

RPE

JUSTIN YIRKA

On

*Complexity Classification of Product State Problems for
Local Hamiltonians*

John Kallaugher, Ojas Parekh, Kevin Thompson, Yipu Wang, and Justin Yirka

arXiv: 2401.06725, January 2024

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Hamiltonians

An n -qubit **Hamiltonian** is a $2^n \times 2^n$ Hermitian matrix.

It encodes constraints, interactions, or “rules” of a physical system, its eigenvectors correspond to physical states of the system, and its eigenvalues are the energies of those states.

$$\langle \psi | H | \psi \rangle = \lambda$$

n -qubit state \leftrightarrow Vector in \mathbb{C}^{2^n} with $\|v\|_2 = 1$

State $|v\rangle \leftrightarrow$ Vector v

$\langle v| \leftrightarrow$ Row vector v^{T*}

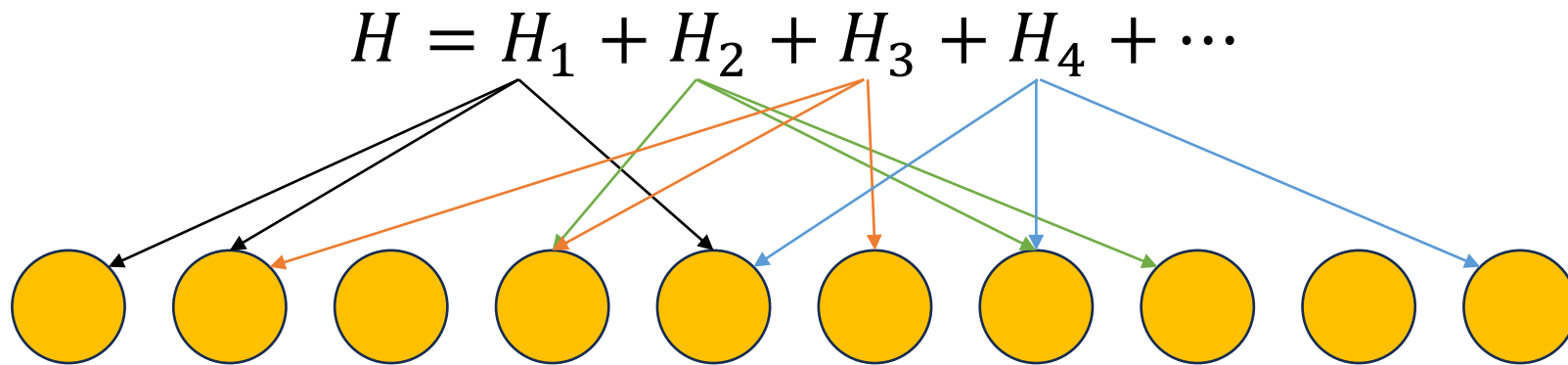
State $\rho \leftrightarrow$ Outer product $|v\rangle\langle v| = v_i^{T*} v_i$

Tensor product $\otimes \leftrightarrow$ “Multiplying” spaces i.e. $\mathbb{R}^4 \otimes \mathbb{R}^4 = \mathbb{R}^{16}$

Local Hamiltonians

A **k -local Hamiltonian** is a sum of Hamiltonian terms each acting on at most k qubits

$$H = \sum_i H_{S_i} \otimes \mathbb{I}_{\bar{S}_i} \quad |S_i| \leq k$$



k -LH

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

Formally: decide if $\lambda_{\min} < a$ (YES) or $\lambda_{\min} > b$ (NO) for $b - a \geq \frac{1}{\text{poly}(n)}$.

Hamiltonian

k -local Hamiltonian

k -LH

$$\begin{bmatrix} 1 & & & \\ & -1 & & \\ & & 0 & \\ & & & 1 \end{bmatrix}_{1,2} + \begin{bmatrix} 0 & & & \\ & 1 & & \\ & & -1 & \\ & & & 0 \end{bmatrix}_{1,3} + \dots$$

Boolean formula

k -CNF

k -Max-SAT

$$(x_1 \vee x_2) \wedge (x_1 \vee \bar{x}_3) \wedge (x_3 \vee x_4) \wedge \dots$$

Complexity

k -Max-SAT is NP-complete for $k \geq 2$

Similarly, k -LH is QMA-complete for $k \geq 2$

Hardness is subtle, though.

Goal: Characterize the complexity of k -LH when the problem is restricted to various subsets of Hamiltonians

Complexity

Just enumerating sets of Hamiltonians seems...

- tedious
- uninformative – what's the underlying structure?
- difficult

So we consider sets of families defined by interesting properties

S -LH

Let a Hamiltonian **family** be defined by the allowed interactions, i.e. by the allowed k -qubit terms.

For a fixed set S of allowed terms/allowed interactions, the **S -LH problem** is k -LH with the additional promise/restriction that any input is of the form

$$H = \sum_i w_i H_i \quad \text{with each } H_i \in S$$

(we will focus on sets S of 2-qubit, 4×4 , terms)

S -LH

For a fixed set S of allowed terms/allowed interactions, the **S -LH problem** is k -LH with the additional promise/restriction that any input is of the form

$$H = \sum_i w_i H_i \quad \text{with each } H_i \in S$$

- S -LH with $S = \{X \otimes X + Y \otimes Y + Z \otimes Z\}$ is the Quantum Max-Cut problem.
- Classically, $\{\neq\}$ -Max-SAT is Max-Cut.
- $\{2\text{-Out-of-4}\}$ -SAT is NP-complete,
used in *The Power of Unentanglement* [ABDSF 08]

