Quantum search-to-decision reductions and the state synthesis problem

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Abstract

It is a useful fact in classical computer science that many search problems are reducible to decision problems; this has led to decision problems being regarded as the \textit{de facto} computational task to study in complexity theory. In this work, we explore search-to-decision reductions for quantum search problems, wherein a quantum algorithm makes queries to a classical decision oracle to output a desired quantum state. In particular, we focus on search-to-decision reductions for QMA, and show that there exists a quantum polynomial-time algorithm that can generate a witness for a QMA problem up to inverse polynomial precision by making one query to a PP decision oracle. We complement this result by showing that QMA-search does not reduce to QMA-decision in polynomial-time, relative to a quantum oracle.

We also explore the more general \textit{state synthesis problem}, in which the goal is to efficiently synthesize a target state by making queries to a classical oracle encoding the state. We prove that there exists a classical oracle with which any quantum state can be synthesized to inverse polynomial precision using only one oracle query and to inverse exponential precision using two oracle queries. This answers an open question of Aaronson\textsuperscript{[Aar16]}, who presented a state synthesis algorithm that makes $O(n)$ queries to a classical oracle to prepare an $n$-qubit state, and asked if the query complexity could be made sublinear.

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1 Introduction

It is a useful fact in classical computer science that search problems are often efficiently reducible to decision problems. For example, the canonical way of constructing a satisfying assignment of a given 3SAT formula $\phi$ (if there exists one) using an oracle for the decision version of 3SAT is to adaptively query the oracle for the satisfiability of $\phi$ conditioned on some partial assignment to the variables of the formula. Based on the oracle answers, the partial assignment can be extended bit-by-bit to a full assignment. Each oracle query reveals an additional bit of the assignment. This strategy generally works for any problem in NP. Likewise, the optimal value of an optimization problem can be calculated to exponential accuracy using binary search. The main consequence of this is that complexity theory often focuses on decision problems (without losing generality) and less on the complexity of search problems.

Quantum information and computation has shifted our perspective on these traditional notions of classical complexity theory. In this paper we consider quantum search problems, where the goal is to output a quantum state (as opposed to a classical bit string) satisfying some condition. In the quantum setting, it is no longer apparent that search-to-decision reductions still hold, and thus it is unclear whether the complexity of quantum search problems can be directly related to the complexity of corresponding quantum decision problems.

To illustrate this, we consider the analogues of P and NP in quantum computing, which are the complexity classes BQP and QMA, respectively. The analogue of the NP-complete problem 3SAT for QMA is the Local Hamiltonian problem, in which one has to decide whether the lowest energy state of a local Hamiltonian $H = H_1 + \cdots + H_m$ acting on $n$ qubits has energy greater than $a$ or less than $b$ for $a - b = 1/poly(n)$, where each term $H_i$ acts non-trivially on only a constant number of qubits. This problem was proven to be QMA-complete by Kitaev [KSVV02]. Is there an efficient search-to-decision reduction for the Local Hamiltonians problem, or more generally for the class QMA? In other words, given quantum query access to an oracle deciding the Local Hamiltonians problem, can a polynomial-time quantum algorithm (i.e. BQP machine) efficiently prepare a low-energy state $|\psi\rangle$ of a given local Hamiltonian?

The classical strategy of incrementally building a partial assignment does not appear to work in the QMA setting. First, there does not appear to be a natural way of “conditioning” a quantum state on a partial assignment. Second, quantum states are exponentially complex: the description size (complexity) of a general quantum state on $n$ qubits is exponential in $n$, and this is suspected to remain true even when considering ground states of local Hamiltonians. This complexity of quantum states poses a significant challenge to finding a search-to-decision reduction for QMA; it is not clear how yes/no answers to QMA decision problems (even when obtained in superposition) can be used to construct exponentially-complex QMA witnesses.

On the other hand, there is a natural quantum analogue of the bit-by-bit search-to-decision algorithm for NP that works for constructing general quantum states. This is due to a general algorithm for state synthesis described by Aaronson in [Aar16] (for which we give an overview of in Section 1.1): there exists a polynomial-time quantum algorithm $A$ such that every $n$-qubit state $|\psi\rangle$ can be encoded into a classical oracle $f$ where, by making $O(n)$ superposition queries to the oracle $f$, the algorithm $A$ will output a state that is exponentially close to $|\psi\rangle$. One can observe

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1Technically speaking, BQP and QMA are better thought of as the quantum analogues of BPP and MA, respectively. However, even in this randomized setting, there are efficient search-to-decision randomized reductions.

