DRAFT: Oracle complexity classes and local measurements on physical Hamiltonians

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Abstract

We study the computational complexity of simulating local measurements on ground states of local Hamiltonians, denoted APX-SIM [Ambainis, CCC 2014]. This natural problem is known to be $\mathrm{P}^{\mathrm{QMA[log]}}$-complete, for $\mathrm{P}^{\mathrm{QMA[log]}}$ the class of problems decidable by a P machine making up to a logarithmic number of adaptive queries to a QMA oracle. We show a sequence of results, which together allow us to prove that APX-SIM remains hard even for physically motivated Hamiltonians, such as the Heisenberg model on the 2D lattice:

1. We first show that for NP, StoqMA, and QMA oracles, a logarithmic number of adaptive queries is equivalent in power to polynomially many parallel queries. Formally, $\mathrm{P}^{\mathrm{NP[log]}} = \mathrm{P}^{||\mathrm{NP}}$, $\mathrm{P}^{\mathrm{StoqMA[log]}} = \mathrm{P}^{||\mathrm{StoqMA}}$, and $\mathrm{P}^{\mathrm{QMA[log]}} = \mathrm{P}^{||\mathrm{QMA}}$.
2. We next show that the hardness of a seemingly weaker problem than APX-SIM, which we denote $\forall$-APX-SIM, is preserved under simulations (in the sense of [Cubitt, Montanaro, Piddock, 2017]). As a byproduct, we obtain a complexity classification of APX-SIM for families of 2-local Hamiltonians built from interactions from one of several fixed sets. Formally, we show that APX-SIM is complete for one of either $\mathrm{P}, \mathrm{P}^{||\mathrm{NP}}, \mathrm{P}^{||\mathrm{StoqMA}}$, or $\mathrm{P}^{||\mathrm{QMA}}$.
3. By leveraging the two previous results, we show that APX-SIM is $\mathrm{P}^{\mathrm{QMA[log]}}$-complete for any family of Hamiltonians which can efficiently simulate spatially sparse Hamiltonians. This implies that APX-SIM remains $\mathrm{P}^{\mathrm{QMA[log]}}$-complete even on physically motivated models, such as the Heisenberg interaction on a 2D square lattice.

1 Introduction

The study of the low energy states of quantum many-body systems is of fundamental physical interest. Estimating the ground state energy of a k-local Hamiltonian, known as the Local Hamiltonian problem (k-LH), was shown by Kitaev [KSV02] to be complete for the class Quantum Merlin Arthur (QMA) — a quantum analogue of the classical complexity class NP. There has been much research on the complexity of the Local Hamiltonian problem, ultimately giving rise to the field of Quantum Hamiltonian Complexity (QHC); see [Osb12, GHLS14]. This, in turn, has led to complexity theoretic research on properties of ground spaces beyond estimating ground state energies. Such work includes, for example, computing ground state degeneracies [BFS11, SZ], minimizing interaction terms yielding frustrated ground spaces [GK12], detecting

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"energy barriers" in ground spaces [GS15, GMV17], deciding if tensor networks represent physical quantum states [GLSW15, SMG$^+$18], estimating spectral gaps of local Hamiltonians [Amb14, CPGW15, GY18], and estimating the free energy of 1D systems [Kim17].

In [Amb14], Ambainis formalised the particularly natural problem of simulating local measurements on low energy states of local Hamiltonians as the problem APPROXIMATE SIMULATION (APX-SIM), defined formally as follows.

Definition 1.1 (APX-SIM$(H, A, k, l, a, b, \delta)$ [Amb14])**.** *Given a k-local Hamiltonian H, an l-local observable A, and real numbers a, b, and δ such that $b - a \geq n^{-c}$ and $\delta \geq n^{-c'}$, for n the number of qubits H acts on and $c, c' > 0$ some constants, decide:*

- *If H has a ground state $|\psi\rangle$ satisfying $\langle\psi| A |\psi\rangle \leq a$, output YES.*
- *If for all $|\psi\rangle$ satisfying $\langle\psi| H |\psi\rangle \leq \lambda(H) + \delta$, it holds that $\langle\psi| A |\psi\rangle \geq b$, output NO.*

[Amb14] showed that APX-SIM is $\mathrm{P}^{\mathrm{QMA[log]}}$-complete for $O(\log n)$-local observables and $O(\log n)$-local Hamiltonians, where n is the number of qubits the Hamiltonian acts on. This was improved in [GY18] to 1-local observables and 5-local Hamiltonians by combining the "query Hamiltonian" construction of Ambainis [Amb14] with the circuit-to-Hamiltonian construction of Kitaev [KSV02]. As an aside, $\mathrm{P}^{\mathrm{QMA[log]}}$ should be thought of as "slightly more difficult than QMA". Formally, one way to see this is that $\mathrm{QMA} \subseteq \mathrm{P}^{\mathrm{QMA[log]}} \subseteq \mathrm{PP}$ [GY18] (where $\mathrm{QMA} \subseteq \mathrm{PP}$ was known [KW00] prior to [GY18]).

That the oracle complexity class $\mathrm{P}^{\mathrm{QMA[log]}}$ is characterized by such a natural physical problem (APX-SIM) raises a new question — how does the complexity of APX-SIM change when restricted to more natural classes of Hamiltonians H? For example, it would be physically appealing if APX-SIM remains $\mathrm{P}^{\mathrm{QMA[log]}}$-complete even for local measurements on well-motivated Hamiltonians, such as the Heisenberg interaction on the 2D lattice. In this work, we show a sequence of results, which we now discuss, which together allow us to positively resolve the question above.

1.1 Parallel versus adaptive queries

A natural question for oracle complexity classes is how the power of the class changes as access to the oracle is varied. In the early 1990's, it was shown [BH91, Hem89, Bei91] that a polynomial number of *parallel* or *non-adaptive* queries to an NP oracle are equivalent in power to a logarithmic number of *adaptive* queries. Formally, letting $\mathrm{P}^{||\mathrm{NP}}$ be the class of languages decidable by a P machine with access to polynomially many parallel queries to an NP oracle, it holds that $\mathrm{P}^{||\mathrm{NP}} = \mathrm{P}^{\mathrm{NP[log]}}$.

We begin by considering an analogue of this question for $\mathrm{P}^{\mathrm{QMA[log]}}$ versus $\mathrm{P}^{||\mathrm{QMA}}$ (defined as $\mathrm{P}^{||\mathrm{NP}}$ but with a QMA oracle). The techniques for showing $\mathrm{P}^{||\mathrm{NP}} \subseteq \mathrm{P}^{\mathrm{NP}}$ do not obviously adapt to the setting of promise problems, so we take a different approach and prove $\mathrm{P}^{||\mathrm{QMA}} \subseteq \mathrm{P}^{\mathrm{QMA[log]}}$ by instead showing a *hardness* result. Specifically, we use a modification to the $\mathrm{P}^{\mathrm{QMA[log]}}$-hardness constructions presented in [Amb14] and [GY18] to show that APX-SIM is $\mathrm{P}^{||\mathrm{QMA}}$-hard. Combined with the known fact that APX-SIM $\in \mathrm{P}^{\mathrm{QMA[log]}}$ [Amb14] then yields the desired containment.

This approach has two benefits: First, it simplifies the "query Hamiltonian" construction of [Amb14] significantly, which we later exploit to prove hardnesss results about physical Hamiltonians (Theorem 1.6). (Our $\mathrm{P}^{||\mathrm{QMA}}$-hardness construction for APX-SIM can hence also be seen as giving a simpler proof of Ambainis' original claim that APX-SIM is $\mathrm{P}^{\mathrm{QMA[log]}}$-hard.) Indeed, with this approach we give a more general statement:

Theorem 1.2. *Let* C *be a class of languages or promise problems. Let $\mathcal{F}$ be a family of Hamiltonians for which k-*LH *is* C*-complete under poly-time many-one reductions for all $k \geq 2$. Suppose $\mathcal{F}$ is closed under positive linear combination of Hamiltonians, and that if $\{H_i\}_{i=1}^m \subset \mathcal{F}$, then $H_{cl} + \sum_{i=1}^m |1\rangle\langle 1|_i \otimes H_i \in \mathcal{F}$, where H_{cl} is any classical Hamiltonian (i.e. diagonal in the standard basis). Then,*

$$\mathrm{P}^{\mathrm{C[log]}} = \mathrm{P}^{||\mathrm{C}},$$

and APX-SIM *is* $\mathrm{P}^{\mathrm{C[log]}}$*-complete when restricted to k-local Hamiltonians and observables from $\mathcal{F}$.*

Applying that k-LH is NP-complete, StoqMA-complete, and QMA-complete when restricted to the families of classical, stoquastic, and arbitrary k-local Hamiltonians, respectively [CM16], Theorem 1.2 yields:

Corollary 1.3. $\mathrm{P}^{\mathrm{NP[log]}} = \mathrm{P}^{||\mathrm{NP}}$, $\mathrm{P}^{\mathrm{StoqMA[log]}} = \mathrm{P}^{||\mathrm{StoqMA}}$, *and* $\mathrm{P}^{\mathrm{QMA[log]}} = \mathrm{P}^{||\mathrm{QMA}}$.

The second benefit of our approach is that, being based on the Cook-Levin theorem [Coo72, Lev73], as opposed to Kitaev's circuit-to-Hamiltonian construction [KSV02] (cf. [GY18]), we obtain a *constant* promise gap for the observable A's threshold values (i.e. $b - a \geq \Omega(1)$, as opposed $b - a \geq 1/\mathrm{poly}$, even when $\|A\| = O(1)$).

1.2 The complexity of APX-SIM for restricted Hamiltonian families

For our next pair of results, we change focus and discuss *simulations* in the sense of [CMP17]. To begin, Kitaev's original paper proved QMA-hardness of k-LH for 5-local Hamiltonians [KSV02]; this was brought down to 2-local Hamiltonians by Kempe, Kitaev and Regev [KKR06] via perturbation theory techniques. Since then, there has been a large body of work showing that QMA-completeness holds for ever simpler systems, much of which uses perturbative gadgets to construct Hamiltonians which have approximately the same ground state energy as a Hamiltonian of an apparently more complicated form. Here, we wish to produce a similarly large number of results for the problem APX-SIM in one go by using the same perturbative gadget constructions and ideas of analogue simulation.

In [CMP17], the authors define a strong notion of simulation which approximately preserves almost all the important properties of a Hamiltonian, and they observe that the perturbative gadget constructions used in the k-LH problem literature are examples of this definition of simulation. They go on to show that there exist simple families of Hamiltonians (such as the 2-qubit Heisenberg interaction) which are *universal* Hamiltonians, in the sense that they can simulate all $O(1)$-local Hamiltonians efficiently.

How do simulations affect the complexity of APX-SIM? Ideally, we would like to show that efficient simulations lead to reductions between classes of Hamiltonians for the problem APX-SIM. However, this is apparently not the case, as the definition of APX-SIM is not robust to small perturbations in the eigenvalues of the system. We instead consider a seemingly easier, closely related problem, which we call $\forall$-APX-SIM.