Complexity classification

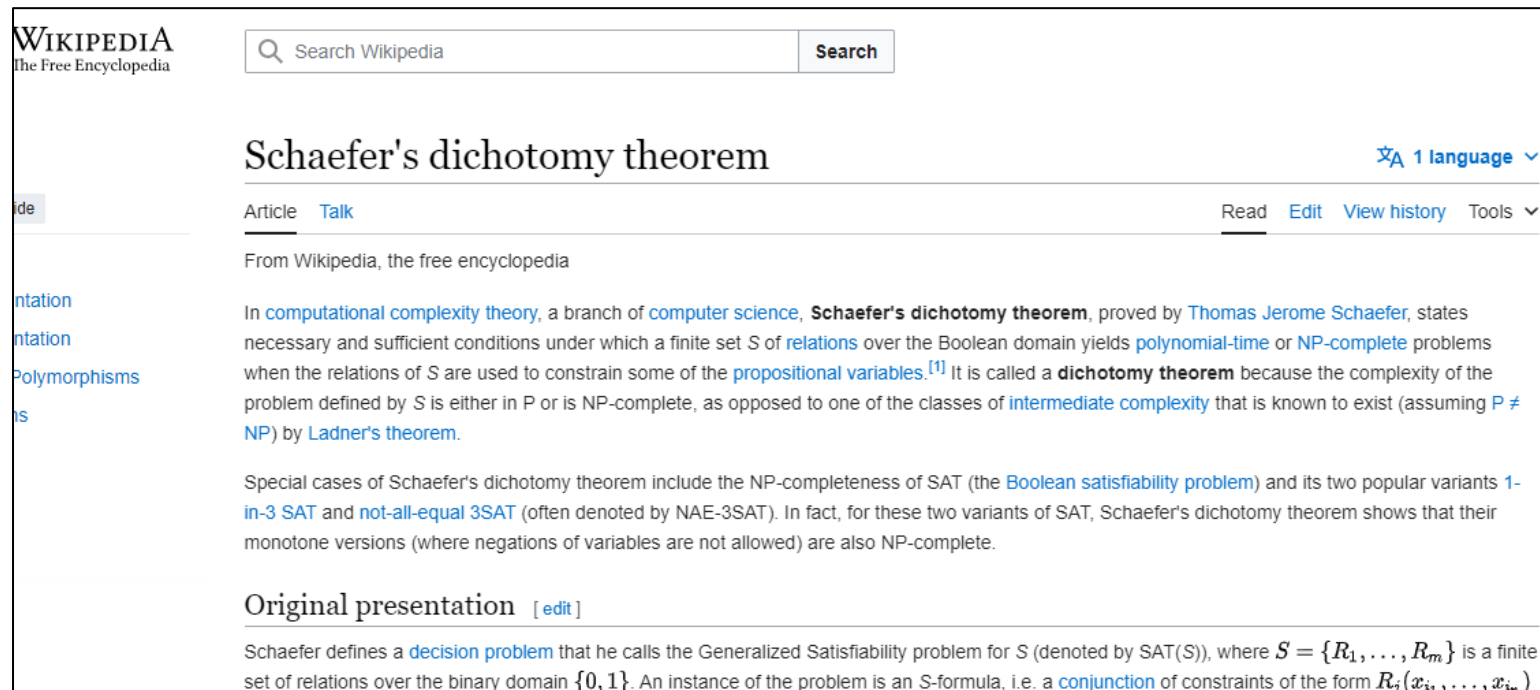
We're interested in classifying the complexity of S -LH *as a function of* the set S of allowed terms.

Detour:

Complexity classifications of constraint satisfaction problems (CSPs) as a function of the allowed constraints

Complexity classification of CSPs

The complexity of satisfiability problems, Schaefer, 1976



The image shows a screenshot of the Wikipedia article titled "Schaefer's dichotomy theorem". At the top left is the Wikipedia logo with the tagline "The Free Encyclopedia". To the right is a search bar with the text "Search Wikipedia" and a "Search" button. Below the search bar is the article title "Schaefer's dichotomy theorem" in a large, bold font. To the right of the title is a language selection dropdown menu showing "1 language". Below the title are navigation tabs for "Article" and "Talk", and on the far right, tabs for "Read", "Edit", "View history", and "Tools". The main content of the article begins with the text "From Wikipedia, the free encyclopedia". The first paragraph explains that in computational complexity theory, Schaefer's dichotomy theorem, proved by Thomas Jerome Schaefer, states necessary and sufficient conditions under which a finite set S of relations over the Boolean domain yields polynomial-time or NP-complete problems. It notes that the problem defined by S is either in P or is NP-complete, as opposed to one of the classes of intermediate complexity. The second paragraph lists special cases, including the NP-completeness of SAT (the Boolean satisfiability problem) and its variants 1-in-3 SAT and not-all-equal 3SAT (often denoted by NAE-3SAT). The article concludes with a section titled "Original presentation" with an edit link, followed by a paragraph defining a decision problem as the Generalized Satisfiability problem for S (denoted by $\text{SAT}(S)$), where $S = \{R_1, \dots, R_m\}$ is a finite set of relations over the binary domain $\{0, 1\}$. An instance of the problem is an S -formula, i.e. a conjunction of constraints of the form $R_j(x_{i_1}, \dots, x_{i_n})$.

Complexity classification of CSPs

Schaefer's dichotomy theorem, 1976:

Given any fixed set S of allowed Boolean constraints,
deciding satisfiability of a formula

$$f(x_1, x_2, \dots, x_n) = \bigwedge_i C_i \text{ for } C_i \in S$$

a.k.a. **S-SAT**

❖ is in P if any of some simple conditions is true,

❖ and otherwise is NP-complete.

- a) " Every relation in S is 0-valid
- b) Every relation in S is 1-valid
- c) Every relation in S is weakly positive
- d) Every relation in S is weakly negative
- e) Every relation in S is affine
- f) Every relation in S is bijunctive "

Complexity classification of CSPs


- [Schaefer 1976] classifies S -SAT
- [Creignou 95] with [Khanna, Sudan, Williamson 97] classify S -Max-SAT
- [Jonsson 00] classifies S -Max-SAT with positive & negative weights.
- [Jonsson, Klasson, Krokhin 06] and [Thapper, Živný 16] extends this to non-binary variables.
 - (Only positive weights)

End of detour, back to quantum

Complexity classification of S -LH

[Cubitt, Montanaro 13] classify S -LH for all sets S of 2-qubit terms:

Given a fixed set S of 2-qubit Hamiltonian terms,
 S -LH is either in P, or is NP-, StoqMA-, or QMA-complete.

