Quantum Hamiltonian Complexity

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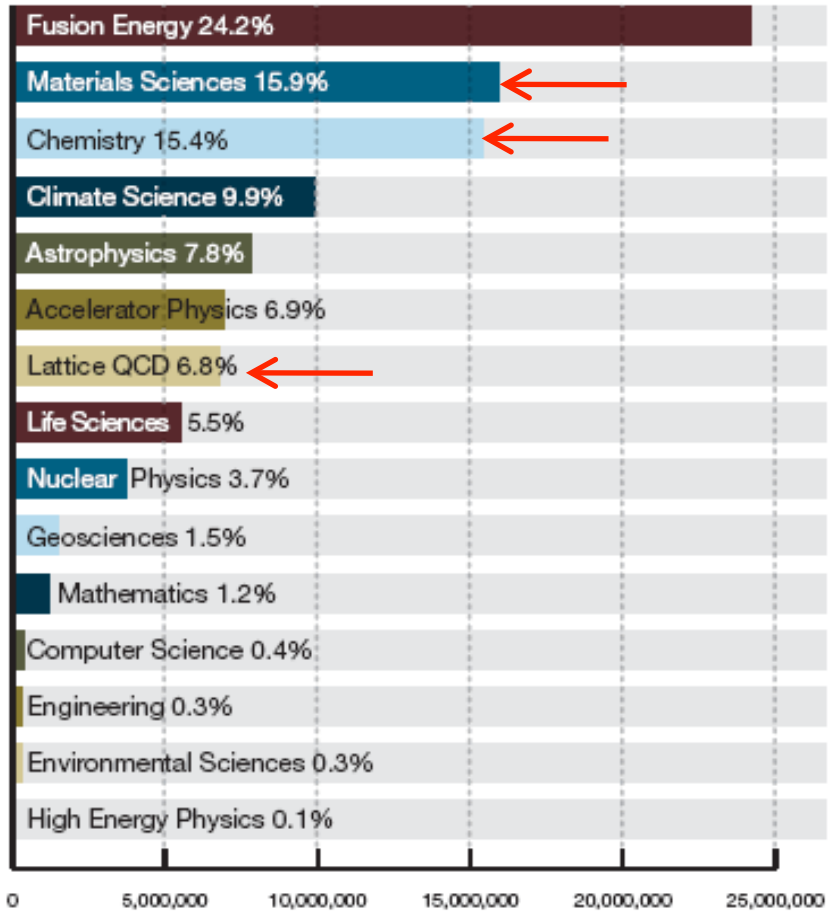
Based on joint work with A. Harrow and M. Horodecki

Quo Vadis Quantum Physics, Natal 2013

Quantum is Hard

Use of DoE supercomputers by area

(from a talk by Alán Aspuru-Guzik)



More than **33%** of DoE **supercomputer power** is devoted to simulating quantum physics

Can we get a better handle on this ***simulation*** problem?

Quantum Information Science

…gives new approaches

1. Quantum computer and quantum simulators

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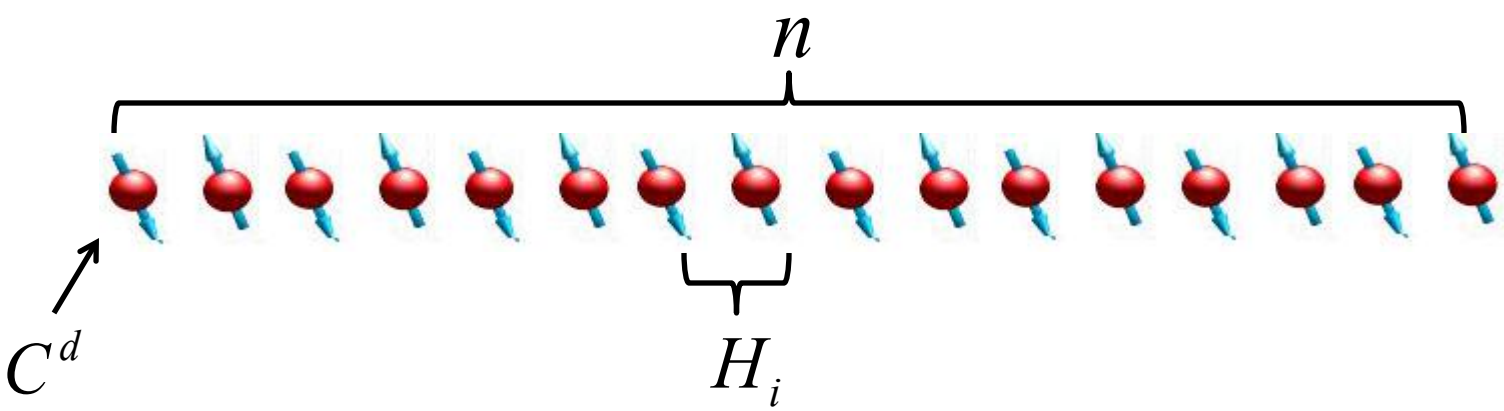
Quantum Many-Body Systems

Quantum Hamiltonian $$H = \sum_{i=1}^{m} H_i \in \left(C^d\right)^{\otimes n}$$



Interested in computing properties such as minimum energy, correlations functions at zero and finite temperature, dynamical properties, …

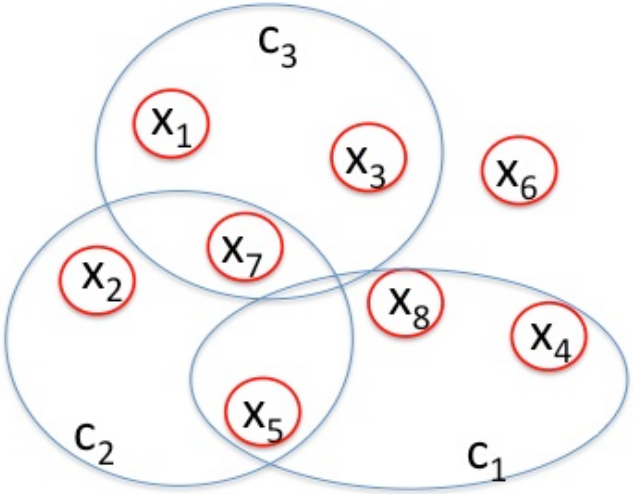
Quantum Hamiltonian Complexity

…analyzes quantum many-body physics through the computational lens

1. Relevant for condensed matter physics, quantum chemistry, statistical mechanics, quantum information

2. Natural generalization of the study of constraint satisfaction problems in theoretical computer science

Constraint Satisfaction Problems vs Local Hamiltonians



k-arity CSP:

Variables $\{x_1, \ldots, x_n\}$, alphabet Σ

Constraints: $c_j : \Sigma^k \to \{0,1\}$

Assignment: $\sigma : [n] \to \Sigma$

Unsat $:= \min_{\sigma} \sum_j c_j(\sigma(x_{j_1}), \ldots, \sigma(x_{j_k}))$

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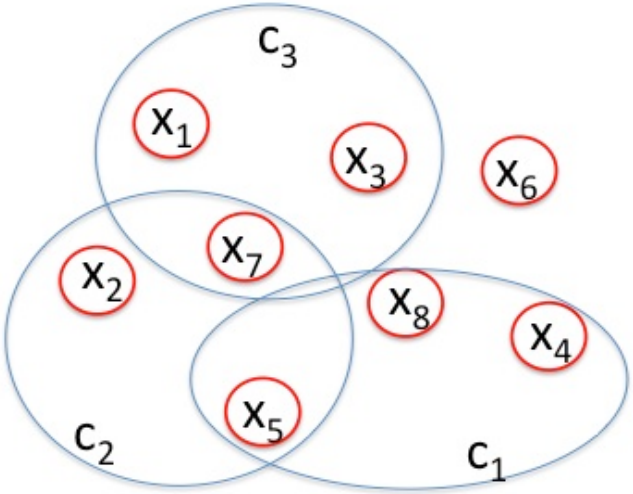

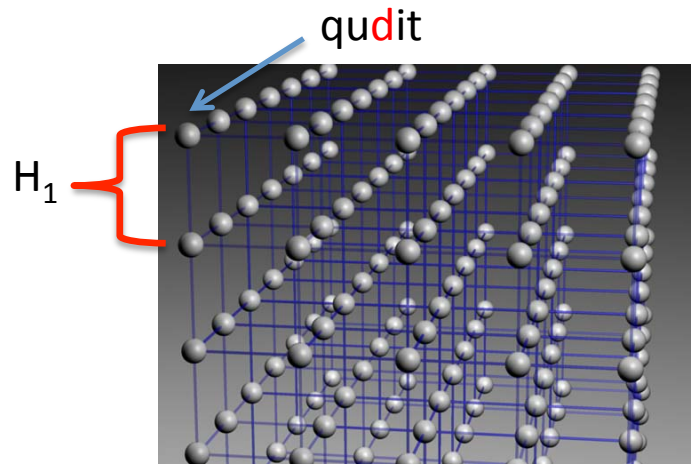

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k-local Hamiltonian H:

n qudits in $\left(C^d\right)^{\otimes n}$

Constraints: $H_j \in Her\left(\left(C^d\right)^{\otimes k}\right)$

qUnsat := $E_0\left(\sum_j H_j\right)$

E_0 : min eigenvalue

C. vs Q. Optimal Assignments

Finding optimal assignment of CSPs can be hard

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(BCS Hamiltonian groundstate, Laughlin states for FQHE,…)

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Main difference: Optimal Assignment can be a highly entangled state (unit vector in $(C^d)^{\otimes n}$)

Optimal Assignments: Entangled States

Non-entangled state: $\left(a_1|0\rangle + b_1|1\rangle\right) \otimes \ldots \otimes \left(a_n|0\rangle + b_n|1\rangle\right)$

e.g. $|\uparrow\rangle \otimes \ldots \otimes |\uparrow\rangle$

Entangled states: $\sum_{i_1,\ldots,i_n} c_{i_1,\ldots,i_n} |i_1,\ldots,i_n\rangle$

e.g. $\left(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle\right) / \sqrt{2}$

To describe a general entangled state of n spins requires exp(O(n)) bits

How Entangled?

Given bipartite entangled state $\left|\psi\right\rangle_{AB} \in C^n \otimes C^m$

the reduced state on A is mixed: $\rho_A \geq 0,\ tr(\rho_A) = 1$

The more mixed ρ_A, the more entangled ψ_{AB}:

Quantitatively: $E(\psi_{AB}) := S(\rho_A) = -tr(\rho_A \log \rho_A)$

Is there a relation between the amount of entanglement in the ground-state and the computational complexity of the model?

Outline

- **Quantum PCP Conjecture**
  What is it?
  Limitations to qPCP
  New algorithms

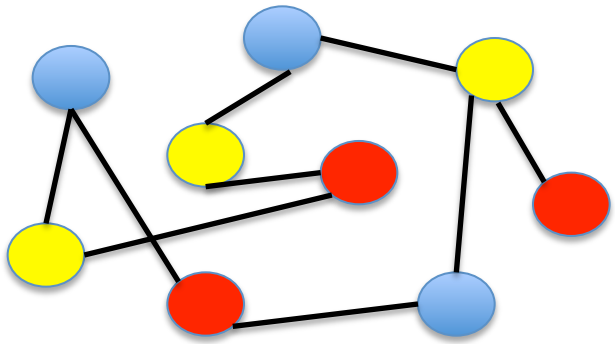
- **Area Law**
  What is it?
  Area Law from Decay of Correlations
  Proof by Quantum Shannon Theory

NP ≠ Non-Polynomial

NP is the class of problems for which one can check the correctness of a potential efficiently (in polynomial time)

E.g. Factoring: Given N, find a number that divides it, N = m x q

E.g. Graph Coloring: Given a graph and k colors, color the graph such that no two neighboring vertices have the same color



3-coloring

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E.g. F

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E.g. G

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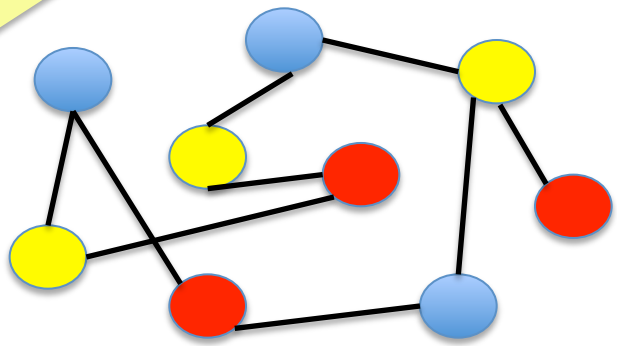
the same colo

The million dollars question:

Is P = NP?