Definition 1.4 ($\forall$-APX-SIM$(H, A, k, l, a, b, \delta)$)**.** *Given a k-local Hamiltonian H, an l-local observable A, and real numbers a, b, and δ such that satisfy $b - a \geq n^{-c}$ and $\delta \geq n^{-c'}$, for n the number of qubits H acts on and $c, c' > 0$ some constants, decide:*

1. *If for all $|\psi\rangle$ satisfying $\langle\psi| H |\psi\rangle \leq \lambda(H) + \delta$, it holds that $\langle\psi| A |\psi\rangle \leq a$, then output YES.*
2. *If for all $|\psi\rangle$ satisfying $\langle\psi| H |\psi\rangle \leq \lambda(H) + \delta$, it holds that $\langle\psi| A |\psi\rangle \geq b$, then output NO.*

Let us emphasize that here we have a stronger promise in the YES case than in APX-SIM — namely, *all* low energy states $|\psi\rangle$ are promised to satisfy $\langle\psi| A |\psi\rangle \leq a$, as opposed to just a single ground state. Thus, $\forall$-APX-SIM is easier than APX-SIM, in that $\forall$-APX-SIM reduces (via polynomial-time many-one reduction) to APX-SIM. We conclude that $\forall$-APX-SIM is contained in $\mathrm{P}^{\mathrm{QMA[log]}}$. Furthermore, the proof of Theorem 1.2 is actually sufficient to show that when restricted to a corresponding family of Hamiltonians for arbitrary class C, $\forall$-APX-SIM is $\mathrm{P}^{||\mathrm{C}}$-complete.

Our second result, Lemma 4.2 in Section 4, is to prove that efficient simulations correspond to reductions between instances of $\forall$-APX-SIM. As a byproduct, we combine this result with Theorem 1.2 and the universality classifications from [CMP17] (cf. Corollary 1.3) in order to obtain complexity classifications for the original APX-SIM problem restricted to several families of Hamiltonians.

Theorem 1.5. *Let $\mathcal{S}$ be an arbitrary fixed subset of Hermitian matrices on at most 2 qubits. Then the* APX-SIM *problem, restricted to Hamiltonians H and measurements A given as a linear combination of terms from $\mathcal{S}$, is*

- P*-complete, if every matrix in $\mathcal{S}$ is 1-local;*
- $\mathrm{P}^{\mathrm{NP[log]}}$*-complete, if $\mathcal{S}$ does not satisfy the previous condition and there exists $U \in SU(2)$ such that U diagonalises all 1-qubit matrices in $\mathcal{S}$ and $U^{\otimes 2}$ diagonalises all 2-qubit matrices in $\mathcal{S}$;*
- $\mathrm{P}^{\mathrm{StoqMA[log]}}$*-complete, if $\mathcal{S}$ does not satisfy the previous condition and 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;*
- $\mathrm{P}^{\mathrm{QMA[log]}}$*-complete, otherwise.*

Hardness of simulating local measurements on lattices and spatially sparse systems. Finally, in Section 5, we use the previous two main results to show that $\forall$-APX-SIM is $\mathrm{P}^{||\mathrm{QMA}}$-hard even when the Hamiltonian is restricted to a spatially sparse interaction graph (in the sense of [OT08]). This is analogous to the equivalent result for k-LH shown in [OT08], which was crucial in showing that the Local Hamiltonian problem is QMA-complete for Hamiltonians on a 2D square lattice. Formally, by exploiting the previously discussed results about parallel queries (Theorem 1.2) and simulations (Lemma 4.2) and developing a variant of the hardness construction from Theorem 1.2, we are able to show the following.

Theorem 1.6. *Let $\mathcal{F}$ be a family of Hamiltonians which can efficiently simulate any spatially sparse Hamiltonian. Then,* APX-SIM *is $\mathrm{P}^{\mathrm{QMA[log]}}$-complete even when restricted to an $O(1)$-local observable and a Hamiltonian from the family $\mathcal{F}$.*

With Theorem 1.6 in hand, we obtain many corollaries via the long line of research using perturbative gadgets to prove QMA-completeness of restricted Hamiltonians; for brevity, here we list a select few such corollaries. We note that the locality of the observable input to APX-SIM may increase after simulation, but only by a constant factor which can be easily calculated based on the simulation used. For example, using the perturbative gadgets constructed in [PM17], the following is an immediate corollary of Theorem 1.6:

Corollary 1.7. *The problem* APX-SIM *is $\mathrm{P}^{\mathrm{QMA[log]}}$-complete even when the observable A is 4-local and the Hamiltonian H is restricted to be of the form:*

$$H = \sum_{(j,k)\in E} a_{(j,k)} h_{(j,k)}, \qquad \text{where } h_{(j,k)} = \alpha X_j X_k + \beta Y_j Y_k + \gamma Z_j Z_k,$$

E is the set of edges of a 2D square lattice, $a_{(j,k)} \in \mathbb{R}$, and at least two of α, β, γ are non-zero. The case $\alpha = \beta = \gamma$ corresponds to $XX + YY + ZZ$, which is known as the Heisenberg interaction.

But, there is not always a blow-up in the locality of A, as is shown by this corollary which follows from Theorem 1.6 and [SV09]:

Corollary 1.8. *The problem* APX-SIM *is* $\mathrm{P}^{\mathrm{QMA[log]}}$*-complete even when the observable A is 1-local and the Hamiltonian H is restricted to be of the form:*

$$H = \sum_{(j,k)\in E} h_{(j,k)} + \sum_j B_j, \qquad \text{where } h_{(j,k)} = X_jX_k + Y_jY_k + Z_jZ_k,$$

E is the set of edges of a 2D square lattice, and B_j is a single qubit operator (that may depend on j).

Finally, we remark that recent work on the simulation power of families of qudit Hamiltonians [PM18] can be used to show the following corollary:

Corollary 1.9. *Let $|\psi\rangle$ be an entangled two qudit state. Then, the problem* APX-SIM *is* $\mathrm{P}^{\mathrm{QMA[log]}}$*-complete even when the Hamiltonian H is restricted to be of the form*

$$H = \sum_{j,k} \alpha_{j,k} |\psi\rangle\langle\psi|_{j,k},$$

where $\alpha_{j,k} \in \mathbb{R}$ and $|\psi\rangle\langle\psi|_{j,k}$ denotes the projector onto $|\psi\rangle$ on qudits j and k.

Each of these corollaries follows immediately from Theorem 1.6, as it is known that the referenced families of Hamiltonians above can efficiently simulate all spatially sparse Hamiltonians.

Our results bring previous hardness results closer to the types of problems studied in the physics literature, where typically observables are $O(1)$-local, allowed interactions physically motivated, and the geometry of the interaction graph is constrained. We note that improving the coupling strengths to $O(1)$, however, remains an important open question, both for our setting and for the complexity classification of k-LH itself [CM16, PM17].

Organization. We first introduce notation and definitions in Section 2. We prove that APX-SIM is contained in $\mathrm{P}^{\mathrm{C[log]}}$ in Section 3.1 for classes C and corresponding restrictions, and that $\forall$-APX-SIM is $\mathrm{P}^{||\mathrm{C}}$-hard in Section 3.2, thereby proving Theorem 1.2. In Section 4, we introduce a special case of the definition of simulation from [CMP17] and show that simulations correspond to reductions of the problem $\forall$-APX-SIM, yielding Theorem 1.5; proofs with regard to the general definition are in Appendix A. Finally, in Section 5 we give a spatially sparse construction with which $\forall$-APX-SIM is $\mathrm{P}^{||\mathrm{QMA}}$-hard, thus proving Theorem 1.6.

2 Preliminaries

Notation. Let $\lambda(H)$ denote the smallest eigenvalue of Hermitian operator H. For a matrix A, $\|A\| := \max\{\|A|v\rangle\|_2 : \||v\rangle\|_2 = 1\}$ is the operator norm or spectral norm of A, and $\|A\|_1 := \mathrm{Tr}\sqrt{A^\dagger A}$ the trace norm. Throughout this paper, we will assume generally that both $H = \sum_{i=1}^m H_i$ and observable $A = \sum_{i=1}^m A_i$ are local Hamiltonians, whose local terms H_i and A_i act non-trivially on at most $O(\log n)$ out of n qubits. This allows natural observables of the form $A = \sum_{i=1}^n X_i$ for Pauli X. We also assume $m, \|H_i\|, \|A_i\| \in O(\mathrm{poly}(n))$ for all $i \in \{1, \ldots, m\}$, and for n the number of qubits in the system.

Definitions. $\mathrm{P}^{\mathrm{QMA[log]}}$, defined in [Amb14], is the set of decision problems decidable by a polynomial-time deterministic Turing machine with the ability to query an oracle for a QMA-complete problem $O(\log n)$ times, where n is the size of the input. For a class C of languages or promise problems, the class $\mathrm{P}^{\mathrm{C[log]}}$ is similarly defined, except with an oracle for a C-complete problem.

$\mathrm{P}^{||\mathrm{C}}$ is the class of problems decidable by a polynomial-time deterministic Turing machine given access to an oracle for a C-complete problem, with the restriction that all (up to $O(n^c)$ for $c \in \Theta(1)$) queries to the oracle must be made in one time step, i.e. in parallel. Such queries are labeled *non-adaptive*, as opposed to the *adaptive* queries allowed to a $\mathrm{P}^{\mathrm{C[log]}}$ machine. We note that $\mathrm{P}^{||\mathrm{NP}}$ has in the past been denoted $\leq_{tt}^{p}$ (NP), in reference to polynomial-time truth-table reductions (e.g. [BH91]).

In this article, for $\mathrm{P}^{\mathrm{QMA[log]}}$ we assume oracle queries made by the P machine are to an oracle for the QMA-complete [KSV02] k-local Hamiltonian problem (k-LH), defined as follows: Given a k-local Hamiltonian H and inverse polynomial-separated thresholds $a, b \in \mathbb{R}$, decide whether $\lambda(H) \leq a$ (YES-instance) or $\lambda(H) \geq b$ (NO-instance) [KKR06]. We shall say an oracle query is *valid* (*invalid*) if it satisfies (violates) the promise gap of the QMA-complete problem the oracle answers. (An invalid query hence satisfies $\lambda(H) \in (a, b)$.) For any invalid query, the oracle can accept or reject arbitrarily. A *correct* query string $y \in \{0,1\}^m$ encodes a sequence of correct answers to all of the m queries made by the P machine, and an *incorrect* query string is one which contains at least one incorrect query answer. Note that for an invalid query, any answer is considered "correct", yielding the possible existence of multiple correct query strings. Nevertheless, the P machine is required to output the same final answer (accept or reject) regardless of how such invalid queries are answered [Gol06]. The above definitions extend analogously when the class QMA is replaced with another class C, with a designated C-complete problem Π_C playing the role of k-LH. (In this paper, the complexity classes C we consider have complete problems.)

3 Parallel versus adaptive queries

We begin by showing Theorem 1.2, i.e. that $\mathrm{P}^{\mathrm{C[log]}} = \mathrm{P}^{||\mathrm{C}}$ for appropriate complexity classes C. Section 3.1 shows containment of the corresponding APX-SIM problem in $\mathrm{P}^{\mathrm{C[log]}}$. Section 3.2 then shows $\mathrm{P}^{||\mathrm{C}}$-hardness of APX-SIM. Theorem 1.2 is restated and proven in Section 3.3.

