# 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

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- An example constraint: $f(a, b, c) = a \vee b \vee \neg c$.
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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.

**Theorem** **[Schaefer '78]**

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

# Local Hamiltonian problems

The natural quantum 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

$$H = \sum_i H^{(i)},$$

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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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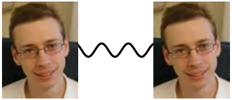
- Later improved to show that even 2-LOCAL HAMILTONIAN is QMA-complete [Kempe, Kitaev and Regev '06].



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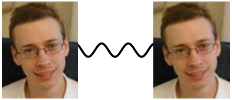

- 1-local Hamiltonian is in P, so is this the end of the line?

# *k*-local Hamiltonian and condensed-matter physics

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

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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

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### $\mathcal{S}$-Hamiltonian

$\mathcal{S}$-Hamiltonian is the special case of $k$-local Hamiltonian where the overall Hamiltonian $H$ is specified by a sum of matrices $H_i$, each of which acts non-trivially on at most $k$ qubits, and whose non-trivial part is proportional to a matrix picked from $\mathcal{S}$.

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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:

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

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. We shorten the title to "transverse Ising model".

# Some more examples

- 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.

# Remarks on the problem

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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").

# Allowing local terms

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

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

$\mathcal{S}$-Hamiltonian with local terms is the special case of $\mathcal{S}$-Hamiltonian where $\mathcal{S}$ is assumed to contain $X$, $Y$, $Z$.

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- For any $\mathcal{S}$, $\mathcal{S}$-Hamiltonian with local terms is at least as hard as $\mathcal{S}$-Hamiltonian.

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]

# Our first result

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.

# Explaining the second case

The second case is stated in terms of "local diagonalisation":

- Let $M$ be a $k$-qubit Hermitian matrix.
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This case is poly-time equivalent to the transverse Ising model $\{ZZ, X\}$-Hamiltonian, i.e. Hamiltonians of the form

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

What is the complexity of solving this model?

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- We have not been able to characterise the complexity of this problem more precisely, so encapsulate it in a new complexity class TIM, where NP $\subseteq$ TIM $\subseteq$ StoqMA.
- Future work: the Transverse Ordered Boson Ynteraction and Anisotropic Symmetric Hamiltonians with Local Extensive Ynteractions...

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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 ($\mathcal{S} = \{XX + YY\}$)

…as well as many other cases.

We can think of this result as a quantum analogue of Schaefer's dichotomy theorem.

# Proof techniques

We follow the standard pattern for proving dichotomy-type theorems:

> “Isolate some special cases and prove that they are easy, then prove that everything else is hard.”

# Proof techniques

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> “Isolate some special cases and prove that they are easy, then prove that everything else is hard.”

- The two results are proven using (fairly) different techniques, but both are based on reductions, rather than direct proofs using clock constructions or similar.

- The starting point for both is a normal form for 2-qubit Hermitian matrices.

# The normal form

We use a very similar normal form to one identified by [Dür et al. '01, Bennett et al. '02]. An important special case:

## 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 next step

The basic idea:

> "To prove QMA-hardness of $\mathcal{A}$-Hamiltonian, approximately simulate some other set of interactions $\mathcal{B}$, where $\mathcal{B}$-Hamiltonian is QMA-hard."

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- To do this, we use two kinds of reductions, both based on perturbation theory.
- 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 $b$.

# Example

**Claim (similar to results of [Schuch and Verstraete '08])**

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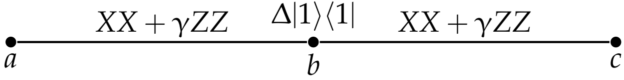

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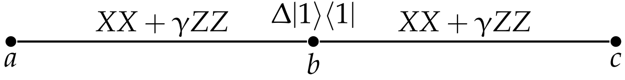


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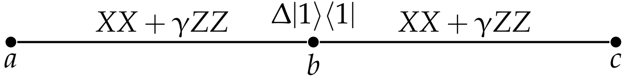


- This forces qubit $b$ to (approximately) be in the state $|0\rangle$.
- It turns out that, up to local and lower-order terms, the effective interaction across the remaining qubits is

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

# Example

- So, given access to terms of the form $XX + \gamma ZZ$, we can effectively make $XX$ terms. By subtracting from $XX + \gamma ZZ$, we can also make $ZZ$ terms.

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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!

# Recap: Our second result

Let $\mathcal{S}$ be an arbitrary fixed subset of Hermitian matrices on at most 2 qubits.

