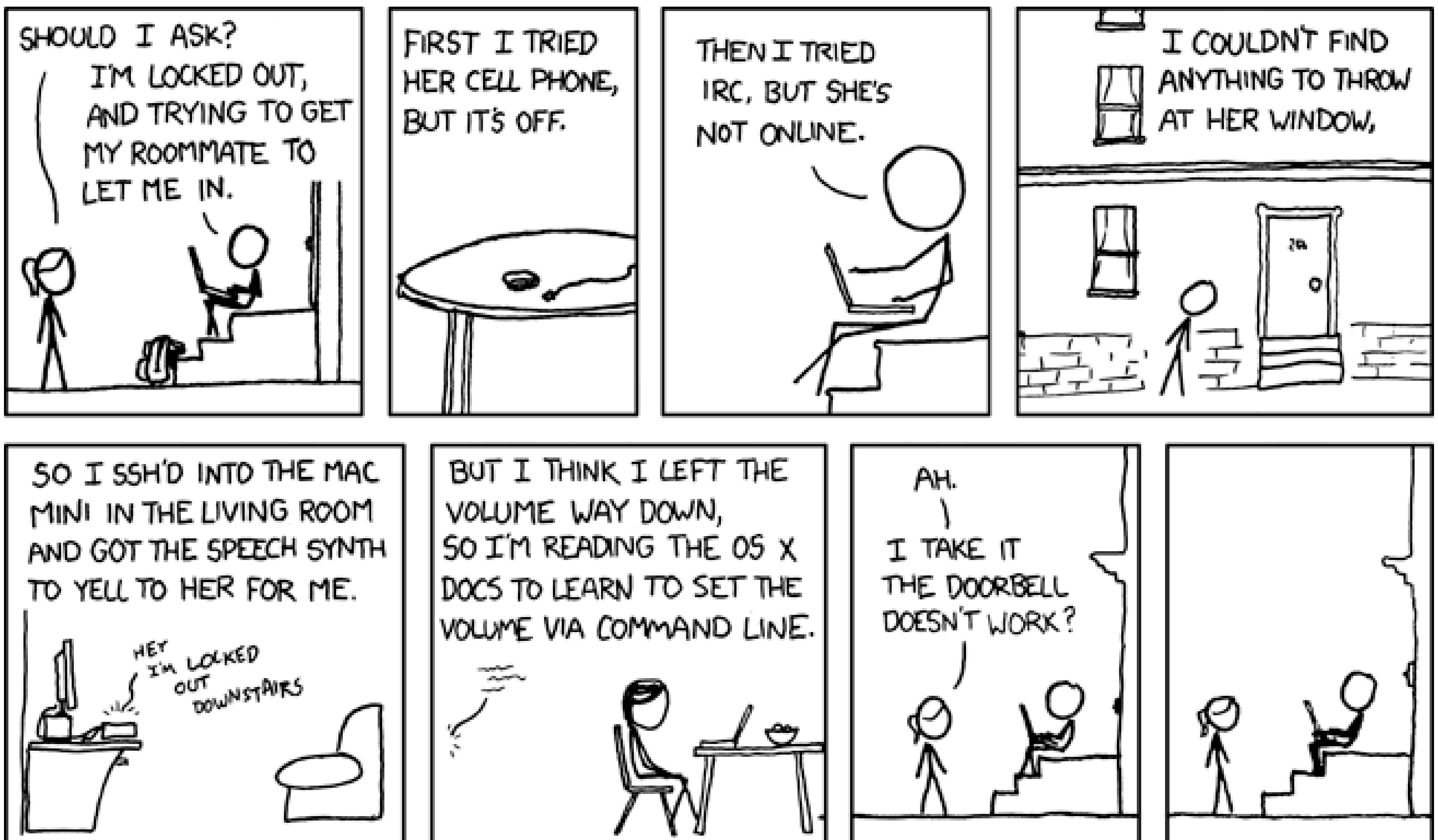
Area Laws for Quantum Many-Body Systems:

Gapped One-Dimensional Quantum Systems are in NP

M. B. Hastings, LANL

Thanks: F. Verstraete, X.-G. Wen, J. Eisert, D. Aharonov



How hard is Quantum Many-Body Theory?