3.1 Containment in $\mathrm{P}^{\mathrm{C[log]}}$

We begin by modifying the containment proof of [Amb14] to show containment of APX-SIM in classes $\mathrm{P}^{\mathrm{C[log]}}$ for C beyond just C = QMA.

Lemma 3.1. *Let H be a k-local Hamiltonian acting on n qudits, and let A be an observable on the same system of n qudits. Suppose k-LH for $\lambda H + \mu A$ is contained in complexity class*[1] C *for any $0 \leq \lambda, \mu \leq \mathrm{poly}(n)$, and for all $k \geq 1$. Then* $\text{APX-SIM}(H, A, k, l, a, b, \delta) \in \mathrm{P}^{\mathrm{C[log]}}$.

Proof. We need to show the existence of a $\mathrm{poly}(n)$ time classical algorithm to decide APX-SIM while making at most $O(\log n)$ queries to an oracle for C. As with the proof in [Amb14], the idea is to use $O(\log n)$ oracle queries to determine the ground space energy $\lambda(H)$ of H by binary search, and then use one final query to determine the answer. In [Amb14] the final query is a QMA query; here we show how this final query can be performed differently so that only an oracle for C is required.

[1] In order to ensure an oracle for C is well-defined, we implicitly assume C has a complete problem, denoted Π_C, under polynomial-time many-one reductions. Thus, by queries to an oracle for C, we implicitly mean queries to an oracle for Π_C.

First calculate a lower bound μ for $\lambda(A)$, the lowest eigenvalue of A. If A acts only on $O(1)$ qudits, then $\lambda(A)$ can be calculated via brute force (up to, say, inverse exponential additive error) in $O(1)$ time. If A acts on many qudits, then $\lambda(A)$ can alternatively be approximated to within inverse polynomial additive error by binary search (á la [Amb14]) by querying the C oracle $O(\log \|A\|) = O(\log n)$ times. (Recall, we assume k-LH for $\lambda H + \mu A$ is contained in C.) Note that without loss of generality, we may assume $0 \leq b - \mu \leq q(n)$ for some efficiently computable polynomial q. The lower bound holds since if $b < \mu \leq \lambda(A)$, we conclude our APX-SIM instance is a NO instance, and we reject. For the upper bound, it holds that $\mu \leq \|A\|$, and we may assume $b \leq \|A\|$, as otherwise our APX-SIM instance is either a YES or invalid instance, and in both cases we can accept. By assumption, $\|A\| \leq q(n)$ for appropriate polynomial q which can be computed efficiently by applying the triangle inequality to the local terms of A; note $\|A\|$ may hence be replaced by q in the bounds above.

Perform binary search with the oracle for C to find λ^* such that $\lambda(H) \in [\lambda^*, \lambda^* + \epsilon]$ where

$$\epsilon = \frac{\delta(b-a)}{2(b-\mu)} \geq 1/\text{poly}(n)$$

since $0 \leq b - \mu \leq \text{poly}(n)$. This requires $O(\log 1/\epsilon) = O(\log n)$ queries to the oracle for C. Next perform one final query to the C oracle to solve k-LH with Hamiltonian H' with thresholds a' and b', where

$$H' = (b-\mu)H + \delta A \quad \text{and} \quad \begin{array}{l} a' = (\lambda^* + \epsilon)(b-\mu) + \delta a \\ b' = \lambda^*(b-\mu) + \delta b \end{array}$$

and accept if and only if this final query accepts. Observe this is an allowed query for the C oracle because H' is of the form required in the statement of the lemma (recall $b - \mu \geq 0$), and also

$$b' - a' = \delta(b-a) - \epsilon(b-\mu) = \delta(b-a)/2 \geq 1/\text{poly}(n).$$

Now, if APX-SIM$(H, A, k, l, a, b, \delta)$ is a YES instance, then there exists $|\psi\rangle$ such that $\langle\psi| H |\psi\rangle = \lambda(H)$ and $\langle\psi| A |\psi\rangle \leq a$. Then

$$\langle\psi| (b-\mu)H + \delta A |\psi\rangle \leq \lambda(H)(b-\mu) + \delta a \leq (\lambda^* + \epsilon)(b-\mu) + \delta a = a'$$

and the algorithm accepts as required.

Now suppose the input is a NO instance. We will show that $\langle\psi| H' |\psi\rangle \geq b'$ for any $|\psi\rangle$ and so the algorithm rejects as required. First, if $|\psi\rangle$ is low energy with $\langle\psi| H |\psi\rangle \leq \lambda(H) + \delta$, then it also satisfies $\langle\psi| A |\psi\rangle \geq b$, and so

$$\langle\psi| (b-\mu)H + \delta A |\psi\rangle \geq \lambda(H)(b-\mu) + \delta b \geq \lambda^*(b-\mu) + \delta b = b'$$

where we have used $\langle\psi| H |\psi\rangle \geq \lambda(H) \geq \lambda^*$ and $b - \mu \geq 0$. Otherwise, if $|\psi\rangle$ is high energy with $\langle\psi| H |\psi\rangle \geq \lambda(H) + \delta$, then

$$\begin{aligned} \langle\psi| (b-\mu)H + \delta A |\psi\rangle &\geq (\lambda(H) + \delta)(b-\mu) + \delta\lambda(A) \\ &= \lambda(H)(b-\mu) + \delta b + \delta(\lambda(A) - \mu) \geq \lambda^*(b-\mu) + \delta b = b' \end{aligned}$$

where we have used $\langle\psi| A |\psi\rangle \geq \lambda(A)$ and $\lambda(A) - \mu \geq 0$. Thus, we reject. □

3.2 Hardness for $\mathrm{P}^{||\mathrm{C}}$

We next modify the proof that APX-SIM is $\mathrm{P}^{\mathrm{QMA[log]}}$-hard to obtain the following lemma. Our modifications include simplifying the "query Hamiltonian" of [Amb14], and improving the construction of [GY18] by using the Cook-Levin theorem, as opposed to Kitaev's circuit-to-Hamiltonian construction. The latter has a nice consequence — in contrast to the QMA-completeness results for k-LH, where the promise gap is inverse polynomial, for APX-SIM we are able to show that the relevant promise gap $b - a$ scales as $\Omega(1)$ in the (e.g.) $\mathrm{P}^{||\mathrm{C}}$-complete regime.

Lemma 3.2. *Let $\mathcal{F}$ be a family of Hamiltonians for which k-LH is C-hard for all $k \geq 2$. Then $\forall$-APX-SIM is $\mathrm{P}^{||\mathrm{C}}$-hard even when $b - a = \Omega(1)$, the observable A is a single Pauli Z measurement, and when restricted to Hamiltonians of the form $H = H_{cl} + \sum_i |1\rangle\langle 1|_i \otimes H_i$, where H_{cl} is a classical Hamiltonian, and the H_i are Hamiltonians from $\mathcal{F}$.*

To show this, we require two tools: in the next two subsections, we show how to simplify [Amb14]'s query Hamiltonian in the context of parallel queries, and discuss how to employ the Cook-Levin reduction, respectively.

3.2.1 Simplifying Ambainis' query Hamiltonian

First, we give a simplified version of the "query Hamiltonian" introduced by Ambainis [Amb14], which will be useful in the following lemmas (see also [GY18], which reduced the locality of the construction of [Amb14] by applying the unary encoding trick of Kitaev [KSV02]; due to the simplified structure of parallel queries, here we do not require this unary encoding to achieve $O(1)$-locality for our Hamiltonian).

Given some $\mathrm{P}^{||\mathrm{C}}$ computation U for an appropriate class C, let $(H_{\mathcal{Y}_i}, a_i, b_i)$ be the instance of (without loss of generality) 2-LH corresponding to the i-th query made by U. Then, our "query Hamiltonian" is

$$H = \sum_{i=1}^{m} M_i := \sum_{i=1}^{m} \left(\frac{a_i + b_i}{2} |0\rangle\langle 0|_{\mathcal{X}_i} \otimes I_{\mathcal{Y}_i} + |1\rangle\langle 1|_{\mathcal{X}_i} \otimes H_{\mathcal{Y}_i} \right), \tag{1}$$

where single qubit register $\mathcal{X}_i$ is intended to encode the answer to query i and $\mathcal{Y}_i$ encodes the ground state of $H_{\mathcal{Y}_i}$. Since each query is 2-local, H is 3-local. Notably, because U makes all of its queries in *parallel*, we are able to weight each of the m terms equally, unlike in [Amb14, GY18] which studied adaptive queries. This significantly eases our later analysis.

The following lemma is analogous to Lemma 3.1 of [GY18], but with an improved spectral gap. The proof is similar to theirs, but is significantly simplified due to our use of parallel queries.

Lemma 3.3. *Define for any $x \in \{0,1\}^m$ the space $\mathcal{H}_{x_1 \cdots x_m} := \bigotimes_{i=1}^{m} |x_i\rangle\langle x_i| \otimes \mathcal{Y}_i$. Then, there exists a correct query string $x \in \{0,1\}^m$ such that the ground state of H lies in $\mathcal{H}_{x_1 \cdots x_m}$. Moreover, suppose this space has minimum eigenvalue λ. Then, for any incorrect query string $y_1 \cdots y_m$, any state in $\mathcal{H}_{y_1 \cdots y_m}$ has energy at least $\lambda + \epsilon$, where $\epsilon = \min_i(b_i - a_i)/2$.*

Proof. We proceed by contradiction. Let $x \in \{0,1\}^m$ ($y \in \{0,1\}^m$) denote a correct (incorrect) query string which has lowest energy among all *correct* (*incorrect*) query strings against H. (Note that x and y are well-defined, though they may not be unique; in this latter case, any such x and y will suffice for our proof.) For any $z \in \{0,1\}^m$, define λ_z as the smallest eigenvalue in $\mathcal{H}_z$.

Since y is an incorrect query string, there exists at least one $i \in \{1, \ldots, m\}$ such that y_i is the wrong answer to a valid query $H_{\mathcal{Y}_i}$. If query i is a YES-instance, the smallest eigenvalue of M_i corresponds to

setting $\mathcal{X}_i$ to (the correct query answer) $|1\rangle$, and is at most a_i. On the other hand, the space with $\mathcal{X}_i$ set to $|0\rangle$ has all eigenvalues equalling $(a_i + b_i)/2$. A similar argument shows that in the NO-case, the $|0\rangle$-space has eigenvalues equalling $(a_i + b_i)/2$, and the $|1\rangle$-space has eigenvalues at least b_i. We conclude that flipping query bit i to the correct query answer $\overline{y}_i$ allows us to "save" an energy penalty of $(b_i - a_i)/2$ against M_i.

