How Hard is Quantum Many-Body Theory?

M. B. Hastings
T-13, Complex Systems Group
Los Alamos National Laboratory

Thanks: X.-G. Wen, F. Verstraete, T. Koma, S. Bravyi

Outline:

- Algorithm overview: perturbation theory, DMRG (matrix product), exact diagonalization.
- Computational complexity classes. Difficulty of the problem depends on entanglement.
- Easy problems (P or almost polynomial): perturbing a system. Can find efficient representation of ground state.
- Harder problems: (NP) 1d gapped systems. Area laws for quantum entanglement imply an efficient representation exists.
- Very hard: (QMA-complete) 1d gapless.

Some common algorithms:

Exact diagonalization:

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

Perturbation theory:

$$H = H_0 + \lambda V$$

$$E_n = E_n^{(0)} + \lambda \langle \Psi_n^{(0)} | V | \Psi_n^{(0)} \rangle + \lambda^2 \sum_{k \neq n} \frac{|\langle \Psi_k^{(0)} | V | \Psi_n^{(0)} \rangle|^2}{E_n^{(0)} - E_k^{(0)}} + \ldots$$

Different ways to compute the terms. Feynman diagrams (physics). Moller-Plesset (quantum chemistry).
Convergence of series?

Matrix product methods (including DMRG):

Based on ground state ansatz of the form:

$$\Psi_(s_1, s_2, s_3, ...) = \sum_{\alpha,\beta,\gamma,\delta,...} A^{(1)}_{\alpha\beta}(s_1) A^{(2)}_{\beta\gamma}(s_2) A^{(3)}_{\gamma\delta}(s_3) ....$$

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

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

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

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

Works extremely well for 1d gapped systems. Why?

Complexity classes:

P: algorithm exists to solve in polynomial time (in the problem size, N).

Examples:

- Sort a list of N numbers
- Find the ground state of a ferromagnetic Ising model of N spins with arbitrary, position-dependent magnetic field
- Determine if an N bit number is prime (but not, as far as we know, factoring it!)

BQP: polynomial algorithm on a quantum computer. Example: factoring.

NP: a yes-no decision problem.
If yes, can check proof in polynomial time.

Example:

- Does a frustrated Ising model $H = \sum J_{ij}\sigma_i\sigma_j$ have a state with energy less than or equal to E, for some E? Proof if yes: just give the configuration of spins.

Also NP-complete: if solvable in polynomial time, then every problem in NP is solvable in polynomial time.
Widely believed impossible!

