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Complexity Classification of Product State Problems for Local Hamiltonians

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Definition

The k-**LH problem** is, given a k-local Hamiltonian, estimate its minimum eigenvalue / ground state energy.

This is analogous to the classical k-Max-SAT problem, where each clause acts on k variables.

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For a fixed set $\mathcal{S}$ of allowed terms / allowed interactions,
the $\mathcal{S}$-**LH problem** is k-LH with the promise that any input is of the form

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$\mathcal{S}$-LH classification

[Cubitt, Montanaro 2015], with [Bravyi, Hastings 2014], give a complete classification of 2-local $\mathcal{S}$-LH as a function of $\mathcal{S}$.

Given any set $\mathcal{S}$ of 2-qubit terms, [CM15] describes properties of the terms which determine whether $\mathcal{S}$-LH is in P or NP-, StoqMA-, or QMA-complete.

What about product states?

What is the complexity of estimating minimum product state energies of various families of local Hamiltonians?

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- Product states can be described efficiently classically.
- They're intermediate between classical states and general quantum states.
- For many natural sets of Hamiltonians, product states are rigorously near-optimal.

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k-LH $\rightarrow$ **prodLH**

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Can we classify the complexity of the product state problem for various families of Hamiltonians?

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Main Theorem ($\mathcal{S}$-prodLH classification)

For any fixed set of 2-qubit Hamiltonian terms $\mathcal{S}$,
if every matrix in $\mathcal{S}$ is 1-local then $\mathcal{S}$-prodLH is in P,
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Corollary

*For any fixed set of 2-qubit Hamiltonian terms $\mathcal{S}$,
the problem $\mathcal{S}$-LH is at least* NP-*hard if and only if* $\mathcal{S}$-prodLH *is* NP-*complete.*

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As an example, consider the 2-qubit term

$$H = X \otimes X + Y \otimes Y + Z \otimes Z$$

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Let

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Then the energy of the interaction between qubits u and v is

$$\mathrm{Tr}\left(H \; |\phi_u\rangle\langle\phi_u| \otimes |\phi_v\rangle\langle\phi_v|\right) = u_1 v_1 + u_2 v_2 + u_3 v_3 = u \cdot v$$

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So for the example $\mathcal{S} = \{X \otimes X + Y \otimes Y + Z \otimes Z\}$, the problem $\mathcal{S}$-prodLH is equivalent to optimizing sums of inner products:

$$\sum_{uv \in E} w_{uv} \; u \cdot v$$

over unit vectors $u, v \in \mathbb{R}^3$.

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New goal: Given arbitrary 2-qubit H, does the optimum product state energy have a nice form like this?
If not, can we force it to?

To Do: show if $\mathcal{S}$ contains a nontrivial 2-qubit term, then $\mathcal{S}$-prodLH is NP-hard.
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Write arbitrary 2-qubit H in Pauli basis:

$$H = \sum_{i,j=1}^{3} M_{ij}\sigma_i \otimes \sigma_j + \sum_{k=1}^{3} c_k\sigma_k \otimes I + w_k I \otimes \sigma_k.$$

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This is not as simple as $u \cdot v$, but we can design gadgets to simplify it.

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Trick 1: Symmetrize
It's nice when the objective function is symmetric, so acting on uv is the same as acting on vu.
Then we can work with *un*-directed graph problems.

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Trick 2: Delete 1-local terms $c^\top u$ and $w^\top v$.

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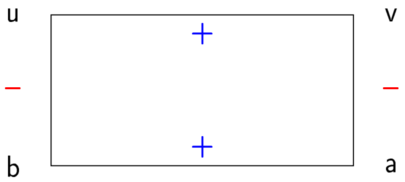
Use 4-qubit gadget with 2 ancilla

$$G^{uv} = H^{uv}_{sym} + H^{ab}_{sym} - H^{ua}_{sym} - H^{bv}_{sym}$$



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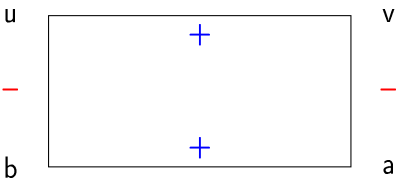
Further analysis of gadget: $G^{uv} = H^{uv}_{sym} + H^{ab}_{sym} - H^{ua}_{sym} - H^{bv}_{sym}$



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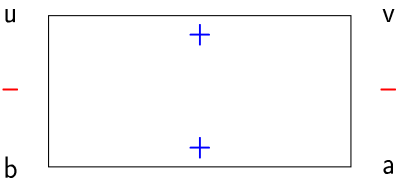

After the tricks, how does the expectation value relate to u and v?

