Title: Unreasonable effectiveness of methods from theoretical computer science in quantum many-body physics

Speakers: Anurag Anshu
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Abstract: A central challenge in quantum many-body physics is a characterization of properties of `natural' quantum states, such as the ground states and Gibbs states of a local hamiltonian. The area-law conjecture, which postulates a remarkably simple structure of entanglement in gapped ground states, has resisted a resolution based on information-theoretic methods. We discuss how the right set of insights may come, quite unexpectedly, from polynomial approximations to boolean functions. Towards this, we describe a 2D sub-volume law for frustration-free locally-gapped ground states and highlight a pathway that could lead to an area law. Similar polynomial approximations have consequences for entanglement in Gibbs states and lead to the first provably linear time algorithm to simulate Gibbs states in 1D. Next, we consider the task of learning a Hamiltonian from a Gibbs state, where many-body entanglement obstructs rigorous algorithms. Here, we find that the effects of entanglement can again be controlled using tools from computer science, namely, strong convexity and sufficient statistics.

The unreasonable effectiveness of the methods from computer science in many-body physics

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January 28, 2021

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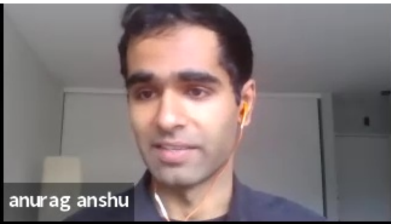
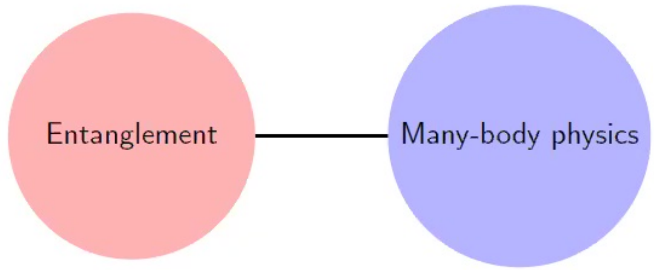
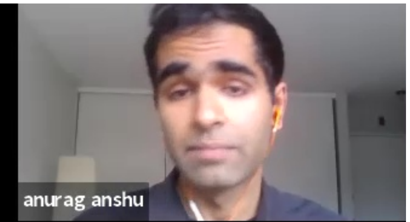
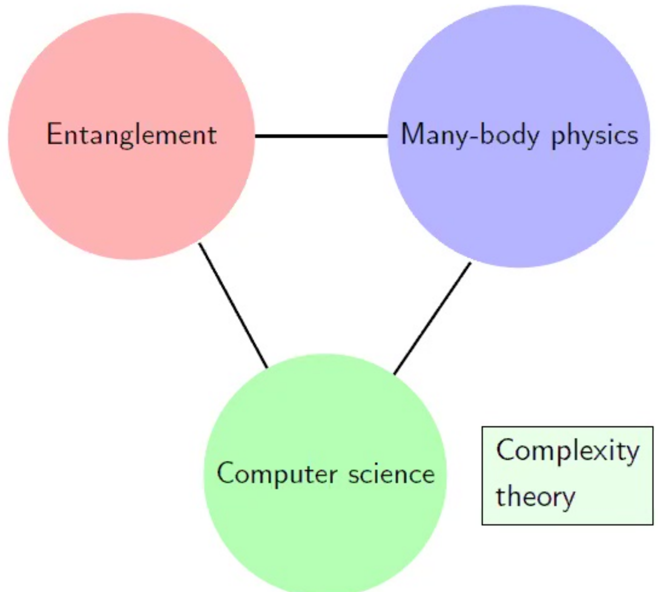


Complexity & entanglement in many-body systems





Complexity & entanglement in many-body systems



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Outline of the talk

- Progress on several questions in quantum many-body physics:
  - Area law in two dimensional gapped ground states.
  - Near-linear time rigorous algorithm for one-dimensional Gibbs states.
  - Learnability of Gibbs state.
- Central theme: *polynomial approximations* and *strong convexity* reveal surprising properties of many-body systems, not captured by prior methods.
- Application: quantum computing & simulation of many-body physics, verification of quantum devices.

