Complexity classification of local Hamiltonian problems

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Joint work with Toby Cubitt: 

Introduction

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- Solving 3-term linear equations: given a system of linear equations over $\mathbb{F}_2$ with at most 3 variables per equation, is there a solution to all the equations?

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$$x_1 + x_2 + x_4 = 0, \quad x_2 + x_3 = 1, \quad x_1 + x_4 = 0$$

The first of these is NP-complete, the second is in P.

General constraint satisfaction problems

A very general way to study these kind of problems is via the framework of the problem $\mathcal{S}$-CSP.

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The complexity of the $\mathcal{S}$-CSP problem depends on the set $\mathcal{S}$.

A dichotomy theorem

A remarkable theorem of Schaefer allows this complexity to be completely characterised.

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- An example problem of this kind is MAX-CUT.

Noncommutative CSPs

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- Each constraint C on k bits gives a $2^k \times 2^k$ diagonal matrix M of 0's and 1's such that $M_{xx} = 1 - C(x)$.

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In this picture, it's natural (?) to generalise by allowing each constraint to be an arbitrary Hermitian $2^k \times 2^k$ matrix.

Local Hamiltonian problems

This natural quantum (noncommutative) generalisation of CSPs is called k-LOCAL HAMILTONIAN [Kitaev, Shen and Vyalyi '02].

- A k-local Hamiltonian is a Hermitian matrix H on the space of n qubits which can be written as

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k-local Hamiltonian

We are given a k-local Hamiltonian $H = \sum_{i=1}^{m} H^{(i)}$ on n qubits, and two numbers $a < b$ such that $b - a \geqslant 1/\operatorname{poly}(n)$. Promised that the smallest eigenvalue of H is either at most a, or at least b, our task is to determine which of these is the case.

NB: we assume throughout that all parameters are "reasonable" (e.g. rational, polynomial in n).

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- 1-local Hamiltonian is easily seen to be in P.

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- For example, the (general) Ising model corresponds to the problem of finding the lowest eigenvalue of a Hamiltonian of the form

$$H = \sum_{i<j} \alpha_{ij} Z_i Z_j.$$

Notation: $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

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- This connection to physics motivates the study of k-local Hamiltonian with restricted types of interactions.
- The aim: to prove QMA-hardness of problems of direct physical interest.

Previously known results

A number of special cases of k-LOCAL HAMILTONIAN have previously been shown to be QMA-complete, e.g.:

- [Schuch and Verstraete '09]:

$$H = \sum_{(i,j) \in E} X_i X_j + Y_i Y_j + Z_i Z_j + \sum_k \alpha_k X_k + \beta_k Y_k + \gamma_k Z_k,$$

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- [Biamonte and Love '08]:

  $$H = \sum_{i<j} J_{ij} X_i X_j + K_{ij} Z_i Z_j + \sum_k \alpha_k X_k + \beta_k Z_k,$$

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…but some other interesting special cases are not thought to be QMA-complete:

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- As AM is in the polynomial hierarchy, it is considered unlikely that k-LOCAL HAMILTONIAN with stoquastic Hamiltonians is QMA-complete.
- Later sharpened by [Bravyi, Bessen and Terhal '06], who showed that this problem is StoqMA-complete, where StoqMA is a complexity class between MA and AM.

The $\mathcal{S}$-Hamiltonian problem

Let $\mathcal{S}$ be a fixed subset of Hermitian matrices on at most k qubits, for some constant k.

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We then have the following general question:

Problem

Given $\mathcal{S}$, characterise the computational complexity of $\mathcal{S}$-Hamiltonian.

Some examples

The $\mathcal{S}$-Hamiltonian problem encapsulates many much-studied problems in physics. For example:

- The (general) Ising model:

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For us this is the problem $\{ZZ\}$-Hamiltonian; it is known to be NP-complete.

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- The (general) Ising model with transverse magnetic fields:

$$H = \sum_{i<j} \alpha_{ij} Z_i Z_j + \sum_k \beta_k X_k.$$

  For us this is the problem $\{ZZ, X\}$-HAMILTONIAN. Its complexity is more interesting…

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- By conjugating any transverse Ising model Hamiltonian by local Z operations on each qubit k such that $\beta_k > 0$, which maps $X \mapsto -X$ and does not change the eigenvalues, we can assume $\beta_k \leqslant 0$.

- The resulting Hamiltonian is stoquastic, so $\{ZZ, X\}$-Hamiltonian $\in$ StoqMA.

