Universal Hamiltonians

We have now developed a mathematical formalism of Hamiltonian simulation, as well as one set of tools (perturbation gadgets) for constructing interesting new simulations.

It is time to apply all this formalism to prove new results. In this course, we will only have time to see one application: universal Hamiltonians. But the Hamiltonian simulation formalism developed here has by now been used to prove a number of other results in quantum information and mathematical physics, in surprisingly diverse areas ranging from AdS/CFT duality in quantum gravity, to position-based verification in quantum cryptography. (Tamara will touch on some of these in her lecture course.)

Here, we will restrict our scope to proving that the Heisenberg model is universal, and close by explaining how this forms the basis of the full classification theorem for 2-local qubit Hamiltonians & some of its consequences.

Def. (Universal Hamiltonian)

We say that a family of Hamiltonians $\mathcal{F}$ is universal if $\forall n \in \mathbb{N}$, $\forall H \in \mathrm{Herm}_n$, $\forall \varepsilon, \eta > 0$, $\Delta > \|H\|$ $\exists H' \in \mathcal{F}$ s.t. H' $(\Delta, \varepsilon, \eta)$-simulates H.

We implicity assume we always have $\mathbb{1} \in \mathcal{F}$.

This is very strong! It says that a universal family of Hamiltonians can simulate all the physics of any other Hamiltonian to arbitrarily good accuracy up to an arbitrarily high energy cut-off.

Note: in fact, we can extend the requirements in this Def. to include simulating any fermionic or bosonic Hamiltonian on any (finite) number of modes, without changing any of the results which follow.

Def. (S-Hamiltonians)

Let S be a set of local interactons.

We call the family of Hamiltonians
$$\{ H : H = \sum_k \alpha_k h_k, \ \forall k \ h_k \in S, \ \alpha_k \in \mathbb{R} \}$$
the "S-Hamiltonians".

Def.
We say that S'-Hamiltonians can simulate S-Hamiltonians if

$\forall\, H \in S\text{-Ham} \;\; \exists\, H' \in S'\text{-Ham}$ s.t. H' simulates H.

Thm. (Universality of Heisenberg model)
Let $S = \{h_{heis}\}$, $h_{heis} = XX + YY + ZZ$ Heisenberg interaction
S-Hamiltonians are universal.

In fact, this result holds even if we restrict the to a 2D square lattice, so $H_{heis} = \sum_{\langle i,j \rangle} \alpha_{ij} h^{heis}_{ij}$.

We will prove this in a sequence of steps, each of which shows that the Hamiltonians from the previous step can simulate Hamiltonians with a more general form, until we reach all Hamiltonians.

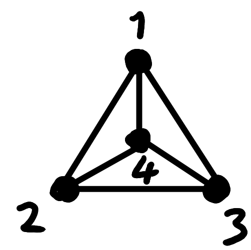
Lemma ([CMP'18])

Let $S = \{XX, XZ, ZX, ZZ, X, Z\}$.
S_{heis}-Ham. simulates S-Ham.

Pf. (sketch)

Heisenberg encoding gadget:

$$H = \sum_{i,j=1}^{4} h_{ij}^{heis} + 6\mathbb{1}$$



Ground states have 0 energy &
g.s. subspace is

$$S_0 = \mathrm{span}\{ |\psi^-\rangle_{12} |\psi^-\rangle_{34}, \ |\psi^-\rangle_{13} |\psi^-\rangle_{24} \}$$

$$|\psi^-\rangle := \frac{1}{\sqrt{2}} (|01\rangle - |10\rangle)$$ singlet

$\Pi_- :=$ projector onto S_0

Let $|0_L\rangle := |\psi^-\rangle_{13} |\psi^-\rangle_{24}$

$$|1_L\rangle := \frac{2}{\sqrt{3}} |\psi^-\rangle_{12} |\psi^-\rangle_{34} - \frac{1}{\sqrt{3}} |\psi^-\rangle_{13} |\psi^-\rangle_{24}$$

Want to construct different H_1's s.t. $\Delta H_0 + H_1$ simulates each of the local terms in S.

