The Computational Complexity of Ground States of Quantum Systems

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Computing Properties of Ground States

The problem:

Given a Hamiltonian $\mathcal{H}$, determine properties of the ground state.
Energy, magnetization, etc...

Basic problem in physics and quantum chemistry.
Often consider Hamiltonians with local two-body interactions:

$$\mathcal{H} = \sum_{ij} h_{ij}$$

Exact Diagonalization

Brute force diagonalization of the Hamiltonian using Lanczos. Effort scales as Hilbert space dimension

$$D \sim 2^N$$

Practical only for small systems. Even using symmetry, $30 - 40$ spins is the limit.

Quantum Monte Carlo

Partition function:

$$Z = \exp[-\beta\mathcal{H}]$$

For large β, gives ground state:

$$\beta \to \infty, \quad Z \to \exp[-\beta E_0]$$

$$\exp[-\beta\mathcal{H}] = 1 - \beta\mathcal{H} + \frac{\beta^2}{2}\mathcal{H}^2 - \ldots$$

If in some product basis, $\mathcal{H}$ has all off-diagonal terms negative, can statistically sample terms in sum.

Works only with no sign-problem: unfrustrated spin systems, fermions at half-filling.
Fails with frustration, most fermion problems, bosons in magnetic field.

DMRG

Invented by Steve White in 1992 for one dimensional systems.
Variational method in class of matrix product states.

$$\psi^{mps}(s_1, s_2, ..., s_N) = A^{(1)}_{\alpha}(s_1) A^{(2)}_{\alpha\beta}(s_2) A^{(3)}_{\beta\gamma}(s_3) ... A^{(N)}_{\sigma}(s_N)$$

Greek indices are bond variables, $\alpha, \beta, ... = 1...k$

s_i has D states

$$s_i = \pm 1/2 \quad , \qquad \text{spin} - 1/2$$
$$s_i = -1, 0, 1 \quad , \qquad \text{spin} - 1$$

A are k-by-k matrices, DNk^2 variational parameters.

DMRG and Matrix Product Methods

Successes:

$S = 1$ Heisenberg ground state energy to 12 digits of accuracy (White and Huse)
Periodic boundary conditions (Verstraete, Porras, Cirac)
Time dependent methods (Vidal)
Time dependent methods to study spin-charge separation (Kollath, Schollwoeck, Zwerger)

Why does it work so well? Especially accurate for systems with a spectral gap.

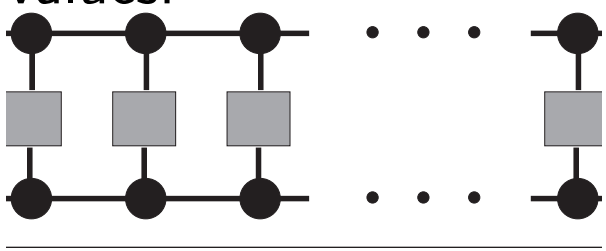
DMRG

Key features: represents large enough class of variational states and easy to compute properties of the state.

$$\psi^{mps}(s_1, s_2, ..., s_N) = A^{(1)}_{\alpha}(s_1) A^{(2)}_{\alpha\beta}(s_2) A^{(3)}_{\beta\gamma}(s_3) ... A^{(N)}_{\sigma}(s_N)$$

MPS:

Computing expectation values:



Computing Properties of Ground States

Methods Used in Practice

Computational Complexity

Hardness results

Easiness results

Conclusion

Complexity classes

P	Class of problems that can be solved on classical computer in polynomial time
NP	Class of problems whose solution can be verified on classical computer in polynomial time
BQP	Class of problems that can be solved on a quantum computer in polynomial time
QMA	Class of problems whose solution can be verified on a quantum computer in polynomial time

Modern Church-Turing thesis: any physical computational process can be simulated by a (probabilistic) Turing machine, i.e., a classical computer. Class P or BPP. "Efficient solution"

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Quantum Church-Turing thesis: any physical computational process can be simulated by a quantum computer. Class BQP.

Complexity class examples:

NP Given a classical Hamiltonian, does it have a state with energy less than E_0?

$$\mathcal{H} = \sum_{i,j} J_{ij} S_i^z S_j^z + \sum_i h_i S_i^z$$

P Same Hamiltonian with $h_i = 0$ on a planar graph

BQP Factoring

QMA Ground state properties of quantum systems, see below

The only general algorithm we gave for quantum systems, exact diagonalization, takes exponential time.