2Due to the QMA $\neq$ QCMA conjecture [AK07]. Formally, there is no known poly-sized description of a witness (proof) for every local Hamiltonian problem.
that for states $|\psi\rangle$ that QMA witnesses (such as ground states of local Hamiltonians), the oracle $f$ corresponds to a PP function (which is at least as powerful as a QMA oracle). This yields a search-to-decision reduction for QMA, albeit with a decision oracle of higher complexity.

In this work, we explore the complexity of search-to-decision procedures in the quantum setting, where the goal is a quantum state synthesis algorithm that outputs a target quantum state (e.g. a ground state of a local Hamiltonian) by making quantum queries to a classical decision oracle. We investigate how the complexity of the state synthesis algorithm and the complexity of the decision oracle depend on the type of states we want to generate. We consider both the generalized state synthesis problem for arbitrary states in the Hilbert space $(\mathbb{C}^2)^\otimes n$ as well as the specific task of generating solutions to QMA problems.

We construct state synthesis and search-to-decision procedures for the quantum setting using only one or two superposition queries as opposed to $O(n)$ superposition queries; for QMA witnesses, the synthesis procedure requires only one query to a PP oracle. Simultaneously, we prove results suggesting the impossibility of any search-to-decision reduction for QMA. More precisely, we show that there exists a quantum oracle $O$ relative to which all efficient query algorithms fail to be a good search-to-decision reduction for QMA$^O$, the relativization of QMA. This stands in contrast to classes such as NP, MA, and QCMA, which all have efficient search to decision reductions, relative to any oracle. As a consequence, proving impossibility of QMA search-to-decision without an oracle is at least as hard as separating QCMA and QMA which is at least as hard as separating P and PP. We believe that the juxtaposition of our results lends further weight to the view that the complexity of tasks where the outputs (and inputs) are quantum states cannot be directly explained by the traditional study of decision problems (which has been the main focus of quantum complexity theory to date). In particular, we believe our results suggest that the relationship between search and decision problems is much more mysterious in the quantum setting. As suggested by Aaronson in [Aar16] and others in some recent works [Kre21, RY21], the complexity of quantum states (and more generally, quantum state transformations) deserves to be studied more deeply as a subject in its own right.

1.1 Starting point

Before describing our results in more detail, we first explain the starting point for our investigations, which is a simple state synthesis algorithm described by Aaronson [Aar16] in his lecture notes. He shows that there exists a poly$(n)$-time quantum algorithm $A$ which makes $O(n)$ quantum queries to a classical oracle such that for every $n$-qubit state $|\psi\rangle = \sum_x \alpha_x |x\rangle$, there exists a classical oracle $f$ for which the algorithm $A^{O_f}$ will output a state that is $\exp(-n)$-close to $|\psi\rangle$. In [Aar16], Aaronson raises the question as to whether his protocol can be improved to a sublinear number of queries. We show, in fact, that 1 query is sufficient to achieve polynomially small error in synthesizing arbitrary states and 2-queries are sufficient for exponentially small error. Both the 1-query and the 2-query algorithms given here require exponential time and polynomial space.

To understand Aaronson’s state synthesis algorithm, we first observe that we can write any quantum state in the form

$$|\psi\rangle = \sum_{x\in\{0,1\}^n} e^{i\theta_x} \sqrt{\Pr[X = x]} |x\rangle$$

(1.1)

where $\Pr[X = x]$ is the probability distribution of some $n$-bit random variable $X$ and $\{\theta_x\}_{\{0,1\}^n}$ are
a set of phases. The synthesis algorithm performs \(2n\) queries to synthesize the “QSample state”.

\[
\sum_{x \in \{0,1\}^n} \sqrt{\Pr[X = x]} \ket{x}
\]  

(1.2)

and then performs two additional queries at the end to apply the phases \(e^{i\theta_x}\) to each basis state \(\ket{x}\).