1-body terms:

Use 1st order simulation Lemma

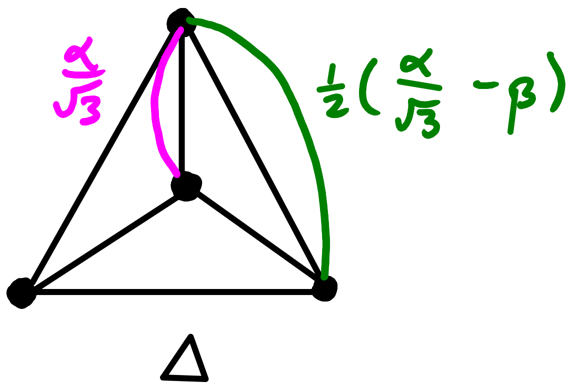
$\Rightarrow$ need H_1 s.t. $H_{eff} = (H_1)_{--} = \Pi_- H_1 \Pi_- = H_{target}$

Let $H_1 := \frac{\alpha}{\sqrt{3}} H_{14} + \frac{1}{2}\left(\frac{\alpha}{\sqrt{3}} - \beta\right) H_{13}$.

$$(H_1)_{--} = \alpha X_L + \beta Z_L + \frac{1}{2}(\beta - \sqrt{3}\alpha)\mathbb{1}$$

$$H_{eff}|_{\mathcal{H}_-} = (H_1)_{--}|_{\mathcal{H}_-} = \alpha X + \beta Z + \frac{1}{2}(\beta - \sqrt{3}\alpha)\mathbb{1}$$

$\Rightarrow$ choosing α, β appropriately lets us simulate 1-qubit Pauli X & Z terms.



vertices = qubits

edges = $h_{heis.}$

2-body terms:

Use 2nd order simulation Lemma on 2 copies of encoding gadget

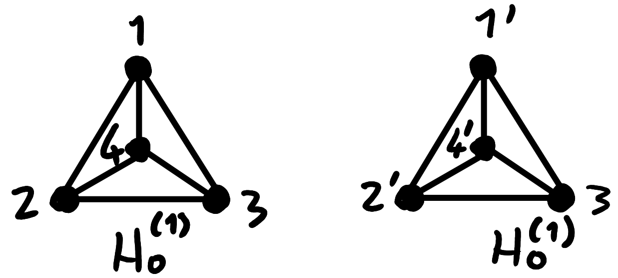
$\Rightarrow$ need H_1, H_2 s.t.

$$(H_1)_{--} - (H_2)_{-+} H_0^{-1} (H_2)_{+-} = H_{target}$$

Note: 2 copies, so now:

$$H_0 = H_0^{(1)} \otimes \mathbb{1} + \mathbb{1} \otimes H_0^{(1)}$$

$$\Pi_- = \Pi_-^{(1)} \otimes \Pi_-^{(1)}$$



Let $H_2 = \sum_{i,j} \alpha_{ij}\, h_{ij}^{heis}$

Lemma $\Rightarrow$ $H_{eff} = (H_1)_{--} - (H_2)_{-+} H_0^{-1} (H_2)_{+-}$

$$(H_2)_{-+} H_0^{-1} (H_2)_{+-} = \frac{1}{8} \sum_{i,j,k,l=1}^{4} 3\, \alpha_{ij}\, \alpha_{kl} (X_i \cdot X_k)_{--} \otimes (X_{j'} \cdot X_{l'})_{--}$$

$H_2 = h_{11'}^{heis} \mp h_{33'}^{heis}$

$\Rightarrow H_{eff} = \pm Z_L Z_L + 1\text{-local terms on } |0\rangle_L, |1\rangle_L$

$\Rightarrow H_{eff}|_{\mathcal{H}_-} = \pm ZZ + 1\text{-local terms}$

$H_2 = h_{13}^{heis} - h_{11'}^{heis} \pm h_{32'}$

$\Rightarrow H_{eff}|_{\mathcal{H}_-} = \pm ZX + 1\text{-local terms}$

$H_2 = h_{11'}^{heis} - 2h_{22'} + h_{33'}$

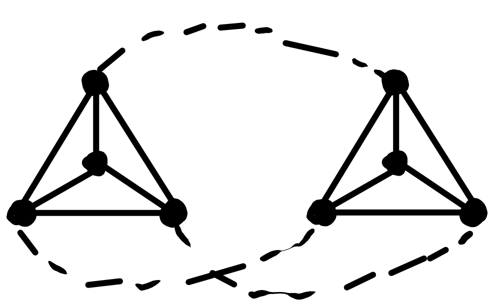
$\Rightarrow H_{eff}|_{\mathcal{H}_-} = XX + 1\text{-local terms}$

$H_2 = 35\, h_{11'}^{heis} + 5\, h_{22'}^{heis} - 3 h_{33'}^{heis} + 5\, h_{44'}^{heis}$

$\Rightarrow H_{eff}|_{\mathcal{H}_-} = -XX + 1\text{-local terms}$

Choosing H_1 as above, can cancel out any 1-local tems. $\square$

$Z_L Z_L$:



Lemma ([OT '08])

Let $S = \{XX, XZ, ZX, ZZ, X, Z\}$.

$$S' = \left\{ \bigotimes_{i=1}^{\leq k} \sigma_i \;:\; \sigma_i \in \{X, Z\} \right\}$$

i.e. all k-local qubit Ham's that contain no Pauli Y's in their Pauli decompositions

S-Ham. simulates S'-Ham.