Answer 1 (computer scientists): Really, really hard. Even in 1d, the problem of approximating the ground state energy to an accuracy of 1/poly(N) is QMA-complete (Aharonov, Gottesman, and Kempe and Irani)

Answer 2 (numerical work): Really, really hard. Brute force simulation of a system of N spins takes a time 2^N

Answer 3 (80 years of practice): In some cases, not that hard. Lots of successes like BCS superconductivity theory, density functional theory, etc... plus even success on strongly interacting problems (matrix product methods)

Two algorithms to find ground states:

Exact diagonalization:

Requires exponentially long time. Even finding ground state is typically limited to 30-40 spin-1/2 spins.

Variational Matrix Product (DMRG):

Remarkably successful in 1d. Works especially well for systems with a spectral gap. Accurate because of limited entanglement

Why does it work and how can we improve?

Matrix product methods (including DMRG):

Based on ground state ansatz of the form:

$$\Psi(s_1, s_2, s_3, ..., s_N) = \sum_{\alpha,\beta,\gamma,\delta,...} \Psi_\alpha^{(1)}(s_1) A_{\alpha\beta}^{(2)}(s_2) A_{\beta\gamma}^{(3)}(s_3) ... \Psi_\tau(s_N)$$

$$= \langle \Psi^{(1)}(s_1) | A^{(2)}(s_2) A^{(3)}(s_3) ... | \Psi^{(N)}(s_N) \rangle$$

Spin 1: $s_i = -1, 0, 1$

$$\alpha, \beta, \gamma = 1...k$$

Spin 1/2: $s_i = -1/2, 1/2$

Matrices A are k-by-k matrices. There are NDk^2 variational parameters.

Works extremely well for 1d gapped systems. Why?

Successes of Matrix Product Methods:

- Heisenberg spin chain ground state (White and Huse)
- Extension to periodic boundary conditions (Verstraete, Porras, Cirac)
- Time dependent methods (Vidal)
- Use of time dependent methods to study spin-charge separation (Kollath, Schollwoeck, Zwerger)

Entanglement in Matrix Product States:

$$\begin{aligned}\Psi(s_1,s_2,s_3,...,s_N) &= \sum_{\alpha,\beta,\gamma,\delta,...} \Psi^{(1)}_\alpha(s_1)A^{(2)}_{\alpha\beta}(s_2)A^{(3)}_{\beta\gamma}(s_3)...\Psi_\tau(s_N) \\ &= \langle\Psi^{(1)}(s_1)|A^{(2)}(s_2)A^{(3)}(s_3)...|\Psi^{(N)}(s_N)\rangle\end{aligned}$$

$$\Psi_{mps} = \sum_{\gamma=1}^{k} A(\gamma)\Psi_L(\gamma)\otimes\Psi_R(\gamma) \qquad \Psi_0 = \sum_{\gamma=1}^{2^N} A^0(\gamma)\Psi^0_L(\gamma)\otimes\Psi^0_R(\gamma)$$

Schmidt rank at most k in matrix product state. Approximately true for ground state? Answer: see the area laws later in this talk!

MPS describes a state (can be used variationally or as a certificate)

Given an MPS, we can compute the expectation value of the energy in a time $\mathcal{O}(Nk^3)$ on a classical computer

A formal result on why quantum many-body theory is "easy" (Hastings, this talk) :

The following problem is in NP: Given a one-dimensional Hamiltonian on N qudits such that

- The interaction strength is O(1)
- The interactions are nearest-neighbor
- The local Hilbert space dimension is O(1)

and given the promises that
(1) the gap ΔE between the ground state and first excited state obeys $1/\Delta E = \mathcal{O}(1)$ and
(2) either the ground state energy is less than zero or at least 1/poly(N)

Decide if the ground state energy is zero or less.