The \(2n\)-query procedure to build the QSample state works in \(n\) stages. Inductively assume that after the \(k\)th stage, for \(k < n\), the intermediate state of the algorithm is the \(k\)-qubit state

\[
\sum_{y \in \{0,1\}^k} \sqrt{\Pr[X_{\leq k} = y]} \ket{y}
\]  

(1.3)

where \(\Pr[X_{\leq k} = y]\) denotes the marginal probability of the first \(k\) bits of \(X\) are equal to \(y\). Controlled on the prefix \(\ket{y}\) the algorithm queries the oracle \(f\) to obtain a (classical description of) the conditional probabilities \(\Pr[X_{k+1} = 0 \mid X_{\leq k} = y]\) and \(\Pr[X_{k+1} = 1 \mid X_{\leq k} = y]\), and prepares a \((k+1)\)st qubit in the state

\[
\sqrt{\Pr[X_{k+1} = 0 \mid X_{\leq k} = y]} \ket{0} + \sqrt{\Pr[X_{k+1} = 1 \mid X_{\leq k} = y]} \ket{1}.
\]  

(1.4)

The algorithm performs another query to \(f\) to uncompute the descriptions of the conditional probabilities. The resulting \(k + 1\) qubit state is then equal to

\[
\sum_{y \in \{0,1\}^{k+1}} \sqrt{\Pr[X_{\leq k} = y]} \cdot \sqrt{\Pr[X_{k+1} = y_{k+1} \mid X_{\leq k} = y]} \ket{y}
\]  

(1.5)

\[
= \sum_{y \in \{0,1\}^{k+1}} \sqrt{\Pr[X_{\leq k+1} = y]} \ket{y}
\]  

(1.6)

which maintains the desired invariant. After the \(n\)th stage, a similar process applies the phases \(\{\theta_x\}\) to generate the output state. The approximations come in when the conditional probabilities and phases are specified with \(\text{poly}(n)\) bits of precision, which result in the final state being at most \(\exp(-n)\) far from the ideal target state \(\ket{\psi}\). With this \(O(n)\)-query state synthesis algorithm in mind, we now proceed to describe our results.

1.2 Our results

A one-query search-to-decision algorithm for QMA with a PP oracle. We show Section 2 that in the case of generating physically relevant states, i.e. solutions to QMA problems, such as the low-energy states of local Hamiltonians, that there exists a one-query search-to-decision algorithm using a PP oracle. While one would hope to find a search-to-decision reduction in which the oracle complexity is only QMA, PP is the smallest complexity class containing QMA for which we can construct an oracular algorithm for search problems. Furthermore, given our no-go result for QMA search-to-decision (see below), this may be the optimal search-to-decision algorithm.

**Theorem 1.1 (QMA-search to PP-decision reduction)** There exists a probabilistic polynomial time quantum algorithm making a single query to a PP phase oracle such that, given as input a QMA problem, either aborts or outputs a witness \(\ket{\phi}\). The algorithm will succeed in outputting a witness (i.e. not abort) with all but inverse exponential (in the system size) probability.
Table 1: Summary of past work and our results on upper bounds for search-to-decision reductions and state synthesis. The “complexity class” column refers to the complexity of the search problem (e.g., computing \( \text{NP} \) witnesses, or \( \text{QMA} \) witnesses). The other columns refer to the algorithmic results known for the specified number of queries; furthermore these are quantum queries performed by quantum algorithms in superposition.

To start sketching the proof, it is fruitful to notice that a single oracle query \( |x\rangle \xrightarrow{O} (-1)^{f(x)} |x\rangle \) for \( x \in \{0,1\}^n \) potentially contains \( 2^n \) bits of information and a quantum state requires \( 2^n \) complex numbers to describe. Furthermore, the collection of \( 2^{2^n} \) states

\[
|p_f\rangle \overset{\text{def}}{=} \bigotimes x \in \{0,1\}^n (-1)^{f(x)} |x\rangle
\]