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NP-hardness

A problem is NP-hard if any other problem in NP can be reduced to it in polynomial time.

E.g. 3-SAT: CSP with binary variables $x_1, \ldots, x_n$ and constraints $\{C_i\}$, $C_i = x_{i_1} \wedge \bar{x}_{i_2} \wedge x_{i_3}$

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E.g. There is an efficient mapping between graphs and 3-SAT formulas such that given a graph G and the associated 3-SAT formula S

G is 3-colarable <-> S is satisfiable

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NP-complete: NP-hard + inside NP

Complexity of qCSP

Since computing the ground-energy of local Hamiltonians is a generalization of solving CSPs, the problem is at least NP-hard.

Is it in NP? Or is it harder?

The fact that the optimal assignment is a highly entangled state might make things harder…

The Local Hamiltonian Problem

Problem

Given a local Hamiltonian H, decide if $E_0(H)=0$ or $E_0(H)>\Delta$

$E_0(H)$: minimum eigenvalue of H

Thm (Kitaev '99) The local Hamiltonian problem is QMA-complete for $\Delta = 1/\mathrm{poly}(n)$

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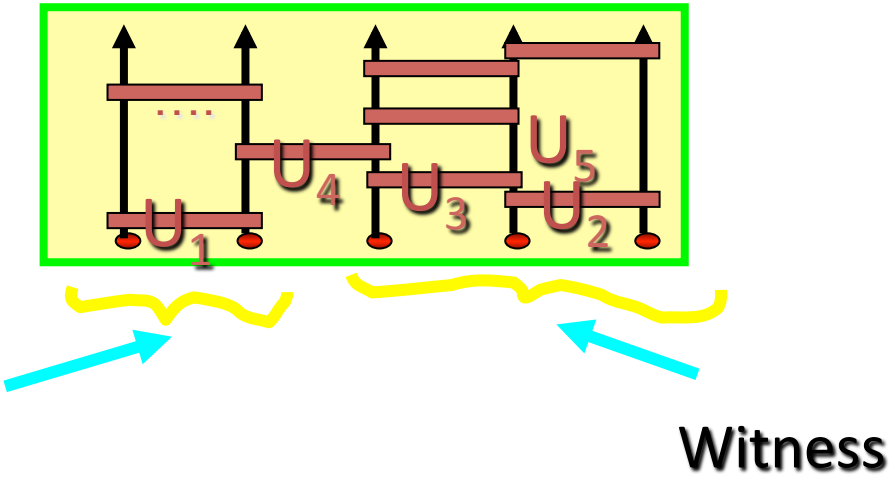
(analogue Cook-Levin thm)

QMA is the quantum analogue of NP, where the proof and the computation are quantum.



The meaning of it

It's widely believed QMA ≠ NP

Thus, there is generally no *efficient* classical description of groundstates of local Hamiltonians

Even very simple models are QMA-complete
E.g.
(Aharonov, Irani, Gottesman, Kempe '07) 1D models

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"1D systems as hard as the general case"

What's the role of the acurracy Δ on the hardness?

… But first what happens classically?

PCP Theorem

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- NP-hard even for $\Delta=\Omega(m)$
- Equivalent to the existence of **P**robabilistically **C**heckable **P**roofs for NP.
- Central tool in the theory of hardness of approximation (optimal threshold for 3-SAT (7/8-factor), max-clique ($n^{1-\varepsilon}$-factor))

Quantum PCP?

The qPCP conjecture: There is $\varepsilon > 0$ s.t. the following problem is QMA-complete: Given 2-local Hamiltonian H with m local terms determine whether

(i) $E_0(H)=0$ or (ii) $E_0(H) > \varepsilon m$.

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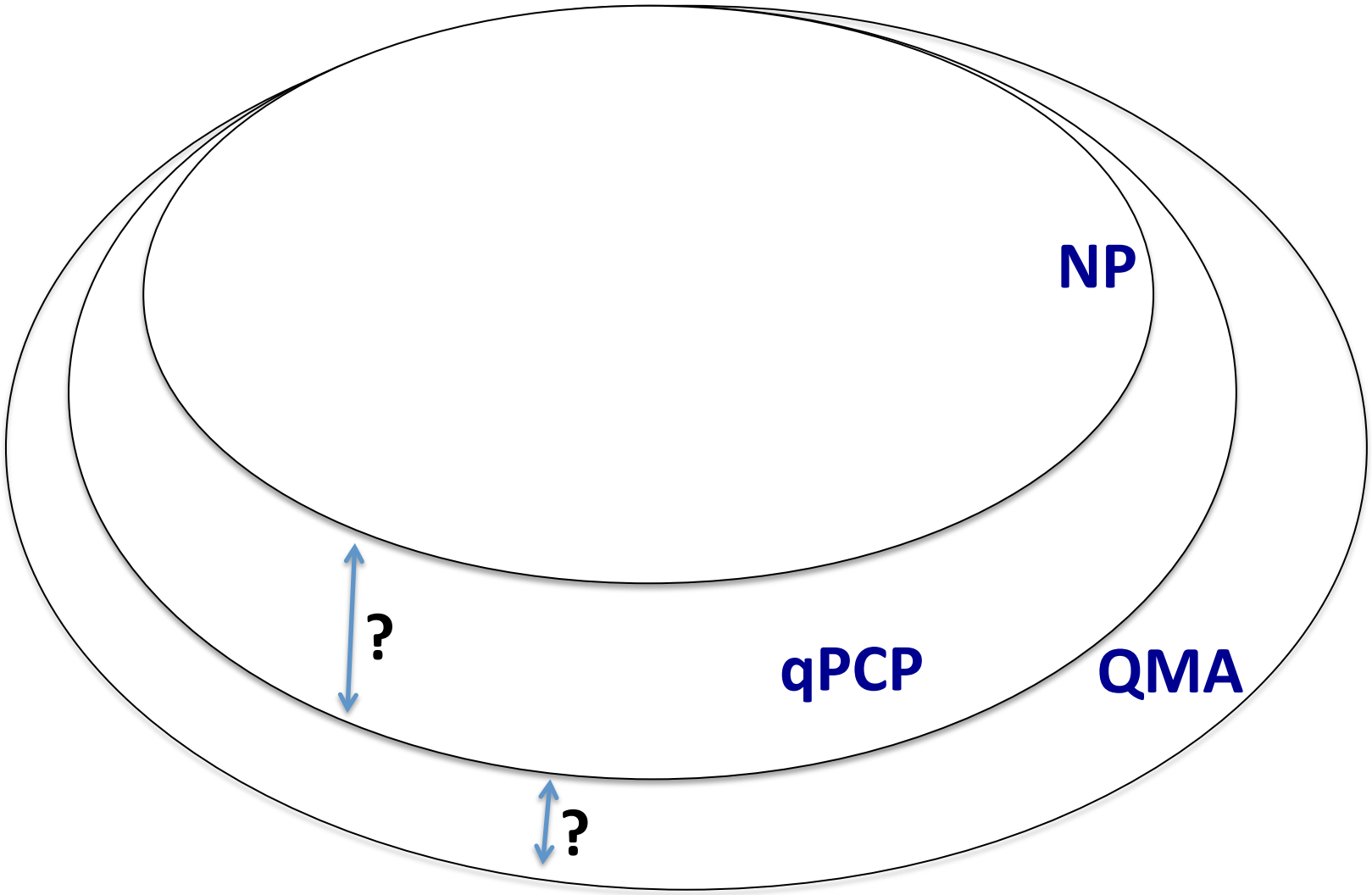
- Related to estimating energy at constant temperature
- At least NP-hard (by PCP Thm) and in QMA

Quantum PCP?



Previous Work and Obstructions

(Aharonov, Arad, Landau, Vazirani '08)
Quantum version of 1 of 3 parts of Dinur's proof of the PCP thm (gap amplification)

But: The other two parts (alphabet and degree reductions) involve massive copying of information; not clear how to do it with a highly entangled assignment

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(Bravyi, Vyalyi '03; Arad '10; Hastings '12; Freedman, Hastings '13; Aharonov, Eldar '13, …)
No-go for large class of commuting Hamiltonians and almost commuting Hamiltonians

But: Commuting case might always be in NP

Going Forward

- Can we understand why got stuck in quantizing the classical proof?
- Can we prove partial no-go beyond commuting case?

Yes, by considering the simplest possible reduction from quantum Hamiltonians to CSPs.

Mean-Field…

…consists in approximating groundstate by a product state $|\psi_1\rangle \otimes \ldots \otimes |\psi_n\rangle$

$$\max_{\psi_1,\ldots,\psi_n} \sum_j \langle \psi_1,\ldots,\psi_n | H_j | \psi_1,\ldots,\psi_n \rangle$$ is a CSP

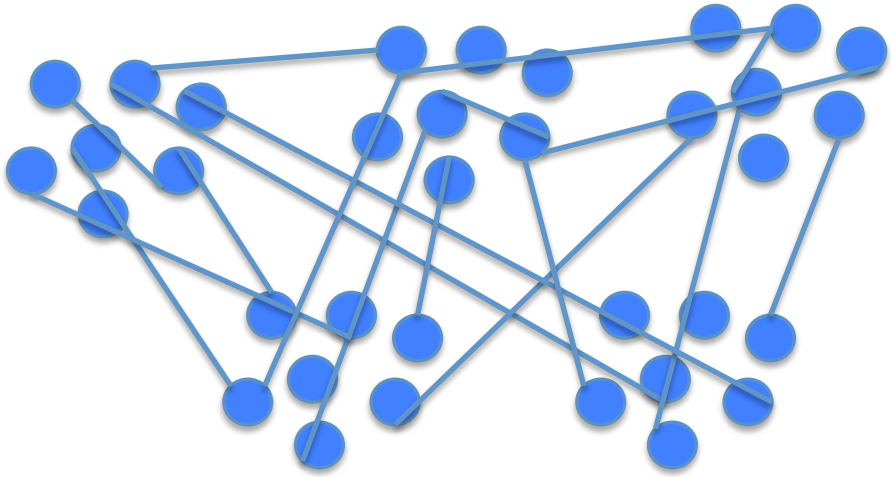
It's a mapping from quantum Hamiltonians to CSPs

Successful heuristic in Quantum Chemistry (Hartree-Fock)
Condensed matter (e.g. BCS theory)

Folklore:
Mean-Field good when Many-particle interactions
Low entanglement in state

Approximation in NP

(B., Harrow '12) Let H be a 2-local Hamiltonian on qudits with interaction graph G(V, E) and |E| local terms.