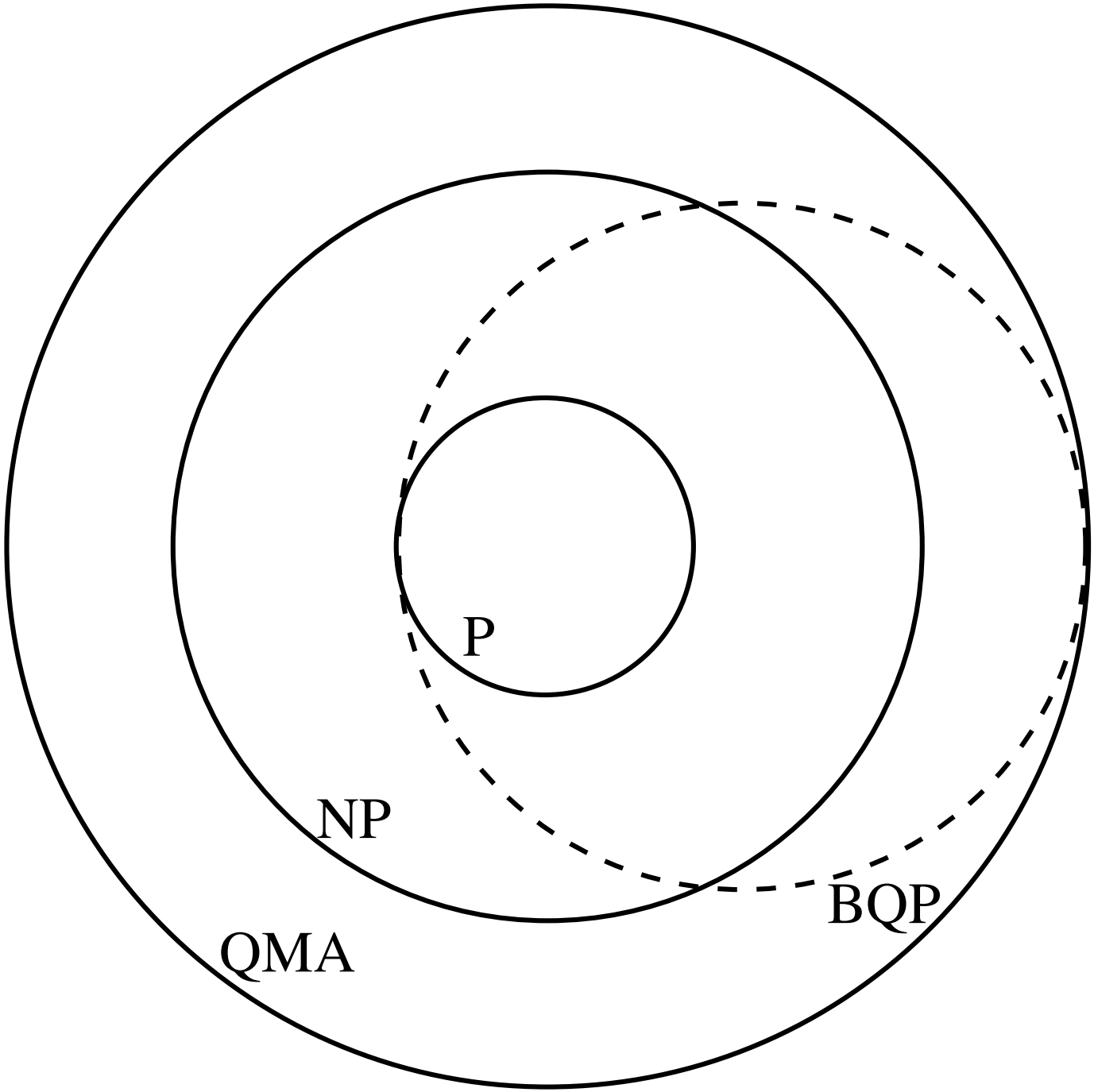
QMA: yes-no decision problem. If yes, can check proof in polynomial time on a quantum computer, with probability at least 2/3 of being right.

- Does a quantum Hamiltonian have a ground state of energy E or less, given a promise that if not, then the energy is at least E+1/N^4. Proof if yes: give the ground state.

Also QMA-complete: if solvable in polynomial time on a quantum computer, then every problem in QMA is solvable in polynomial time. Also believed impossible!

Kitaev 02; Aharonov, Gottesman, Kempe 07; Irani 07.

Relation of complexity classes:



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Perturbation of gapped, decoupled Hamiltonian is in P:

$$H = H_0 + \lambda V \qquad H_0 = \Delta E \sum_i S_i^z$$

$$E_n = E_n^{(0)} + \lambda \langle \Psi_n^{(0)} | V | \Psi_n^{(0)} \rangle + \lambda^2 \sum_{k \neq n} \frac{|\langle \Psi_k^{(0)} | V | \Psi_n^{(0)} \rangle|^2}{E_n^{(0)} - E_k^{(0)}} + \ldots$$

Time to compute m-th coefficient is exponential in m:

Coupled cluster (Bravyi, DiVincenzo, Loss 07)

Rayleigh-Schrodinger (Hastings 07)

Perturbation of gapped, interacting Hamiltonian is exp(polylog(N))

Quasi-adiabatic continuation (Hastings-Wen 05; Osborne 07)

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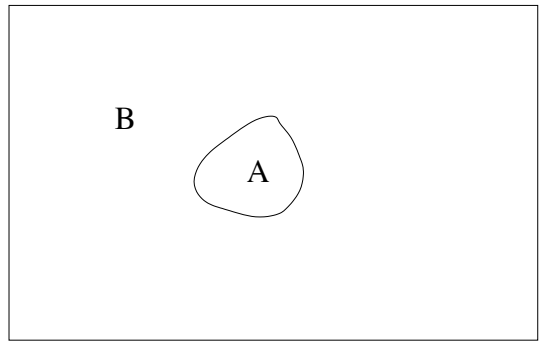
Entanglement in Matrix Product States:

$$\Psi_(s_1, s_2, s_3, ...) = \sum_{\alpha,\beta,\gamma,\delta,...} A^{(1)}_{\alpha\beta}(s_1) A^{(2)}_{\beta\gamma}(s_2) A^{(3)}_{\gamma\delta}(s_3) ....$$

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

Schmidt rank at most k in matrix product state. Approximately true for ground state?