Let y' denote y with bit i flipped. If y' is also an incorrect query string, we have $\lambda_{y'} < \lambda_y$, a contradiction due to the minimality of y. Conversely, if y' is a correct query string, then we must have $\lambda_{y'} \geq \lambda_x + (b_i - a_i)/2 \geq \lambda + \epsilon$, as otherwise we contradict the minimality of x. □

3.2.2 Cook-Levin construction

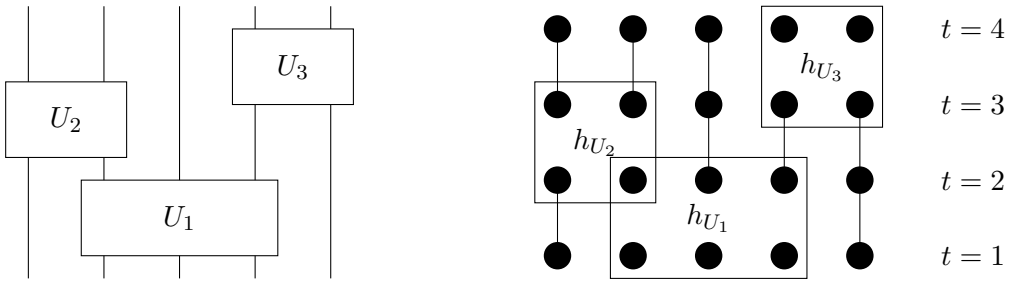

Figure 1: Cook-Levin construction of classical Hamiltonian to simulate a P machine. On the left is a picture of the gates U_i in the circuit of the P machine; the figure on the right shows the Hamiltonian terms h_{U_t} encoding each gate. Each straight line edge on the right represents the interaction $|01\rangle\langle 01| + |10\rangle\langle 10|$. The initialization terms H_{in} on qubits in time step $t = 0$ are omitted in the diagram.

We now show how to model the Cook-Levin construction in our setting. For this, we consider the P machine to be given as a circuit of classical reversible gates $U = U_m \dots U_1$, in which one gate occurs at each time step. The evolution of the circuit is encoded into a 2D grid of qubits, where the t-th row of qubits corresponds to the state of the system at time step t; the output of the circuit is copied to a dedicated output bit in the final timestep. The overall Hamiltonian is diagonal in the computational basis with a groundspace of states corresponding to the correct evolution of the P machine.

Let I_t be the set of qubits which U_t acts non-trivially on. If a qubit $i \notin I_t$ (i.e. it is not acted on by the circuit at time step t), then there is an interaction $|01\rangle\langle 01| + |10\rangle\langle 10|$ on qubits (i, t) and $(i, t + 1)$, to penalise states which encode a change on qubit i. To encode a classical reversible gate $U_t : x \mapsto U_t(x)$ acting at time t, we define an interaction $h_{U_t} = I - \sum_x |x\rangle\langle x|_t \otimes |U_t(x)\rangle\langle U_t(x)|_{t+1}$ acting non-trivially only on qubits (i, t') for $i \in I_t$ and t' equal to t or $t + 1$. See Figure 1 for a pictorial representation of this Hamiltonian. Then

$$H_{\text{prop}} = \sum_{t=1}^{m} \left(h_{U_t} + \sum_{i \notin I_t} |0\rangle\langle 0|_{(i,t)} |1\rangle\langle 1|_{(i,t+1)} + |1\rangle\langle 1|_{(i,t)} |0\rangle\langle 0|_{(i,t+1)} \right) \tag{2}$$

is positive semi-definite and has ground space spanned by states of the form:

$$|w(x)\rangle = |x\rangle_{t=1} \otimes |U_1 x\rangle_{t=2} \otimes \cdots \otimes |U_m \dots U_1 x\rangle_{t=m+1}$$

Typically, there is an additional term H_{in} consisting of 1-local $|1\rangle\langle 1|$ terms on all qubits in the first ($t = 1$) row. Then the Hamiltonian $H_{\text{prop}} + H_{\text{in}}$ has (1) unique ground state $|w(0^n)\rangle$ encoding the action of the

circuit on the 0^n string, (2) ground state energy 0, and (3) spectral gap at least 1, since the Hamiltonian is a sum of projectors. We will later show how we adapt H_{in} given our uninitialized query register.

3.2.3 Proof of hardness

We are almost ready to prove the main result of this section, Lemma 3.2. Before doing so, we require a final technical lemma.

Lemma 3.4. *Let H be a Hamiltonian and ρ a density matrix satisfying $\operatorname{Tr}(H\rho) \leq \lambda(H) + \delta$. Let P be the projector onto the space of eigenvectors of H with energy less than $\lambda(H) + \delta'$. Then,*

$$\frac{1}{2}\|\rho - \rho'\|_1 \leq \sqrt{\frac{\delta}{\delta'}}, \quad \text{where } \rho' = P\rho P / \operatorname{Tr}(P\rho).$$

Proof. First, bound the trace distance by the fidelity in the usual way (using one of the Fuchs-van de Graf inequalities [FvdG99]):

$$\frac{1}{2}\|\rho - \rho'\|_1 \leq \sqrt{1 - F(\rho, \rho')^2} \tag{3}$$

where

$$F(\rho, \rho') = \operatorname{Tr}\left(\sqrt{\sqrt{\rho}\rho'\sqrt{\rho}}\right) = \operatorname{Tr}\left(\sqrt{\frac{\sqrt{\rho}P\rho P\sqrt{\rho}}{\operatorname{Tr}(P\rho)}}\right) = \frac{1}{\sqrt{\operatorname{Tr}(P\rho)}}\operatorname{Tr}(\sqrt{\rho}P\sqrt{\rho}) = \sqrt{\operatorname{Tr}(P\rho)},$$

where the third equality follows since $(\sqrt{\rho}P\sqrt{\rho})^2 = \sqrt{\rho}P\rho P\sqrt{\rho}$ and since the latter is positive semi-definite. Now, it remains to bound $\operatorname{Tr}(P\rho)$. We note that H has eigenvalues at least $\lambda(H) + \delta'$ on the space annihilated by P and eigenvalues at least $\lambda(H)$ everywhere else, and so $H \succeq (\lambda(H)+\delta')(I-P)+\lambda(H)P = (\lambda(H) + \delta')I - \delta' P$. Therefore, using the bound on $\operatorname{Tr}(H\rho)$, we have

$$\lambda(H) + \delta \geq \operatorname{Tr}(H\rho) \geq (\lambda(H) + \delta')\operatorname{Tr}(\rho) - \delta'\operatorname{Tr}(P\rho) \quad \Leftrightarrow \quad 1 - \operatorname{Tr}(P\rho) \leq \frac{\delta}{\delta'}.$$

Substituting this back into Equation (3) proves the result. □

We are now ready to prove the main result of this section, Lemma 3.2, which we restate below for convenience.

Lemma 3.2. *Let $\mathcal{F}$ be a family of Hamiltonians for which k-LH is* C*-hard for all $k \geq 2$. Then $\forall$-APX-SIM is $\mathrm{P}^{\|\mathrm{C}}$-hard even when $b - a = \Omega(1)$, the observable A is a single Pauli Z measurement, and when restricted to Hamiltonians of the form $H = H_{cl} + \sum_i |1\rangle\langle 1|_i \otimes H_i$, where H_{cl} is a classical Hamiltonian, and the H_i are Hamiltonians from $\mathcal{F}$.*

Proof. We split the Hilbert space into three parts $\mathcal{W}$, $\mathcal{X} = \bigotimes_i \mathcal{X}_i$, $\mathcal{Y} = \bigotimes_i \mathcal{Y}_i$ and have a Hamiltonian of the form $H = H_1 + H_2$, where H_1 acts on $\mathcal{W}$ and $\mathcal{X}$, and H_2 acts on $\mathcal{X}$ and $\mathcal{Y}$. H_2 is the query Hamiltonian of Equation (1), and therefore by Lemma 3.3 the space of eigenvectors of H_2 with eigenvalues less than $\lambda(H_2) + \epsilon$ is spanned by states of the form: $|x\rangle_{\mathcal{X}} \otimes |\phi\rangle_{\mathcal{Y}}$, where x is a correct string of answers for the queries to the C oracle.

$H_1 = H_{\text{prop}} + H_{\text{in}}$ is the classical Hamiltonian encoding the evolution of a classical P circuit, using the Cook-Levin construction of Section 3.2.2, where H_{prop} is as defined in Equation (2). For clarity, H_{prop} and H_{in} act on $\mathcal{W}$ and $\mathcal{W} \otimes \mathcal{X}$, respectively. We think of $\mathcal{W}$ as "laid out in a 2D grid" as in Figure 1, and

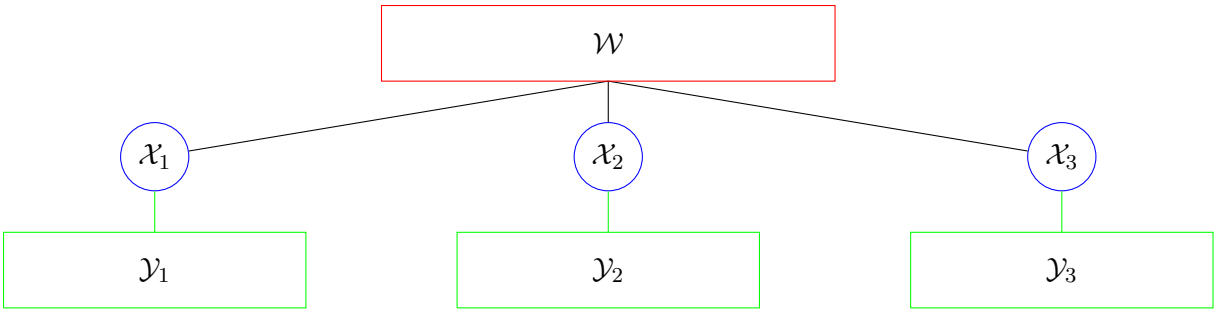

Figure 2: The structure of the Hamiltonian $H = H_1 + H_2$ used in Lemma 3.2, for the case of 3 queries. H_1 acts on the space $\mathcal{W} \otimes \mathcal{X}$ and H_2 acts on $\mathcal{X} \otimes \mathcal{Y}$, where $\mathcal{X} = \bigotimes_i \mathcal{X}_i$ and $\mathcal{Y} = \bigotimes_i \mathcal{Y}_i$

of $\mathcal{X}$ as playing the role of a "message" register passing information between H_1 and H_2. We modify the Hamiltonian H_{in} which initialises the qubits at the start of the classical circuit. For each qubit $\mathcal{X}_i$ in $\mathcal{X}$, we initialise a corresponding qubit of the first ($t = 0$) row of $\mathcal{W}$ into the same state with a penalty term $|1\rangle\langle 1|_{\mathcal{X}_i} \otimes |0\rangle\langle 0|_{\mathcal{W}_i} + |0\rangle\langle 0|_{\mathcal{X}_i} \otimes |1\rangle\langle 1|_{\mathcal{W}_i}$. All other qubits in the first ($t = 0$) row of $\mathcal{W}$ are initialised to $|0\rangle$ with a penalty $|1\rangle\langle 1|$. The full construction is depicted diagrammatically in Figure 2. Note that as stated in the claim, H is of the form $H = H_{\text{cl}} + \sum_i |1\rangle\langle 1|_i \otimes H_i$, where H_{cl} contains H_1 and the local terms of H_2 which are tagged with $|0\rangle\langle 0|$ in registers $\mathcal{X}_i$.