- If every matrix in S is 1-local, S -LH is in P;
- Otherwise, if there exists $U \in SU(2)$ such that U locally diagonalises S , then S -LH is NP-complete;
- Otherwise, if there exists $U \in SU(2)$ such that, for each 2-qubit matrix $H_i \in S$, $U^{\otimes 2} H_i U^{\dagger \otimes 2} = \alpha_i Z^{\otimes 2} + A_i \otimes I + I \otimes B_i$ where $\alpha_i \in \mathbb{R}$ and A_i, B_i are arbitrary single-qubit Hermitian matrices, then S -LH is StoqMA-complete; 
- Otherwise, S -LH is QMA-complete. [Bravyi, Hastings 2014]

What about product states?

What about product states?

We have a full classification of S -LH for 2-qubit terms, i.e. estimating the minimum eigenvalue.

What about other Hamiltonian problems?

- Other ground state properties
- Constrained optimization
- Thermal limit
- ...
- **Product states**

Product states

A **product state** is an unentangled tensor product of single-qubit states

$$\rho = \rho_1 \otimes \rho_2 \otimes \rho_3 \otimes \cdots \otimes \rho_n$$

- Product states can be described efficiently classically.

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} \otimes \begin{bmatrix} e & f \\ g & h \end{bmatrix} \otimes \begin{bmatrix} i & j \\ k & l \end{bmatrix} \otimes \cdots \otimes \begin{bmatrix} w & x \\ y & z \end{bmatrix}$$

Product states

A **product state** is an unentangled tensor product of single-qubit states

$$\rho = \rho_1 \otimes \rho_2 \otimes \rho_3 \otimes \cdots \otimes \rho_n$$

- Product states can be described efficiently classically.
- They're intermediate between classical and general quantum states.
- For many natural sets of Hamiltonians, product states are rigorously near-optimal.
 - [Brandao, Harrow 13]: “High”-degree Hamiltonians' ground states are close to product states (monogamy of entanglement!)
- They're a popular ansatz in classical Hamiltonian approximation algorithms

Product state problems

A **product state** is an unentangled tensor product of single-qubit states

$$\rho = \rho_1 \otimes \rho_2 \otimes \rho_3 \otimes \cdots \otimes \rho_n$$

k -LH \rightarrow **prodLH**

given a local Hamiltonian, estimate the minimum energy over all product states:

$$\min_{\rho = \rho_1 \rho_2 \cdots \rho_n} \text{Tr}(H\rho)$$

S -LH \rightarrow **S-prodLH**

the problem prodLH restricted to $H = \sum_i w_i H_i$ with $H_i \in S$.

Main Theorem

Drum roll...

Complexity classification of product state problems

Main Theorem

For any fixed set of 2-qubit Hamiltonian terms S ,

- if every matrix in S is 1-local then S -prodLH is in P,
- and otherwise S -prodLH is NP-complete.

Corollary

For any fixed set of 2-qubit Hamiltonian terms S ,

- the problem S -LH is at least NP-hard iff S -prodLH is NP-complete.
- the problem S -LH is in P iff S -prodLH is in P.

Proof outline

Main Theorem

For any fixed set of 2-qubit Hamiltonian terms S ,

- if every matrix in S is 1-local then S -prodLH is in P,
 - and otherwise S -prodLH is NP-complete.
-

✓ If every term is 1-local, then we can optimize the state of each qubit individually, so the problem is in P.

✓ prodLH is always contained in NP, using product states' concise classical descriptions

$$\text{Tr}(H\rho) = \sum_{ij} \text{Tr}(H_{ij} \rho_i \rho_j)$$

□ **To Do:** show if S contains a nontrivial 2-qubit term, then S -prodLH is NP-hard.

- Design Hamiltonian gadgets to embed “nice” objective into optimal product state.
- That objective defines a variant of Vector Max-Cut, which we show is NP-complete.

Questions?

Analyzing product state energies

As a warmup, consider the example 2-qubit term

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

where X, Y, Z are the Pauli matrices.

$$\left\{ X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right\}$$

is a basis for 2×2 Hermitian matrices

Analyzing product state energies

As a warmup, consider the example 2-qubit term

$$H = XX + YY + ZZ$$

where X, Y, Z are the Pauli matrices.

Write states using **Bloch vectors**:

$$\rho^a = \frac{1}{2} (I + a_1 X + a_2 Y + a_3 Z), \quad \hat{a} \in \mathbb{R}^3, |\hat{a}| = 1$$

Then

$$\text{Tr}(H \rho^a \rho^b) = \frac{1}{4} \sum_{ij} a_i b_j \text{Tr}[H \sigma_i \sigma_j] \quad \text{for } \sigma_i \in \{X, Y, Z, I\}$$

Cross terms disappear!

$$\text{Tr}[H \sigma_i \sigma_j] \neq 0 \text{ iff } \text{Tr}[H \sigma_i \sigma_j] = \text{Tr}[II], \text{ which requires } i = j$$

Analyzing product state energies

As a warmup, consider the example 2-qubit term

$$H = XX + YY + ZZ$$

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Write states using **Bloch vectors**:

$$\rho^a = \frac{1}{2} (I + a_1 X + a_2 Y + a_3 Z) \quad \hat{a} \in \mathbb{R}^3, |\hat{a}| = 1$$

Cross terms disappear!

$$\begin{aligned} \text{Tr}(H \rho^a \rho^b) &= \\ & \frac{1}{4} \text{Tr}[a_1 b_1 XX \cdot XX + a_2 b_2 YY \cdot YY + a_3 b_3 ZZ \cdot ZZ] \\ &= a_1 b_1 + a_2 b_2 + a_3 b_3 = \hat{a} \cdot \hat{b} \end{aligned}$$

Analyzing product state energies

$$H = XX + YY + ZZ$$
$$\text{Tr}(H \rho^a \rho^b) = \hat{\mathbf{a}} \cdot \hat{\mathbf{b}}$$

Product state problems become optimization problems over Bloch vectors!