Easy vs. Hard

The traditional view (pre-quantum): P is easy, NP is hard

When we have a quantum computer: P and BQP are easy, NP and QMA are hard

Simulating quantum mechanics using a classical computer (like the one on your desk): P and NP are easy, BQP and QMA are hard

Computing Properties of Ground States

Finding quantum ground states can be very hard!

Question: given a one-dimensional Hamiltonian, determine whether the ground state has energy zero or less, given a promise that if not, then the energy is at least $1/poly(N)$.

This is QMA-hard in general (Aharonov, Gottesman and Kempe, 2007 and Irani, 2007, building on previous work by Kitaev (hardness on a graph), Oliveira and Terhal (hardness in 2d)

Consequences: other hard problems

$$\mathcal{H} = \sum_{ij} h_{ij}$$

Energy determined by reduced density matrices:

$$E = \sum_{ij} \mathrm{Tr}(h_{ij}\rho_{ij})$$

Determine if 2-body reduced density matrices are consistent (Liu, Christandl, and Verstraete, 2006) is QMA-hard

$$\rho_{12} = \mathrm{Tr}_{34\ldots N}\Big(\rho\Big) \tag{1}$$

Note, determining possible one-particle density matrices was recently solved. Different problem (Klyachko, 2009)

$$\langle \psi_i^\dagger \psi_j \rangle \tag{2}$$

(1) determines (2) but not the other way round.

Consequences: other hard problems

Universal functional of density functional theory

$$E_0 = \min_\rho \{\mathrm{Tr}(V\rho) + F_N[\rho]\},$$

$$F_N[\rho] = \min_{\psi \to \rho} \left(\int \Psi^\dagger H \Psi \right)$$

No efficiently computable universal functional in density functional theory (Schuch and Verstraete, 2007)

Computing Properties of Ground States

One dimensional gapped Hamiltonian is in NP.

Specifically: $\mathcal{H}$ is one-dimensional, nearest neighbor Hamiltonian.

$$\mathcal{H} = \sum_i h_{i,i+1}$$

$$\|h_{i,i+1}\| \leq 1$$

Low dimension on each site:

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

Determine if ground state energy is zero or less, given a promise that if not then it is at least $1/\mathrm{poly}(N)$ and given a promise on energy gap:

$$\Delta E \geq \mathcal{O}(1).$$

One dimensional gapped Hamiltonian in NP

Consequence of the following result:

$$\mathcal{H} = \sum_i h_{i,i+1}$$

$$\|h_{i,i+1}\| \leq 1$$

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

Then, for any ϵ, there exists a matrix product state with Ψ^{mps} with

$$|\Psi^{mps} - \Psi^0| \leq \epsilon$$

with rank

$$k = \mathrm{poly}(N/\epsilon),$$

where the power in the poly depends on $1/\Delta E$.

Entanglement entropy

Given pure state ψ,

$$\rho = |\psi\rangle\langle\psi|$$

Reduced density matrix by partial trace:

$$\rho_A = \mathrm{Tr}_B(\rho)$$

Entanglement entropy:

$$S = -\mathrm{Tr}\Big(\rho_A \log_2(\rho_A)\Big)$$

Example:

$$\psi = \frac{1}{\sqrt{2}}\Big(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\Big),$$

$$\rho_A = \begin{pmatrix} 1/2 & \\ & 1/2 \end{pmatrix}$$

$$S = \log_2(2) = 1.$$

Entanglement in matrix product state

$$\psi^{mps}(s_1, s_2, ..., s_N) = A^{(1)}_{\alpha}(s_1) A^{(2)}_{\alpha\beta}(s_2) A^{(3)}_{\beta\gamma}(s_3) ... A^{(N)}_{\sigma}(s_N)$$