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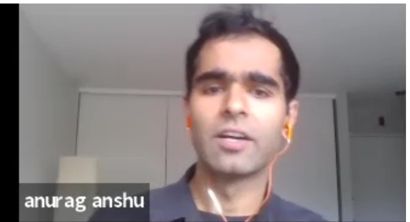
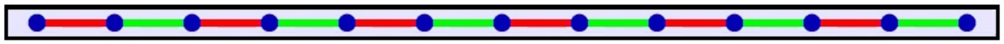


Many-body systems



$h_{8,9}$

Particles

Interactions

Hamiltonian: $\sum_{i=1}^{n-1} \mathsf{I} \otimes \mathsf{I} \ldots h_{i,i+1} \otimes \mathsf{I} \ldots \mathsf{I}$

Physical quantum states

- Ground states: lowest energy states of the hamiltonian.
- Gibbs state: describes the state of the system in contact with a heat bath at some temperature.
- Question: can these states be simulated via an efficient algorithm on a classical computer?

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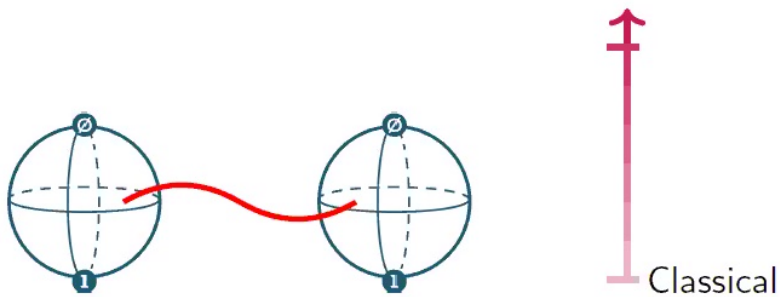
Quantum entanglement



Entanglement is typically associated with complexity

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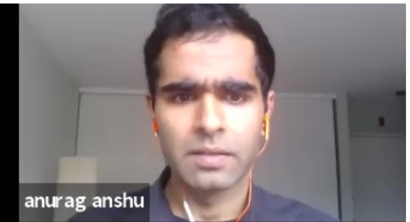
A different notion of complexity

- Polynomial approximations to the ground state and Gibbs state, as functions of the hamiltonian.
- Example: Taylor expansion of $e^{-\beta H}$ up to certain degree to obtain $p(H) = a_0 + a_1 H + \ldots a_d H^d$.
- More generally, multi-variate polynomials that look like

$$a h_{1,2} h_{3,4} \ldots h_{2,3} + \ldots + c h_{5,6} h_{3,4} \ldots h_{21,23}.$$

- A recent picture : the smallest degree of a polynomial approximation as a new notion of complexity.



The talk so far...

- Entanglement is viewed as a measure of complexity.
- Less entanglement intuitively suggests efficient algorithms for the corresponding state.
- We can look at the polynomial degree as a different notion of complexity.
- Up next: area laws and the power of low degree polynomial approximations.

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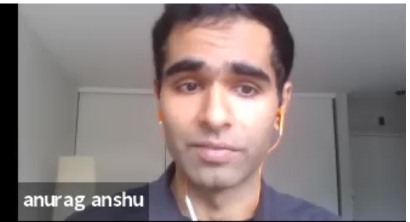
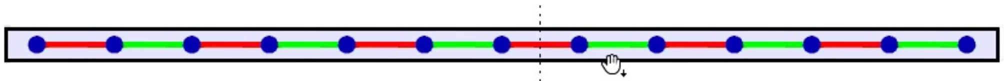
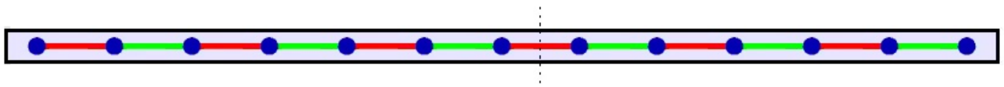


1D entanglement structure: area law



- Area law: entanglement (measured as entropy) between the two parts scales as the size of the partition (a constant).