Colloquially: approximate the ground state energy to accuracy 1/poly(N)

E_1 $\Omega(1)$

NO

1/poly(N)

E_0

0

YES

This problem is in P: Given a one-dimensional parameter-dependent Hamiltonian $\mathcal{H}_s$ on N qudits such that $\mathcal{H}_0$ is trivial and such that for all $0 \leq s \leq 1$

- The interaction strength is O(1)
- The interactions are nearest-neighbor
- The local Hilbert space dimension is O(1)

and given the promises that

(1) the gap ΔE between the ground state and first excited state obeys $1/\Delta E = \mathcal{O}(1)$ for all $0 \leq s \leq 1$ and

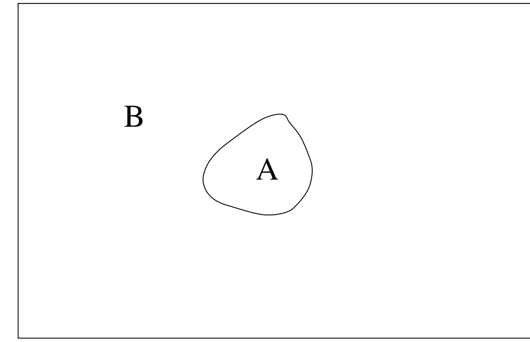
(2) either the ground state energy is less than zero or at least 1/poly(N) at s=1

Decide if the ground state energy at s=1 is zero or less.

Outline:

- What is an area law and why is it important for simulation?
- Correlations vs. Entanglement: Why Quantum Expanders make it tough to prove an area law
- Proof of an area law for one-dimensional systems, and implications for simulation
- A conjecture relating certain correlations to entanglement

Area laws:



How much entanglement between A and B?
Less entanglement means easier to simulate.

$$\Psi_0 = \sum_\alpha A(\alpha)\Psi_A(\alpha) \otimes \Psi_B(\alpha); \quad S = -\sum_\alpha |A(\alpha)|^2 \ln(|A(\alpha)|^2)$$

Von Neumann and Renyi entropy of a density matrix:

$$S = -\mathrm{tr}(\rho \ln(\rho))$$
$$S_\alpha(\rho) = \frac{1}{1-\alpha} \ln(\mathrm{tr}(\rho^\alpha))$$

Entropy of reduced density matrix on a region A for an arbitrary state is of order the volume of A. Area law means that it is of order the surface area.

Relation between area law and existence of MPS for one-dimensional systems:

Bound on Renyi entropy implies bound on truncation error:

$$\epsilon(k) = \sum_{\alpha=k+1}^{\infty} |A(\alpha)|^2$$

$$\log(\epsilon(k)) \leq \frac{1-\alpha}{\alpha}\Big(S_\alpha(\rho) - \log(\frac{k}{1-\alpha})\Big)$$