(1.7)
defined for any function \( f : \{0,1\}^n \rightarrow \{0,1\} \) are a diverse set of states in the Hilbert space. These states, referred to as phase states henceforth, despite not forming an \( \epsilon \)-net for \( (\mathbb{C}^2)^{\otimes n} \), turn out to provide a good approximation for \( (\mathbb{C}^2)^{\otimes n} \) when considering the Haar-random distribution. It follows that if we wanted to synthesize the witness to a QMA-complete problem, such as a low-energy state \( |\tau\rangle \) for a local Hamiltonian problem, it suffices to build phase state \( |p_f\rangle \) with constant overlap with the low-energy subspace. Finding a state with constant overlap with the target state is sufficient because QMA is efficiently verifiable, and given a state with constant overlap with the low-energy subspace, it is possible to distill a low-energy state with constant probability (by performing an energy measurement). However, it is not necessarily the case that a low-energy state of QMA problem will have a good approximation by a phase state. To solve this issue, we prove that for any state \( |\tau\rangle \), with high probability \( C |\tau\rangle \) will have a good approximation by a phase state.

\[3\]Recall, the Haar-measure is the unique left- and right- invariant distribution over unitary matrices over \( (\mathbb{C}^2)^{\otimes n} \) and the Haar-random distribution is the distribution over quantum states \( U |0^n\rangle \) where \( U \) is sampled according to the Haar-measure.
state where \( C \) is a random Clifford unitary. Therefore, we can instead attempt to synthesize \( C |\tau\rangle \) which is the result of Theorem 1.1. In particular, if we can synthesize a phase state \( |p\rangle \) that has constant overlap with \( C |\tau\rangle \), then \( C^\dagger |p\rangle \) will have constant overlap with the target \( |\tau\rangle \).

Furthermore, we show that, using a slight modification of the same algorithm, we can perform a somewhat weaker one-query search-to-decision reduction for \( \text{QMA}_{\exp} \) (Theorem 2.4), the class of non-deterministic quantum computations with only an inverse exponential gap between completeness and soundness. \( \text{QMA}_{\exp} \) is known to equal \( \text{PSPACE} \) [FL16, DGF20], and our algorithm prepares a witness state with constant overlap with a low-energy state with one query to a \( \text{PSPACE} \) oracle (note that here, we cannot efficiently amplify the overlap with an energy measurement due to the inverse-exponential energy gap). As a further observation, we also show that quantum query access to a classical oracle gives one-query search-to-decision reductions when the witness is classical: in particular, for \( \text{QCMA} \) (Theorem 2.7), and also for \( \text{NP} \). The one-query algorithm preparing the witness first reduces \( \text{QCMA} \) to \( \text{unique QCMA} \) (UQCMA) using the Valiant-Vazirani reduction [ABOBS08], and then uses the Bernstein-Vazirani algorithm to extract the unique polynomial length witness with a single query.

A no-go result for search-to-decision for \( \text{QMA} \). The previous result shows that search-to-decision reductions for \( \text{QMA} \) are possible with a \( \text{PP} \) decision oracle. However, the optimal search-to-decision reduction for \( \text{QMA} \) is with a \( \text{QMA} \) decision oracle (rather than a stronger \( \text{PP} \) oracle). We provide evidence that this is unlikely to exist: we prove that there is a quantum oracle relative to which \( \text{QMA} \) search-to-decision is impossible. This stands in contrast to classes such as \( \text{NP}, \text{MA}, \) and \( \text{QCMA} \), which all have efficient search to decision reductions, relative to any oracle.

More precisely, we show that there exists a quantum oracle \( \mathcal{O} \) relative to which all \( \text{poly}(n) \)-time query algorithms fail to be a good search-to-decision reduction for \( \text{QMA}^\mathcal{O} \), the relativization of \( \text{QMA} \). The oracle \( \mathcal{O} \) is a reflection \( I - 2|\psi\rangle\langle\psi| \) about a Haar-random state \( |\psi\rangle \); we rely on the concentration of measure phenomenon of the Haar measure to prove this oracle no-go result. We formalize and prove this result in Section 3.

Theorem 1.2 (Oracle impossibility for \( \text{QMA} \) search-to-decision) There exists a quantum oracle \( \mathcal{O} \) relative to which all \( \text{poly}(n) \)-time query algorithms fail to be a good search-to-decision reduction for \( \text{QMA}^\mathcal{O} \).