1D entanglement structure: area law



- Area law: entanglement (measured as entropy) between the two parts scales as the size of the partition (a constant).
- Hastings [J. Stat. Mech, 2008]: holds for 1D *gapped* ground states.
- Introduced information theoretic tools.

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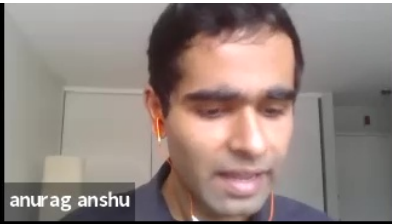
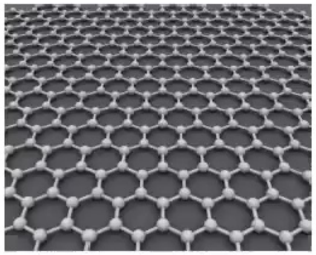
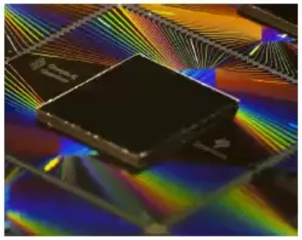
Simulating quantum many-body system on a quantum computer



- Following Feynman [IJTP 1982], a programmable quantum system can be used to prepare the ground state or Gibbs state of any system.
- Given this, properties can be predicted via measurements.



Program $\longrightarrow$



Measure $\longrightarrow$ Properties

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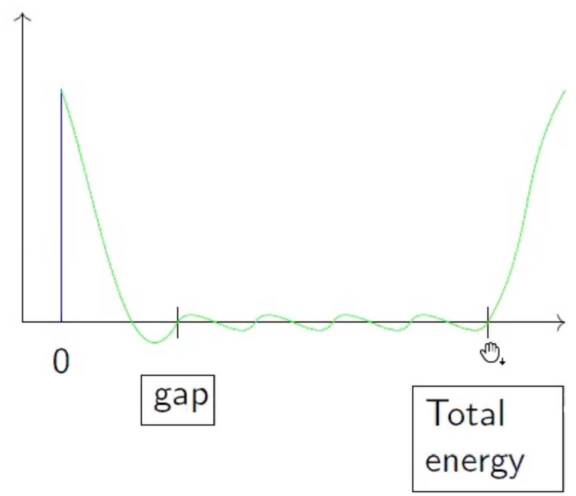
1D entanglement structure: area law and classical algorithm

- Arad, Kitaev, Landau, Vazirani [2013] showed the best known 1D area law.
- Introduced the notion of *Chebyshev-based* polynomial approximation to ground states. Established connection between polynomial degree and entanglement.
- First provably efficient algorithm for 1D ground states (Landau, Vidick, Vazirani [Nature Physics, 2015]).

Chebyshev-based polynomial approximation



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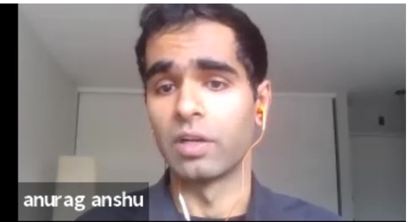

