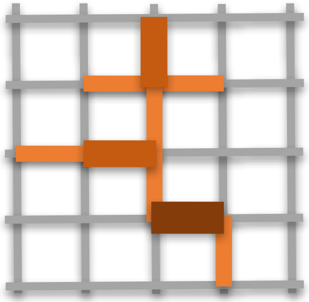
  -Works for many different interaction graphs.

- Here: it also works for problems of **quantum dynamics**.

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

- Versatile technique for classical simulation of many quantum problems.





Conclusions

- Cluster expansion: versatile and well-studied tool for partition functions + related problems.

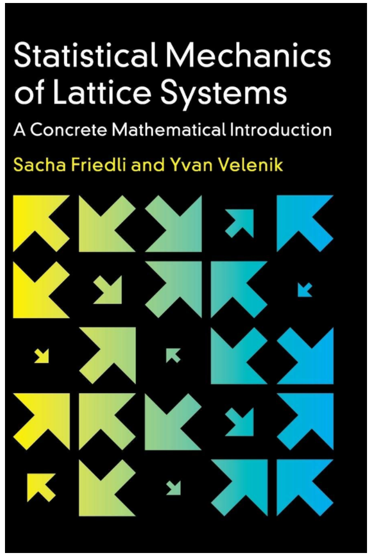
  -Shows convergence of Taylor approximation and yields efficient algorithms.

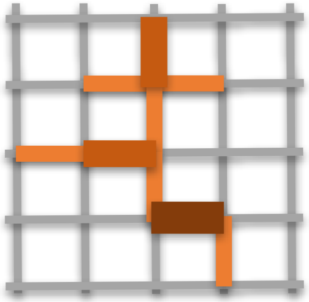
  -Works for many different interaction graphs.

- Here: it also works for problems of **quantum dynamics**.

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

- Versatile technique for classical simulation of many quantum problems.





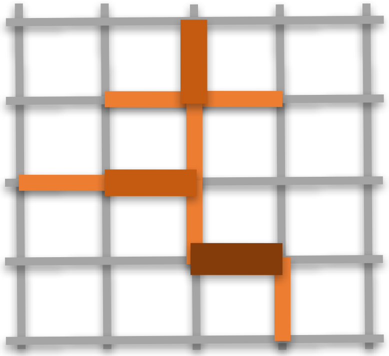
arXiv:2210.11490

Thanks!!

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)
- Efficient sampling of high temperature Gibbs states (Yin & Lucas 2305.18514)



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

- 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....