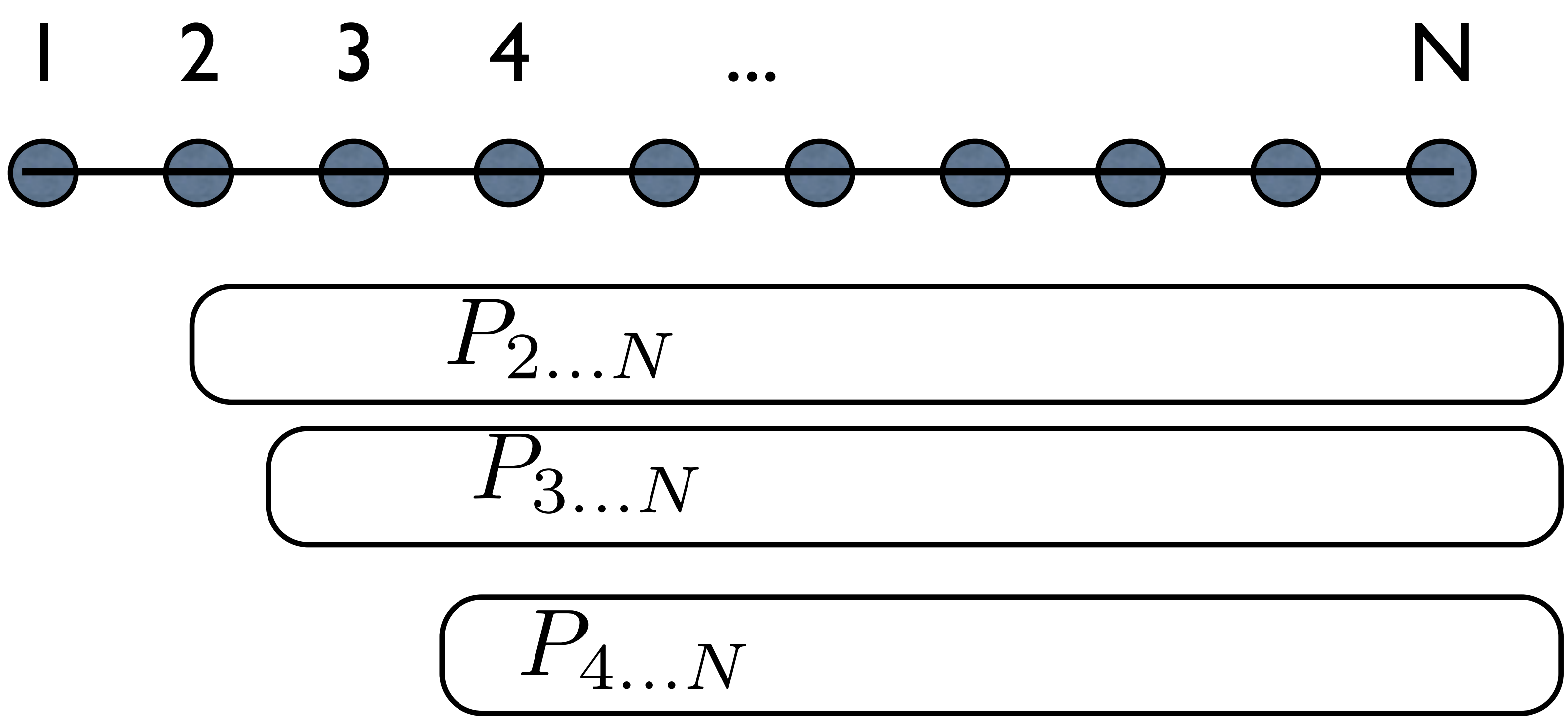
Prove this by minimizing entropy subject to constraint on truncation error. Bound for $\alpha \leq 1$ implies that truncation error scales as 1/poly(k) (Verstraete and Cirac).

Relation between area law and existence of MPS for one-dimensional systems:

We have bound on truncation error on a given cut. Repeat across all cuts. Error is N/poly(k).

$P_{i \dots N}$ projects onto k largest eigenvalues of ground state reduced density matrix on sites i...N

$$\Psi_{mps} = P_{N-1,N} P_{N-2,N} \dots P_{2,N} \Psi_0$$



Handwaving argument for an area law:

Assumptions: short-range Hamiltonian, unique ground state, spectral gap.

- If there is a gap, correlations are short-ranged.
- Therefore, only the degrees of freedom near the surface of A are entangled with the degrees of freedom in B.
- Therefore, there is an area law.

Can we make this rigorous? (why area laws are tricky)

- Given the assumption of a gap and short-range Hamiltonian, it is possible to prove that the correlations are short-range.

M. B. Hastings, PRB 69, 104431 (2004); M. B. Hastings, PRL 93, 140402 (2004).

- However, even in one-dimension, there exist states with short-range correlations but arbitrarily large entanglement. This is based on quantum expanders.

M. B. Hastings, cond-mat/0701055; A. Ben-Aroya and A. TaShma, quant-ph/0702129.

Need to consider more than correlations to prove an area law!