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 for an arbitrary state is of order the volume of A.
Area law means that entropy is of order the surface area.

Handwaving argument for an area law:

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

- Gap implies short-range correlations.
- 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)

- Assuming a gap and short-range Hamiltonian, can prove that the correlations are short-range.

M. B. Hastings, PRB 2004;
M. B. Hastings, PRL 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, PRB 2007;
A. Ben-Aroya and A. TaShma, quant-ph/0702129.

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

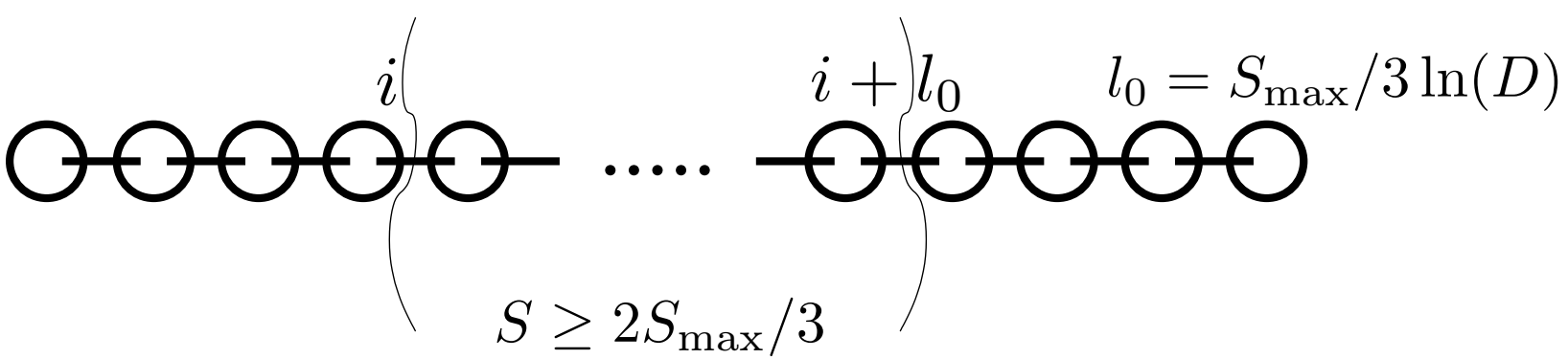
An area law in 1-d

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, JSTAT 2007.

(Sketched) proof:

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



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 $i, i+l$

Some trivial properties:

$$S_1 \leq \ln(D)$$
$$S_{2l} \leq 2S_l$$

Araki, Lieb 1970

If second inequality saturates, $\rho_{i,i+2l} = \rho_{i,i+l} \otimes \rho_{i+l+1,i+2l}$
Then ground state factorizes, contradicting assumption of non-vanishing entanglement entropy.