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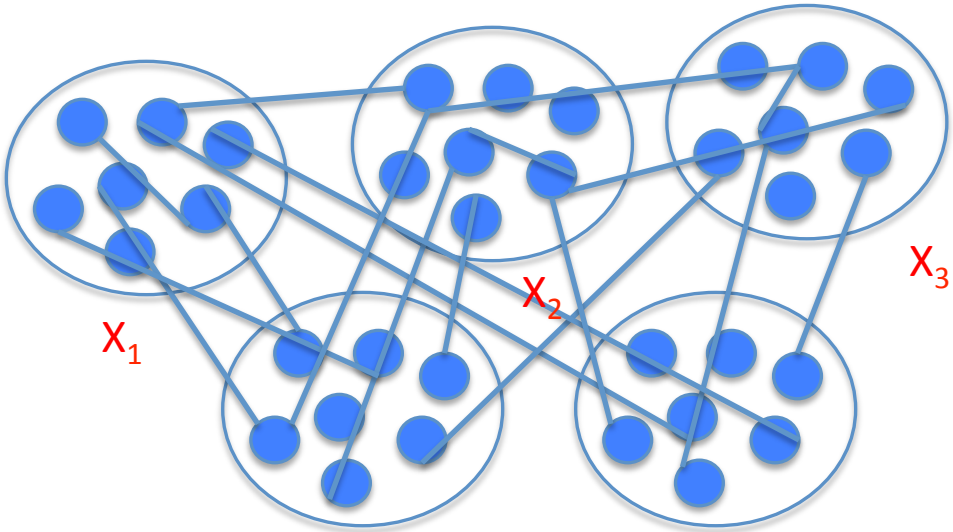

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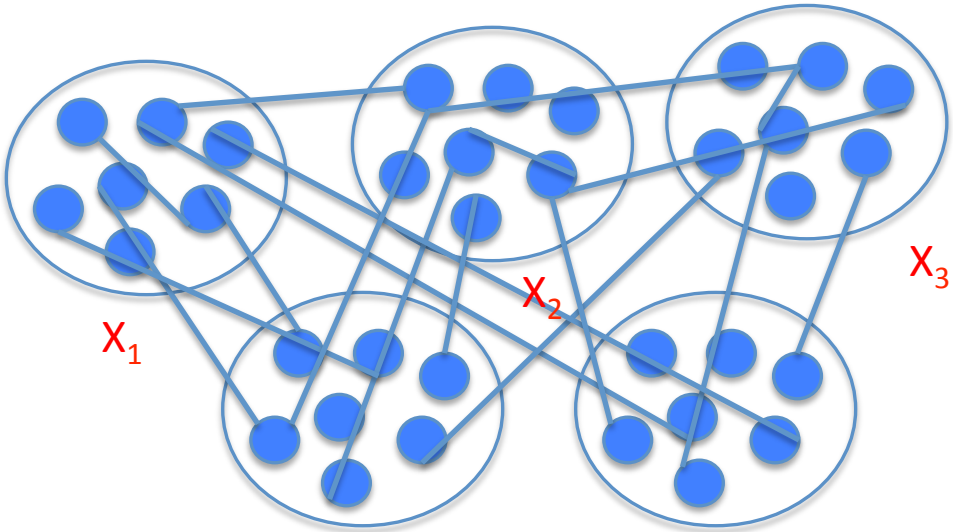

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$$\frac{1}{|E|}\langle\psi_1,\ldots,\psi_m|H|\psi_1,\ldots,\psi_m\rangle \le e_0(H)+\Omega\left(d^6 E_i \Phi(X_i)\frac{1}{\deg(G)}E_i\frac{S(X_i)}{m}\right)^{1/8}$$

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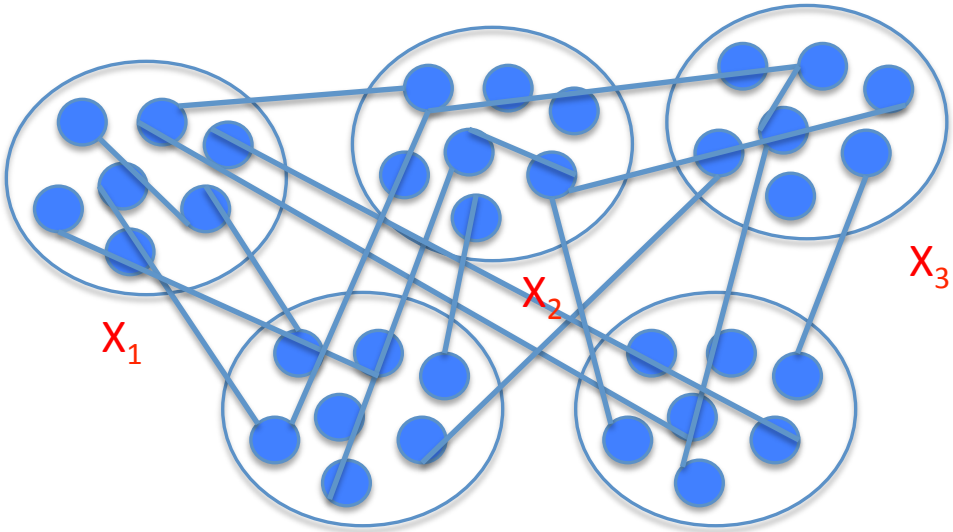

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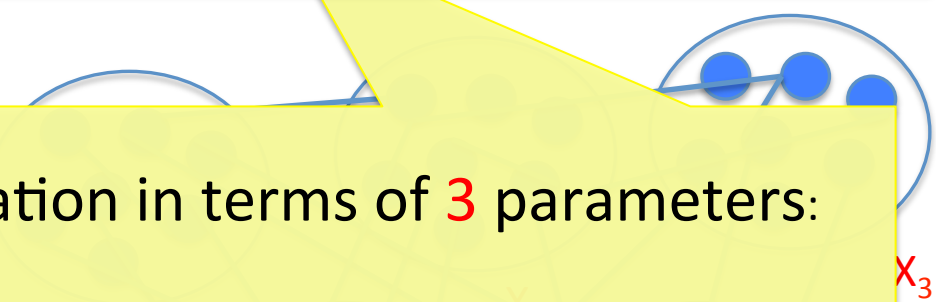


Approximation in terms of 3 parameters:

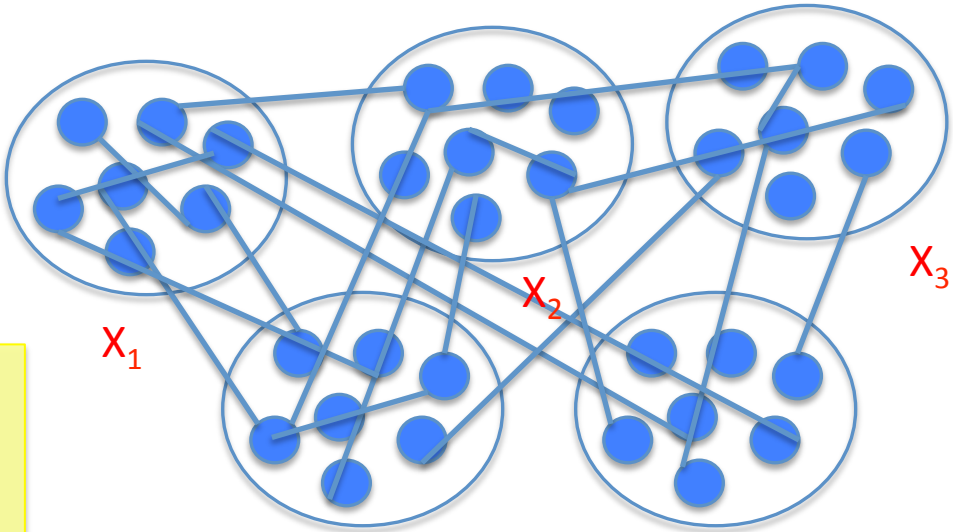
1. Average expansion
2. Degree interaction graph
3. Average entanglement groundstate

Approximation in terms of average expansion

$$\frac{1}{|E|}\langle\psi_1,\ldots,\psi_m|H|\psi_1,\ldots,\psi_m\rangle \le e_0(H)+\Omega\left(d^6 \boxed{E_i\Phi(X_i)}\frac{1}{\deg(G)}E_i\frac{S(X_i)}{m}\right)^{1/8}$$

Average Expansion: $E_i\Phi(X_i) = E_i \Pr_{(u,v)\in E}\left(v \notin X_i \,|\, u \in X_i\right)$

Well known fact:  's divide and conquer



Potential hard instances must be based on expanding graphs

$m < O(\log(n))$

Approximation in terms of degree

$$\frac{1}{|E|}\langle\psi_1,\ldots,\psi_m|H|\psi_1,\ldots,\psi_m\rangle \le e_0(H)+\Omega\left(d^6 E_i \Phi(X_i)\boxed{\frac{1}{\deg(G)}}E_i\frac{S(X_i)}{m}\right)^{1/8}$$

No classical analogue:

(PCP + parallel repetition) For all $\alpha, \beta, \gamma > 0$ it's NP-complete to determine whether a CSP *C* is s.t.

Unsat = 0 or Unsat > $\alpha\, \Sigma^{\beta}/\deg(G)^{\gamma}$

Parallel repetition: *C* -> *C'*

i. $\deg(G') = \deg(G)^k$
ii. $\Sigma' = \Sigma^k$
ii. Unsat(G') > Unsat(G)

(Raz '00) even showed Unsat(G') approaches 1 exponentially fast

Approximation in terms of degree

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Q. Parallel repetition: *H* -> *H'*

?????

i. $\deg(H') = \deg(H)^k$

ii. $d' = d^k$

iii. $e_0(H') > e_0(H)$

Approximation in terms of degree

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Contrast: It's in NP determine whether a Hamiltonian H is s.t

$e_0(H)=0$ or $e_0(H) > \alpha d^{3/4}/\deg(G)^{1/8}$

Quantum generalizations of PCP *and* parallel repetition *cannot* both be true (assuming QMA not in NP)

Approximation in terms of degree

$$\frac{1}{|E|}\langle\psi_1,\ldots,\psi_m|H|\psi_1,\ldots,\psi_m\rangle \le e_0(H)+\Omega\left(d^6 E_i \Phi(X_i)\boxed{\frac{1}{\deg(G)}}E_i\frac{S(X_i)}{m}\right)^{1/8}$$

Bound: $\Phi_G < ½ - \Omega(1/\deg)$ implies

Highly expanding graphs (Φ_G -> 1/2) are not hard instances

Obs: Restricted to 2-local models

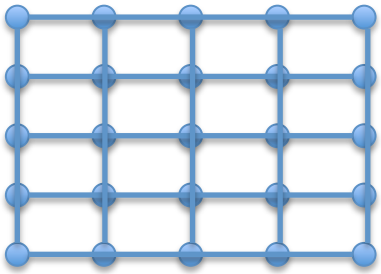
(Aharonov, Eldar '13) k-local, commuting models

Approximation in terms of degree

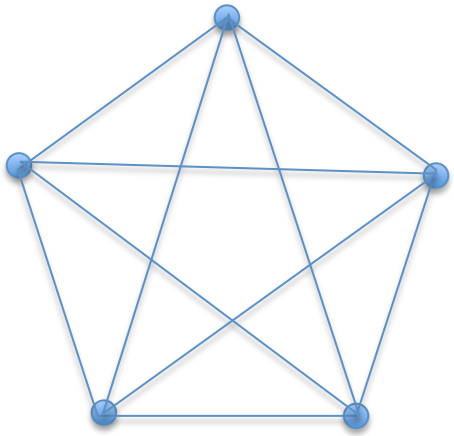
...shows mean field becomes exact in high dim