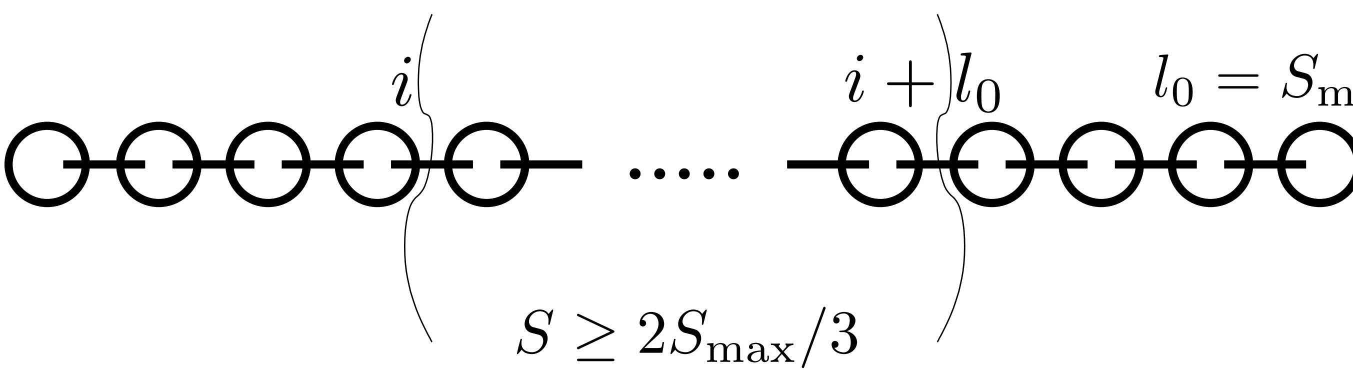
An area law in 1-d

Assumptions: nearest neighbor Hamiltonian with interaction strength bounded by J, finite dimensional Hilbert space D on each site, unique ground state, spectral gap.

$$S \leq S_{\max} = \exp(\mathcal{O}(v/\Delta E))$$ M. B. Hastings, arXiv:0705.2024.

(Sketched) proof:

Suppose not. Then, the entropy is large over a range of cuts of the chain, not just one.



$l_0 = S_{\max}/3\ln(D)$

We will derive a contradiction from this based on relative entropy.

Define S_l to be the maximum entropy of an interval of length l contained in the interval between $i, i + l_0$

Some trivial properties:
$$S_1 \leq \ln(D)$$
$$S_{2l} \leq 2S_l$$

The second inequality cannot be saturated, as then the density matrix on the interval of length 2l factorizes exactly, and so the ground state factorizes, contradicting the assumption of non-vanishing entanglement entropy.

We will go further and use the large entanglement entropy to show: $S_{2l} \leq 2S_l - \mathcal{O}(l\Delta E/v)$

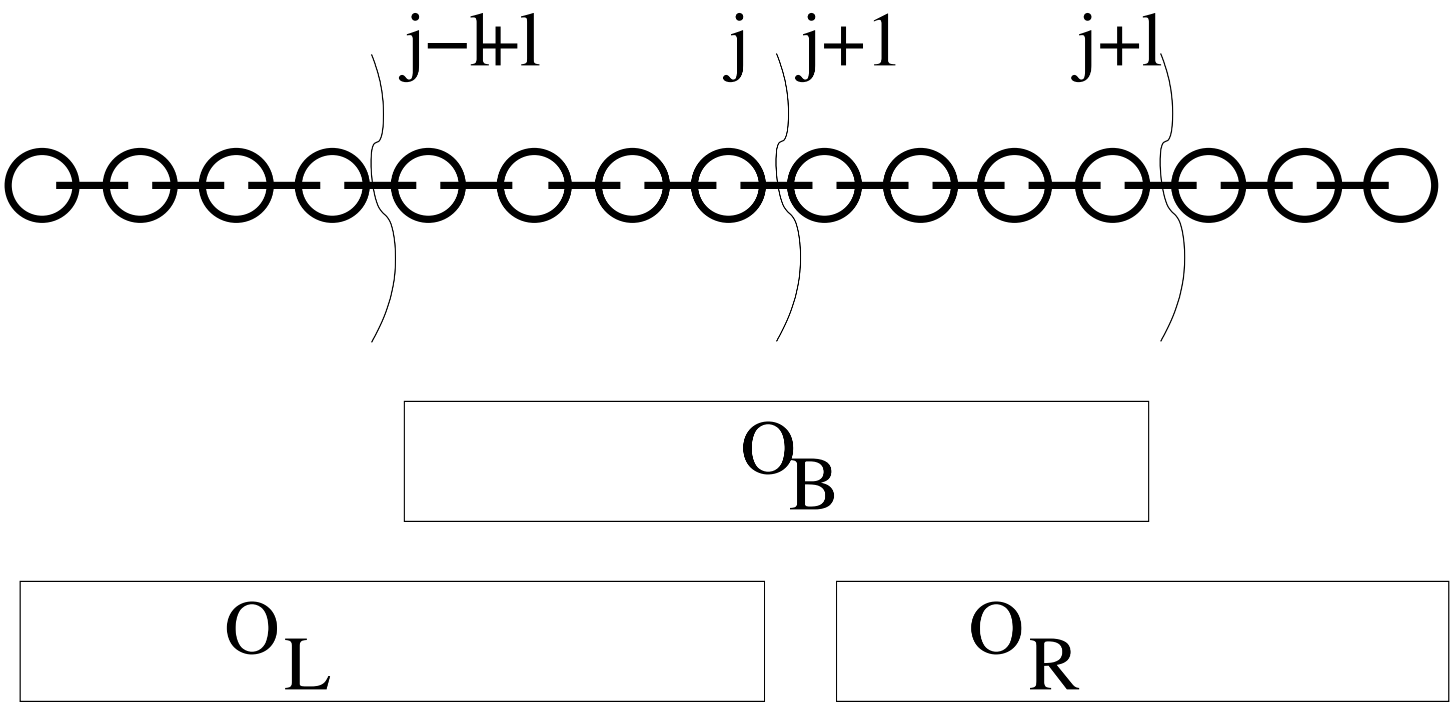
This gives a contradiction for large l and proves the main theorem.