A one-query state synthesis algorithm with inverse polynomial error. We also investigate the query complexity of synthesizing an arbitrary state, in the same spirit as Aaronson’s adaptive state synthesis algorithm outlined in Section 1.1. In particular, we show that that every state \( |\tau\rangle \) can be encoded into a classical oracle \( f_\tau \) such that by making one query to \( |\tau\rangle \), a quantum algorithm can prepare \( |\tau\rangle \) with inverse polynomial error. The space complexity of the synthesis algorithm is polynomial in \( n \), the number of qubits in the target state \( |\tau\rangle \), but the time complexity is exponential. The starting point for the 1-query algorithm is the same observation used in the protocol for synthesizing \( \text{QMA} \) witnesses, which is that a random state has an expected constant overlap with some phase state. We can think of the oracle function \( f_\tau \) as hard-coding the target \( |\tau\rangle \), but parameterized by unitary \( U \) and standard basis state \( x \). The oracle \( f_\tau(U, x) = \text{sgn}(\text{Re}(\langle x|U\tau\rangle)) \) can be used to create a phase state \( |p_U\rangle \) which has constant overlap with \( U |\tau\rangle \) with high probability for random \( U \). The state \( U^\dagger |p_U\rangle \) is already then a decent approximation for \( |\tau\rangle \).

There are two remaining techniques to improve upon this basic synthesis protocol. First, we use a novel distillation procedure based on the swap test (explained below) to take a polynomial
number of states generated in this manner, using unitaries $U_1, \ldots, U_m$, to create a single aggregated output state with greater overlap with the target state. Note that since the target state $|\tau\rangle$ is arbitrary, we do not have a means of measuring the overlap of an output state with $|\tau\rangle$ to boost the overlap as we did when the target state is a QMA witness. Secondly, we address the fact that the algorithm described above suffers from needing exponential space complexity; this is because specifying a Haar-random unitary on $n$ qubits requires $\exp(\Omega(n))$ space, and thus the oracle $f_{\tau}(U, x)$ needs to act on exponentially many input bits. We derandomize this construction, and show via the probabilistic method that there exists a single choice of unitaries $U_1, \ldots, U_m$ that works for all $n$-qubit states. This will reduce the space complexity of the algorithm to polynomial, although implementing the unitaries will still require exponential time.

**Theorem 1.3 (One Query State Synthesis - Informal)** There is a 1-query algorithm that uses polynomial space and exponential time that synthesizes a state $\rho$ such that $\text{Tr}\{\rho |\tau\rangle\langle\tau|\} \geq 1 - 1/q(n)$ for some polynomial $q$ and an arbitrary target state $|\tau\rangle$.

**The Swap Test Distillation Algorithm.** This procedure takes in a polynomial number of states each of which has at least a constant overlap with the target state and outputs a state whose overlap with the target is at least $1 - 1/\text{poly}$. In some sense, the Swap Test Distillation algorithm provides a way to take the “mean” of a collection of quantum samples where each state can be decomposed into a “signal” component and a “noise” component such that (1) the signal is some constant fraction of the mass and (2) the noise is roughly random. This may be useful in other contexts in quantum algorithms.

For formally, the algorithm requires that the sequence of input states $|\psi_1\rangle, \ldots, |\psi_m\rangle$ satisfies two properties. The first is that there is a constant $a$ such that $|\langle\psi_j|\tau\rangle|^2 \geq a$ for all $j$. (We also show that this condition can be relaxed so that the expected overlap of each input state with the target state is at least $a$, as long as the input states are independently generated.) The second condition is that for every pair of input states, their components orthogonal to $|\tau\rangle$ are close to orthogonal to each other:

$$|\langle\psi_j| (I - |\tau\rangle\langle\tau|) |\psi_i\rangle|^2 \leq \delta,$$

for $\delta$ exponentially small in $n$. Intuitively, one can imagine that if the $|\psi_i\rangle$ are generated independently, then the error vectors (the components perpendicular to $|\tau\rangle$) would be random and uncorrelated. We prove that under these two conditions, if the number of states is a sufficiently large polynomial, then the overlap of the resulting aggregated state with $|\tau\rangle$ is at least $1 - 1/\text{poly}$. The algorithm is based on the observation that if the swap test is applied to a pair of states which each have overlap at least $a$ with the target state, then conditioning on the swap test succeeding (measuring a 0 in the output bit), the state in each register has an overlap with the target state that is strictly larger than $a$. In each round of the algorithm, the surviving states are paired up and the swap test is applied to each pair. One state from every pair that succeeds the swap test advances to the next round.