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

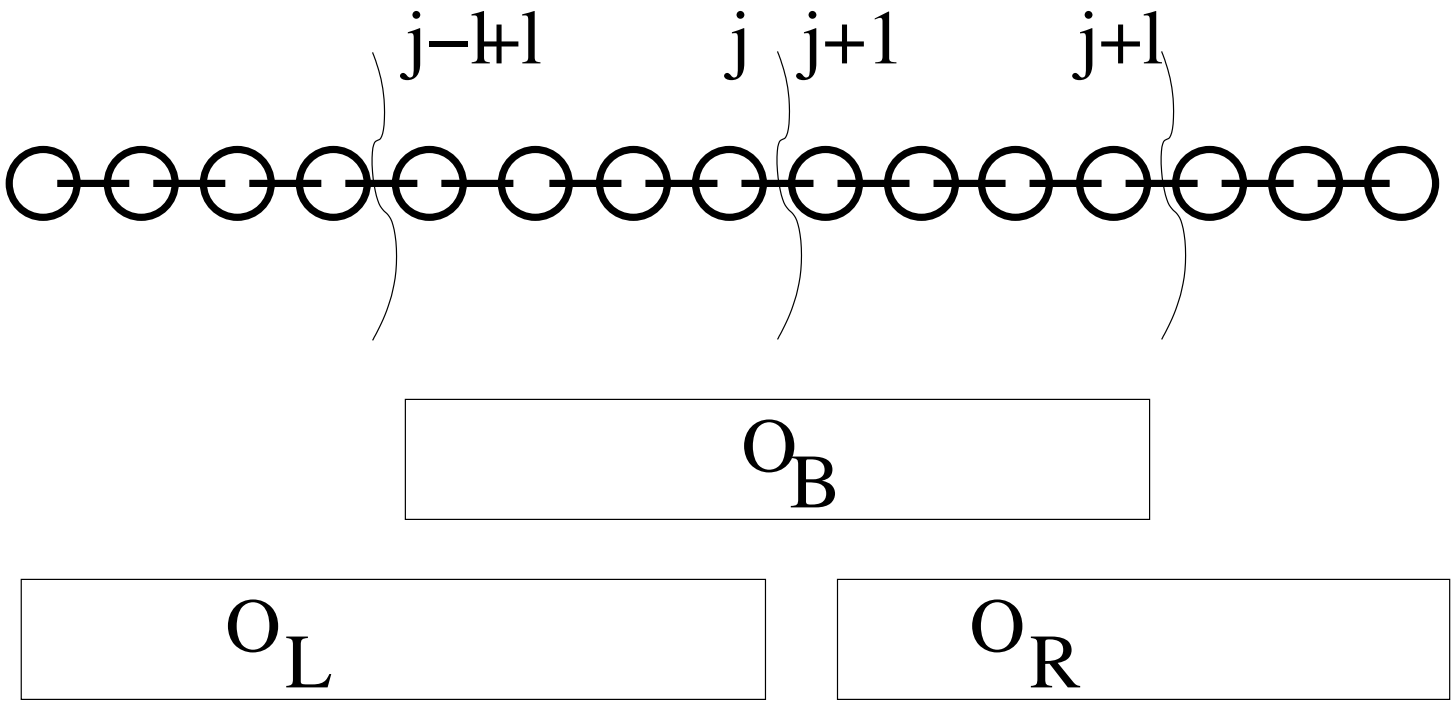
This gives a contradiction for large l and proves the main theorem.

Two lemmas:

1) Given assumptions above, 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 assumptions above, suppose exists factorized density matrix $\rho = \rho_L \otimes \rho_R$ such that

$$\langle \Psi_0 | \rho | \Psi_0 \rangle = P > 0.$$

Then, the entropy S across the cut is bounded by

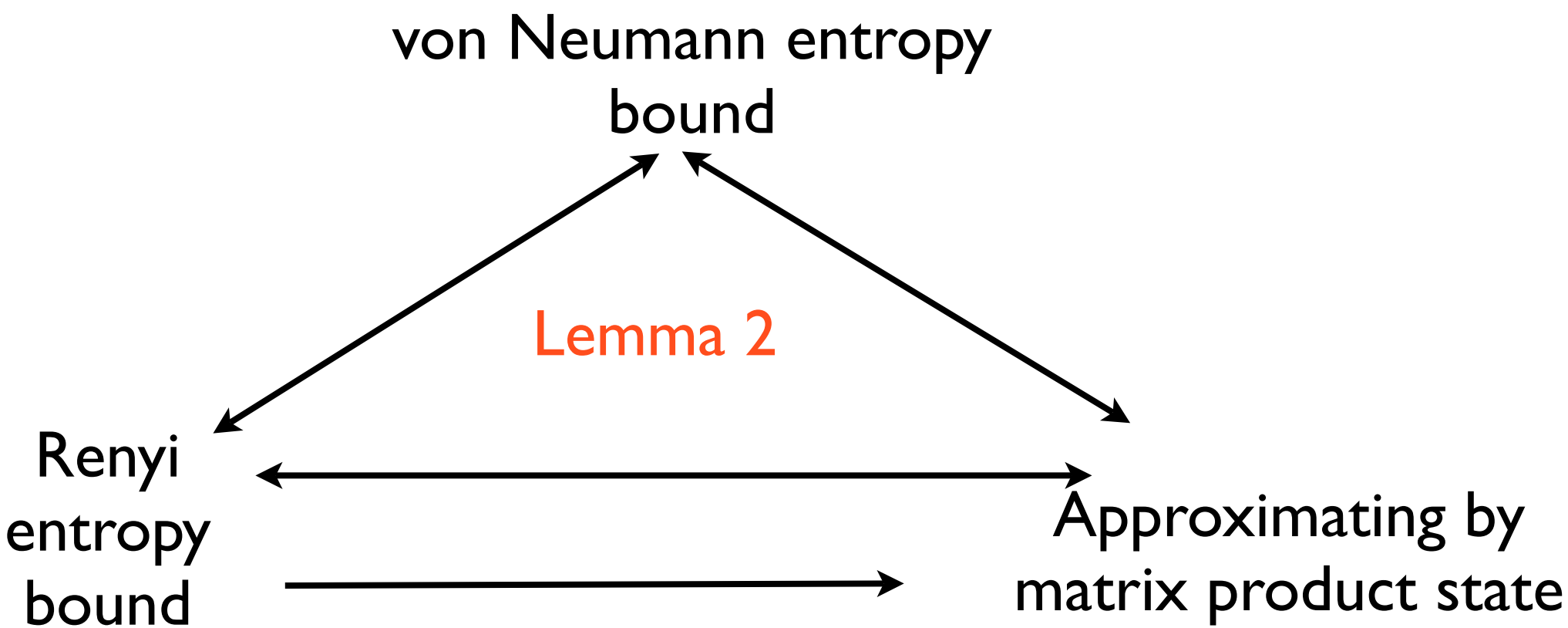
$$\begin{aligned} S &\leq \mathcal{O}(v/\Delta E) \ln(D) \ln(1/P) \\ &+ \mathcal{O}(v/\Delta E) \ln(v/\Delta E) \ln(D) \end{aligned}$$