Split: $A = 1, 2, 3$, $B = 4, ..., N$

$$\psi^{mps} = \sum_{\gamma=1}^{k} \psi^{A}_{\gamma} \psi^{B}_{\gamma}$$

If A is k dimensional system,

$$S \leq \log_2(k)$$

Entanglement in matrix product state

Rényi entropy:

$$S_\alpha(\rho) = \frac{1}{1-\alpha} \log_2\Big(\mathrm{Tr}(\rho^\alpha)\Big)$$

Schmidt decomposition:

$$\psi = \sum_\gamma A(\gamma) \Psi_A^\gamma \otimes \Psi_B^\gamma,$$

orthonormal basis: $\langle \Psi_A^\mu, \Psi_A^\nu \rangle = \langle \Psi_B^\mu, \Psi_B^\nu \rangle \rangle = \delta_{\mu\nu}$

$$S_\alpha = \frac{1}{1-\alpha} \log_2\Big(\sum_\gamma |A(\gamma)|^{2\alpha}\Big)$$

Rényi entropy and matrix product states

$$S_\alpha = \frac{1}{1-\alpha} \log_2 \left(\sum_\gamma |A(\gamma)|^{2\alpha} \right)$$

For $\alpha < 1$, sensitive to small eigenvalues.

For $\alpha > 1$, sensitive to large eigenvalues.

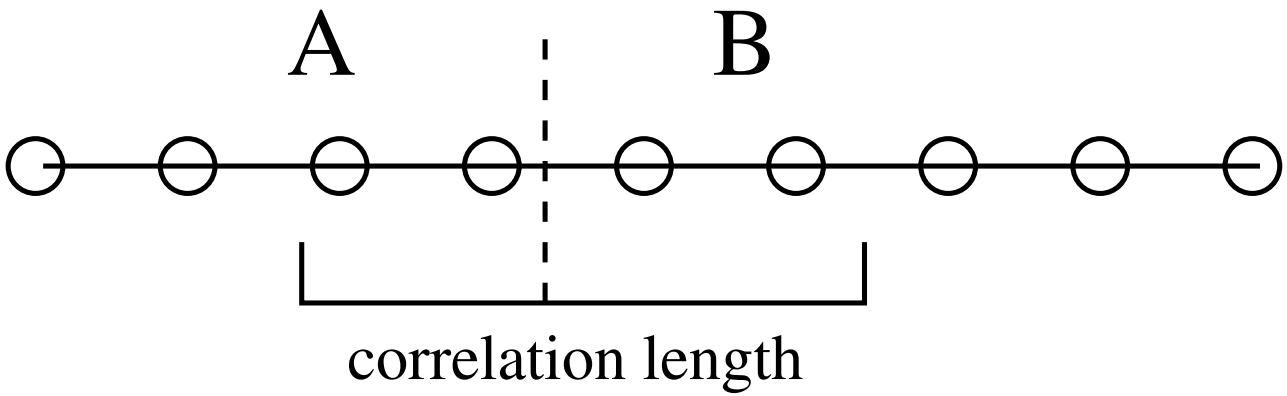
Rényi entropy bound for $\alpha < 1$ implies ability to approximate by mps (Verstraete and Cirac, 2006).

Idea: truncate sequentially across each cut.

$$\psi = \sum_\gamma A(\gamma) \Psi_A^\gamma \otimes \Psi_B^\gamma \rightarrow \psi \approx \sum_{\gamma=1}^{k} A(\gamma) \Psi_A^\gamma \otimes \Psi_B^\gamma$$

Handwaving argument for an area law

1. Assume we have a one dimensional Hamiltonian with nearest neighbor interactions and a spectral gap.
2. Since there is a gap, correlations decay exponentially.
3. Therefore, there is an area law.



Guess:

$$S \overset{?}{\leq} \log_2(D)\xi$$

Handwaving argument for an area law

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Can we make it precise?

2. Follows from 1 in any dimension. (Hastings, 2004). $\xi \sim 1/\Delta E$
3. Does *not* follow from 2. Counterexample: quantum expanders (Hastings; Ben-Aroya and Ta-Shma, 2007).