$\{H\}$ -prodLH is equivalent to optimizing sums of inner products:

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

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

General product state energies

Write an arbitrary 2-qubit term in the Pauli basis:

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

3×3 matrix M vectors \hat{c} \hat{w}

Then

$$\text{Tr}(H \rho^u \rho^v) = \hat{u}^T M \hat{v} + \hat{u}^T \hat{c} + \hat{v}^T \hat{w}$$

General product state energies

$$\text{Tr}(H \rho^u \rho^v) = \hat{u}^T M \hat{v} + \hat{u}^T \hat{c} + \hat{v}^T \hat{w}$$

For a general 2-qubit H , we still have a sum of inner products,
but with extra terms
and warped by extra coefficients

Can we make this “nicer”?

Hamiltonian gadgets

Trick 1: Symmetrize

In general, the orientation of interactions matters: $H^{ab} \neq H^{ba}$.

It eases analysis if the term is symmetric.

From now on, if we apply H to qubits a, b , we apply it in both directions:

$$H_{sym} = H^{ab} + H^{ba} = H^{ab} + \text{SWAP } H^{ab} \text{ SWAP}$$

Since H_{sym} is symmetric, M' is symmetric, and we can analyze assuming

$$M' = \begin{bmatrix} \alpha & & \\ & \beta & \\ & & \gamma \end{bmatrix}$$

$$H_{sym} = \sum_{i,j=1}^3 M'_{ij} \sigma_i \otimes \sigma_j + \sum_{k=1}^3 (c_k + w_k) (\sigma_k \otimes I + I \otimes \sigma_k)$$

Trick 2: Delete 1-local terms

$$H_{\text{sym}} = \sum_{i=1}^3 M'_{ii} \sigma_i \otimes \sigma_i + \sum_{k=1}^3 (c_k + w_k) (\sigma_k \otimes I + I \otimes \sigma_k)$$

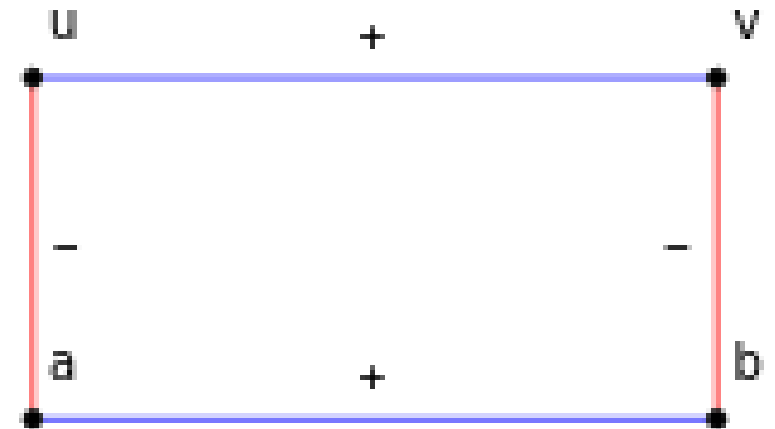
$$\text{Tr}(H \rho^u \rho^v) = \hat{u}^T M' \hat{v} + (\hat{c} + \hat{w})^T (\hat{u} + \hat{v})$$

We borrow a nice gadget from [CM14].

To interact two qubits u, v , we add two ancilla qubits a, b :

$$G^{uv} = H_{\text{sym}}^{uv} + H_{\text{sym}}^{ab} - H_{\text{sym}}^{ua} - H_{\text{sym}}^{vb}$$

Negative weights cause all the 1-local terms to cancel



Result of Trick 2

$$H_{\text{sym}} = \sum_{i=1}^3 M'_{ii} \sigma_i \otimes \sigma_i + \sum_{k=1}^3 (c_k + w_k) (\sigma_k \otimes I + I \otimes \sigma_k)$$

To interact two qubits u, v , we add two ancilla qubits a, b :

$$G^{uv} = H_{\text{sym}}^{uv} + H_{\text{sym}}^{ab} - H_{\text{sym}}^{ua} - H_{\text{sym}}^{vb}$$

= \dots \dots \dots

Then,

$$\text{Tr}[G^{uv} \rho_u \rho_v \rho_a \rho_b] = (\hat{\mathbf{u}} - \hat{\mathbf{v}})^T \mathbf{M}' (\hat{\mathbf{a}} - \hat{\mathbf{b}})$$

Bloch vectors

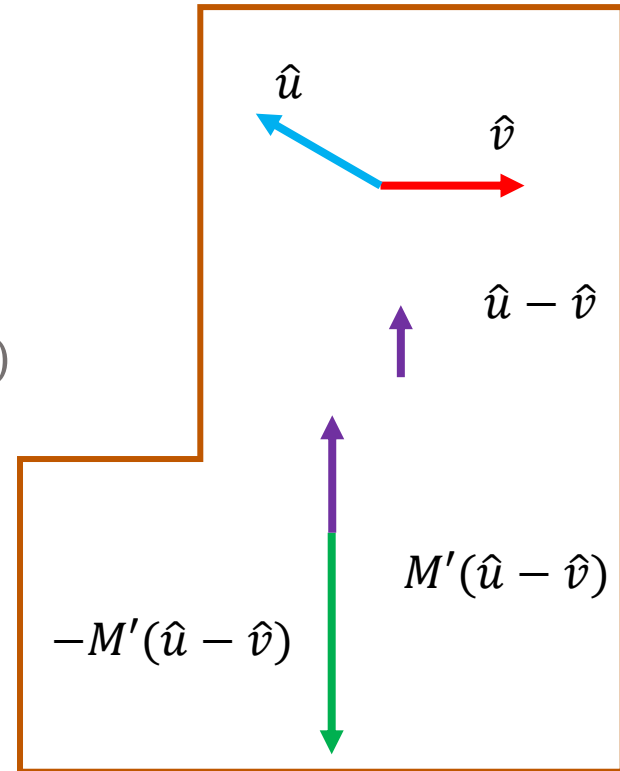
$$\mathbf{M}' = \begin{bmatrix} \alpha & & \\ & \beta & \\ & & \gamma \end{bmatrix}$$

Result of tricks

$$H_{sym} = \sum_{i=1}^3 M'_{ii} \sigma_i \otimes \sigma_i + \sum_{k=1}^3 (c_k + w_k) (\sigma_k \otimes I + I \otimes \sigma_k)$$

To interact two qubits u, v , we add two ancilla qubits a, b , and construct gadget G .

$$\text{Tr}[G^{uv} \rho_u \rho_v \rho_a \rho_b] = (\hat{u} - \hat{v})^T M'(\hat{a} - \hat{b})$$



Given u, v are constrained, what is the minimum value of $(\hat{u} - \hat{v})^T M'(\hat{a} - \hat{b})$?