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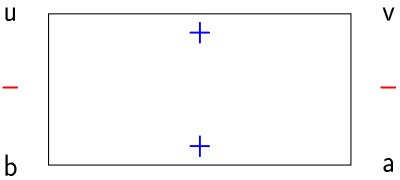

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Recall for $H = X \otimes X + Y \otimes Y + Z \otimes Z$,

$$\mathrm{Tr}\left(H \ |\phi_u\rangle\langle\phi_u| \otimes |\phi_v\rangle\langle\phi_v|\right) = u \cdot v.$$

Here, each edge/interaction H_{sym} also contributes

$$\mathrm{Tr}(H^{uv}_{sym} |\phi_u\rangle\langle\phi_u| \otimes |\phi_v\rangle\langle\phi_v|) \approx u^\top M v.$$

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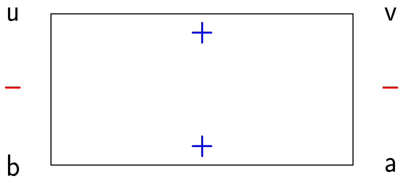

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$$\mathrm{Tr}(H^{uv}_{sym} \, |\phi_u\rangle\langle\phi_u| \otimes |\phi_v\rangle\langle\phi_v|) \approx u^\top M v \approx 1 - \|Mu - Mv\|^2.$$

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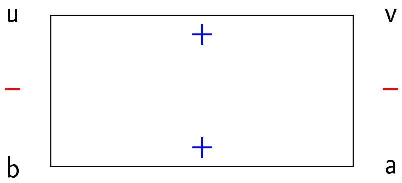

After the tricks, how does the expectation value relate to u and v?

Letting the ancilla a, b take optimal values, and summing the four contributions, we get

$$\|Mu - Mv\|$$

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New goal: Given arbitrary 2-qubit H, does the optimum product state energy have a nice form?

We've used Hamiltonian gadgets to embed an objective function of the form

$$\sum_{uv \in E} \|Mu - Mv\|$$

into the minimum product state energy.

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Now, we can focus on this completely classical graph & vector problem.

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Stretched linear Vector Max-Cut ($\mathrm{MC}^{\mathrm{L}}_{W}$)

For W a fixed diagonal matrix,
and a graph $G = (V, E)$,
estimate

$$\mathrm{MC}^{\mathrm{L}}_{W}(G) = \frac{1}{2} \max_{\hat{u} \in S^{k-1}} \sum_{uv \in E} \|W\hat{u} - W\hat{v}\|$$

In words, assign unit vectors $\hat{v} \in \mathbb{R}^k$ to each vertex v in order to maximize the difference along each edge.

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In words, assign unit vectors $\hat{v} \in \mathbb{R}^k$ to each vertex v in order to maximize the difference along each edge.

Theorem

For any fixed non-negative nonzero $W = \mathrm{diag}(\alpha, \beta, \gamma)$
$\mathrm{MC}^{\mathrm{L}}_{W}$ *is* NP*-complete.*

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Intuition: W defines an ellipsoid (if $W = I$, then its the unit sphere).
Given some graph, the problem is to embed the vertices onto the ellipsoid's surface to maximize the sum of the edge lengths.

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Proof sketch:

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Proof sketch:

1. Given a graph G, construct a new graph G' by replacing each edge with a 3-clique (triangle) gadget.

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This relates the $\mathsf{MC}^{\mathsf{L}}_{W}$ value of G' to the 3-colorability of G.
And 3-Coloring is NP-complete.

Main Theorem ($\mathcal{S}$-prodLH classification)

For $\mathcal{S}$ any fixed set of 2-qubit Hamiltonian terms,
if every matrix in $\mathcal{S}$ is 1-local then $\mathcal{S}$-prodLH is in P,
and otherwise $\mathcal{S}$-prodLH is NP-complete.

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- If every term is 1-local, then we can optimize the state of each qubit individually, so the problem is in P.
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  1. Construct Hamiltonian gadgets so the minimum product state energy has a nice form, like $\|Wu - Wv\|$.
  2. Show $\mathrm{MC}^{\mathrm{L}}_{W}$ is NP-hard by a reduction from 3-Coloring.

Corollary: Quantum Max-Cut

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Definition

Quantum Max-Cut is equivalent to $\mathcal{S}$-LH with $\mathcal{S} = \{XX + YY + ZZ\}$.

Our classification theorem implies the following.

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3D-Vector-Max-Cut is NP-complete.

Complexity Classification of Product State Problems for Local Hamiltonians
arXiv: 2401.06725
John Kallaugher, Ojas Parekh, Kevin Thompson, Yipu Wang, **Justin Yirka**

1. **Product state complexity**: Given any set $\mathcal{S}$ of allowed 2-qubit terms, estimating the minimum product state energy on the family of Hamiltonians is either in P or is NP-complete.
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Open problems:

1. Can we use complexity of product state problem to prove the *general* ground states of a class of Hamiltonians are *not* hard?
2. Classify $\mathcal{S}$-prodLH with additional restrictions, e.g. only positive weights, spatial geometry?