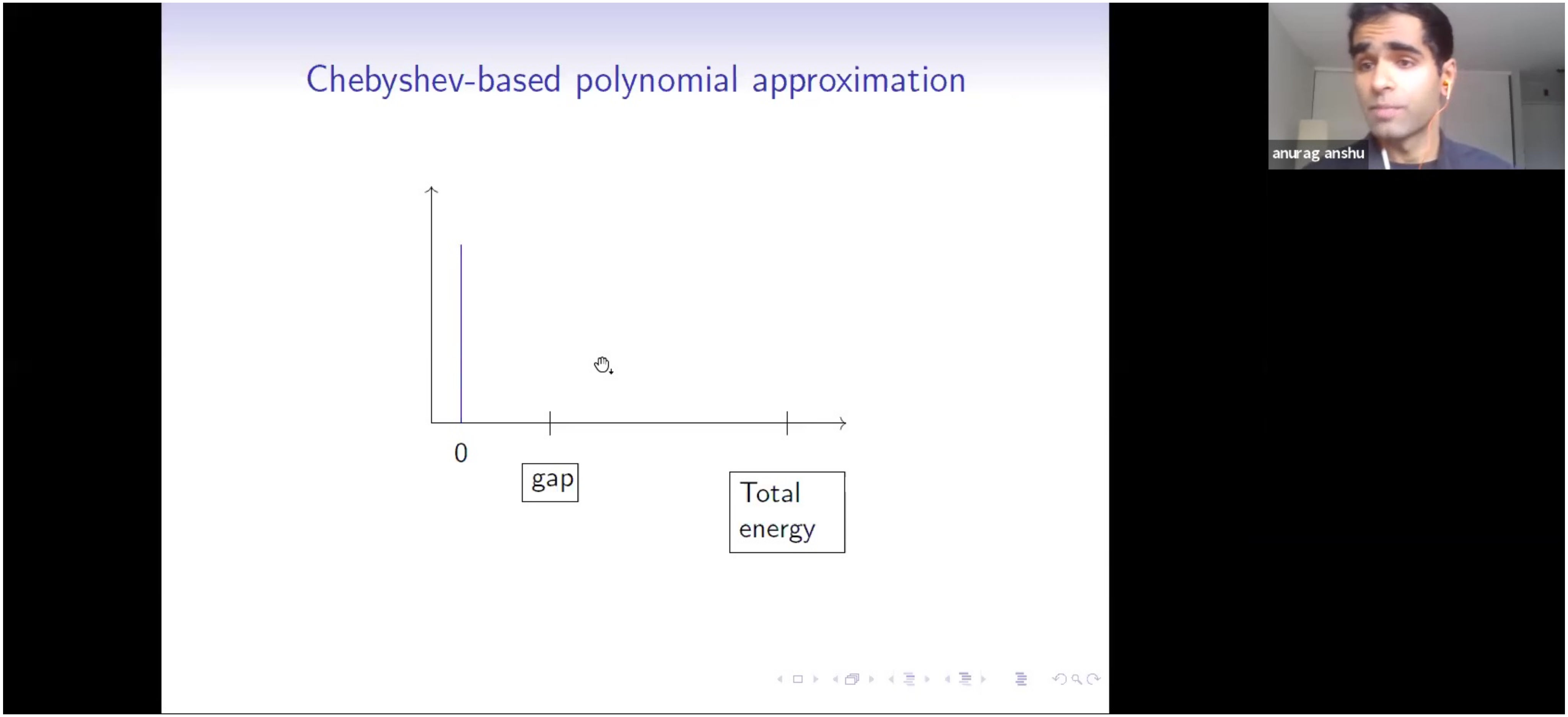
Chebyshev-based polynomial approximation
0
gap
Total energy
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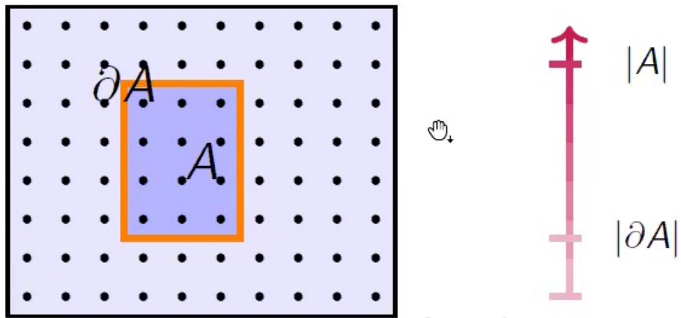
Area law conjecture in two dimensions