Qubits a, b are free, each become proportional to $-M'(\hat{u} - \hat{v})$,

So minimum value is... $-2(\hat{u} - \hat{v})^T M'' \frac{M''(\hat{u} - \hat{v})}{\|M''(\hat{u} - \hat{v})\|} = -2\|M''(\hat{u} - \hat{v})\|$ for $M'' = |M'|$

Stop thinking about inner products...

Start thinking about distances

Result of tricks

Using only a given term $H \in S$,

Construct a Hamiltonian $H_{\text{final}} = \sum_{uv} G^{uv}$,

Such that the minimum energy of a product state is

$$\min_{\rho = \rho_1 \rho_2 \dots \rho_n} \text{Tr}[H_{\text{final}} \rho_1 \dots \rho_n]$$

$$= \min_{|\hat{u}|=1} \sum_{uv} -2 \|M''(\hat{u} - \hat{v})\| = -2 \max_{|\hat{u}|=1} \sum_{uv} \|M''(\hat{u} - \hat{v})\|$$

Call this sufficiently “nice”, and try to prove such a function is NP-hard.

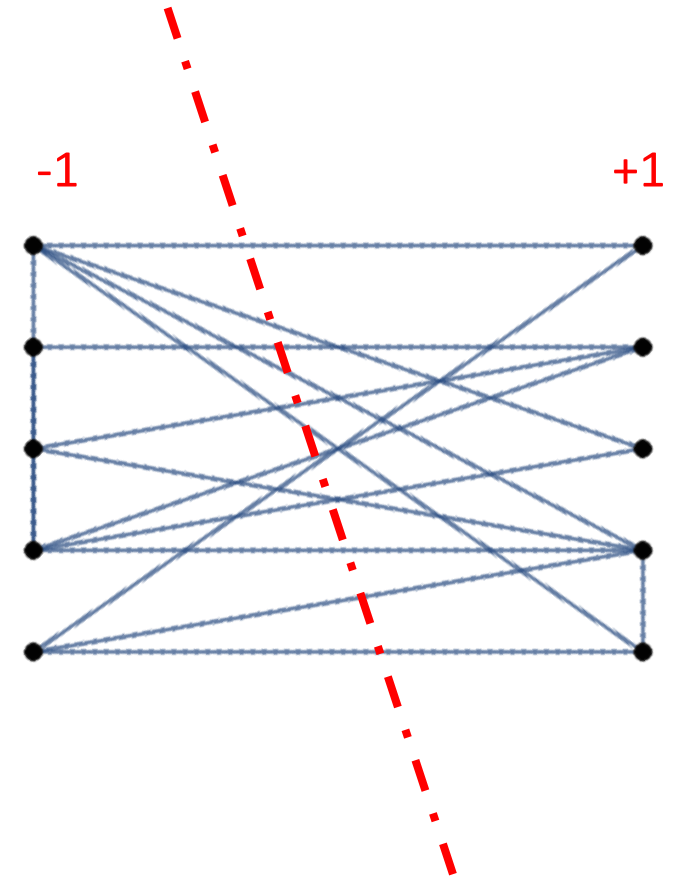
Vector Max-Cut Problems

All classical TCS from here – no more quantum

Max-Cut

Max-Cut

$$\begin{aligned} \text{MC}(G) &= \frac{1}{2} \max_{\hat{i}=\pm 1} \sum_{ij \in E} 1 - \hat{i}\hat{j} \\ &= \frac{1}{2} \max_{\hat{i}=\pm 1} \sum_{ij \in E} |\hat{i} - \hat{j}| \end{aligned}$$