Pf. (sketch)

Apply subdivision gadget + observation that this doesn't introduce any Pauli Y's if there were none present initially, to get to 3-local.

But for $k=3$, $\lceil k/2 \rceil + 1 = 3$, so subdivision gadget can't reduce below 3-local.

Need to use (third order) 3-to-2 gadget from [OT '08] to complete last step, + observation this doesn't introduce new Pauli Y's either.

Lemma

$$S = \left\{ \bigotimes_{i=1}^{\leq k+1} \sigma_i \ : \ \sigma_i \in \{X, Z\} \right\}$$

$$S' = \left\{ \bigotimes_{i=1}^{\leq k} h_i \in \mathrm{Herm}_{2^{2k}}(\mathbb{R}) \right\}$$

S-Ham. simulates S'-Ham.

Pf.

h_i real $\Rightarrow$ even # Pauli Y's

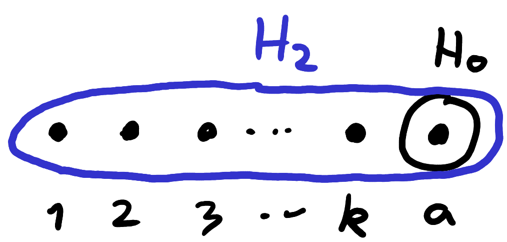
Wlog. assume $h_i = Y^{\otimes 2m} \otimes A$

where $A = \bigotimes_{j=1}^{k-2m} \sigma_j$, $\sigma_i \in \{X, Z\}$.

Use 2nd-order simulation Lemma

$$H_0 = \frac{\mathbb{1} + Z_a}{2} = |0\rangle\langle 0|_a$$

$$H_2 = X_a \otimes \left(X^{\otimes 2m} \otimes \mathbb{1} + (-1)^{m+1} Z^{\otimes m} \otimes A \right)$$



$$H_{\mathrm{eff}} = -(H_2)_{-+} H_0^{-1} (H_2)_{+-}$$

$$= -|0\rangle\langle 0|_a \otimes \left(X^{\otimes 2m} \otimes \mathbb{1} + (-1)^{m+1} Z^{\otimes 2m} \otimes A \right)^2$$

$$= 2\, |0\rangle\langle 0|_a \otimes \left(Y^{\otimes 2m} \otimes A + \mathbb{1} \right)$$

$$H_{\mathrm{eff}}\big|_{\mathcal{H}_-} = 2\, Y^{\otimes 2m} \otimes A + 2\mathbb{1}$$

$\square$

Lemma

$$S = \left\{ \bigotimes_{i=1}^{\leq 2k} h_i \ : \ h_i \in \mathrm{Herm}_2(\mathbb{R}) \right\}$$

$$S' = \left\{ \bigotimes_{i=1}^{k} h_i \ : \ h_i \in \mathrm{Herm}_2(\mathbb{C}) \right\}$$

S-Ham. simulates S'-Ham.

Pf.

This is just the local complex-to-real simulation we've already seen previously.

Note: k is arbitrary, and all qubit Hamiltonians can be decomposed into Paulis

$\Rightarrow$ S' = all qubit Hamiltonians

Exercise: Show that $\forall n$, $\forall$ sufficiently large Δ, & $\forall\, \varepsilon, \eta > 0$, any $H \in \mathrm{Herm}_n$ can be simulated by a qubit Hamiltonian.

Chaining these Lemmas together, we have proven the claimed universality of the Heisenberg model:

<u>Thm.</u> (restated)
$S_{heis} = \{XX + YY + ZZ\}$
S_{heis}-Hamiltonians are universal.

In fact, with slightly more effort, one can show that this result remains true even if all the local Heisenberg interactions are restricted to a 2D square lattice.

We call also extend this to include simulation of any bosonic or fermionic (or supersymmetric) Hamiltonian on any (finite) number of modes:

<u>Thm.</u>
$S = \{ \mathrm{Herm}_n : n < \infty \}$
$S' = \{$n-mode bosonic or fermionic Ham's: $n < \infty \}$
S-Ham. simulates S'-Ham.