1-D

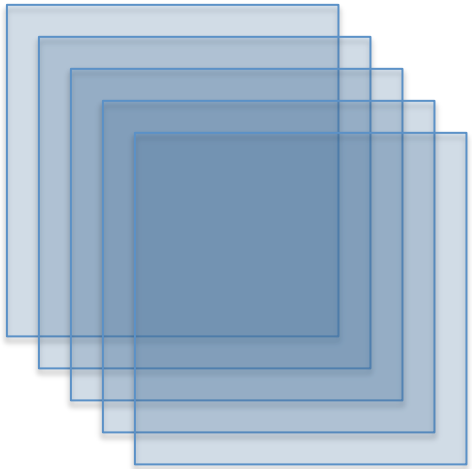
2-D



∞-D



3-D



Rigorous justification to folklore in condensed matter physics

Approximation in terms of average entanglement

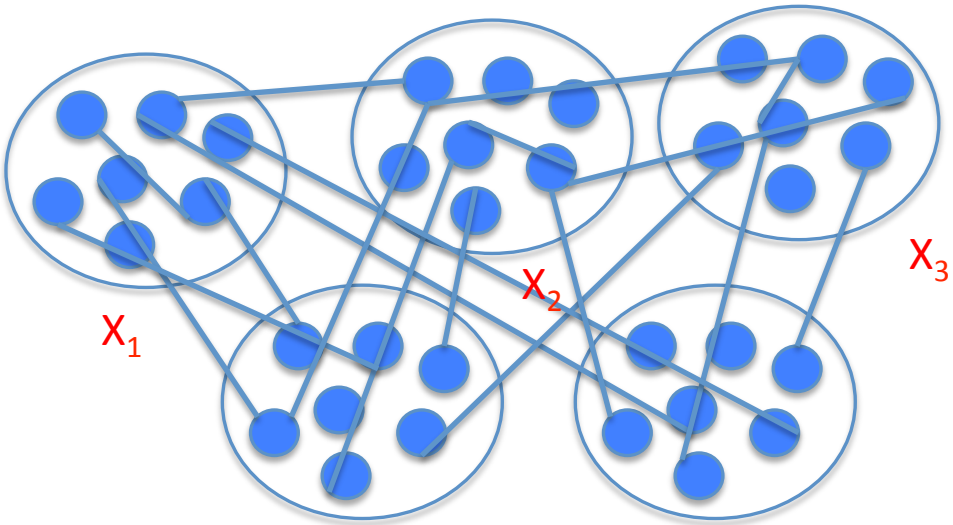
$$\frac{1}{|E|}\langle\psi_1,\ldots,\psi_m|H|\psi_1,\ldots,\psi_m\rangle \le e_0(H)+\Omega\left(d^6 E_i \Phi(X_i)\frac{1}{\deg(G)}\boxed{E_i\frac{S(X_i)}{m}}\right)^{1/8}$$

Mean field works well if entanglement of groundstate satisfies a subvolume law:

$$E_i\frac{S(X_i)}{m}=o(1)$$

Connection of amount of entanglement in groundstate and computational complexity of the model

m < O(log(n))



Approximation in terms of average entanglement

$$\frac{1}{|E|}\langle\psi_1,\ldots,\psi_m|H|\psi_1,\ldots,\psi_m\rangle \le e_0(H)+\Omega\left(d^6 E_i \Phi(X_i)\frac{1}{\deg(G)}\boxed{E_i\frac{S(X_i)}{m}}\right)^{1/8}$$

Systems with low entanglement are expected to be easy

So far only precise in 1D:

Area law for entanglement -> MPS description

Here:

Good: arbitrary lattice, only subvolume law

Bad: Only mean energy approximated well

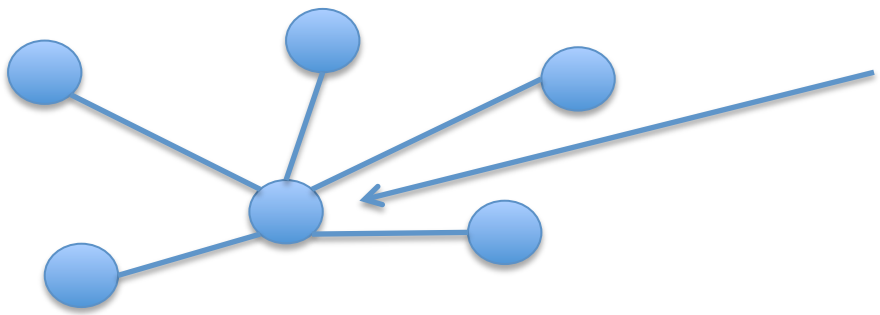
New Classical Algorithms for Quantum Hamiltonians

Following same approach we also obtain polynomial time algorithms for approximating the groundstate energy of

1. Planar Hamiltonians, improving on (Bansal, Bravyi, Terhal '07)
2. Dense Hamiltonians, improving on (Gharibian, Kempe '10)
3. Hamiltonians on graphs with low threshold rank, building on (Barak, Raghavendra, Steurer '10)

In all cases we prove that a product state does a good job and use efficient algorithms for CSPs.

Proof Idea: Monogamy of Entanglement



Cannot be highly entangled with too many neighbors

Entropy quantifies how entangled it can be

Proof uses information-theoretic techniques to make this intuition precise

Inspired by classical information-theoretic ideas for bounding convergence of SoS hierarchy for CSPs
(Tan, Raghavendra '10, Barak, Raghavendra, Steurer '10)

Outline

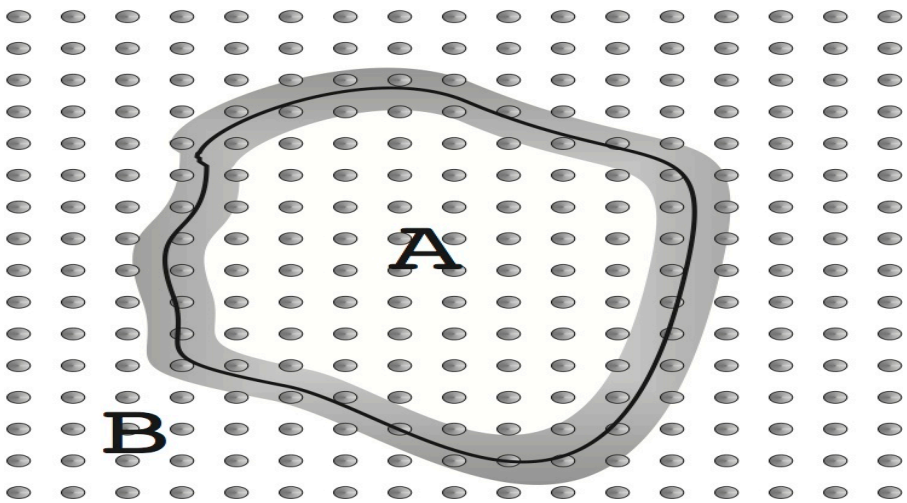
- Quantum PCP Conjecture
  What is it?
  Limitations to qPCP
  New algorithms

- Area Law
  What is it?
  Area Law from Decay of Correlations
  Proof by Quantum Information Theory

Area Law

How complex are groundstates of local models?

Given $|\psi_0\rangle$, how much entanglement does it have?



Area law means the entanglement is proportional to the perimeter of A only (stepping stone to many approximation schemes based on tensor network states (PEPS, MERA, etc))

Why Area Law?

The intuition comes from the fact that correlations decay exponentially in groundstates of *non-critical* models

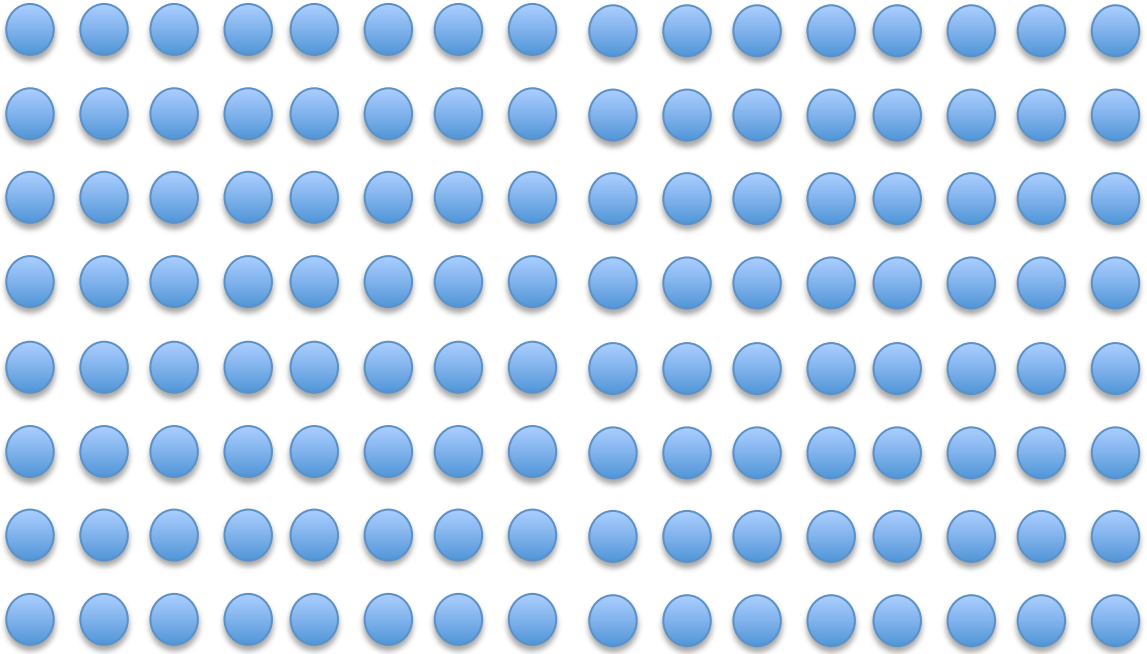
(Hastings '04, Nachtergaele, Sims '06, Koma '06)

Spectral Gap: $\Delta(H) := E_1 - E_0$

Non critical Hamiltonians are *gapped*

Condensed (matter) version of Area Law from Exponential Decay of Correlations

$|\psi\rangle$



- Finite correlation length implies correlations are short ranged

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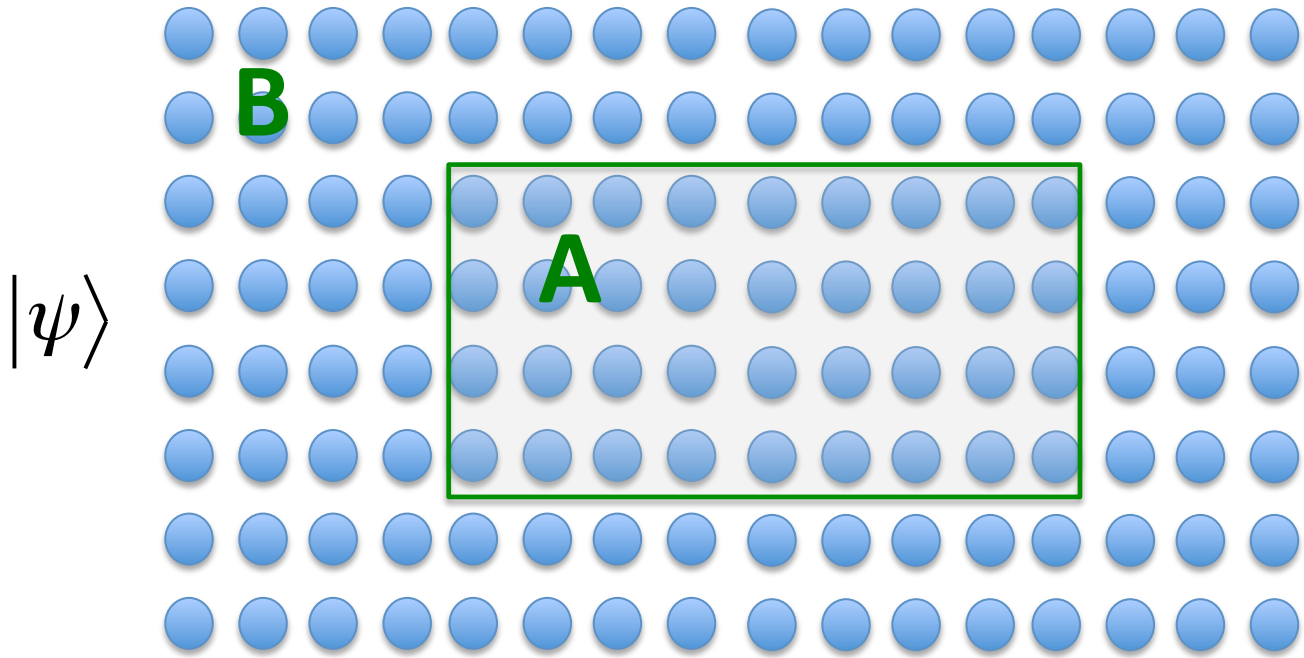