We can argue about the low energy eigenspace of H as follows. Since the ground spaces of H_1 and H_2 have non-trivial intersection, $\lambda(H) = \lambda(H_1) + \lambda(H_2) = \lambda(H_2)$. Moreover, since $[H_1, H_2] = 0$ (they overlap only on the $\mathcal{X}$ register, on which they are both diagonal in the standard basis), and since we may assume without loss of generality that $\lambda(H_2) + \epsilon$ is inverse polynomially bounded below 1 (otherwise, we can scale H_1 by an appropriate fixed polynomial), we conclude the space of eigenstates of H with eigenvalue less than $\lambda(H) + \epsilon$, henceforth denoted $\mathcal{H}_{\text{low}}$, is spanned by states of the form $|\Phi\rangle = |w\rangle_{\mathcal{W}} \otimes |x\rangle_{\mathcal{X}} \otimes |\phi\rangle_{\mathcal{Y}}$, where x is a string of correct answers to the oracle queries and w is the classical string encoding the correct computation of the P circuit acting on x. The qubit corresponding to the output bit of the P circuit will be in the state $|1\rangle$ (resp. $|0\rangle$) in a YES (resp. NO) instance of $\forall$-APX-SIM.

To complete the proof let the observable $A = Z_{\text{out}}$, a Pauli Z measurement on the qubit corresponding to the output bit of the P circuit, and let $\delta = \epsilon/16$ and $\delta' = \epsilon$. Consider any state $|\psi\rangle$ with $\langle\psi| H |\psi\rangle \leq \lambda(H) + \delta$. Then by Lemma 3.4, there exists a state $|\psi'\rangle \in \mathcal{H}_{\text{low}}$ such that $\langle\psi'| H |\psi'\rangle \leq \lambda(H) + \delta' = \lambda(H) + \epsilon$ which satisfies $\| |\psi\rangle\langle\psi| - |\psi'\rangle\langle\psi'| \|_1 \leq 1/2$. So,

$$\langle\psi'| Z_{\text{out}} |\psi'\rangle = \begin{cases} -1 & \text{in a YES instance} \\ 1 & \text{in a NO instance} \end{cases}$$

which implies by Hölder's inequality that $\langle\psi| A |\psi\rangle$ is $\leq -1/2$ in a YES instance and $\geq 1/2$ in a NO instance, as required. □

3.3 Final result

Theorem 1.2 is now a straightforward consequence of Lemma 3.1 and Lemma 3.2.

Theorem 1.2. *Let* C *be a class of languages or promise problems. Let $\mathcal{F}$ be a family of Hamiltonians for which k-*LH *is* C*-complete under poly-time many-one reductions for all $k \geq 2$. Suppose $\mathcal{F}$ is closed under*

positive linear combination of Hamiltonians, and that if $\{H_i\}_{i=1}^m \subset \mathcal{F}$*, then* $H_{cl} + \sum_{i=1}^m |1\rangle\langle 1|_i \otimes H_i \in \mathcal{F}$*, where* H_{cl} *is any classical Hamiltonian (i.e. diagonal in the standard basis). Then,*

$$\mathrm{P}^{\mathrm{C[log]}} = \mathrm{P}^{||\mathrm{C}},$$

and APX-SIM *is* $\mathrm{P}^{\mathrm{C[log]}}$*-complete when restricted to* k*-local Hamiltonians and observables from* $\mathcal{F}$*.*

Proof. The containment $\mathrm{P}^{\mathrm{C[log]}} \subseteq \mathrm{P}^{||\mathrm{C}}$ follows directly from the same argument that $\mathrm{P}^{\mathrm{NP[log]}} \subseteq \mathrm{P}^{||\mathrm{NP}}$ of [Bei91]. (Briefly, a P machine making a logarithmic number of adaptive queries to a C oracle can make only polynomially many distinct queries, each of which can be computed beforehand in poly-time since the machine is deterministic. The values for all such queries can simply be queried in parallel by the $\mathrm{P}^{||\mathrm{C}}$ machine.) By Lemma 3.1, APX-SIM is contained in $\mathrm{P}^{\mathrm{C[log]}}$ for Hamiltonians and observables from $\mathcal{F}$. And by Lemma 3.2 $\forall$-APX-SIM is $\mathrm{P}^{||\mathrm{C}}$-hard for Hamiltonians from $\mathcal{F}$, and when the observable is a single Pauli Z measurement, which is contained in $\mathcal{F}$ by the assumption that $\mathcal{F}$ contains any classical Hamiltonian H_{cl}. The proof is completed by recalling that $\forall$-APX-SIM reduces to APX-SIM. □

4 Simulations and APX-SIM for physical classes of Hamiltonians

In order to study the complexity of APX-SIM for physically motivated Hamiltonians in Section 5, we require two tools: First, hardness results for parallel query classes $\mathrm{P}^{||\mathrm{C}}$, given in Section 3, and second, an understanding of how *simulations* affect the hardness of the problem APX-SIM, which this section focuses on. Specifically, we consider a simplified notion of simulation, defined below, which is a special case of the full definition given in [CMP17]. This simpler case includes all of the important details necessary for the general case. For full proofs with regard to the general definition of simulation, see Appendix A.

Definition 4.1 (Special case of definition in [CMP17]; variant of definition in [BH17])**.** *We say that* H' *is a* (Δ, η, ϵ)*-simulation of* H *if there exists a local isometry* $V = \bigotimes_i V_i$ *such that*

1. *There exists an isometry* $\widetilde{V}$ *such that* $\widetilde{V}\widetilde{V}^\dagger = P_{\leq \Delta(H')}$*, where* $P_{\leq \Delta(H')}$ *is the projector onto the space of eigenvectors of* H' *with eigenvalues less than* Δ*, and* $\|\widetilde{V} - V\| \leq \eta$*;*
2. $\|H'_{\leq \Delta} - \widetilde{V} H \widetilde{V}^\dagger\| \leq \epsilon$*, where* $H'_{\leq \Delta} = P_{\leq \Delta(H')} H' P_{\leq \Delta(H')}$*.*

We say that a family $\mathcal{F}'$ *of Hamiltonians can simulate a family* $\mathcal{F}$ *of Hamiltonians if, for any* $H \in \mathcal{F}$ *and any* $\eta, \epsilon > 0$*, and* $\Delta \geq \Delta_0$ *for some* $\Delta_0 > 0$*, there exists* $H' \in \mathcal{F}'$ *such that* H' *is a* (Δ, η, ϵ)*-simulation of* H*. We say that the simulation is efficient if, for* H *acting on* n *qudits,* $\|H'\| = \mathrm{poly}(n, 1/\eta, 1/\epsilon, \Delta)$*;* H' *and* $\{V_i\}$ *are computable in polynomial-time given* H*,* Δ*,* η *and* ϵ *and provided that* $\Delta, 1/\eta, 1/\epsilon$ *are* $O(\mathrm{poly}(n))$*; and each isometry* V_i *maps from at most one qudit to* $O(1)$ *qudits.*

Remark: Unlike in [CMP17], here we have the additional requirement that the local isometry V is efficiently computable. This ensures that given some input Hamiltonian H and local observable A, we can use the notion of simulation to efficiently produce a simulating Hamiltonian H' *and* a simulating observable A' (see proof of Lemma 4.2 below). As far as we are aware, all known constructions satisfying the notion efficient of simulation from [CMP17] fulfill this additional requirement (see proof of Theorem 1.5 for examples).

Note that eigenvalues are preserved up to a small additive factor ϵ in a simulation, but that the YES instance in the definition of APX-SIM is not robust to such perturbations of eigenvalues when the spectral gap is very small. We therefore do not expect to show directly that hardness of APX-SIM is preserved by simulations, and instead we work with the alternative computational problem $\forall$-APX-SIM defined in

Definition 1.4. Let $\mathcal{F}$-$\forall$-APXSIM denote the problem $\forall$-APX-SIM restricted to Hamiltonians taken from the family $\mathcal{F}$.

Lemma 4.2 (Simulations preserve hardness of $\forall$-APX-SIM)**.** *Let $\mathcal{F}$ be a family of Hamiltonians which can be efficiently simulated by another family $\mathcal{F}'$. Then, $\mathcal{F}$-$\forall$-APXSIM reduces to $\mathcal{F}'$-$\forall$-APXSIM via polynomial-time many-one reductions. Specifically, any instance $\Pi = (H, A, k, l, a, b, \delta)$ of $\mathcal{F}$-$\forall$-APXSIM is mapped to an instance $\Pi' = (H', A', k', l', a', b', \delta')$ of $\mathcal{F}'$-$\forall$-APXSIM satisfying $l' \in O(l)$, $a' = a + (b-a)/3$, $b' = b - (b-a)/3$, and $\delta - \delta' \geq 1/\mathrm{poly}(n)$.*

Here, we provide a proof only for the special case where the simulation is of the form given in Definition 4.1; for a full proof of the general case, see Appendix A.

Proof. Let $\Pi = (H, A, k, l, a, b, \delta)$ be an instance of $\mathcal{F}$-$\forall$-APXSIM. We will demonstrate that one can efficiently compute $H' \in \mathcal{F}'$ and A', k', l', a', b', and δ' such that $\Pi' = (H', A', k', l', a', b', \delta')$ is a YES (respectively NO) instance of $\forall$-APX-SIM if Π is a YES (resp. NO) instance of $\forall$-APX-SIM. To do so, we shall pick parameters Δ, η, ϵ so that $\Delta, 1/\eta, 1/\epsilon$ are $O(\mathrm{poly}(n))$, upon which the definition of efficient simulation (Definition 4.1) guarantees we can efficiently compute a Hamiltonian H' being a (Δ, η, ϵ)-simulation of H, which we claim will preserve YES and NO instances H.

Let us leave Δ, η, ϵ arbitrary for now, and assume we have a simulation of the form given in Definition 4.1. Then, there exists an isometry $\widetilde{V} : \mathcal{H} \to \mathcal{H}'$ ($\mathcal{H}$ and $\mathcal{H}'$ are the spaces H and H' act on, respectively) which maps onto the space of eigenvectors of H' with eigenvalues less than Δ, i.e. onto $S_{\leq\Delta} := \mathrm{Span}\{|\psi\rangle : H'|\psi\rangle = \lambda|\psi\rangle, \lambda \leq \Delta\}$. In addition, $\widetilde{V}$ satisfies $\|\widetilde{V} - \bigotimes_i V_i\| \leqslant \eta$ and $\|H_{\leqslant\Delta} - \widetilde{V}H\widetilde{V}^\dagger\| \leqslant \epsilon$.

Let $|\psi'\rangle$ be a low energy state of H' satisfying $\langle\psi'|H'|\psi'\rangle \leq \lambda(H') + \delta'$ for δ' to be set later. First, we show that $|\psi'\rangle$ is close to a state $\widetilde{V}|\psi\rangle$ where $|\psi\rangle$ is a low energy state of H; then, we will show that there exists an observable A', depending only on A and the isometries V_i, such that $\langle\psi'|A'|\psi'\rangle$ approximates $\langle\psi|A|\psi\rangle$ for any choice of $|\psi\rangle$. Since by Definition 4.1 A is efficiently computable, our choice of A' will be as well.