Vector Max-Cut

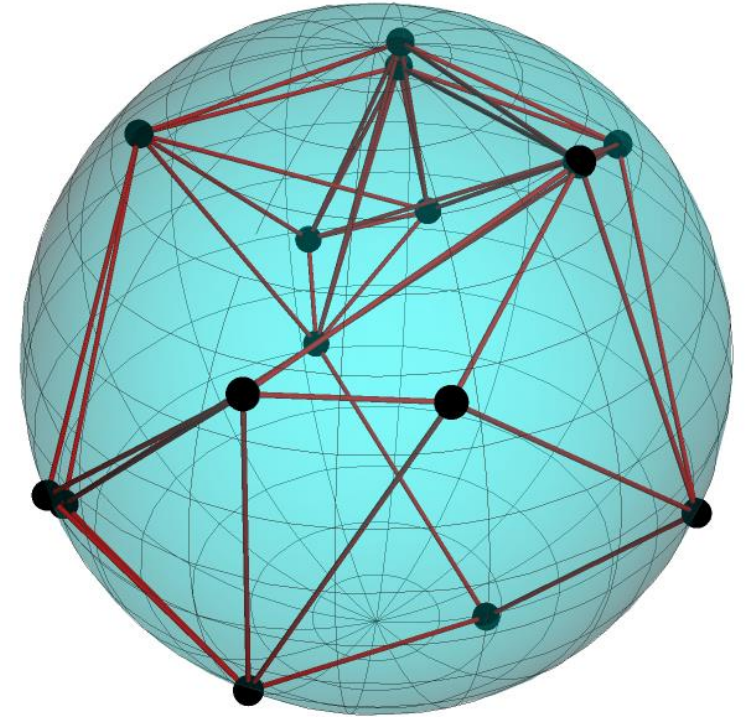
Max-Cut

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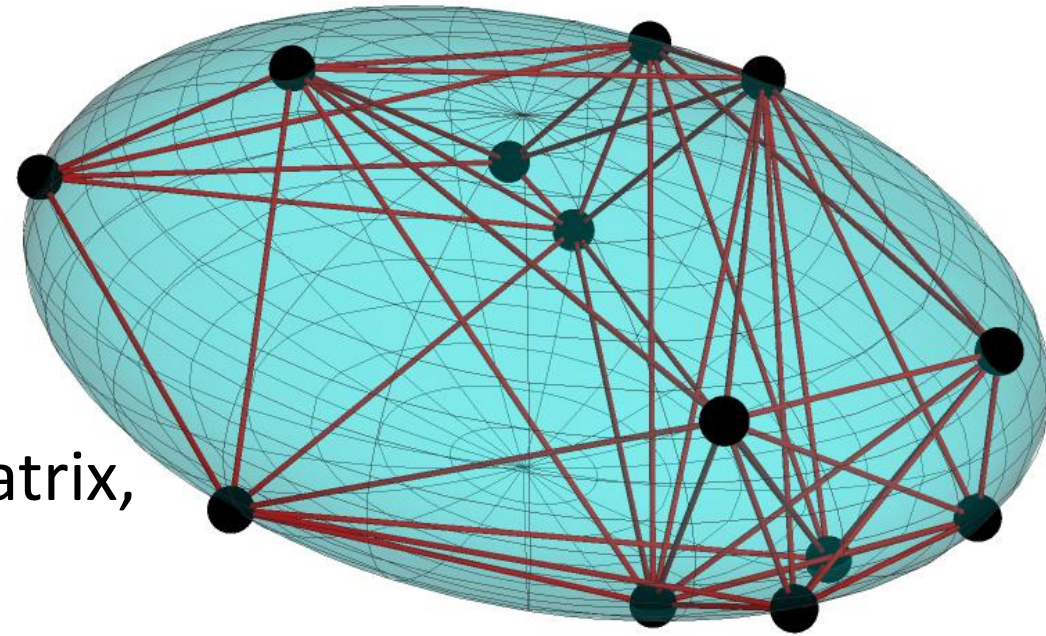
Vector Max-Cut

$$\begin{aligned}\text{MC}_k(G) &= \frac{1}{2} \max_{\hat{i} \in S^{k-1}} \sum_{ij \in E} 1 - \hat{i}\hat{j} \\ &= \frac{1}{4} \max_{\hat{i} \in S^{k-1}} \sum_{ij \in E} \|\hat{i} - \hat{j}\|^2\end{aligned}$$

Intuition: Embed a graph onto unit sphere S^{k-1} in \mathbb{R}^k to maximize the sum of the squared distances



Stretched linear Vector Max-Cut



For $W = \begin{bmatrix} \alpha & & \\ & \beta & \\ & & \gamma \end{bmatrix}$ a fixed diagonal matrix,

given a graph $G = (V, E)$,

estimate

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

Intuition: Embed a graph onto ~~unit sphere~~ ellipsoid in \mathbb{R}^k to maximize the sum of the squared distances

Stretched linear Vector Max-Cut is NP-hard

Theorem: For any fixed non-negative nonzero $W = \text{diag}(\alpha, \beta, \gamma)$, MC_W^L is NP-complete.

Earlier, we showed how to reduce an instance of MC_W^L to $S\text{-prodLH}$.

✓ So, this theorem will complete our main result: $S\text{-prodLH}$ is NP-hard.

Proof sketch 1

Theorem: For any fixed non-negative nonzero $W = \text{diag}(\alpha, \beta, \gamma)$, MC_W^L is NP-complete.

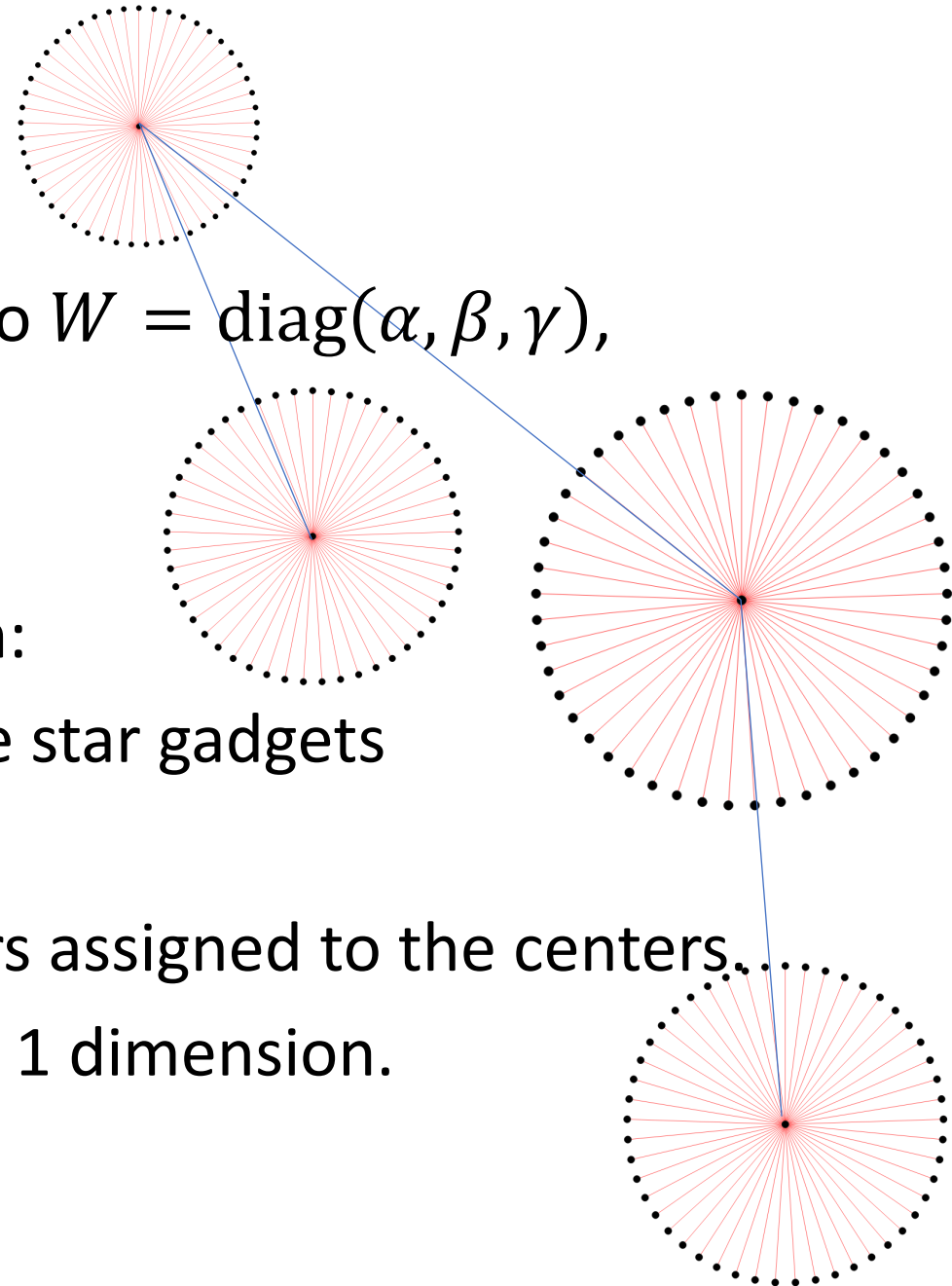
If $\alpha > \beta, \gamma$, we can use a simple construction:

- Given graph G , construct G' by adding large star gadgets

The star gadgets *amplify* the length of vectors assigned to the centers.

To maximize the lengths, vectors must live in 1 dimension.

→ Reduction from standard Max-Cut

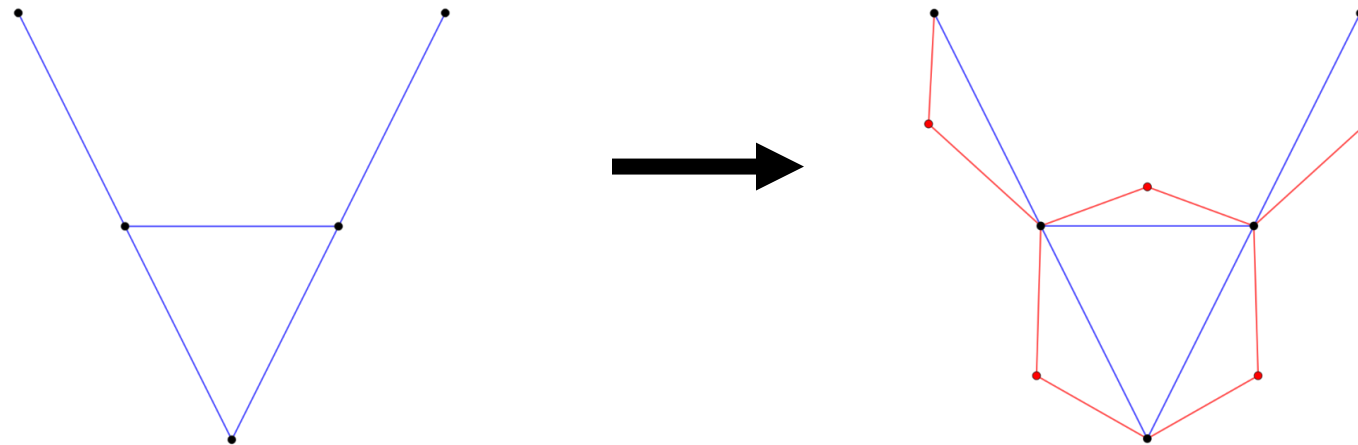


Proof sketch 2

Theorem: For any fixed non-negative nonzero $W = \text{diag}(\alpha, \beta, \gamma)$, MC_W^L is NP-complete.

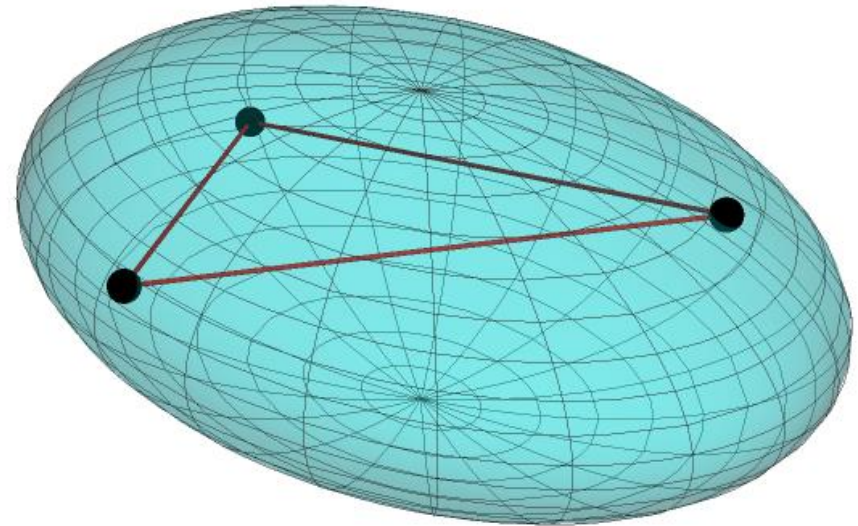
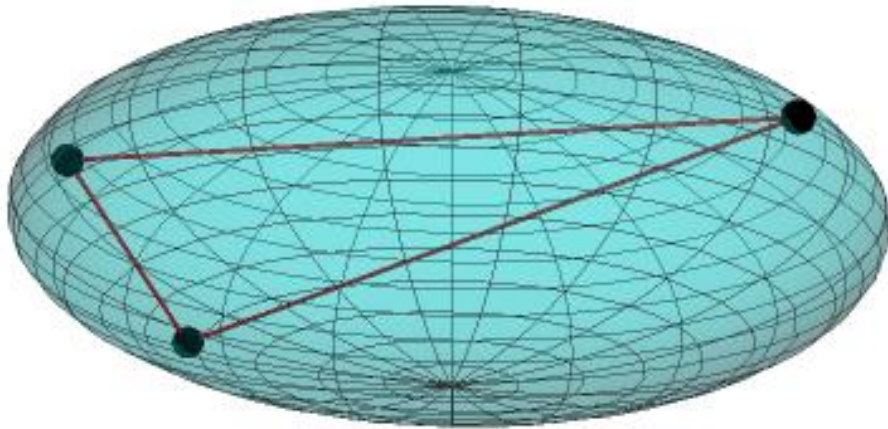
If $\alpha \neq \beta, \gamma$, we use a lengthier, but easy-to-analyze, construction.