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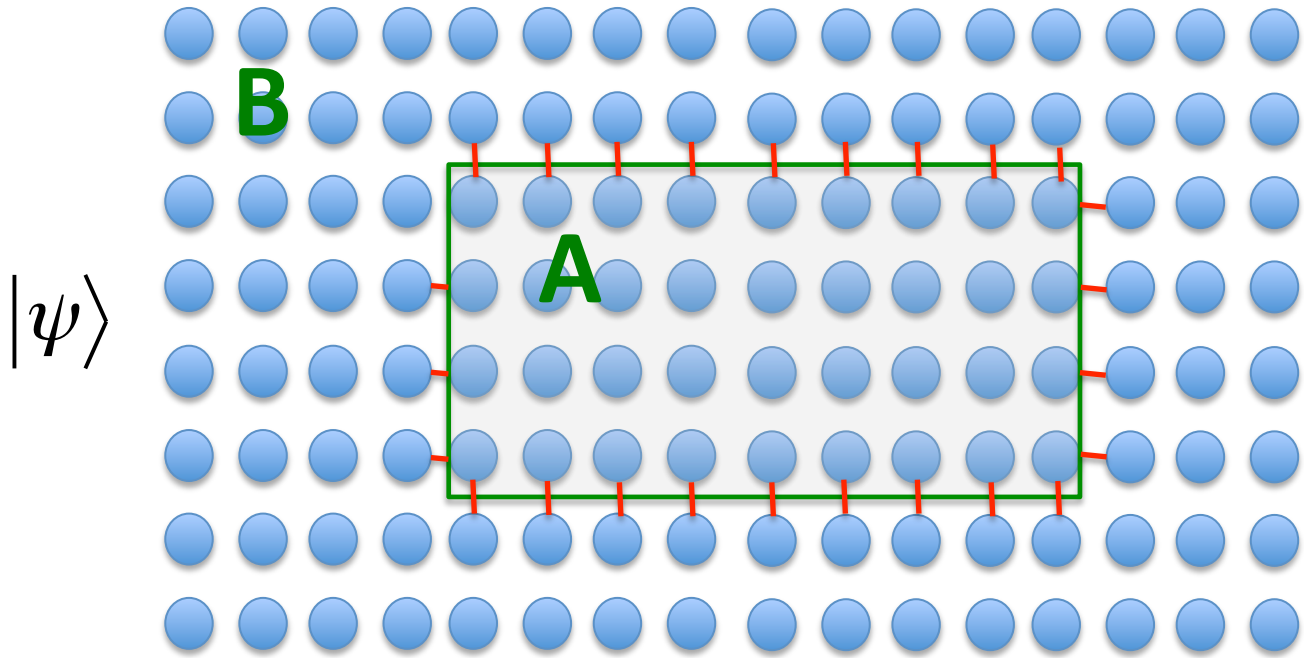

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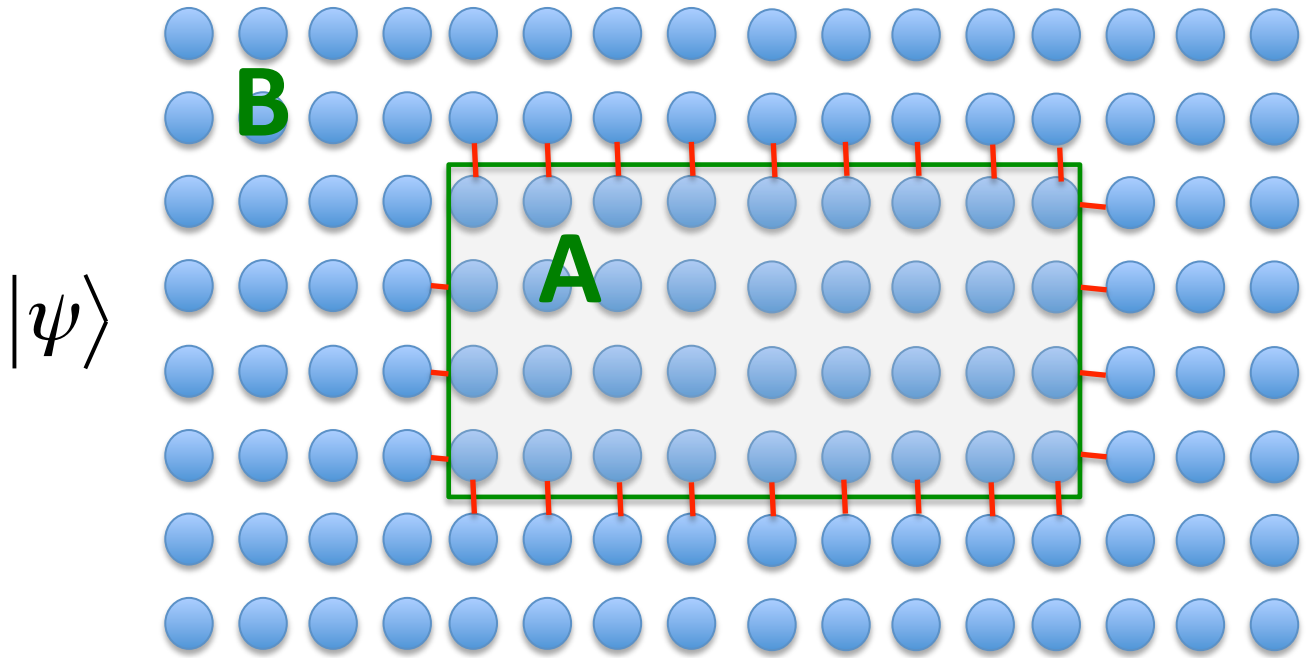
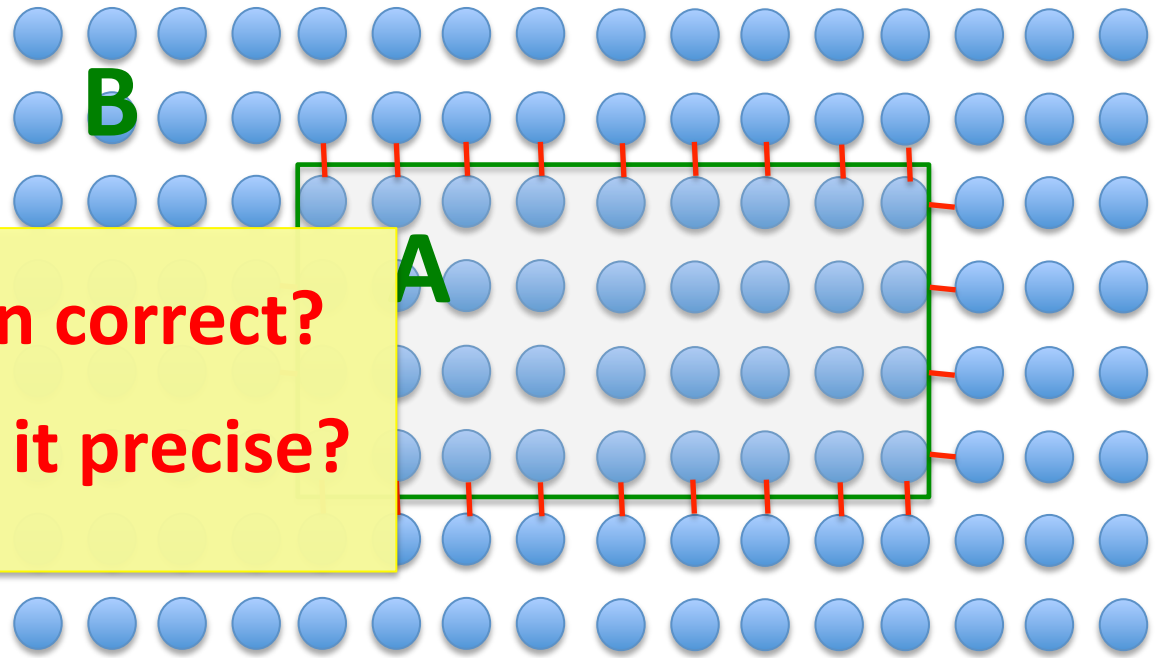


- Finite correlation length implies correlations are short ranged
- A is only entangled with B at the boundary: **area law**

Condensed (matter) version of Area Law from Exponential Decay of Correlations

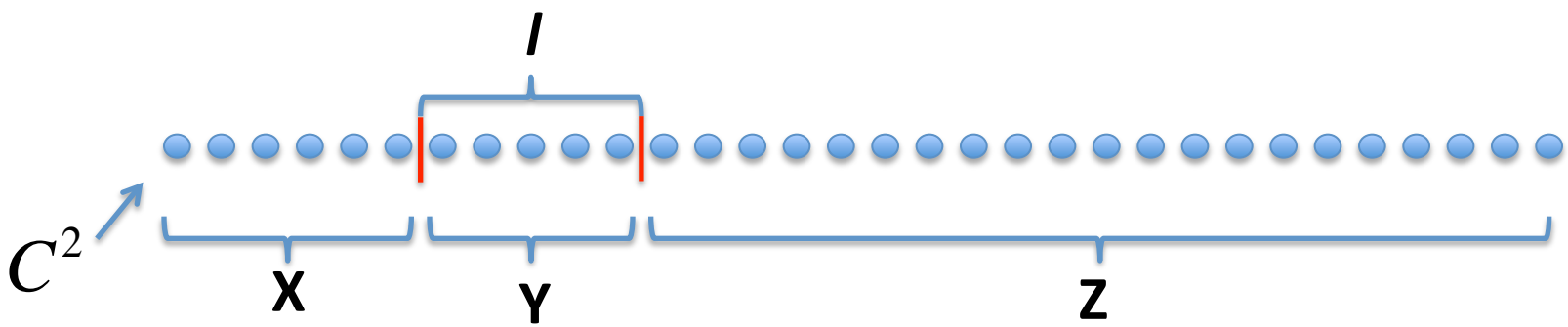


- Is the intuition correct?
- Can we make it precise?