Two lemmas:

1) Given the assumptions before, for any j,l we can define Hermitian, positive definite operators, $O_B(j,l), O_L(j,l), O_R(j,l)$, with operator norms bounded by unity such that

$$\|O_B(j,l)O_L(j,l)O_R(j,l) - |\Psi_0\rangle\langle\Psi_0|\| \leq \exp(-\mathcal{O}(l\Delta E/v))$$

and such that the operators are supported like this:



2) Given the assumptions before, suppose we can find a density matrix ρ which is a mixture of pure states of Schmidt rank k across some cut, such that $\langle \Psi_0 | \rho | \Psi_0 \rangle = P > 0.$

Then, the entropy S across the cut is bounded by

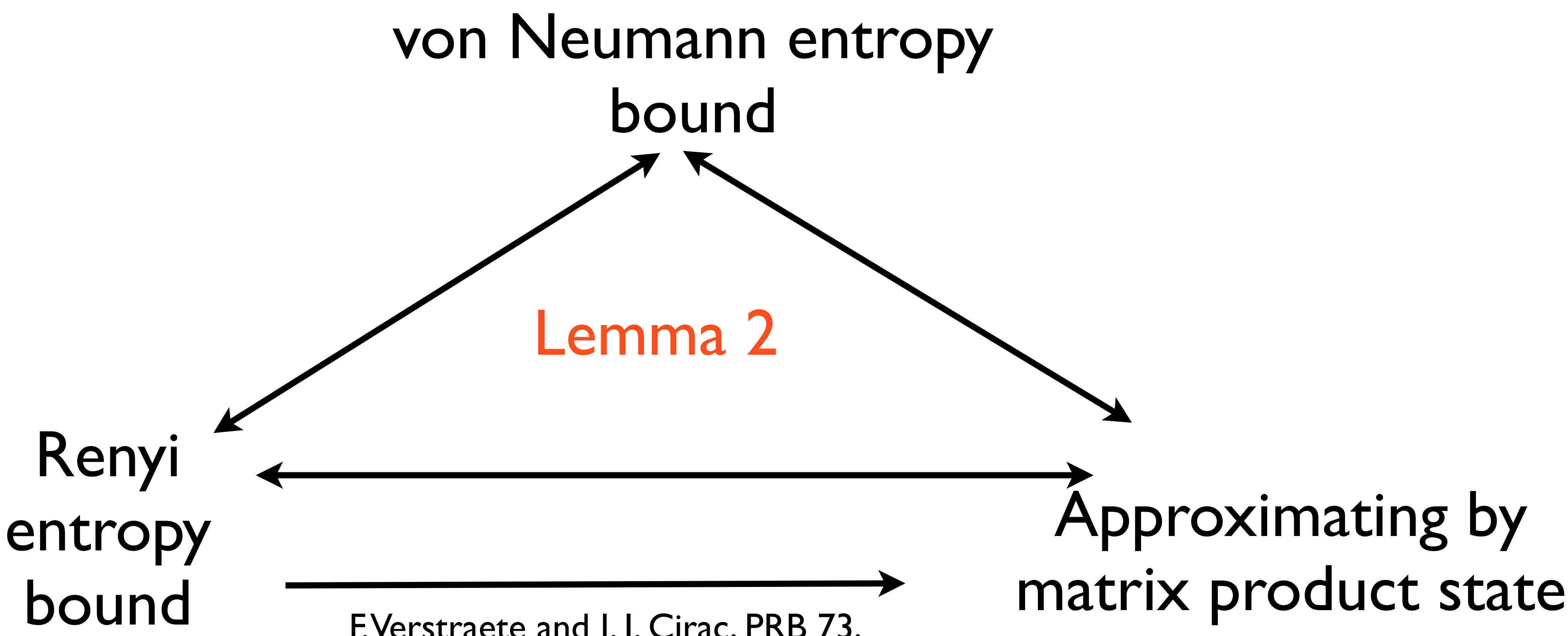
$$S \leq \ln(k) + \mathcal{O}(v/\Delta E) \ln(D) \ln(1/P) + \mathcal{O}((v/\Delta E) \ln(v/\Delta E) \ln(D))$$