Area law conjecture

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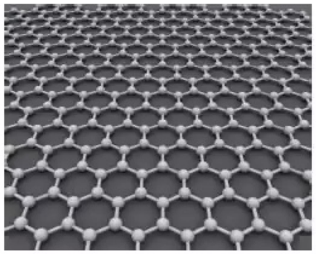
Area law conjecture in two dimensions



- Area law for ground states on two-dimensional lattice is not known.
- Chebyshev polynomial approximations to ground states do not seem to suffice.

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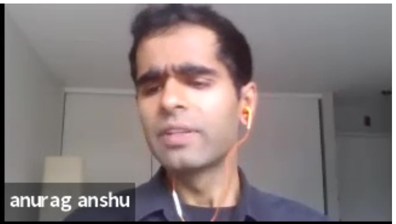
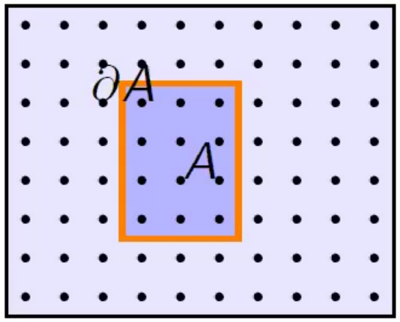
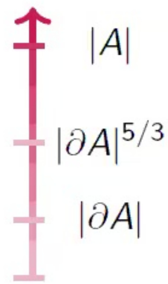
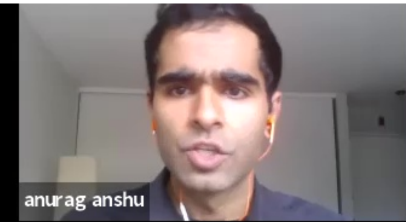


Entanglement structure in two dimensions





Sub-volume law

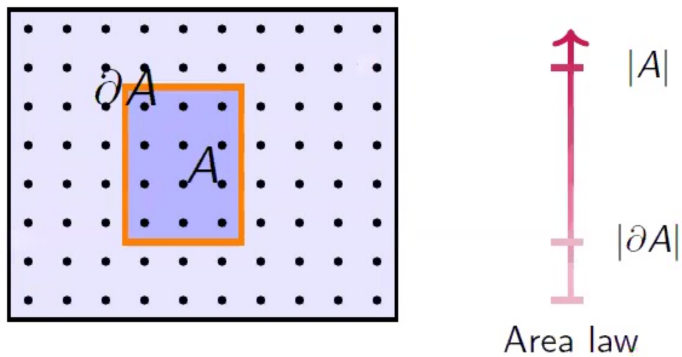


Theorem (**A.**, Arad, Gosset, STOC 2020)

Frustration-free 2D ground states[1] *satisfy a* <u>*sub-volume law*</u> *of* $|\partial A|^{5/3}$.

[1]with constant local spectral gap.

Entanglement structure in two dimensions

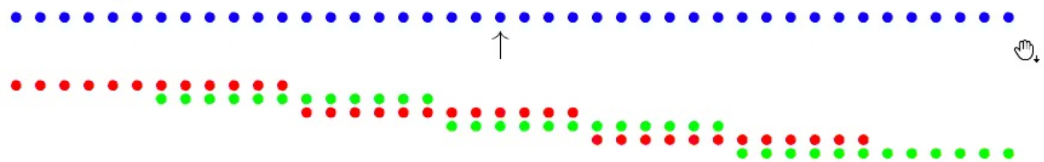


A., Arad, Gosset (Work in progress): Frustration-free 2D ground states[2] satisfy an area law with entanglement scaling as $|\partial A|^{1+o(1)}$.

[2] with constant local spectral gap.