Let $|\phi\rangle = P_{\leq\Delta(H')}|\psi'\rangle / \|P_{\leq\Delta(H')}|\psi'\rangle\|$ be the (normalised) component of $|\psi'\rangle$ in $S_{\leq\Delta}$. By Lemma 3.4, we have

$$\frac{1}{2}\left\||\psi'\rangle\langle\psi'| - |\phi\rangle\langle\phi|\right\|_1 \leq \sqrt{\frac{\delta'}{\Delta - \lambda(H')}}.$$

Since $S_{\leq\Delta} = \mathrm{Im}(\widetilde{V})$, there must exist a state $|\psi\rangle$ in $\mathcal{H}$ such that $\widetilde{V}|\psi\rangle = |\phi\rangle$; next, we will show that $|\psi\rangle$ has low energy with respect to H. Note that $|\psi'\rangle = \sqrt{p}|\phi\rangle + \sqrt{1-p}|\phi^\perp\rangle$ for some $p \in [0,1]$ and a state $|\phi^\perp\rangle$ in $S^\perp_{\leq\Delta}$ which has higher energy: $\langle\phi^\perp|H'|\phi^\perp\rangle \geq \Delta \geq \langle\phi|H'|\phi\rangle$. Therefore,

$$\langle\psi'|H'|\psi'\rangle = p\langle\phi|H'|\phi\rangle + (1-p)\langle\phi^\perp|H'|\phi^\perp\rangle \geqslant \langle\phi|H'|\phi\rangle,$$

which implies that

$$\begin{aligned}
\langle\psi|H|\psi\rangle - \langle\psi'|H'|\psi'\rangle &\leqslant \langle\psi|H|\psi\rangle - \langle\phi|H'|\phi\rangle &(4)\\
&= \langle\phi|\widetilde{V}H\widetilde{V}^\dagger|\phi\rangle - \langle\phi|H'|\phi\rangle &(5)\\
&\leqslant \|H'_{\leq\Delta} - \widetilde{V}H\widetilde{V}^\dagger\| \leqslant \epsilon. &(6)
\end{aligned}$$

So, $\langle\psi|H|\psi\rangle \leqslant \lambda(H') + \delta' + \epsilon \leqslant \lambda(H) + \delta' + 2\epsilon$, where the final inequality follows from Lemma 27 of [CMP17], which roughly states that eigenvalues are preserved up to error ϵ in a simulation (in particular, the minimum eigenvalues satisfy $|\lambda(H') - \lambda(H)| \leq \epsilon$).

For any local measurement A_S acting on subset of S qubits $\mathcal{H}_S$ (here $\mathcal{H}_S$ is the Hilbert space for qudits in set $S \subseteq [n]$), we can define the local measurement $A'_S = V_S A_S V_S^\dagger$ on $\mathcal{H}'_S$ where $V = \bigotimes V_i$ is the local isometry in the definition of simulation and $V_S := \bigotimes_{i \in S} V_i$. Note that A'_S acts only on the $O(|S|)$ qudits which V_S maps to. Furthermore, $V^\dagger(A'_S \otimes I)V = A_S \otimes I$ and so

$$
\begin{aligned}
|\langle\psi'| A'_S \otimes I |\psi'\rangle - \langle\psi| A_S \otimes I |\psi\rangle| &= |\langle\psi'| A'_S \otimes I |\psi'\rangle - \langle\psi| V^\dagger(A'_S \otimes I)V |\psi\rangle| && (7)\\
&\leqslant \|A'_S\| \| |\psi'\rangle\langle\psi'| - V|\psi\rangle\langle\psi|V^\dagger\|_1 && (8)\\
&\leqslant \|A_S\| \left(\| |\psi'\rangle\langle\psi'| - |\phi\rangle\langle\phi| \|_1 + \|\widetilde{V}|\psi\rangle\langle\psi|\widetilde{V}^\dagger - V|\psi\rangle\langle\psi|V^\dagger\|_1 \right) && (9)\\
&\leqslant \|A_S\| \left(\| |\psi'\rangle\langle\psi'| - |\phi\rangle\langle\phi| \|_1 + 2\|\widetilde{V} - V\| \right) && (10)\\
&\leqslant \|A_S\| \left(2\sqrt{\frac{\delta'}{\Delta - \lambda(H')}} + 2\eta \right) && (11)
\end{aligned}
$$

where to get to (10), we have used the triangle inequality to bound:

$$
\begin{aligned}
\|\widetilde{V}|\psi\rangle\langle\psi|\widetilde{V}^\dagger - V|\psi\rangle\langle\psi|V^\dagger\|_1 &\leq \|\widetilde{V}|\psi\rangle\langle\psi|\widetilde{V}^\dagger - V|\psi\rangle\langle\psi|\widetilde{V}^\dagger\|_1 + \|V|\psi\rangle\langle\psi|\widetilde{V}^\dagger - V|\psi\rangle\langle\psi|V^\dagger\|_1 && (12)\\
&= \|\widetilde{V} - V\| \left(\| |\psi\rangle\langle\psi|\widetilde{V}^\dagger\|_1 + \|V|\psi\rangle\langle\psi|\|_1 \right) = 2\|\widetilde{V} - V\| && (13)
\end{aligned}
$$

Therefore, to ensure that Π' is a YES (resp. NO) instance if Π is a YES (resp. NO) instance, we will choose $a' = a + (b-a)/3$ and $b' = b - (b-a)/3$. Choosing $\delta', \Delta, \epsilon, \eta$ such that

$$
0 < \delta' + 2\epsilon < \delta \qquad \text{and} \qquad 0 < \|A\| \left(2\sqrt{\frac{\delta'}{\Delta - \lambda(H')}} + 2\eta \right) < \frac{b-a}{3}
$$

completes the proof. □

As a fairly simple corollary of our results, we obtain Theorem 1.5, which gives a complete classification of the complexity of APX-SIM when restricted to families of Hamiltonians and measurements built up from a set of interactions $\mathcal{S}$.

Theorem 1.5. *Let $\mathcal{S}$ be an arbitrary fixed subset of Hermitian matrices on at most 2 qubits. Then the* APX-SIM *problem, restricted to Hamiltonians H and measurements A given as a linear combination of terms from $\mathcal{S}$ and the identity I, is*

- P*-complete, if every matrix in $\mathcal{S}$ is 1-local;*
- $\mathrm{P}^{\mathrm{NP[log]}}$*-complete, if $\mathcal{S}$ does not satisfy the previous condition and there exists $U \in SU(2)$ such that U diagonalises all 1-qubit matrices in $\mathcal{S}$ and $U^{\otimes 2}$ diagonalises all 2-qubit matrices in $\mathcal{S}$;*
- $\mathrm{P}^{\mathrm{StoqMA[log]}}$*-complete, if $\mathcal{S}$ does not satisfy the previous condition and 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;*
- $\mathrm{P}^{\mathrm{QMA[log]}}$*-complete, otherwise.*

Proof. In the first case it is clearly trivial to simulate the outcome of 1-local measurements on the ground state of a 1-local Hamiltonian, as the ground state is an easily calculated product state. For the other three cases, it was shown in [CM16] and [BH17], that the Local Hamiltonian problem for these three families of Hamiltonians is complete for the classes NP, StoqMA, QMA, respectively. Therefore by Lemma 3.1, APX-SIM is contained in $\mathrm{P}^{\mathrm{NP}[\log]}, \mathrm{P}^{\mathrm{StoqMA}[\log]}$ and $\mathrm{P}^{\mathrm{QMA}[\log]}$, respectively. It was also shown in [CMP17] that these families of Hamiltonians can efficiently simulate all classical, stoquastic and arbitrary local Hamiltonians, respectively, and thus by Lemma 3.2 $\forall$-APX-SIM is hard for $\mathrm{P}^{||\mathrm{NP}}, \mathrm{P}^{||\mathrm{StoqMA}}$ and $\mathrm{P}^{||\mathrm{QMA}}$ respectively.

It remains to check that the observable A in the hardness proof of Lemma 3.2 can be performed by an $\mathcal{S}$-Hamiltonian. That hardness proof requires a single Z measurement; in principle, however, we may (without loss of generality) alter the starting P machine to encode its output in any function on two bits (such as the parity function), rather than just 1 bit, as will be assumed below. This is trivial in the second (classical) case, where we have direct access to a 2-local classical measurement. For the third case, one can check that the reductions in [BH17] correspond to a simulation with an isometry V which maps each qubit $|0\rangle \mapsto |0011\rangle$ and $|1\rangle \mapsto |1100\rangle$. For two logical qubits encoded in physical qubits $1, 2, 3, 4$ and $5, 6, 7, 8$ respectively, it is possible to simulate a 2-local classical measurement with $ZZ + AI + IB$, because

$$(V \otimes V)^\dagger (Z_1 Z_5 + A_1 + B_5)(V \otimes V) = Z \otimes Z + \mathrm{diag}(A) \otimes I + I \otimes \mathrm{diag}(B)$$

where $\mathrm{diag}(A)$ denotes the diagonal part of A, i.e. $\mathrm{diag}(A) = \sum_{i=0}^{1} |i\rangle\langle i|A|i\rangle\langle i|$.

The final case is slightly more complicated. When showing that these Hamiltonians are universal the one non-trivial step is simulating $\{X, Z, XX, ZZ\}$-Hamiltonians with $\{XX + YY\}$-Hamiltonians or $\{XX + YY + ZZ\}$-Hamiltonians in Theorem 41 of [CMP17]. In both of these cases, the isometry V maps each qubit

$$|0\rangle \mapsto |\Psi^-\rangle_{13} |\Psi^-\rangle_{24} \qquad |1\rangle \mapsto \tfrac{2}{\sqrt{3}} |\Psi^-\rangle_{12} |\Psi^-\rangle_{34} - \tfrac{1}{\sqrt{3}} |\Psi^-\rangle_{13} |\Psi^-\rangle_{24}$$

In the proof of Theorem 41 of [CMP17], it is shown that a single Z observable can be reproduced by choosing $A = h_{13}$ (where h is $XX + YY$ or $XX + YY + ZZ$), that is $V^\dagger h_{13} V$ is proportional to Z. Here h_{13} is an operator on 4 qubits although it only acts non-trivially on qubits 1 and 3.