Prove this using lemma 1. Can approximate ground state better and better using the state

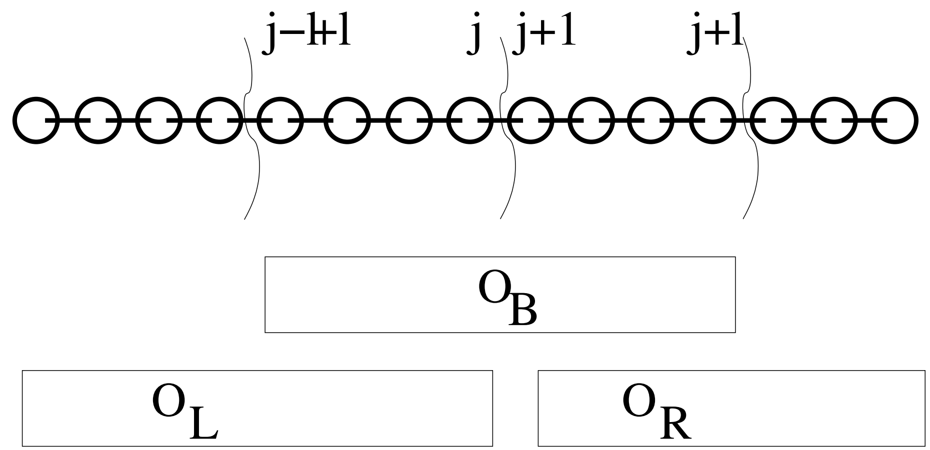
$$O_B(j,l) O_L(j,l) O_R(j,l) \rho O_R(j,l) O_L(j,l) O_B(j,l)$$

for larger and larger l. Each such state has Schmidt rank bounded by kD^{2l}.

Lemma 2 works for Renyi entropies also. Also, Lemma 2 gives ability to approximate ground state by a matrix product state. Finally, an upper bound on Renyi or von Neumann entropy gives a lower bound on the largest Schmidt coefficient across a cut and hence a lower bound on P for k=1 in Lemma 2.



Back to proving the main theorem:



The expectation value $\langle \Psi_0 | O_B(j,l) | \Psi_0 \rangle = \mathrm{tr}(\rho_{j-l+1,j+l} O_B(j,l))$ must be close to unity.

But the expectation value $\mathrm{tr}(\rho_{j-l+1,j} \otimes \rho_{j+1,j+l}\ O_B(j,l))$ must be small since the entropy across the cut is large.

So, by the Lindblad-Uhlmann theorem, the relative entropy $S(\rho_{j-l+1,j+l} || \rho_{j-l+1,j} \otimes \rho_{j+1,j+l})$ must be large.

But this is bounded by $2S_l - S_{2l}$

Putting in the constants gives the desired result.

Is this entropy bound tight?