New tools

- RG flow-type polynomial approximation: a framework to map polynomial approximations at smaller scales to polynomial approximations at larger scale.
- Robust polynomial method: a key constituent of the RG-flow argument.



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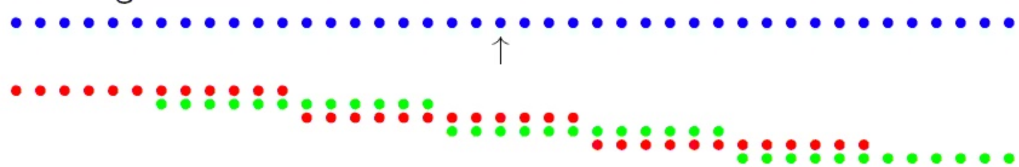

- Locality at the boundary: crucial use of the local structure of the hamiltonian at the boundary.

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The polynomial approximation picture

- Chebyshev-based polynomials are optimal at constant error. But this not true when error is tiny, such as, $e^{-\text{total energy}}$.
- In the classical case, best degree polynomial approximations for tiny errors is well known (Kahn, Linial, Samorodnitsy [Comb. 1993], Buhrman, Cleve, de Wolf, Zalka [FOCS 1999]).
- Area law follows if the same can be reproduced for the ground states:

  Complexity of 2D ground states $\equiv$ Complexity in the classical case

  as measured by the polynomial degree.

Future directions for ground state entanglement

- How far can the tiny error polynomial approximations be pushed? Would they possibly lead to a 2D area law for frustrated systems?
- New tools to remove the local gap assumption (which would generalize to the frustrated case).
- If 2D area law for frustration-free systems holds, can the ground state be represented as a PEPS?
- Would the resulting tools suffice to construct new heuristic classical algorithms for such ground states?

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Near-linear time algorithm for 1D Gibbs states

- Several heuristic algorithms achieve near linear time algorithms for 1D Gibbs states at low temperatures (iTEBD, METTS; Orus [A. Phys, 2014])
- But no rigorous proof of the run-time of the algorithms.

Theorem (Kuwahara, Alhambra, **A.**, PRX 2021)

For a 1D Gibbs state on n particles at inverse temperature $\beta = o(\log n)$, there is a classical algorithm that runs in time $n^{1+o(1)}$ and outputs an MPO approximation of the state.

Near-linear time algorithm for 1D Gibbs states

- Key tool: polynomial approximation to the function $e^{-\beta x}$.
- Truncated Taylor series is known since 1715 AD. So what's new?
- Chebyshev-based approximations that improve upon Taylor series (Sachdeva, Vishnoi [FTCS, 2014]).

Theorem (Kuwahara, Alhambra, **A.**, PRX 2021)

Gibbs states on a lattice satisfy an area law of $O(\beta^{2/3})|\partial A|$.

- Improves upon the prior area law $O(\beta)|\partial A|$ (Wolf, Verstraete, Hastings, Cirac [PRL, 2008]).
- Suggests that entanglement in imaginary time evolution spreads as $O(\beta^{2/3})$, instead of $O(\beta)$.

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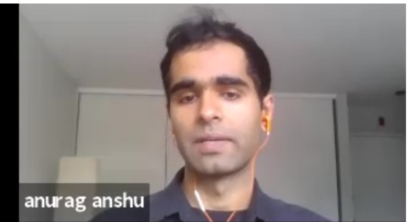
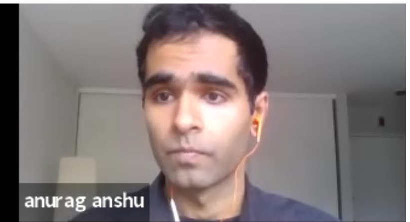


The talk so far...

- Polynomial approximations to the ground state are leading to powerful insights into the entanglement structure of the ground states, not accessible by information theoretic tools.
- Polynomial approximations to the Gibbs states have similar consequences, along with efficient algorithms for their simulation.
- Up next: learnability of Gibbs states.