Some more examples

Two other cases previously studied in condensed-matter physics:

- The (general) Heisenberg model:

$$H = \sum_{i<j} \alpha_{ij}(X_i X_j + Y_i Y_j + Z_i Z_j).$$

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We use "general" in the titles to emphasise that there is no implied spatial locality or underlying interaction graph.

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3. Otherwise, if there exists $U \in SU(2)$ such that, for each 2-qubit matrix $H_i \in \mathcal{S}$, $U^{\otimes 2} H_i (U^\dagger)^{\otimes 2} = \alpha_i Z^{\otimes 2} + A_i I + I B_i$, where $\alpha_i \in \mathbb{R}$ and A_i, B_i are arbitrary 2×2 Hermitian matrices, then $\mathcal{S}$-HAMILTONIAN is polytime-equivalent to the transverse Ising model;

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4. Otherwise, $\mathcal{S}$-Hamiltonian is QMA-complete.

Corollaries

In particular, we have that:

- The (general) Heisenberg model is QMA-complete ($\mathcal{S} = \{XX + YY + ZZ\}$)
- The (general) XY model is QMA-complete ($\mathcal{S} = \{XX + YY\}$)

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- Note that matrices in $\mathcal{S}$ may be of different sizes.

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- We can assume without loss of generality that the identity matrix $I \in \mathcal{S}$ (we can add an arbitrary "energy shift").

The proof: easy parts

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1. The minimal eigenvalue of a sum of 1-local terms is the sum of the minimal eigenvalues.
2. If every interaction in $\mathcal{S}$ is diagonal, the minimal eigenvalue is achieved on a computational basis state; NP-completeness follows from showing that any 2-body diagonal interaction can be produced.

Case (3) isn't too difficult either:

- It's clearly no harder than $\{ZZ\}$-Hamiltonian with arbitrary local terms; these arbitrary terms turn out to give no additional power.

The proof: easy parts

Cases (1) and (2) are the easiest:

1. The minimal eigenvalue of a sum of 1-local terms is the sum of the minimal eigenvalues.
2. If every interaction in $\mathcal{S}$ is diagonal, the minimal eigenvalue is achieved on a computational basis state; NP-completeness follows from showing that any 2-body diagonal interaction can be produced.

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The most interesting case is (4)…

Proof techniques

The basic idea behind the proof is to use reductions.

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- Given two Hamiltonians H and V, we form $\widetilde{H} = V + \Delta H$, where Δ is a large parameter.
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Projection Lemma (informal, based on [Oliveira-Terhal '08])

If $\Delta = \delta \|V\|^2$, then

$$\|\widetilde{H}_{<\Delta/2} - V_-\| = O(1/\delta).$$

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The case $\mathcal{S} = \{XX + YY + ZZ\}$ illustrates the difficulties that we face. Let

$$H = \sum_{i<j} \alpha_{ij}(X_iX_j + Y_iY_j + Z_iZ_j).$$

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Just as with classical CSPs, the way round this is to use encodings.

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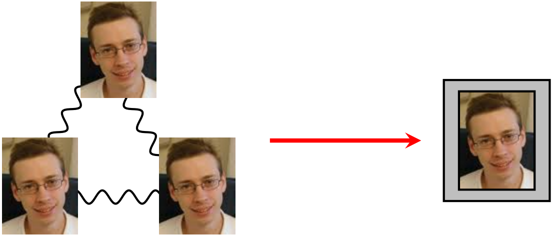

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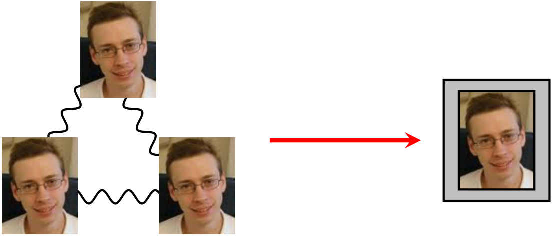

- This is inspired by previous work on universality of the exchange interaction [Kempe et al. ’00].

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- Then we can apply Z and X on two logical pseudo-qubits.

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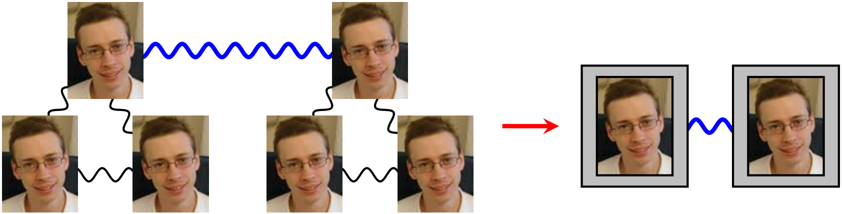
We would now like to apply pairwise interactions across logical qubits.