Area Law

Theorem

Consider a one-dimensional nearest-neighbor Hamiltonian with spectral gap ΔE, and interactions strength bounded by unity:

$$\mathcal{H} = \sum_i h_{i,i+1}$$

$$\|h_{i,i+1}\| \leq 1$$

Let the Hilbert space dimension on each site be D. Then, the entanglement entropy across any cut is bounded by S_{max} where

$$S_{max} = \exp[\mathcal{O}(\log(D)/\Delta E)].$$

(Hastings, 2007)
Similar bounds hold for Rényi entropies also

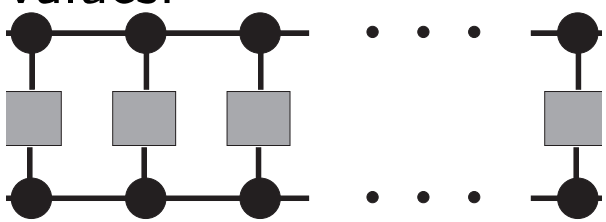
Consequence of area law

One dimensional gapped Hamiltonian: in NP because there is an efficient (polynomial size) representation of an approximation to the ground state as an MPS and the energy can be computed efficiently (in polynomial time) on a classical computer

$$\psi^{mps}(s_1, s_2, ..., s_N) = A^{(1)}_{\alpha}(s_1)A^{(2)}_{\alpha\beta}(s_2)A^{(3)}_{\beta\gamma}(s_3)...A^{(N)}_{\sigma}(s_N)$$

MPS:

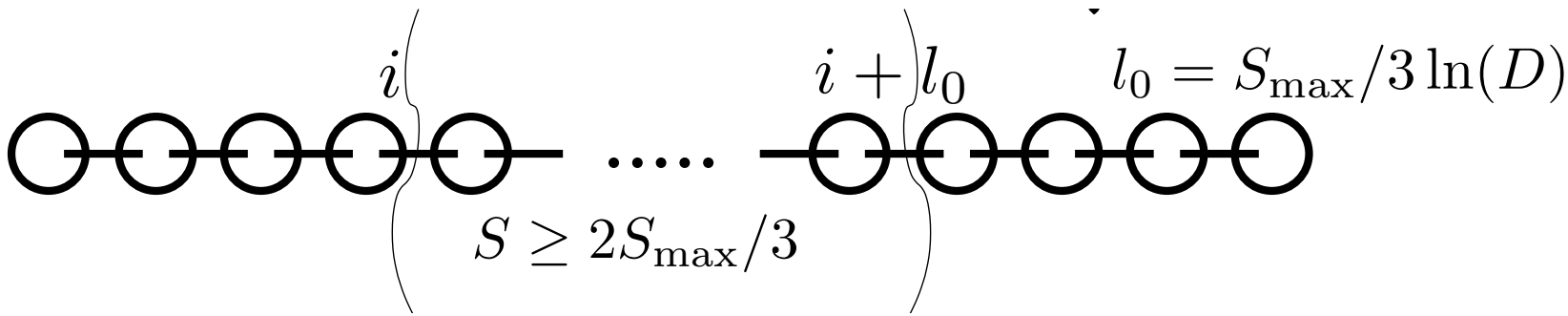
Computing expectation values:



Sketch of area law proof (by contradiction)

If the entropy is more than S_{max} across some cut, then it is large across many nearby cuts by subadditivity:

$$S_{AB} \leq S_A + S_B \tag{3}$$



Define S_l to be the maximum entropy of an interval of length l within distance l_0 of i.
Some properties:

$$S_1 \leq \log(D)$$

$$S_{2l} \leq 2S_l$$

If the second inequality saturates, $\rho_{i,i+2l} = \rho_{i,i+l} \otimes \rho_{i+l+1,i,2l}$ implying that the state $\rho_L \otimes \rho_R$ has same energy as ground state, contradicting assumption of large entanglement.
We will go further and use the large entanglement entropy to show:

$$S_{2l} \leq 2S_l - \mathcal{O}(l\Delta E/v)$$

Sketch of area law proof (by contradiction)

$$S_{2l} \leq 2S_l - \mathcal{O}(l\Delta E/v)$$

So,

$$\begin{aligned}
S_l &\leq 2S_{l/2} - \mathcal{O}(l\Delta E/v) \\
&\leq 2\left(2S_{l/4} - \frac{1}{2}\mathcal{O}(l\Delta E/v)\right) - \mathcal{O}(l\Delta E/v) \\
&\leq 2\left\{2\left(2S_{l/8} - \frac{1}{4}\mathcal{O}(l\Delta E/v)\right) - \frac{1}{2}\mathcal{O}(l\Delta E/v)\right\} - \mathcal{O}(l\Delta E/v) \\
&\leq \ldots \\
&\leq lS_1 - \log_2(l)\mathcal{O}(l\Delta E/v)
\end{aligned}$$