The proof is completed by Corollary 1.3 (i.e. logarithmic adaptive queries are equivalent to polynomially many parallel queries). □

5 Spatially sparse construction

We now combine the tools developed in the previous sections to study the complexity of APX-SIM for physical Hamiltonians. Our approach is to show that $\forall$-APX-SIM is $\mathrm{P}^{||\mathrm{QMA}}$-hard even for Hamiltonians on a *spatially sparse interaction graph*, defined below:

Definition 5.1 (Spatial sparsity [OT08])**.** *A spatially sparse interaction (hyper)graph G on n vertices is defined as a (hyper)graph in which 1. every vertex participates in $O(1)$ hyper-edges, 2. there is a straight-line drawing in the plane such that every hyper-edge overlaps with $O(1)$ other hyper-edges and the surface covered by every hyper-edge is $O(1)$.*

Lemma 5.2. *$\forall$-APX-SIM is $\mathrm{P}^{||\mathrm{QMA}}$-hard even when $b - a = \Omega(1)$, the observable A is 1-local, and the Hamiltonian H is 4-local and is restricted to a spatially sparse interaction graph.*

Here, we adapt the proof of Lemma 3.2. Recall that the Hamiltonian H in Lemma 3.2 is composed of two parts $H = H_1 + H_2$, where H_2 uses (a simplification of) Ambainis's query Hamiltonian on each of the

registers $\mathcal{X}_i \otimes \mathcal{Y}_i$ to encode the answer to that query into the state of $\mathcal{X}_i$ (see Equation (1)), and H_1 encodes the evolution of the P circuit using the Cook-Levin construction on the $\mathcal{W}$ register (controlling on the states of the $\mathcal{X}_i$ registers). This is represented by Figure 2.

We arrange the qubits of the $\mathcal{W}$ register on a square lattice and note that H_1 is already manifestly spatially sparse. This is one of the advantages of using the Cook-Levin construction over the Kitaev history state construction. Furthermore, the Hamiltonian $H_{\mathcal{Y}_i}$, corresponding to the ith QMA query, can always be chosen to be spatially sparse – in fact it can be chosen to have its interactions on the edges of a 2D square lattice [OT08], and so we also lay out the qubits of each $\mathcal{Y}_i$ register on a square lattice.

But the interaction graph of this Hamiltonian is still far from spatially sparse because in (the modified version of) Ambainis's query Hamiltonian H_2, every qubit of $\mathcal{Y}_i$ interacts with $\mathcal{X}_i$. We will solve this problem by replacing each single qubit $\mathcal{X}_i$ register with a multi-qubit register of n_i qubits labelled by $\{\mathcal{X}_i(j)\}_{j=1}^{n_i}$, for n_i the number of qubits of $\mathcal{Y}_i$. We spread out the qubits of the $\mathcal{X}_i$ register in space around the $\mathcal{Y}_i$ register, and modify H_2 so that each term is controlled only on a nearby qubit in the $\mathcal{X}_i$ register. To make this work we need to introduce a third term H_3 which ensures that all the qubits in each $\mathcal{X}_i$ register are either all 0 or all 1.

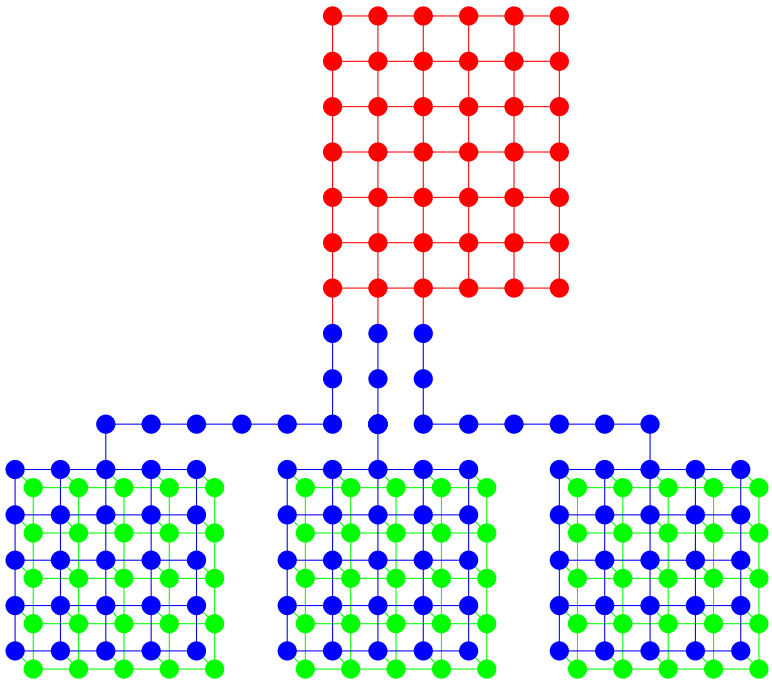

Figure 3: (Color figure) Geometric structure of total Hamiltonian $H = H_1 + H_2 + H_3$ for the case of 3 queries. In words, H_1 is the top square, H_3 is the set of connecting wires, along with the bottom three squares to which they are connected. H_2 is the remaining set of three squares at the bottom of the diagram.

Proof of Lemma 5.2. We will construct a Hamiltonian on the registers $\mathcal{W}$, $\mathcal{X}_i$ and $\mathcal{Y}_i$ for $i \in \{1, \ldots m\}$, for which the problem $\forall$-APX-SIM encodes the output of a $\mathrm{P}^{||\mathrm{QMA}}$ circuit, where m is the number of parallel queries to the QMA oracle.

Let the qubits of $\mathcal{W}$ and $\mathcal{Y}_i$ be arranged on distinct parts of a square lattice. For each qubit of $\mathcal{Y}_i$, there is a corresponding qubit in $\mathcal{X}_i$, and $\mathcal{X}_i$ contains a path of qubits leading from $\mathcal{Y}_i$ to $\mathcal{W}$. See Figure 3 for an example layout in the case $m = 3$.

Let E_i be the set of edges of the square lattice of qubits of $\mathcal{Y}_i$ (i.e. not including the edges connecting $\mathcal{Y}_i$ to $\mathcal{X}_i$ in Figure 3) and let $H_{\mathcal{Y}_i} = \sum_{(j,k)\in E_i} h^i_{\mathcal{Y}_i(j,k)}$ be a 2D nearest neighbour Hamiltonian on $\mathcal{Y}_i$ corresponding to the ith query. We have used the subscript notation $\mathcal{Y}_i(j,k)$ to denote the action of an operator on the jth and kth qubits of the $\mathcal{Y}_i$ register. $H_{\mathcal{Y}_i}$ has ground state energy less than a_i if query i is a YES instance and energy greater than b_i in a NO instance. Then, let $H_2 = \sum_i H_2^{(i)}$ where

$$H_2^{(i)} = \frac{a_i + b_i}{2}|0\rangle\langle 0|_{\mathcal{X}_i(1)} \otimes I_{\mathcal{Y}_i} + \sum_{(j,k)\in E_i} \left(|1\rangle\langle 1|_{\mathcal{X}_i(g(j,k))} \otimes h^i_{\mathcal{Y}_i(j,k)}\right),$$

where $g(j,k)$ is the location of the "nearest" qubit in $\mathcal{X}_i$ to edge (j,k) in $\mathcal{Y}_i$. Here, the choice "nearest" is somewhat arbitrary; for concreteness, one can set $g(j,k) = j$, i.e. pick the vertex in $\mathcal{X}_i$ which aligns with the first coordinate of the edge (j,k). (Aside: In this sense, Figure 3 is not entirely accurate, since it depicts the 3-local constraint $|1\rangle\langle 1|_{\mathcal{X}_i(g(j,k))} \otimes h^i_{\mathcal{Y}_i(j,k)}$ as a pair of 2-local constraints. This is done solely for the purpose of simplifying the illustration, as otherwise one would need to draw hyperedges of size 3.)

Let $H_1 = H_{\text{prop}} + H_{\text{in}}$ be the Cook-Levin Hamiltonian where H_{prop} is exactly as in Lemma 3.2. Let H_{in} initialise the qubits of the first ($t = 1$) row of the qubits in $\mathcal{W}$. For each query i, we have a penalty term $|1\rangle\langle 1|_{\mathcal{X}_i(1)}|0\rangle\langle 0| + |0\rangle\langle 0|_{\mathcal{X}_i(1)}|1\rangle\langle 1|$ which effectively copies the state of $\mathcal{X}_i(1)$, the qubit in $\mathcal{X}_i$ nearest to $\mathcal{W}$, onto the ith qubit of the first row of $\mathcal{W}$. For all the remaining qubits in the first ($t = 1$) row of $\mathcal{W}$, we have a penalty term $|1\rangle\langle 1|$, effectively initialising the qubit into the $|0\rangle$ state.

Restricted to the subspace $\mathcal{H}$ where each $\mathcal{X}_i$ register is either all $|0\rangle$ or all $|1\rangle$, $H_1 + H_2$ is exactly the same Hamiltonian as in Lemma 3.2. It remains to give a high energy penalty to all other states not in this subspace. We do this with $H_3 = \sum_{i=1}^m H_3^{(i)}$ where each term $H_3^{(i)}$ acts on $\mathcal{X}_i$:

$$H_3^{(i)} = \Delta_i \sum_{(j,k)\in G_i} \left(|0\rangle\langle 0|_{\mathcal{X}_i(j)}|1\rangle\langle 1|_{\mathcal{X}_i(k)} + |1\rangle\langle 1|_{\mathcal{X}_i(j)}|0\rangle\langle 0|_{\mathcal{X}_i(k)}\right)$$

where G_i is the set of edges between the qubits of the $\mathcal{X}_i$ register. G_i consists of edges between nearest neighbours on the square lattice E_i and on the path of qubits from $\mathcal{Y}_i$ to $\mathcal{W}$. The overall Hamiltonian $H = H_1 + H_2 + H_3$ is therefore spatially sparse.

$H_3^{(i)}$ is a classical Hamiltonian, so all of its eigenstates can be taken to be of form $|x\rangle$ for some $x \in \{0,1\}^{n_i}$. Its ground space $\mathcal{G}_i$ contains $|0\rangle^{\otimes n_i}$ and $|1\rangle^{\otimes n_i}$; and all states in $\mathcal{G}_i^\perp$ have energy at least Δ_i. Choosing $\Delta_i > \delta + \sum_{(j,k)\in E_i} \|h^i_{\mathcal{Y}_i(j,k)}\|$ ensures that all states in $\mathcal{G}_i^\perp$ have energy greater than $\lambda(H) + \delta$.

Then $H = H_1 + H_2 + H_3$ is block diagonal with respect to the split of each subspace $\mathcal{G}_i \oplus \mathcal{G}_i^\perp$; restricted to the spaces $\mathcal{G}_i$, H is exactly the Hamiltonian from Lemma 3.2, and all states in spaces $\mathcal{G}_i^\perp$ have energy greater than $\lambda(H) + \delta$. The result then follows just as in the proof of Lemma 3.2. □

Finally we restate Theorem 1.6 which shows APX-SIM is hard not only for families of Hamiltonians which are universal – that is, families that can efficiently simulate any k-local Hamiltonian – but also for more restricted families of Hamiltonians which can only efficiently simulate the family of spatially sparse Hamiltonians. As stated in Section 1.2, this then yields the desired hardness results for APX-SIM on physical Hamiltonians such as the Heisenberg interaction on a 2D lattice (see, e.g., Corollary 1.7).