- Finite correlation length implies correlations are short ranged
- A is only entangled with B at the boundary: **area law**

Exponential Decay of Correlations

Let $|\psi\rangle_{1,\ldots,n} \in (C^2)^{\otimes n}$ **be a *n*-qubit quantum state**



Correlation Function:

$$Cor(X:Z) := \max_{\|M\|,\|N\|\le 1} \left| tr\left((M \otimes N)(\rho_{XZ} - \rho_X \otimes \rho_Z) \right) \right|$$

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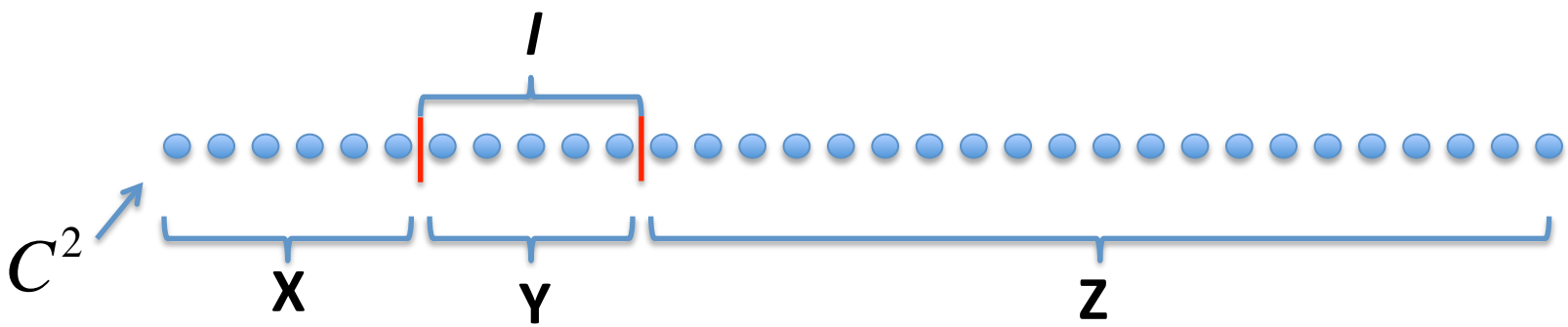

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$$= \max_{\|M\|,\|N\|\le 1} \langle M_X N_Z \rangle_\psi - \langle M_X \rangle_\psi \langle N_Z \rangle_\psi$$

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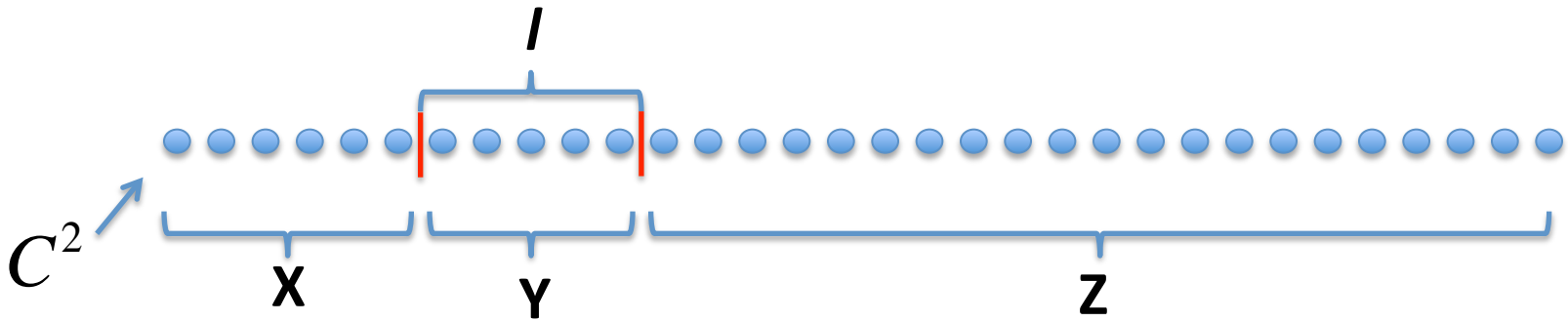

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Exponential Decay of Correlations: There is **ξ > 0** s.t. for all cuts X, Y, Z with |Y| = l

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ξ: correlation length

Area Law in 1D

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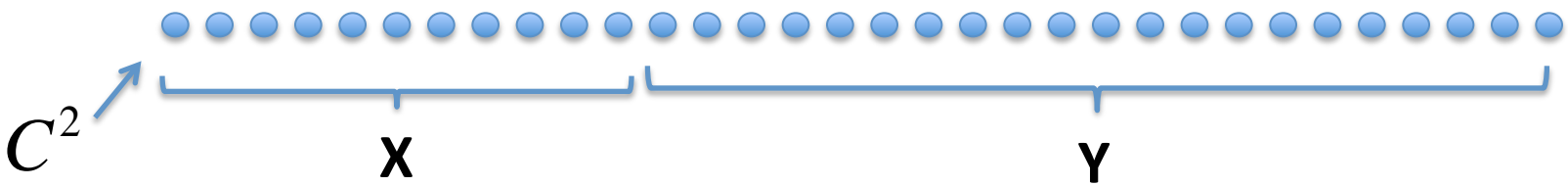

Entanglement Entropy: $E(|\psi_{XY}\rangle) := S(\rho_X)$

Area Law: For all partitions of the chain (X, Y)

$$S(\rho_X) \leq const$$

Area Law in 1D

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$$S(\rho_X) \leq const$$

For the majority of quantum states: $S(\rho_X) \approx size(X) = r$

Area Law puts severe constraints on the amount of entanglement of the state

States that satisfy Area Law

Intuition - based on concrete examples (XY model, harmomic systems, etc.) and general non-rigorous arguments:

Model		Spectral Gap		Area Law
Non-critical	⇔	Gapped	⇒	$S(X) \leq O(\text{Area}(X))$
Critical	⇔	Non-gapped	⇒	$S(X) \leq O(\text{Area}(X)\log(n))$

States that satisfy Area Law

(Aharonov *et al* '07; Irani '09, Irani, Gottesman '09)

Groundstates 1D Ham. with *volume* law $S(X) \geq \Omega(\mathrm{vol}(X))$

Connection to QMA-hardness

(Hastings '07)

Groundstates 1D *gapped* local Ham. $S(X) \leq 2^{O(1/\Delta)}$

Analytical Proof: Lieb-Robinson bounds, etc…

(Wolf, Verstraete, Hastings, Cirac '07)

Thermal states of local Ham. $I(X:Y) \leq O(\mathrm{Area}(X)/\beta)$

Proof from Jaynes' principle

(Arad, Kitaev, Landau, Vazirani '12) $S(X) \leq O(1/\Delta)$

Groundstates 1D *gapped* local Ham.

Combinatorial Proof: Chebyshev polynomials, etc…

Area Law and MPS

Matrix Product State (MPS):

$$|\psi\rangle_{1,\ldots,n} = \sum_{i_1=1}^{2} \ldots \sum_{i_n=1}^{2} tr\left(A_{i_1}^{[1]} \ldots A_{i_n}^{[n]}\right) |i_1,\ldots,i_n\rangle, \quad A_j^{[l]} \in Mat(D,D)$$

D : bond dimension

- Only **nD^2** parameters.
- Local expectation values computed in **poly(D, n)** time
- Variational class of states for powerful **DMRG**

In 1D: Area Law → State has an efficient classical description MPS with D = poly(n)

(Vidal '03, Verstraete, Cirac '05, Schuch, Wolf, Verstraete, Cirac '07, Hastings '07)

Area Law in 1D

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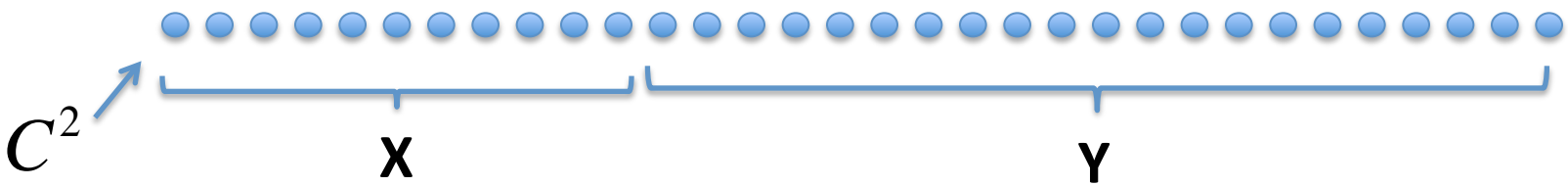

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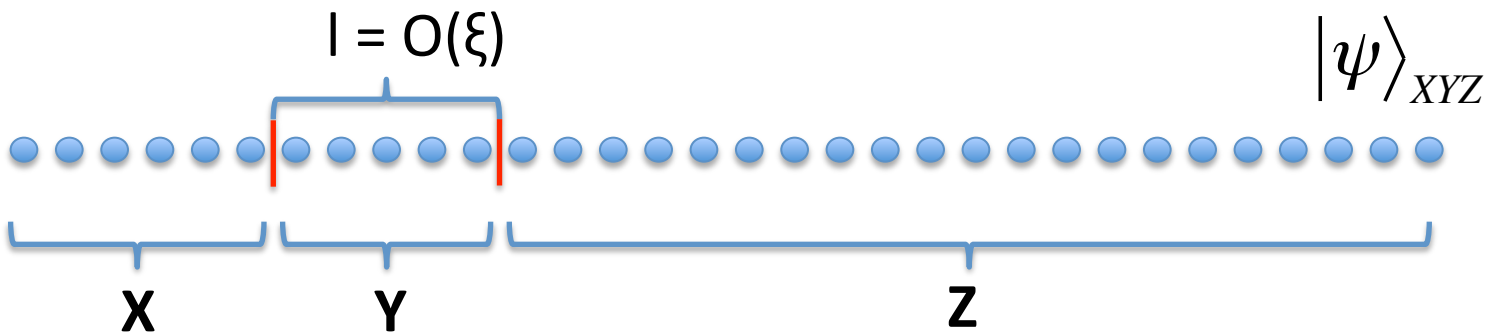

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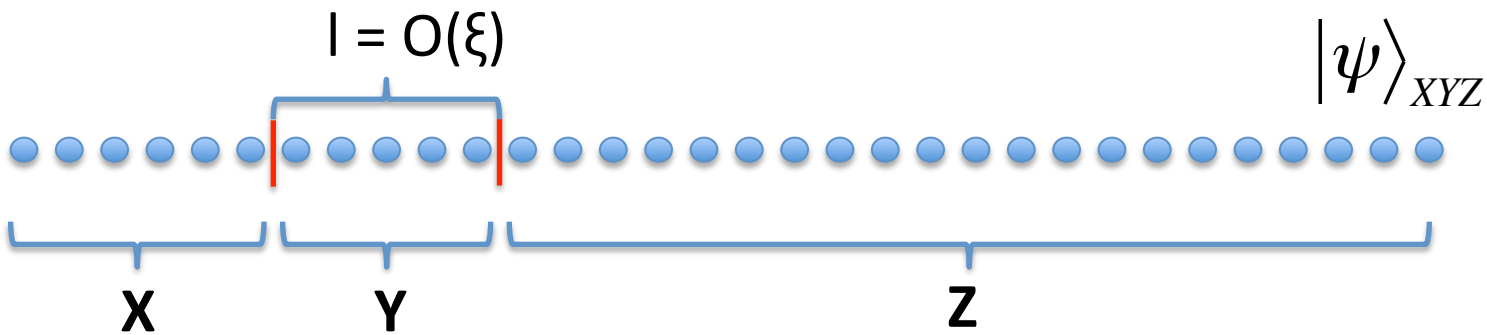

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$|\psi\rangle_{XYZ} \approx_{2^{-l/\xi}} \left(U_{Y_1Y_2 \to Y} \otimes I_{XZ}\right) |\pi\rangle_{XY_1} |\upsilon\rangle_{Y_2Z}$ (by Uhlmann's theorem)

X is only entangled with Y!