We have $S \leq \exp(\mathcal{O}(v/\Delta E))$

Conjecture: $S \leq \mathcal{O}(v/\Delta E)$

and maybe even: $S \leq \mathcal{O}(\sqrt{v/\Delta E})$

See talk by Irani and related work by Gottesman and Hastings

Results and Open Questions:

- Given a gap in 1-d, an area law follows.
- Does this apply in higher dimensions?
- Can we tighten the bound? (see talk by Irani and related work by Gottesman and Hastings)

Hamiltonian Complexity Theory:

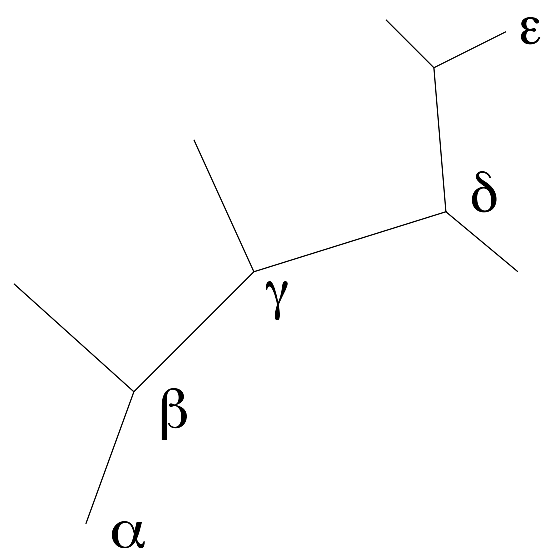
- QMA-hardness of 1d problems: Aharonov, Gottesman, and Kempe and Irani
- Gapped 1d problems are in NP: Hastings (this talk)
- Simulation of dynamics in 1d for log time is in P: Osborne
- Hardness of finding MPS ground states (NP-complete with 1/poly gap and poly bond dimensions): Schuch, Cirac, and Verstraete

Sidetrack: a conjecture

Matrix product state:

$$\Psi(s_1, s_2, ...s_N) = \sum_{\alpha,\beta,...} A_{\alpha,\beta}(s_1) A_{\beta,\gamma}(s_2) A_{\gamma,\delta}(s_3)...$$

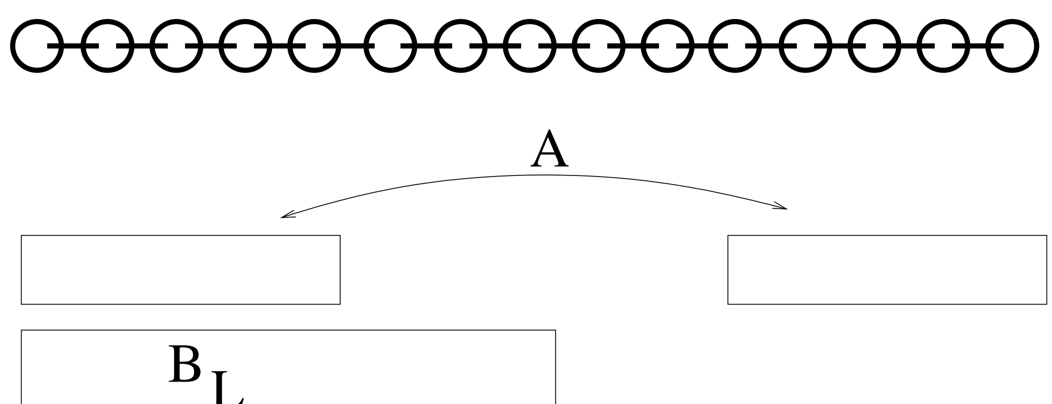
Expander graph to get large entropy for mps but small correlations:



Sidetrack: a conjecture (continued)

This particular state cannot be ground state of local Hamiltonian as there is no mutual information between nearby sites. But also, it has a certain kind of correlation: knowledge of α, ϵ gives knowledge of γ.

Not only do two point correlations decay exponentially in gapped, local systems, but also correlations of operators A,B where B is diagonal in Schmidt basis and support is like this:



Sidetrack: a conjecture (continued)

We conjecture that exponential decay of these more general correlations implies a bound on entropy for an mps. See arXiv:0705.2024.

Expand, but not too fast!