<u>Pf.</u>
Bosons: Holstein–Primakoff transformation.
Fermions: any <u>local</u> fermion-to-qubit mapping (Jordan–Wigner insufficient)

This is a remarkable result! It shows, in a fully rigorous sense, that the entire physics of <u>any</u> Hamiltonian, in any spatial dimension — 3d, 4d, 11d... (cf. holography ⇝ Tamara's lectures), or even on interaction graphs with no geometric embedding) — Hamiltonians with <u>any</u> local or global symmetry, or no symmetries at all, every phase of matter, indeed any physical phenomenon whatsoever*, can all be seen in the 2d Heisenberg model.

This is all the more remarkable given the Heisenberg model has all-real matrix elements and full local $SU(2)$ invariance.

We can prove the analogous result for the XY-model:

<u>Thm.</u> (universality of XY-model)
$S_{xy} = \{XX + YY\}$
S_{xy} - Ham's are universal.

<u>Pf.</u>
Very similar to the Heisenberg case.

Complete classification of 2-qubit Ham's

Thm.
Let S be any fixed set of 1- and 2-local qubit interactions $\{h_1\} \cup \{h_2\}$ s.t. $\exists$ at least one 2-local $h \in S$. Then S falls into exactly one of the following categories:

(1) If $\exists\ U \in SU(2)$ s.t. $\forall\ h_1, h_2 \in S$

$$U h_1 U^\dagger = \text{diag}, \quad (U \otimes U) h_2 (U \otimes U)^\dagger = \text{diag}.$$

(i.e. S is "locally simultaneously diagonalisable")

S- Ham's are universal <u>classical</u> Hamiltonian simulators.

(2) Otherwise, if $\exists\ U \in SU(2)$ s.t. $\forall\ h_2 \in S$

$$(U \otimes U) h_2 (U \otimes U)^\dagger = \alpha ZZ + A \otimes \mathbb{1} + \mathbb{1} \otimes B$$

for some $\alpha \in \mathbb{R}$, $A, B \in \text{Herm}_2$

(i.e. S is "locally simultaneously equivalent to the transverse Ising model")

S- Ham's are universal <u>stoquastic</u> Hamiltonian simulators.

(3) Otherwise, S- Ham's are universal quantum Hamiltonian simulators.

Pf. (sketch)

(1) [de las Cuevas, Cubitt '14] proved that any classical Hamiltonian with NP-complete g.s. energy problem is a universal classical simulator.

Claim then follows from fact classical Ising model is NP-complete.

(2) Essentially proven by [BDOT'08] + checking that each step in their g.s. complexity reduction in fact gives a simulation.

(3) Follows from following Lemma + + universality of Heisenberg + XY.

Lemma

For S from case (3), S-Ham. simulates either S_{heis}-Ham. or S_{XY}-Ham.

Pf.

Follows from [Cubitt-Montanaro '16] + checking that each step in the g.s. complexity reduction in fact gives a simulation.

We haven't said anything in this lecture course about <u>efficiency</u> of simulations. One can define an efficient local simulation to be one where all parametes (Δ, ε, η, # qubits in H'...) scale as poly(N) or $1/\text{poly}(N)$ (as appropriate) in the bit-complexity of H, i.e. N = # bits required to describe H.

All of the simulations we have constructed in this course are in fact efficient.

Whence we recover the following quantum generalisation of Schaeffer's seminal dichotomy theorem from classical complexity theory, originally proven by [CM'16] & [BH'17] (the Cubitt-Montanaro quadrichotomy theorem!)

__Corollary.__

Let S be any fixed set of 1- and 2-local qubit interactions $\{h_1\} \cup \{h_2\}$.

Then the complexity of the ground state energy problem for S-Ham.'s falls into exactly one of the following categories:

(0) P if S does not contain any 2-local terms; otherwise

(1) NP-complete if S is locally simultaneously diagonalisable; otherwise

(2) StoqMA-complete if simultaneously locally equivalent to the transverse Ising model; otherwise

(3) QMA-complete.

Note: This is sometimes said to be the first known result showing that StoqMA is a "natural" complexity class after all.

These two classification theorems, in particular the fact that both are exhaustive and the cases match up exactly, hints at a deep connection between complexity of the ground state & universal simulation.

Indeed, for the classical case, this connection was proven by [dlCC'14]:

Thm [dlCC'14]

NP-hardess of g.s. energy under faithful reduction
$\Rightarrow$ universal classical simulation

Somewhat later, we finally managed to prove the quantum generalisation of this result:

Thm [Kohler, Piddock, Bausch, Cubitt '22]

QMA-completeness of g.s. energy under faithful reductions
$\Rightarrow$ universal quantum simulation

The proof uses all the Hamiltonian simulation theory we've built up, together with a completely different way of constructing simulations that also has its roots in Hamiltonian complexity and computability theory (in particular [GI'09] and [CPW'15]), but doesn't use perturbation theory at all.

For all that & more, go to Tamara's lectures!