Prove this using lemma 1. Approximate ground state with

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

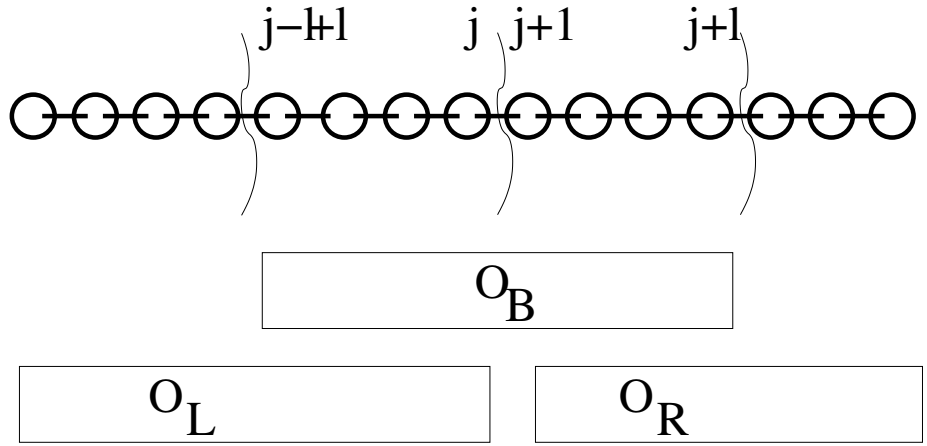
Approximation improves with larger l. State is mixture of pure states with Schmidt rank D^{2l}.

- Lemma 2 works for Renyi entropies also.
- Lemma 2 enables approximating ground state by matrix product state.
- Upper bound on Renyi or von Neumann entropy gives lower bound on the largest Schmidt coefficient across a cut and hence lower bound on P in Lemma 2.



F. Verstraete and J. I. Cirac, PRB 2006.

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 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 $S_{2l} - 2S_l$.

Putting in the constants gives the desired result.

1d gapped systems are in NP

- Represent ground state as matrix product state $k \gtrsim \exp(S)$
- Hard to find matrix product state in certain cases (NP-complete, Eisert 2006)
- In practice, DMRG or variational matrix product methods work well.

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What if no gap in 1d? How hard is it to compute ground state energy to accuracy 1/N^4?

If gap vanishes at quantum critical point described by conformal field theory, Renyi entropy is log(N).
Problem is still in P!
Examples: spin-1/2 Heisenberg chain, 1d transverse field Ising model, etc...

Verstraete, Cirac 05

But with arbitrary interactions the problem is QMA-complete. So, there is probably no hope of an efficient algorithm in general.

Aharonov, Gottesman, Kempe 07; Irani 07.

Other methods:

- Quantum Monte Carlo
- Density functional theory: Hohenberg-Kohn theorem implies exact functional exists. But, unless NP=QMA, exact functional is not tractable.
- Coupled cluster method

Conclusion:

- The difficulty of solving different problems seems to be closely related to the entanglement.
- Can we make the area law bound tight?
- What happens in higher dimensions to the area law?
- Do matrix product states work well in higher dimensions? Are there other better algorithms?