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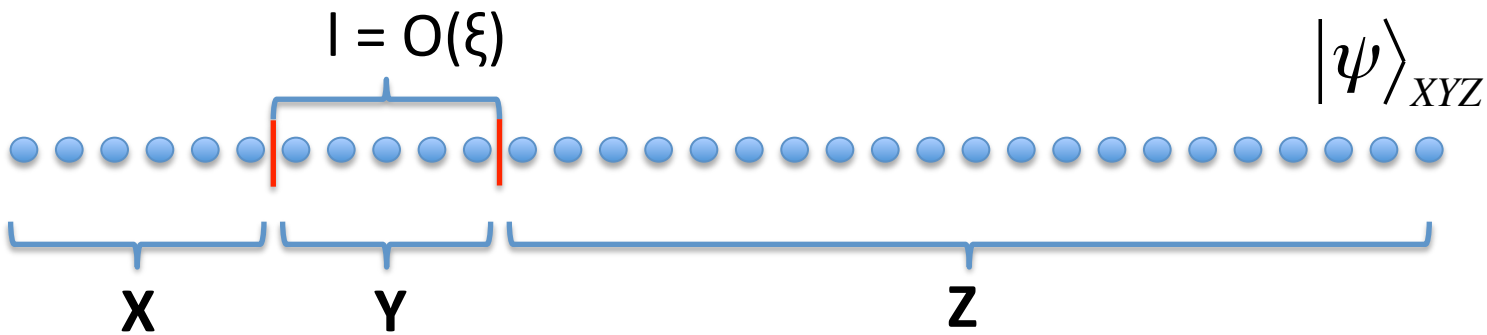

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Uhlmann's thm require 1-norm:

$$\left\|\rho_{AC} - \rho_A \otimes \rho_C\right\|_1 = 2\max_{0<M<I} tr\left(M\left(\rho_{AC} - \rho_A \otimes \rho_C\right)\right)$$

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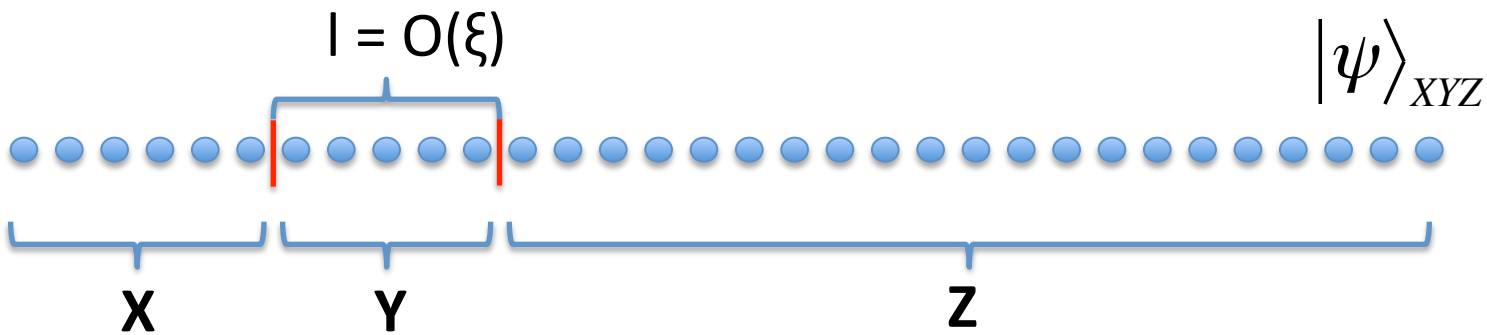

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Data Hiding States

Well distinguishable globally, bur poorly distinguishable locally

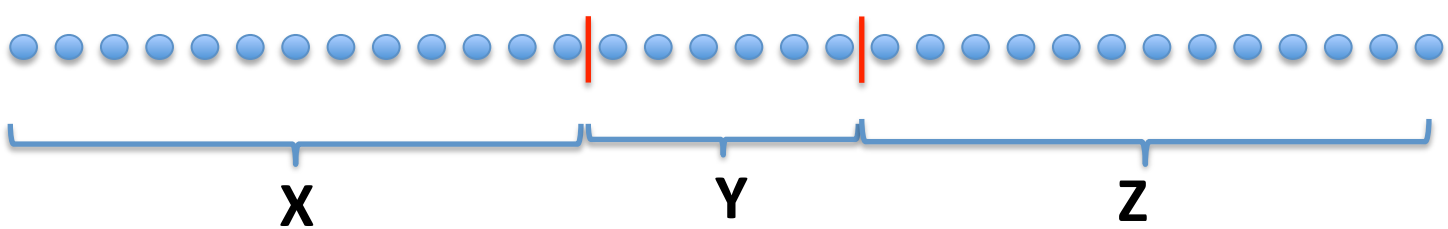
(DiVincenzo, Hayden, Leung, Terhal '02)

Ex. 1 Antisymmetric Werner state $\omega_{AB} = (I - F)/(d^2-d)$

$$Cor(A:B) \le 1/d, \qquad \left\| \omega_{AB} - \omega_A \otimes \omega_B \right\|_1 \approx 1/2$$

Ex. 2 Random state $|\psi\rangle_{XYZ}$ with $|X|=|Z|$ and $|Y|=l$

$$Cor(X:Y) \le 2^{-\Omega(l)}, \qquad S(X) \approx (n-l)/2$$



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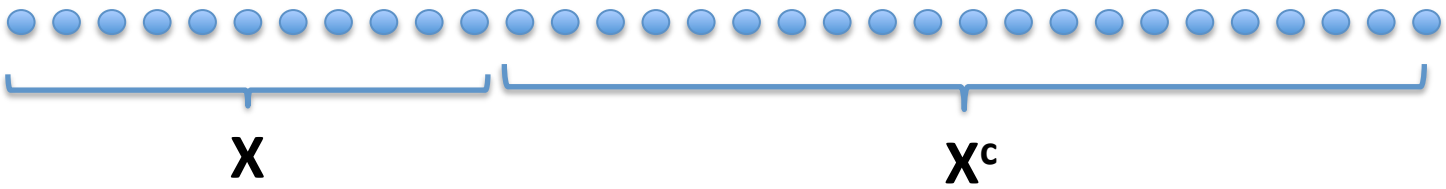
3. Cop out: data hiding states are unnatural; "physical" states are well behaved.

4. We fixed a partition; EDC gives us more…

5. It's an interesting quantum information problem:
   How strong is data hiding in quantum states?

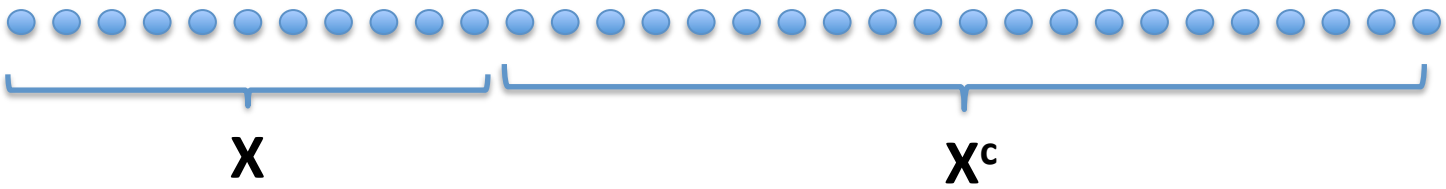
Exponential Decaying Correlations Imply Area Law



Thm 1 (B., Horodecki '12) If $|\psi\rangle_{1,\ldots,n}$ has ξ-EDC then for every X,

$$S(X) \leq 2^{O(\xi \log(\xi))}$$

Efficient Classical Description



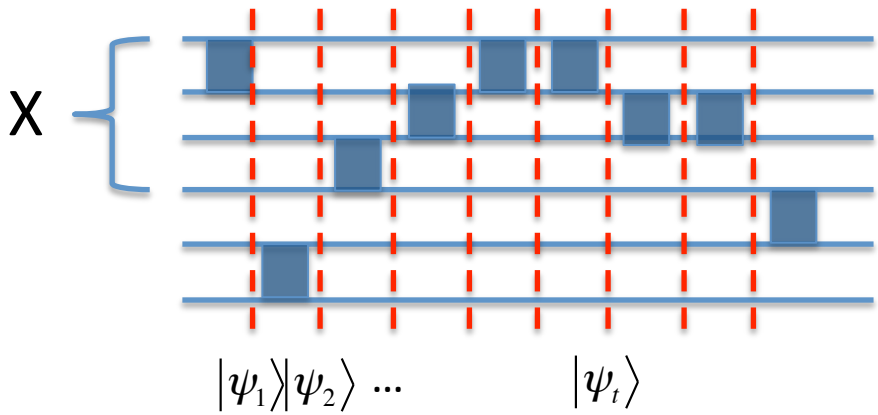
(Cor. Thm 1) If $|\psi\rangle_{1,\ldots,n}$ has ξ-EDC then for every ε>0 there is MPS $|\psi_\varepsilon\rangle$ with poly(n, 1/ε) bound dim. s.t.

$$\left|\langle\psi|\psi_\varepsilon\rangle\right| \geq 1-\varepsilon$$

States with exponential decaying correlations are *simple* in a precise sense

Correlations in Q. Computation

What kind of correlations are necessary for exponential speed-ups?



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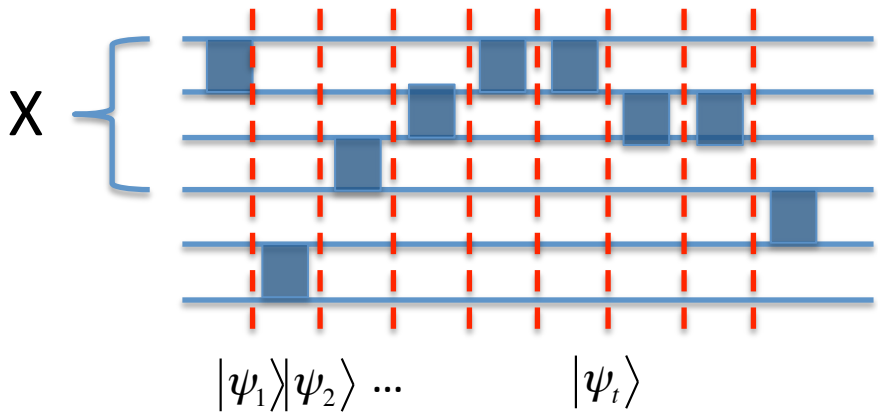
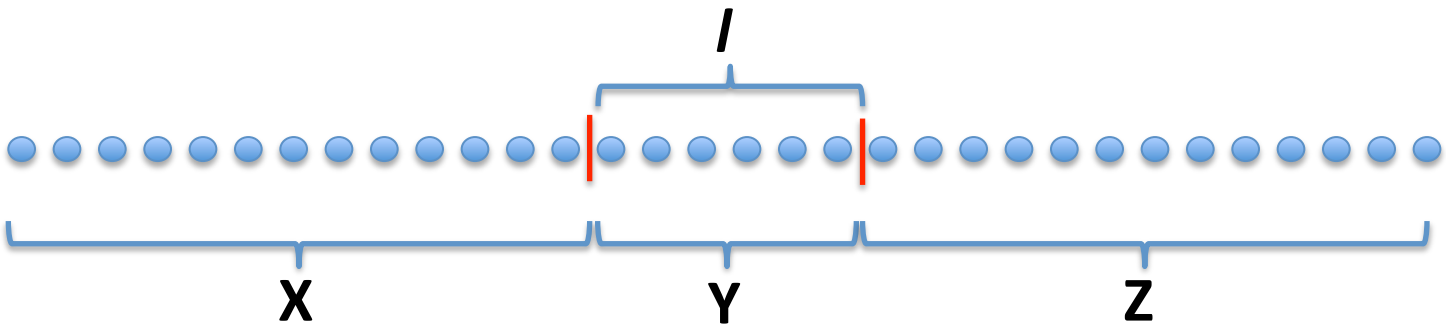


1. (Vidal '03) Must exist *t* and X = [1,r] s.t. $S^{\varepsilon}_{\max}(\rho_{t,X}) \geq n^{\delta}$

2. (Cor. Thm 1) At some time step state must have long range correlations (at least algebraically decaying)
   - Quantum Computing happens in "critical phase"
   - Cannot hide information everywhere

Random States Have EDC?