Theorem 1.6. *Let $\mathcal{F}$ be a family of Hamiltonians which can efficiently simulate any spatially sparse Hamiltonian. Then,* APX-SIM *is* $\mathrm{P}^{\mathrm{QMA}[\log]}$*-complete even when restricted to an $O(1)$-local observable and a Hamiltonian from the family $\mathcal{F}$.*

Proof. This follows from Lemma 4.2, Lemma 5.2 and Corollary 1.3. □

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A General simulations

In this section we will give a full proof of Lemma 4.2 and show that *any* efficient simulation will preserve hardness of ∀-APX-SIM, not just the special case considered in Definition 4.1. To state the full definition of simulation, we must first introduce the notion of an encoding.

Definition A.1 ([CMP17])**.** *We say a map $\mathcal{E} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H}')$ is an encoding if it is of the form*

$$\mathcal{E}(M) = V(M \otimes P + \overline{M} \otimes Q)V^\dagger$$

where $\overline{M}$ denotes the complex conjugate of M, P and Q are orthogonal projectors (i.e. $PQ = 0$) on an ancilla space E; and V is an isometry $V : \mathcal{H} \otimes E \to \mathcal{H}'$.

When $\mathcal{H}$ is a many body system with a decomposition $\mathcal{H} = \bigotimes_{i=1}^n \mathcal{H}_i$, we say $\mathcal{E}$ is a local encoding if $E = \bigotimes_{i=1}^n E_i$ such that:

- *$V = \bigotimes_{i=1}^n V_i$ where each V_i acts on $\mathcal{H}_i \otimes E_i$.*
- *for each i, there exist orthogonal projectors P_{E_i} and Q_{E_i} on E which act non-trivially only on E_i, and satisfy $PP_{E_i} = P$ and $QQ_{E_i} = Q$.*

We are now ready to give the full definition of simulation.

Definition A.2 ([CMP17])**.** *We say that H' is a (Δ, η, ϵ)-simulation of H if there exists a local encoding $\mathcal{E}(M) = V(M \otimes P + \overline{M} \otimes Q)V^\dagger$ such that:*

1. *There exists an isometry $\widetilde{V} : \mathcal{H} \otimes E \to \mathcal{H}'$ such that $\|\widetilde{V} - V\| \leq \eta$; and that the encoding $\widetilde{\mathcal{E}}(M) = \widetilde{V}(M \otimes P + \overline{M} \otimes Q)\widetilde{V}^\dagger$ satisfies $\widetilde{\mathcal{E}}(I) = P_{\leq \Delta(H')}$.*
2. *$\|H'_{\leq \Delta} - \widetilde{\mathcal{E}}(H)\| \leq \epsilon$.*

We say that a family $\mathcal{F}'$ of Hamiltonians can simulate a family $\mathcal{F}$ of Hamiltonians if, for any $H \in \mathcal{F}$ and any $\eta, \epsilon > 0$ and $\Delta \geq \Delta_0$ (for some $\Delta_0 > 0$), there exists $H' \in \mathcal{F}'$ such that H' is a (Δ, η, ϵ)-simulation of H. We say that the simulation is efficient if, in addition, for H acting on n qudits, $\|H'\| = \mathrm{poly}(n, 1/\eta, 1/\epsilon, \Delta)$; H' and $\{ V_i \}$ are efficiently computable given H, Δ, η and ϵ; and each local isometry V_i in the decomposition $V = \bigotimes_i V_i$ maps to $O(1)$ qudits.

We note that Definition 4.1 is just the special case of Definition A.2 where $\mathcal{E}(M) = VMV^\dagger$. We are now ready to restate and prove Lemma 4.2.

Lemma 4.2 (Simulations preserve hardness of ∀-APX-SIM)**.** *Let $\mathcal{F}$ be a family of Hamiltonians which can be efficiently simulated by another family $\mathcal{F}'$. Then $\mathcal{F}$-∀-APXSIM reduces to $\mathcal{F}'$-∀-APXSIM.*

Proof. For brevity, let $P_{\leq \Delta} := P_{\leq \Delta(H')}$. Let $\rho' = |\psi'\rangle\langle\psi'|$ be a state on $\mathcal{H}'$ such that $\langle\psi'| H' |\psi'\rangle \leq \delta'$ and let $\widetilde{\rho} = P_{\leq \Delta}\rho' P_{\leq \Delta} / \operatorname{Tr}(P_{\leq \Delta}\rho')$, so that by Lemma 3.4, we have $\|\rho' - \widetilde{\rho}\|_1 \leq 2\sqrt{\frac{\delta'}{\Delta - \lambda(H')}}$.

Since $P_{\leq \Delta}$ commutes with H', we have

$$\operatorname{Tr}(H'\rho') = \operatorname{Tr}(H' P_{\leq \Delta}\rho' P_{\leq \Delta}) + \operatorname{Tr}(H'(I - P_{\leq \Delta})\rho'(I - P_{\leq \Delta})) \tag{14}$$

$$= p \operatorname{Tr}(H'\widetilde{\rho}) + (1 - p) \operatorname{Tr}(H'\widetilde{\rho}^\perp) \geq \operatorname{Tr}(H'\widetilde{\rho}) \tag{15}$$

where $p = \mathrm{Tr}(P_{\leq\Delta}\rho')$, $\widetilde{\rho}^{\perp} = (I - P_{\leq\Delta})\rho'(I - P_{\leq\Delta})/\mathrm{Tr}((I - P_{\leq\Delta})\rho')$; and the final inequality follows because $\mathrm{Tr}(H'\widetilde{\rho}^{\perp}) \geq \Delta \geq \mathrm{Tr}(H'\widetilde{\rho})$.

Now let

$$\rho = \mathrm{Tr}_E\left(\widetilde{V}^{\dagger}\widetilde{\rho}\widetilde{V}(I \otimes P)\right) + \mathrm{Tr}_E\left(\overline{\widetilde{V}^{\dagger}\widetilde{\rho}\widetilde{V}(I \otimes Q)}\right)$$

and note that for any operator A on $\mathcal{H}$, we have

$$\mathrm{Tr}(\widetilde{\mathcal{E}}(A)\widetilde{\rho}) = \mathrm{Tr}\left(\widetilde{V}(A \otimes P + \overline{A} \otimes Q)\widetilde{V}^{\dagger}\widetilde{\rho}\right) = \mathrm{Tr}\left(A \otimes P\widetilde{V}^{\dagger}\widetilde{\rho}\widetilde{V}\right) + \mathrm{Tr}\left(\overline{A} \otimes Q\widetilde{V}^{\dagger}\widetilde{\rho}\widetilde{V}\right) = \mathrm{Tr}(A\rho).$$

Therefore,

$$\mathrm{Tr}(H\rho) = \mathrm{Tr}(\widetilde{\mathcal{E}}(H)\widetilde{\rho}) \leq \mathrm{Tr}(H'\widetilde{\rho}) + \|H'_{\leq\Delta} - \widetilde{\mathcal{E}}(H)\| \leq \mathrm{Tr}(H'\rho') + \epsilon \leq \lambda(H') + \delta' + \epsilon \leq \lambda(H) + \delta' + 2\epsilon,$$

where the second inequality follows from Equation (15) and the last inequality from Lemma 27 of [CMP17], which roughly states that eigenvalues are preserved up to additive error ϵ in a simulation.

At this point the proof diverges from the simpler case because ρ may be a mixed state, even when $\rho' = |\psi'\rangle\langle\psi'|$ is pure. Despite having a bound on $\mathrm{Tr}(H\rho)$, this bound may not hold for all pure states in the spectral decomposition of ρ. Let $\rho_{\delta} = P_{\delta}\rho P_{\delta}/\mathrm{Tr}(P_{\delta})$, where P_{δ} is the projector onto eigenvectors of H with energy less than δ. By Lemma 3.4, $\|\rho - \rho_{\delta}\|_1 \leq 2\sqrt{\frac{\delta'+2\epsilon}{\delta}}$. We will use the spectral decomposition of $\rho_{\delta} = \sum_i \mu_i|\phi_i\rangle\langle\phi_i|$ where the $|\phi_i\rangle$ are orthogonal states with energy $\langle\phi_i| H |\phi_i\rangle \leq \lambda(H) + \delta$ and thus, for observable A given as part of of $\mathcal{F}$-$\forall$-APXSIM input,

$$\mathrm{Tr}(A\rho_{\delta}) = \sum_i \mu_i \langle\phi_i| A |\phi_i\rangle \quad \begin{cases} \leq a \text{ in a YES instance} \\ \geq b \text{ in a NO instance.} \end{cases}$$

Let $U = V\widetilde{V}^{\dagger}$, which satisfies $U\widetilde{\mathcal{E}}(A) = \mathcal{E}(A)U$ for any A, and so $\mathcal{E}(I)U\widetilde{\rho}U^{\dagger} = U\widetilde{\mathcal{E}}(I)\widetilde{\rho}U^{\dagger} = U\widetilde{\rho}U^{\dagger}$. Now we need to choose A' such that $A'\mathcal{E}(I) = \mathcal{E}(A)$. For example if $A = B_i \otimes I$, let $A' = V_i(B_i \otimes P_{E_i} + \overline{B_i} \otimes Q_{E_i})V_i^{\dagger} \otimes I$. We note that the locality of A' depends on the number of qudits which V_i maps to, which is $O(1)$ by the definition of efficient simulation. Then

$$\mathrm{Tr}(A\rho) = \mathrm{Tr}\left(\widetilde{\mathcal{E}}(A)\widetilde{\rho}\right) = \mathrm{Tr}\left(\mathcal{E}(A)U\widetilde{\rho}U^{\dagger}\right) = \mathrm{Tr}(A'\mathcal{E}(I)U\widetilde{\rho}U^{\dagger}) = \mathrm{Tr}(A'U\widetilde{\rho}U^{\dagger})$$

and therefore

$$\begin{aligned} |\mathrm{Tr}(A'\rho') - \mathrm{Tr}(A\rho_{\delta})| &\leq |\mathrm{Tr}(A'\rho') - \mathrm{Tr}(A'U\widetilde{\rho}U^{\dagger})| + |\mathrm{Tr}(A\rho) - \mathrm{Tr}(A\rho_{\delta})| \\ &\leq \|A'\|\left(\|\rho' - \widetilde{\rho}\|_1 + \|\widetilde{\rho} - U\widetilde{\rho}U^{\dagger}\|_1\right) + \|A\|\|\rho - \rho_{\delta}\|_1 \\ &\leq \|A\|\left(2\sqrt{\frac{\delta'}{\Delta - \lambda(H')}} + 2\eta + 2\sqrt{\frac{\delta' + 2\epsilon}{\delta}}\right), \end{aligned}$$

We note that $\|\widetilde{\rho} - U\widetilde{\rho}U^{\dagger}\|_1 \leq 2\eta$ follows from $\|U - \widetilde{V}\widetilde{V}^{\dagger}\| \leq \eta$, and that $\widetilde{V}\widetilde{V}^{\dagger}\widetilde{\rho} = P_{\leq\Delta}\widetilde{\rho} = \widetilde{\rho}$. Therefore we just need to choose $\Delta, \epsilon, \eta, \delta'$ such that this is less than $(b - a)/3$ and then set $a' = a + (b - a)/3$ and $b' = b - (b - a)/3$.

□