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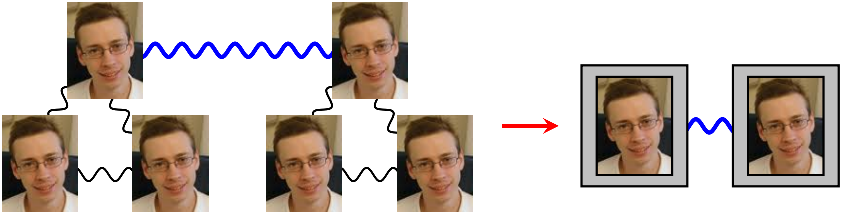

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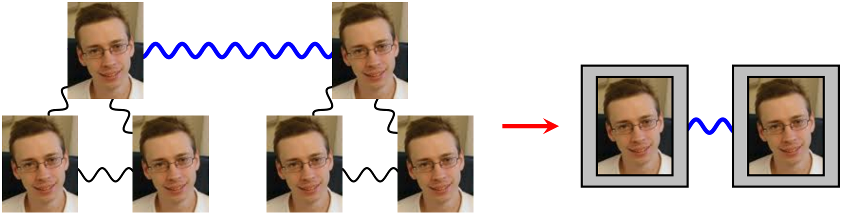

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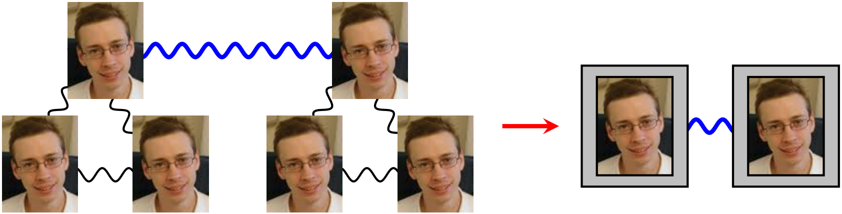

- This can almost be done by applying F interactions across different choices of physical qubits.
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- It turns out that, by applying suitable linear combinations across qubits, we can effectively make

$$X_1 X_3 (2F - I)_{24}, \quad Z_1 Z_3 (2F - I)_{24}, \quad I_1 I_3 (2F - I)_{24}.$$

Example: the Heisenberg model

So, using Heisenberg interactions alone, we can implement an arbitrary (logical) Hamiltonian of the form

$$H = \sum_{k=1}^{n} (\alpha_k X_k + \beta_k Z_k) I_{k'} + \sum_{i<j} (\gamma_{ij} X_i X_j + \delta_{ij} Z_i Z_j)(2F - I)_{i'j'},$$

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- To do this, we force the primed qubits to be in some state by very strong $F_{i'j'}$ interactions: we add the (logical) term

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- We can do this by making $I_i I_j (2F - I)_{i'j'}$ as on last slide.

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If the ground state $|\psi\rangle$ of G is non-degenerate, the primed qubits will all be effectively projected onto the ground state, and H will become (up to a small additive error)

$$\widetilde{H} = \sum_{k=1}^{n} \alpha_k X_k + \beta_k Z_k + \sum_{i<j} (\gamma_{ij} X_i X_j + \delta_{ij} Z_i Z_j) \langle\psi|(2F - I)_{i'j'}|\psi\rangle.$$

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- Not so easy! This corresponds to an exactly solvable special case of the Heisenberg model, and not many of these are known.
- Luckily for us, the Lieb-Mattis model [Lieb and Mattis '62] has precisely the properties we need.

The Lieb-Mattis model

The Lieb-Mattis model describes Hamiltonians of the form

$$H_{LM} = \sum_{i\in A, j\in B} X_i X_j + Y_i Y_j + Z_i Z_j,$$

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Claim **[Lieb and Mattis '62, . . .]**

If $|A| = |B| = n$, the ground state $|\phi\rangle$ of H_{LM} is unique. For i and j such that $i, j \in A$ or $i, j \in B$, $\langle\phi|F_{ij}|\phi\rangle = 1$. Otherwise, $\langle\phi|F_{ij}|\phi\rangle = -2/n$.