$|\psi\rangle_{XYZ}$: Drawn from Haar measure

w.h.p, if size(X) ≈ size(Z): $cor(X:Z) \leq 2^{-\Omega(l)}$

and $S(X) \approx S(Z) \approx (n-l)/2$

Small correlations in a *fixed* partition do not imply area law.

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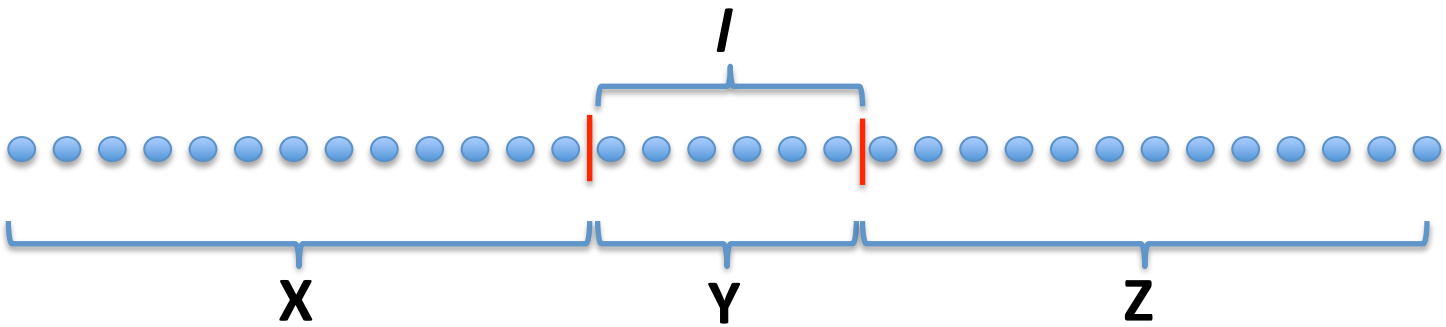

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Small correlations in a *fixed* partition do not imply area law.

But we can **move the partition freely**...

Random States Have Big Correl.

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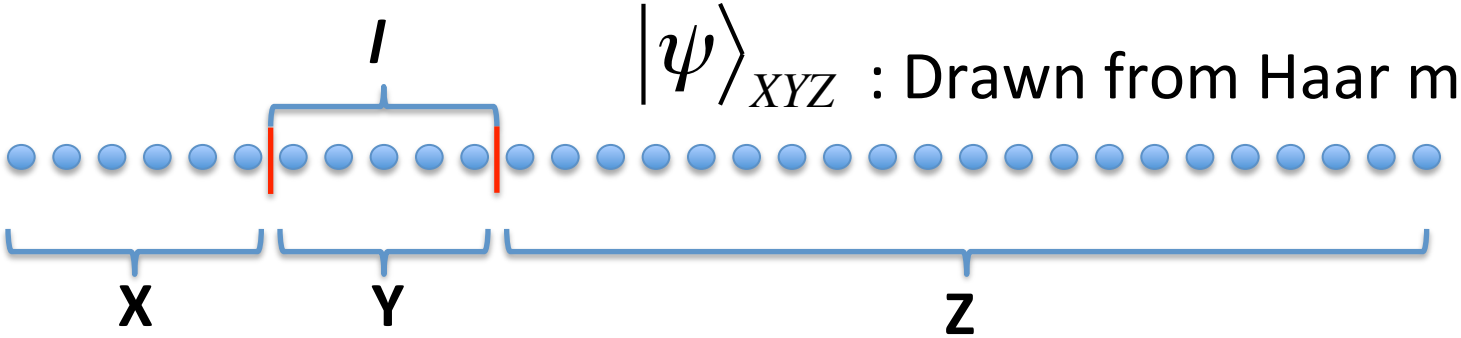

Let size(XY) < size(Z). W.h.p. $\left\|\rho_{XY} - \tau_X \otimes \tau_Y\right\|_1 \leq 2^{-\Omega(n)}$, $\tau_X := \frac{I}{|X|}$

X is **decoupled** from *Y*.

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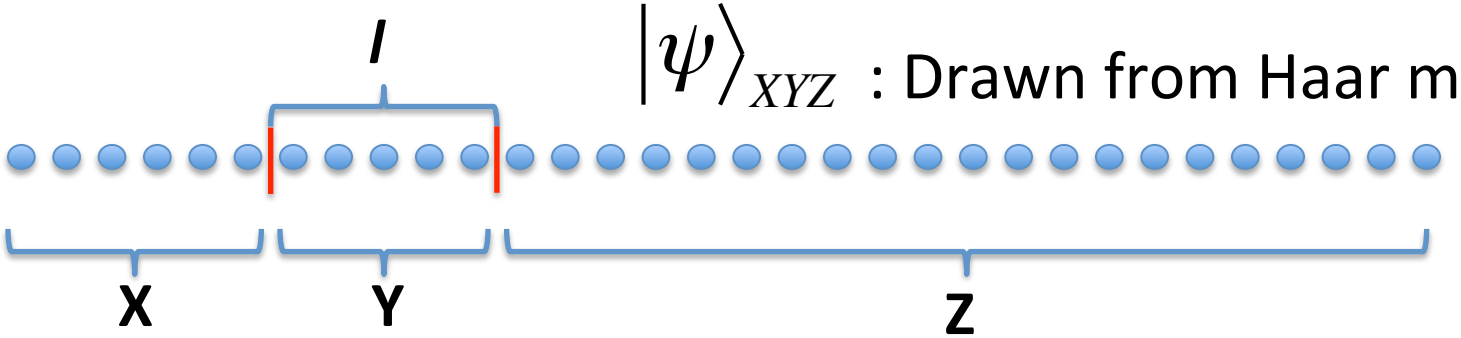

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Extensive entropy, but
also *large* correlations:

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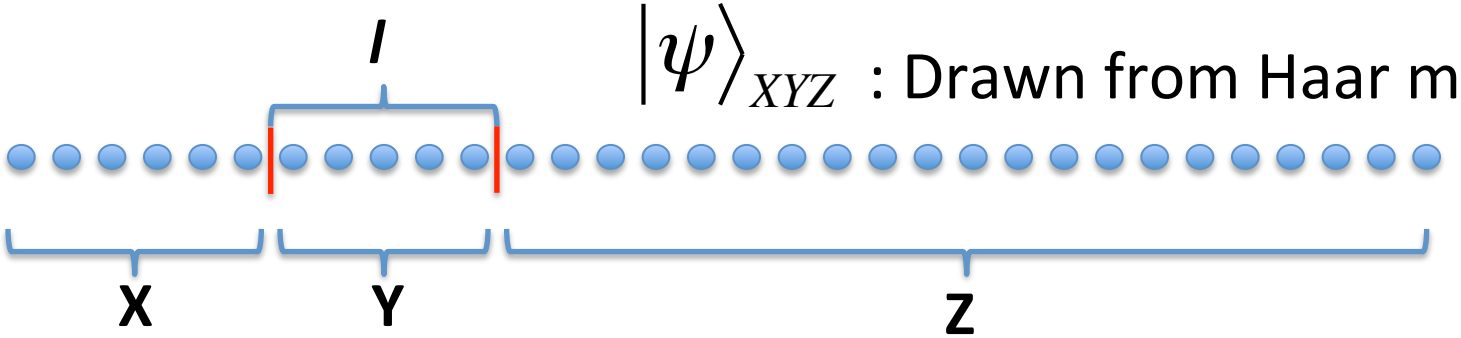

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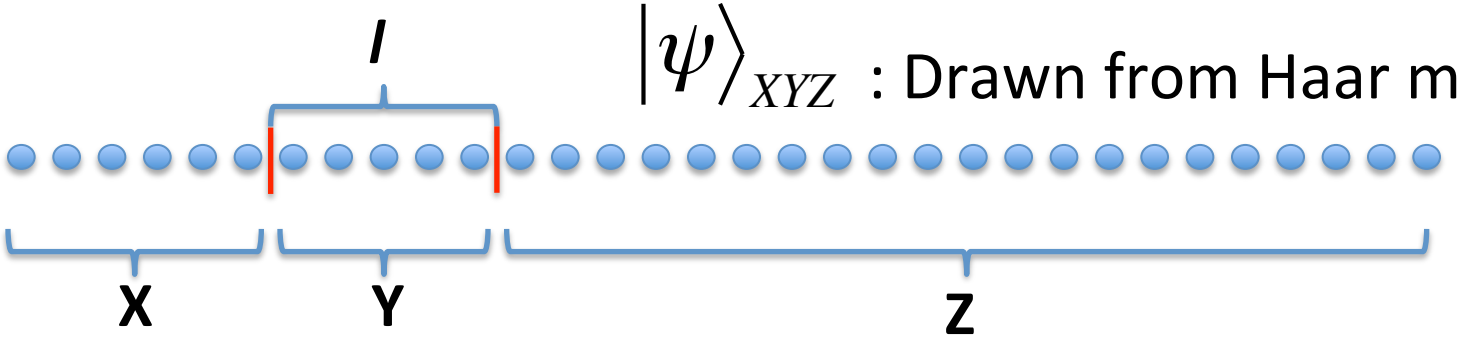
Extensive entropy, but also *large* correlations:

$$U_{Z \to Z_1 Z_2} |\psi\rangle_{XYZ} \approx |\Phi\rangle_{XZ_1} \otimes |\Phi\rangle_{YZ_2}$$

(Uhlmann's theorem)

$|\Phi\rangle_{XZ_1}$: Maximally entangled state between XZ_1.

Random States Have Big Correl.



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X is **decoupled** from *Y*.

Extensive entropy, but also *large* correlations:

$$U_{Z \to Z_1 Z_2} |\psi\rangle_{XYZ} \approx |\Phi\rangle_{XZ_1} \otimes |\Phi\rangle_{YZ_2}$$

(Uhlmann's theorem)

$|\Phi\rangle_{XZ_1}$: Maximally entangled state between XZ_1.

$\mathrm{Cor}(X{:}Z) \geq \mathrm{Cor}(X{:}Z_1) = \Omega(1) \gg 2^{-\Omega(n)}$: **long-range correlations!**

Random States Have Big Correl.

It was thought random states were counterexamples to area law from EDC.

Not true; reason hints at the idea of the general proof:

We show large entropy leads to large correlations by choosing a **random measurement that decouples *A* and *B***

Extensive entropy, but also *large* correlations:

$$U_{Z\to Z_1Z_2}\left|\psi\right\rangle_{XYZ} \approx \left|\Phi\right\rangle_{XZ_1} \otimes \left|\Phi\right\rangle_{YZ_2}$$

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$\left|\Phi\right\rangle_{XZ_1}$: Maximally entangled state between XZ_1.

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The ingredients

We need to analyse decoupling and state merging in a single copy of a state. For that we use

single-shot information theory (Renner *et al* '03, …)

State Merging →	**Single-Shot State Merging** (Dupuis, Berta, Wullschleger, Renner '10) **+ New bound on correlations by random measurements**
Saturation Mutual Info. →	**Saturation max- Mutual Info.** Proof much more involved; based on - Quantum substate theorem, - Quantum equipartition property, - Min- and Max-Entropies Calculus - EDC Assumption

Conclusions

- Quantum Hamiltonian Complexity studies quantum many-body physics through the computational lens

- Two major open problems there are (i) the existence of a quantum PCP theorem and (ii) to prove area laws

- Both are concerned with understanding better entanglement in groundstates.
  Quantum information theory is a powerful tool

Thank you!