Contradiction: goes negative for sufficiently large l

Approximating projector onto ground state

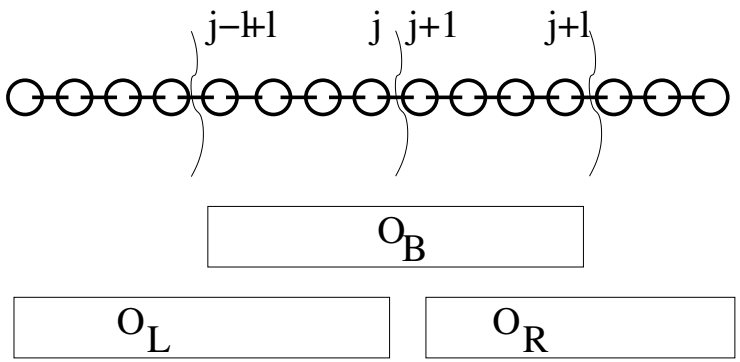
A lemma:

Given the existence of a spectral gap, for any j, l there exist Hermitian operators O_L, O_R, O_B such that

- $\|O_L\|, \|O_R\|, \|O_B\| \leq 1$
- The product $O_L O_R O_B$ approximates the projector P_0 onto the ground state:

$$\|O_L O_R O_B - P_0\| \leq \exp[-\mathcal{O}(l\Delta E / v_{LR})]$$

- Operators are supported as shown: O_L supported on $1...j$, O_R supported on $j+1...N$, O_B supported on $j-l...j+l$.



Proof relies on Lieb-Robinson bounds (discussed in next talk) for velocity v_{LR} and spectal gap

Bootstrapping a good approximation to the ground state

Suppose a factorized state $\rho_L \otimes \rho_R$ had high overlap with the ground state:

$$\mathrm{Tr}\Big(\rho_L \otimes \rho_R P_0\Big) = P > 0$$

Then, the state

$$\rho' \equiv O_L O_R O_B \rho_L \rho_R O_L O_R O_B$$

has even higher overlap.
Rank of ρ' is bounded by D^{2l}
However since there is high entanglement across all cuts locally, the factorized state $\rho_L \otimes \rho_R$ must have very low entanglement with ground state: P is small

Sketch of area law proof (by contradiction)

However since there is high entanglement across all cuts locally, the factorized state $\rho_L \otimes \rho_R$ must have very low entanglement with ground state: P is small
Therefore,

$$\mathrm{Tr}(O_L O_R O_B \rho_L \otimes \rho_R) << 1$$

However,

$$\mathrm{Tr}(O_L \rho_L), \mathrm{Tr}(O_R \rho_R) \approx 1$$

Thus,

$$\mathrm{Tr}(\rho_L \otimes \rho_R O_B) << 1$$

but

$$\mathrm{Tr}(P_0 O_B) \approx 1$$

Sketch of area law proof (by contradiction)

Therefore, operator O_B detects entanglement locally in the ground state:

$$\mathrm{Tr}(\rho_{j-l\ldots j} \otimes \rho_{j+1\ldots j+l} O_B) << 1$$

$$\mathrm{Tr}(\rho_{j-l\ldots j+l} O_B) \approx 1$$

By Lindblad-Uhlmann theorem, this means that there is large mutual information between $j-l\ldots j$ and $j+1\ldots j+l$. But this is bounded by $S_{2l} - 2S_l$

Computing Properties of Ground States

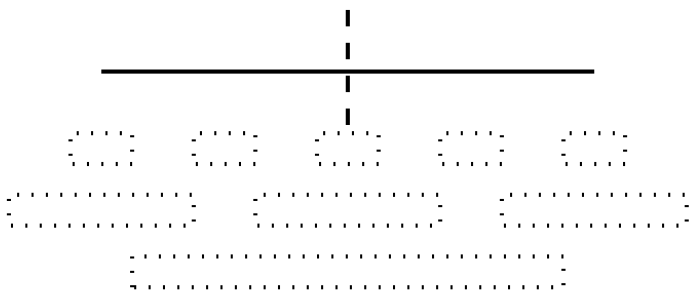
Open questions:

How hard is it to find a matrix product ground state for a gapped Hamiltonian? (exist Hamiltonians with $k = poly(N)$ mps ground states which are NP-hard to find but they are not gapped, Schuch and Verstraete 2008)

Can we prove an area law in 2D for all gapped systems?