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



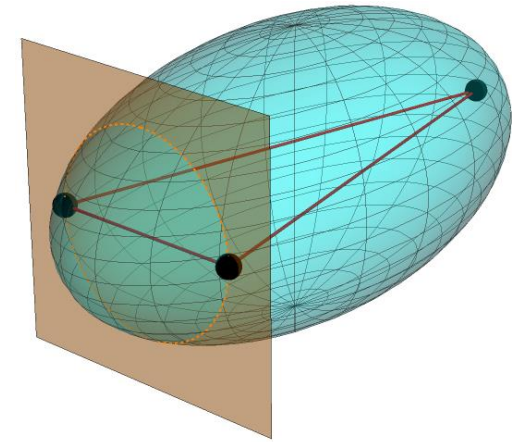
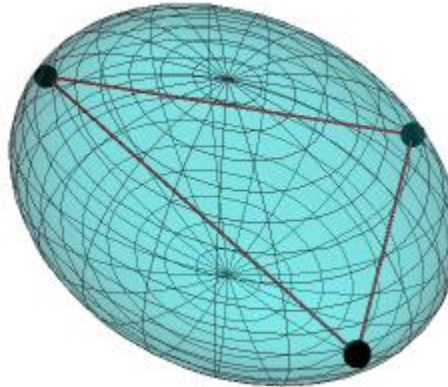
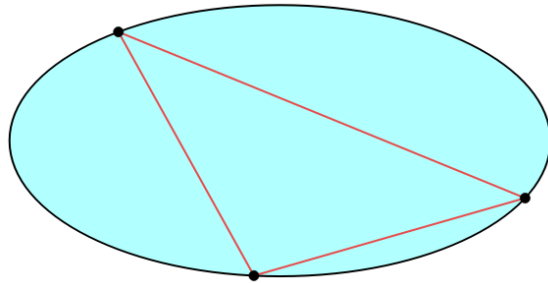
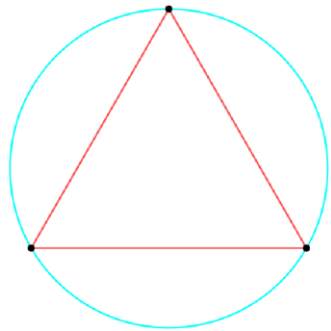
Proof sketch 2

2. Observe that maximizing the total distance between the vectors in a 3-clique is equivalent to picking 3 points on an ellipsoid which inscribe a triangle with maximum perimeter.



Proof sketch 2

3. Use the fact that maximum perimeter inscribed triangles are (somewhat) unique.



Circle, Ellipse, Ellipsoid: fix any 1 point, there is exactly 1 max perimeter triangle.

Centroid: must fix **2** points to fully determine max perimeter triangle.

Proof sketch 2

4. Every 3-clique gadget shares a vertex with another 3-clique gadget.
 - a) So, every gadget is assigned at least 1 vector shared with another gadget.
 - b) Given 1 fixed point, there's a unique pair of other points giving maximum length...
5. Conclude that G' can maximally satisfy *every* 3-clique gadget iff the *same* set of 3 optimal vectors can be assigned to all 3-cliques.

The NP-complete **3-Coloring** problem reduces to the **Stretched linear Vector Max-Cut** problem. □

Summary of proof of main theorem

Proof summary

Main Theorem

For any fixed set of 2-qubit Hamiltonian terms S ,

- if every matrix in S is 1-local then S -prodLH is in P,
 - and otherwise S -prodLH is NP-complete.
-

- ✓ If every term is 1-local, then we can optimize the state of each qubit individually, so the problem is in P.
- ✓ prodLH is always contained in NP, using product states' concise classical descriptions $\text{Tr}(H\rho) = \sum_{ij} \text{Tr}(H_{ij} \rho_i \rho_j)$
- **To Do:** show if S contains a nontrivial 2-qubit term, then S -prodLH is NP-hard.

Proof summary

- **To Do:** show if S contains a nontrivial 2-qubit term, then S -prodLH is NP-hard.
- Product state problems can be viewed as optimization over single-qubit Bloch vectors.
- Given an arbitrary non-trivial 2-qubit term, we construct gadgets to make the product state energy “nice”.
- Call this new objective value **Stretched linear Vector Max Cut** ($\text{MC}_{\mathcal{W}}^L$).
- Show $\text{MC}_{\mathcal{W}}^L$ is NP-complete by reductions from 3-coloring or Max-Cut.

What's next?

1. Can we use the complexity of product state problems to suggest the general ground states of a class of Hamiltonians are *not* hard?
2. Classify S-prodLH with additional restrictions, e.g. only positive weights, spatial geometry?
3. Hamiltonian Constrained-Optimization problems, e.g. Quantum Vertex Cover

RPE

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On

Complexity Classification of Product State Problems for Local Hamiltonians

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arXiv: 2401.06725, January 2024

Main Theorem: For any fixed set of 2-qubit Hamiltonian terms S ,

- if every matrix in S is 1-local then S -prodLH is in P,
- and otherwise S -prodLH is NP-complete.

Corollary: For any fixed set of 2-qubit Hamiltonian terms S ,

- the problem S -LH is at least NP-hard iff S -prodLH is NP-complete.
- the problem S -LH is in P iff S -prodLH is in P.