**Theorem**

1. If every matrix in $\mathcal{S}$ is 1-local, $\mathcal{S}$-Hamiltonian is in P;
2. Otherwise, if there exists $U \in SU(2)$ such that $U$ locally diagonalises $\mathcal{S}$, then $\mathcal{S}$-Hamiltonian is NP-complete;
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 single-qubit Hermitian matrices, then $\mathcal{S}$-Hamiltonian is TIM-complete;
4. Otherwise, $\mathcal{S}$-Hamiltonian is QMA-complete.

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The most interesting case is (4)...

# Proof techniques

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- The basic idea: encode interactions within a subspace.
- Given two Hamiltonians $H$ and $V$, we form $\widetilde{H} = V + \Delta H$, where $\Delta$ is a large parameter.
- Then $\widetilde{H}_{<\Delta/2}$, the low-energy part of $\widetilde{H}$, is effectively the same as $V_-$, the projection of $V$ onto the lowest-energy eigenspace of $H$.

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**Projection Lemma (informal, based on [Oliveira+Terhal '08])**

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

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

# Example: the Heisenberg model

The case $\mathcal{S} = \{XX + YY + ZZ\}$ illustrates the difficulties that we face when we do not have access to all 1-local terms. Let

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

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

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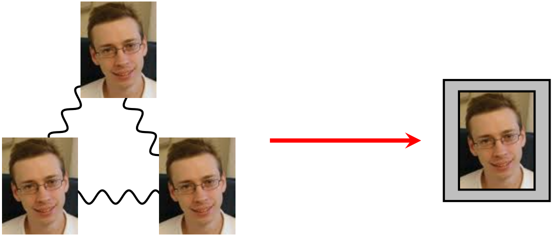

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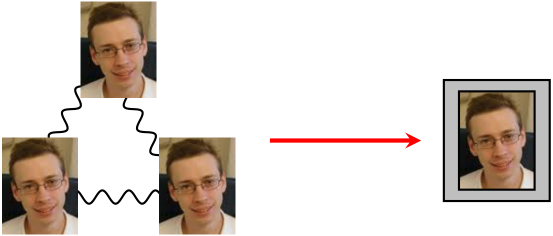

- This is inspired by previous work on universality of the exchange interaction [Kempe et al. '00].

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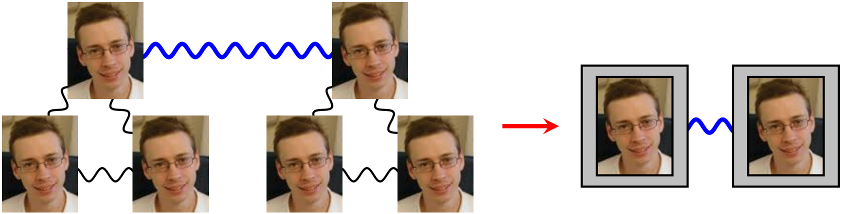
- By applying strong $F$ interactions across all pairs of qubits, we can effectively project onto $S_2$.
- Then we can apply $Z$ and $X$ on two logical pseudo-qubits.

# Example: the Heisenberg model

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



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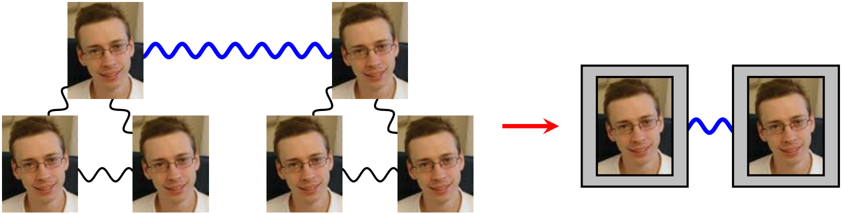

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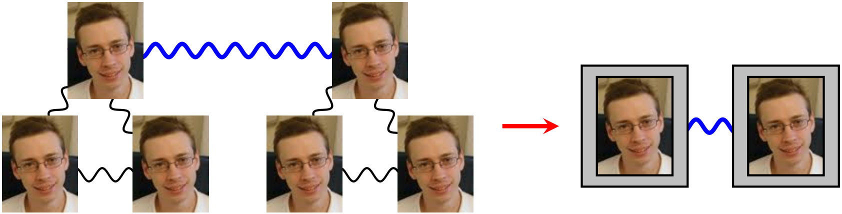