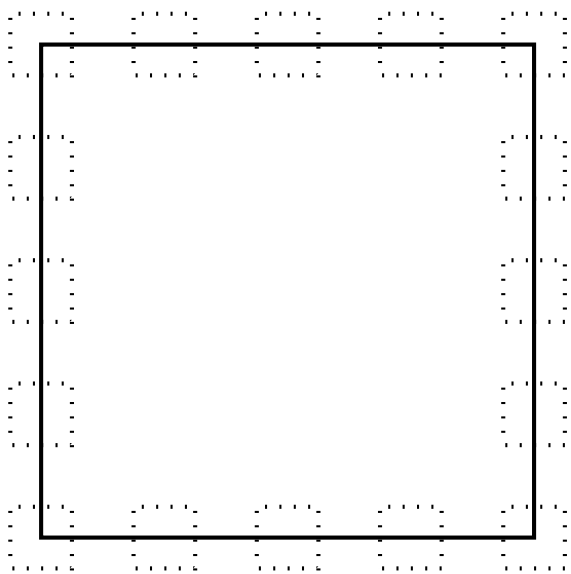
And even some gapless systems?

1D: $1 + 1 + ... = \log(L)$



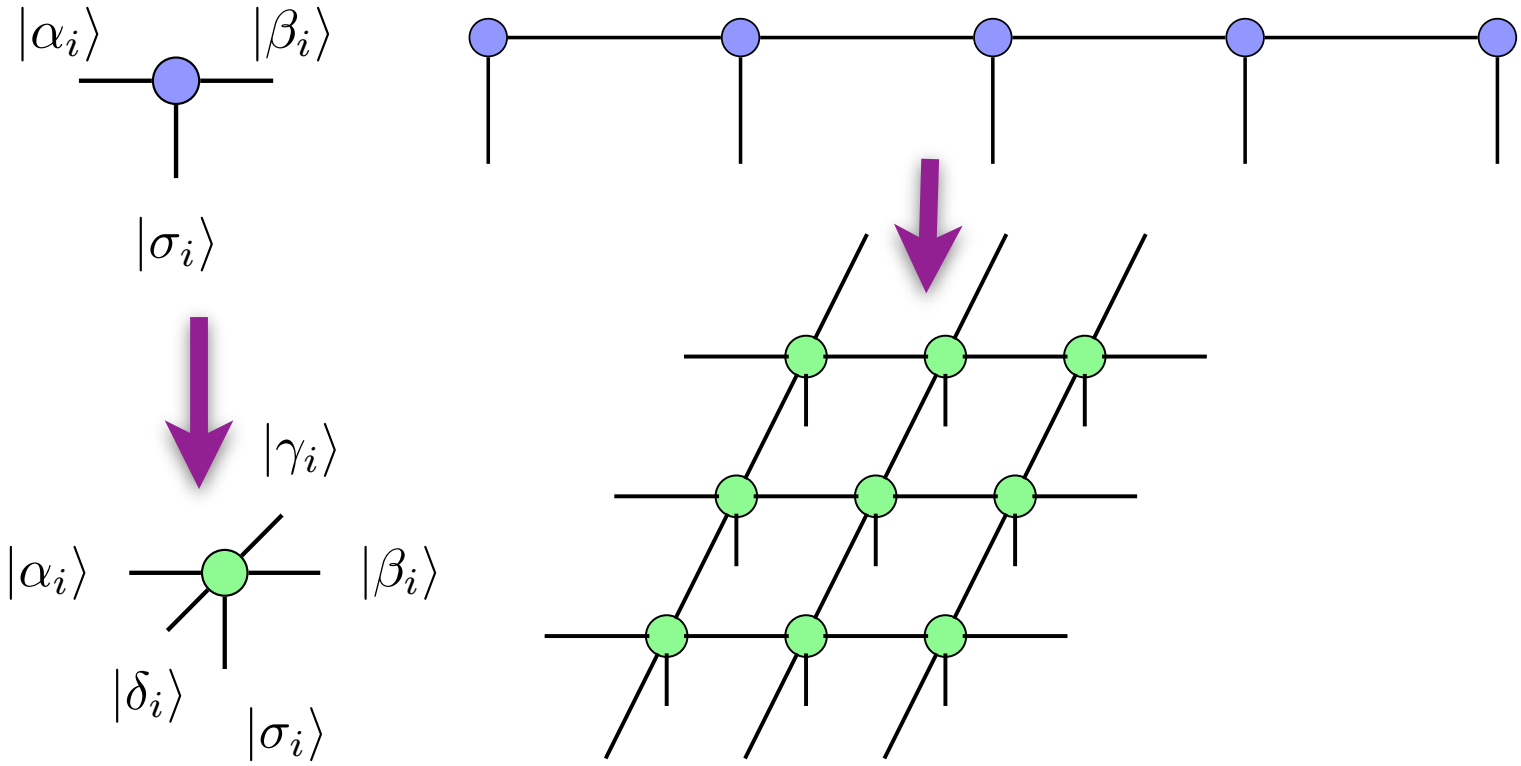
2D:

$L + L/2 + L/4 + ... = 2L$



Open Questions: 2D

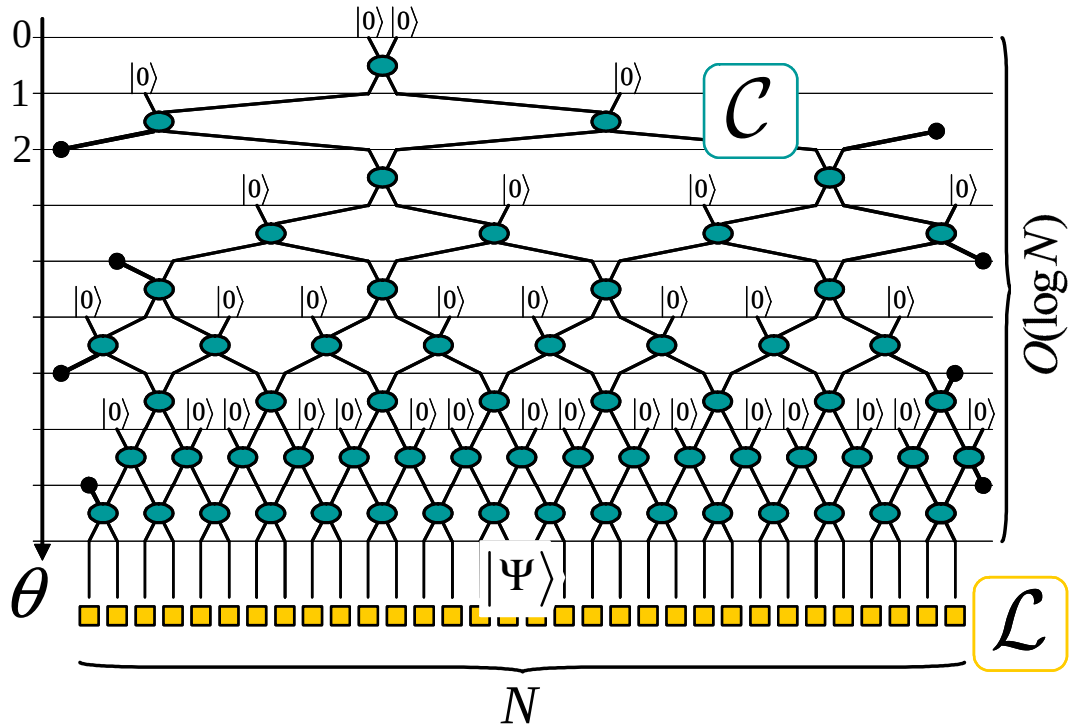
Is there an efficient classical representation of an approximation to the ground state of a gapped system in 2D?
Example: a PEPS state



Note: while PEPS implies area law, the reverse is not true.
Example of gapless system 2D Heisenberg AFM

Open Questions: 2D

Is there an efficient classical representation where expectation values can be efficiently computed?
Example: MERA (Vidal)



Open questions

Better area law in 1D? (Current 1D area law has **exponential** dependence of entropy on gap)

What is the best upper bound?

$S \sim \log(1/\Delta E)$	conformal field theory (Calabrese and Cardy, 2004; Casini and Huerta, 2005)
$S \sim (1/\Delta E)^{1/4}$	model system (Gottesman and Hastings, 2009, Irani, 2009)
$S \sim 1/\Delta E$	naive guess
$S \sim \exp(1/\Delta E)$	current most general bound