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Using this claim, we can effectively implement any Hamiltonian of the form

$$\widetilde{H} = \sum_{k=1}^{n} \alpha_k X_k + \beta_k Z_k + \sum_{i<j} \gamma_{ij} X_i X_j + \delta_{ij} Z_i Z_j,$$

which suffices for QMA-completeness [Biamonte and Love '08].

The normal form

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We've dealt with the Heisenberg model. . . what about everything else? We can simplify things using a very similar normal form to one identified by [Dür et al. '01, Bennett et al. '02]:

Lemma

Let H be a 2-qubit interaction which is symmetric under swapping qubits. Then there exists $U \in SU(2)$ such that the 2-local part of $U^{\otimes 2} H (U^\dagger)^{\otimes 2}$ is of the form

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Why is this useful? If we conjugate each term by $U^{\otimes 2}$ in a 2-local Hamiltonian with only H interactions, it doesn't change the eigenvalues:

$$\sum_{i \neq j} \alpha_{ij} (U^{\otimes 2} H (U^\dagger)^{\otimes 2})_{ij} = U^{\otimes n} \left(\sum_{i \neq j} \alpha_{ij} H_{ij} \right) (U^\dagger)^{\otimes n}.$$

The other QMA-complete cases

Our normal form drastically reduces the number of interactions we have to consider to a few special cases:

- The XY model $\mathcal{S} = \{XX + YY\}$ uses similar techniques to the Heisenberg model, but the gadgets are a bit simpler.
- For $\mathcal{S} = \{XX + \alpha YY + \beta ZZ\}$, we can reduce from the XY model.
- We also need to deal with the antisymmetric case $\mathcal{S} = \{XZ - ZX\}$.
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Finding and verifying each of the gadgets required was somewhat painful and required the use of a computer algebra package.

Conclusions and open problems

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Despite this, our work is only just beginning. . .

- What about k-qubit interactions for $k > 2$? We have a complete characterisation here in the special case where we assume that we are allowed access to arbitrary local terms.

- What about local dimension $d > 2$? Classically, the complexity of d-ary CSPs is still unresolved.

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- What about quantum k-SAT?

- Finally, what is the complexity of the transverse Ising model? Our intuition: at least MA-hard...for now, we encapsulate it as a new complexity class TIM.

Thanks!

arXiv:1311.3161

- For other further reading, several recent surveys on Hamiltonian complexity are arXiv:1401.3916, arXiv:1212.6312, arXiv:1106.5875.

Allowing local terms

One variant of this framework is to allow arbitrary local terms ("magnetic fields").

$\mathcal{S}$-Hamiltonian with local terms

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It is known that $\mathcal{S}$-Hamiltonian with local terms is QMA-complete when:

- $\mathcal{S} = \{XX + YY + ZZ\}$ [Schuch and Verstraete '09]
- $\mathcal{S} = \{XX, ZZ\}$ or $\mathcal{S} = \{XZ\}$ [Biamonte and Love '08]

The case with local terms

Let $\mathcal{S}$ be a fixed subset of Hermitian matrices on at most k qubits, for some constant k.

Theorem

Let $\mathcal{S}'$ be the subset formed by removing all 1-local terms from each element of $\mathcal{S}$, and then deleting all 0-local matrices. Then:

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3. Otherwise, $\mathcal{S}$-Hamiltonian with local terms is QMA-complete.

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- The first-order perturbative gadgets we use are based on ideas going back to [Oliveira and Terhal '08] and [Schuch and Verstraete '08].
- The basic idea: to implement an effective interaction across two qubits a and c, add a new mediator qubit b interacting with each of a and c, and put a strong 1-local interaction on b.

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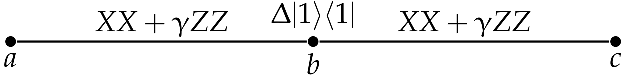

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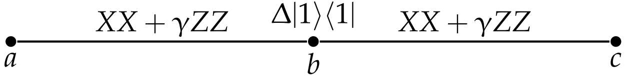

- This forces qubit b to (approximately) be in the state $|0\rangle$.

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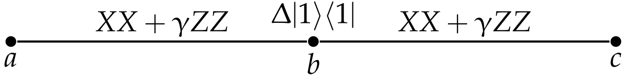

- This forces qubit b to (approximately) be in the state $|0\rangle$.
- It turns out that, up to local and lower-order terms, the effective interaction across the remaining qubits is

$$H_{\text{eff}} \propto X_a X_c.$$

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We can similarly show that:

- For any $\beta, \gamma \neq 0$, $\{XX + \beta YY + \gamma ZZ\}$-Hamiltonian with local terms is QMA-complete.
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This turns out to be all the cases we need to complete the characterisation of $\mathcal{S}$-Hamiltonian with local terms!