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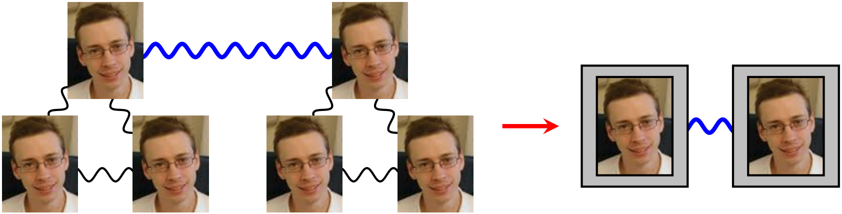

- This can almost be done by applying $F$ interactions across different choices of physical qubits.
- Let the logical qubits in the first (resp. second) triangle be labelled (1,2) (resp. (3,4)).
- It turns out that, by applying suitable linear combinations across qubits, we can effectively make

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

# Example: the Heisenberg model

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

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

where we identify the $i$'th logical qubit pair with indices $(i, i')$.

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- We would like to remove the $(2F - I)$ operators.
- 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

$$G = \Delta \sum_{i<j} w_{ij} F_{i'j'}$$

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

# Example: the Heisenberg model

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

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

where $A$ and $B$ are disjoint subsets of qubits.

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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 other QMA-complete cases

We've dealt with the Heisenberg model…what about everything else?

- 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.
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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

We have (almost) completely characterised the complexity of 2-local qubit Hamiltonians.

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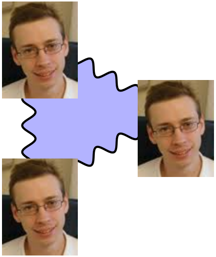
- What about $k$-qubit interactions for $k > 2$? We only resolved this case for $\mathcal{S}$-Hamiltonian with local terms.



# Conclusions and open problems

We have (almost) completely characterised the complexity of 2-local qubit Hamiltonians.

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

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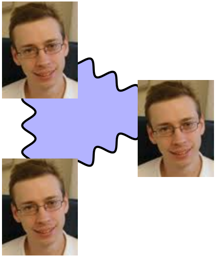

- What about local dimension $d > 2$? Classically, the complexity of $d$-ary CSPs is still unresolved.

# More open problems

- What about restrictions on the interaction pattern or weights? e.g. the antiferromagnetic Heisenberg model etc.
- See very recent independent work proving QMA-hardness for $\mathcal{S} = \{XX + YY, Z\}$ when weights of $XX + YY$ terms are positive and weights of $Z$ terms are negative [Childs, Gosset and Webb '13]...
- What about quantum $k$-SAT?
- Finally, what is the complexity of TIM? Our intuition: at least MA-hard...

# Thanks!

arXiv:1311.3161

# 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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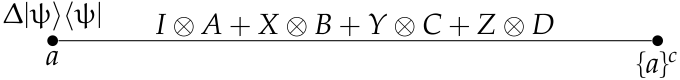

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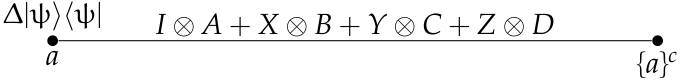


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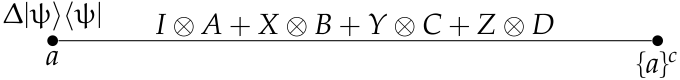


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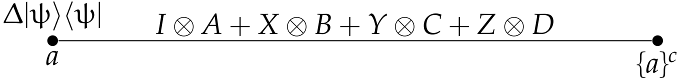


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- By adding/subtracting these matrices we can make each of $\{A, B, C, D\}$.
- So either $\mathcal{S}$ is QMA-complete, or all 2-local "parts" of each interaction in $\mathcal{S}$ are simultaneously diagonalisable by local unitaries. This case turns 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, $\beta$, $\gamma$ are real numbers such that at least one of $\beta$ and $\gamma$ 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.

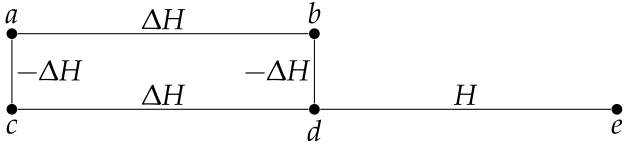
# Example gadget for cases with 1-local terms

Let $H := XX + \beta YY + \gamma ZZ + AI + IA$, where $\beta$ or $\gamma$ 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 $H$.