Learning interactions from the Gibbs state

- A system or device prepares a Gibbs state based on some interactions, which are not known to us.
- Imagine that the system or device can prepare several independent samples of the Gibbs state.
- Goal: learn the interactions by quantum measurements, with as few samples as possible.

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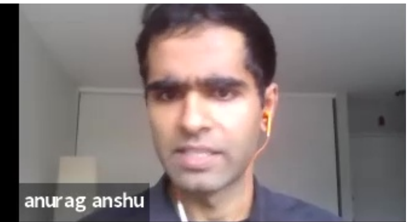

Learning interactions from the Gibbs state: relevance

- Inherent in the method of physics itself: interactions need to be discovered and samples are naturally Gibbs states.
- A good learning algorithm ensures verification of quantum devices. Gibbs states are crucially used in recent quantum algorithms (SDP solvers, Brandao, Svore [FOCS 2017]).
- A central problem for quantum learning theory (Amin et. al. [PRX 2018]). Several heuristic results that work very well in practice (Wiebe et. al. [PRL 2014]; Bairey, Arad, Lindner [PRL 2019])

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Why Gibbs states should be learnable?

- Gibbs states on lattices have a simple entanglement structure and have low degree polynomial approximation.
- Thus, their complexity is low in both notions discussed here.
- Learning family of states with low complexity is expected.

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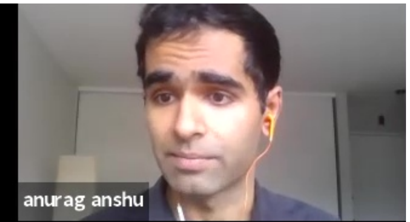
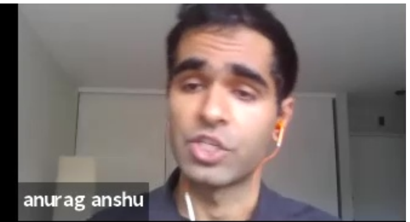


The bottleneck for rigorous algorithms

- Entanglement can completely delocalise the information about each interaction.
- The quantum Gibbs states violate the Markov condition.



Learning interactions from the Gibbs state: results

Theorem (**A.**, Arunachalam, Kuwahara, Solemanifar, FOCS 2020)

The hamiltonian can be learned with good accuracy, with number of samples polynomial in the number of particles.

- The algorithm is time efficient at high temperatures and for sign-free hamiltonians.
- The sample complexity is tight up to polynomial factors.
- Intuition: information about the interactions, however delocalized by entanglement, can be accessed via simple quantum measurement.
- Technical core: strong convexity of the quantum partition function.

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Future directions in learnability

- Is time-efficient hamiltonian learning possible at all temperatures?
- Can a hamiltonian be learned from Gibbs states over arbitrary interaction hypergraphs?
- Learning theory for other quantum many-body states of low complexity?

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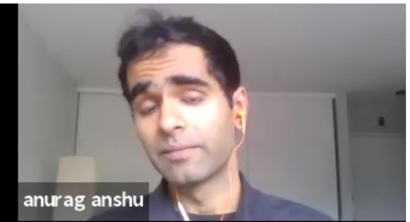
Outlook

- There are notions natural to both physics and computer science: time efficiency, randomness (Glauber dynamics), non-locality, etc.
- We highlighted some notions that are inherent to computer science: efficiency in terms of polynomial approximations, the concept of strong convexity; and effective in many-body physics.
- As observed by E. Wigner in "The Unreasonable Effectiveness of Mathematics in the Natural Sciences", such connection between fields require a deeper understanding, or a legendary essay.



Outlook

- Going back in history, these concepts originated from the physical world.
    - Chebyshev was "comparing different mechanisms of motion transfer, especially in a steam engine" (Goncharov [J. Approx. Theory, 2000]).
- Are we coming full circle, or spiralling into a deeper connection?

Thank you for your attention!

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