The different cases in the characterisation

To finish off the 2-local special case of $\mathcal{S}$-Hamiltonian with local terms:

- If the 2-local part of any interaction in $\mathcal{S}$ is locally equivalent to $XX + \beta YY + \gamma ZZ$ or $XZ - ZX$, we have QMA-completeness;

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- So we can make $XX + AA$, which suffices for QMA-completeness.

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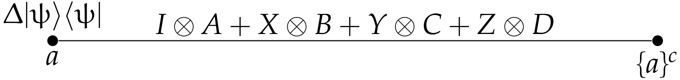

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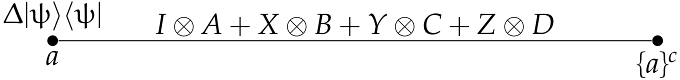

- By letting $|\psi\rangle$ be the eigenvector of X, Y or Z with eigenvalue ± 1, we can produce the effective interactions $A \pm B$, $A \pm C$ and $A \pm D$ (up to a small additive error).

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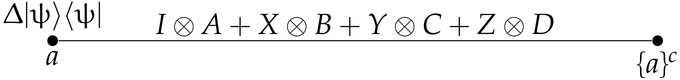

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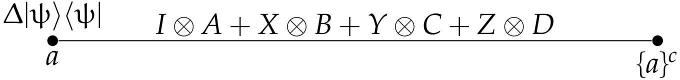

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- By adding/subtracting these matrices we can make each of $\{A, B, C, D\}$.
- So either $\mathcal{S}$ is QMA-complete, or all 2-local "parts" of each interaction in $\mathcal{S}$ are simultaneously diagonalisable by local unitaries. This case turns out to be in TIM.

$\mathcal{S}$-Hamiltonian: The list of lemmas

It suffices to prove QMA-completeness of the following cases:

1. $\{XX + YY + ZZ\}$-Hamiltonian;
2. $\{XX + YY\}$-Hamiltonian;
3. $\{XZ - ZX\}$-Hamiltonian;
4. $\{XX + \beta YY + \gamma ZZ\}$-Hamiltonian;
5. $\{XX + \beta YY + \gamma ZZ + AI + IA\}$-Hamiltonian;
6. $\{XZ - ZX + AI - IA\}$-Hamiltonian.

In the above, β, γ are real numbers such that at least one of β and γ is non-zero, and A is an arbitrary single-qubit Hermitian matrix.

$\mathcal{S}$-Hamiltonian: The list of lemmas

We also need some reductions from cases which are not necessarily QMA-complete:

- $\{ZZ, X, Z\}$-Hamiltonian reduces to $\{ZZ + AI + IA\}$-Hamiltonian;
- $\{ZZ, X, Z\}$-Hamiltonian reduces to $\{ZZ, AI - IA\}$-Hamiltonian.

In the above, A is any single-qubit Hermitian matrix which does not commute with Z.

And the very final case to consider:

- Let $\mathcal{S}$ be a set of diagonal Hermitian matrices on at most 2 qubits. Then, if every matrix in $\mathcal{S}$ is 1-local, $\mathcal{S}$-Hamiltonian is in P. Otherwise, $\mathcal{S}$-Hamiltonian is NP-complete.

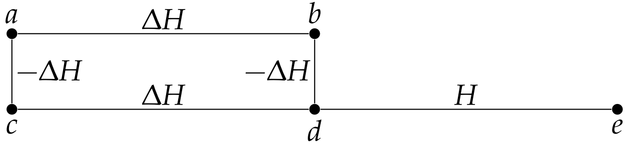
Example gadget for cases with 1-local terms

Let $H := XX + \beta YY + \gamma ZZ + AI + IA$, where β or γ is non-zero.

Lemma

$\{H\}$-Hamiltonian is QMA-complete.

The gadget used looks like:



- The ground state of $G := H_{ab} + H_{cd} - H_{ac} - H_{bd}$ is maximally entangled across the split $(a\text{-}c : d)$.
- So if we project H_{de} onto this state, the effective interaction produced is A on qubit e.
- This allows us to effectively delete the 1-local part of H.