**A two-query state synthesis algorithm with inverse exponential error.** While we do not know how to improve the error of the previous one-query algorithm beyond inverse polynomial, we show that there is a two-query state synthesis algorithm that achieves inverse exponential error.
Theorem 1.4 (Two Query State Synthesis - Informal) There is a 2-query algorithm that uses polynomial space and exponential time that with high probability synthesizes a state ρ such that \( \text{Tr}\{\rho |\tau\rangle\langle\tau|\} \geq 1 - 1/r(n) \) for some function \( r = \exp(n) \) and an arbitrary target state \( |\tau\rangle \).

Like with the one-query synthesis algorithm, we take advantage of the properties of Haar-random unitaries. Let \( |\tau\rangle \) denote the target state to be synthesized. Whereas the basic building block of the one-query algorithm described is to synthesize the phase state corresponding to \( U |\tau\rangle \) where \( U \) is a Haar-random unitary, the two-query algorithm attempts to directly synthesize the state \( U |\tau\rangle \), and then apply the inverse unitary \( U^\dagger \) to recover \( |\tau\rangle \). Since \( U \) is Haar-random, the distribution of \( U |\tau\rangle \) is that of a Haar-random state.

We then argue that with overwhelmingly high probability, a Haar-random state can be synthesized via two queries to a classical oracle. This relies on the observation that the amplitude profile of a Haar-random state concentrates extremely tightly around a fixed profile. By profile, we mean the list of absolute values of amplitudes of the state in sorted order. In other words, there exists a fixed, universal state \( |\theta\rangle = \sum_x \beta_x |x\rangle \) such that, with very high probability, a Haar-random state \( |\psi\rangle = \sum_x \alpha_x |x\rangle \) satisfies the following: there exists a permutation \( \sigma \) on the set of basis states \( |x\rangle \) such that the distance

\[
\left\| |\theta\rangle - \sum_x |\alpha_x \sigma(x)\rangle \right\| \tag{1.9}
\]

is exponentially small. To prove this, we utilize bounds from the theory of optimal transport that control the convergence of the Wasserstein distance (also known as the Earth Mover Distance) between a log-concave distribution and the empirical distribution resulting from sampling from the distribution.

Given this, the two-query algorithm to synthesize \( |\tau\rangle \) to exponential precision is clear: the algorithm first prepares the universal state \( |\theta\rangle \). It then queries the classical oracle to determine how to permute the basis states \( |x\rangle \) and what phase to apply to all the basis states. The algorithm applies the permutation and the phases in superposition. Finally, the algorithm queries the oracle again to uncompute the permutation/phase information.

Just as with the one-query algorithm, we also perform a derandomization step in order to make the query algorithm space-efficient (but not necessarily time-efficient). By expanding the dimension of the random unitary \( U \), we show that there exists (via the probabilistic method) a single unitary \( U^\star \) that maps every target state \( |\tau\rangle \) to one whose amplitude profile is exponentially close to the universal one.

Open Questions. We conclude with some open questions which are elaborated in greater detail in Section 7. Can the 1- and 2-query algorithms for general state synthesis be improved to polynomial time by using random Cliffords instead of Haar-random unitaries? Is there a 1-query algorithm for state synthesis that also achieves inverse exponential error? What is the power of a QMA decision oracle? In particular, what states can be synthesized with queries to a QMA oracle in superposition? Is there a weaker oracle class than PP that can achieve search-to-decision for QMA witnesses?

Preliminaries. Preliminaries and definitions necessary for the proofs are listed in Appendix A.
2 Search-to-decision for QMA problems

In the traditional search-to-decision paradigm, the goal is to create a witness $|\psi\rangle$ which could convince a verifier that indeed some string is in a particular QMA language. The creation of this witness should be carried out by a quantum machine running in polynomial time with access to a QMA oracle. There are multiple ways to relax this paradigm; here we consider using a PP oracle instead of a QMA oracle and show that there is a polynomial time quantum algorithm which makes only one PP oracle call and generates a solution to a QMA-complete problem.

Our algorithm proceeds from two observations:

1. Any phase state $|p_f\rangle = 2^{-n/2} \sum_{x \in \{0,1\}^n} (-1)^{f(x)} |x\rangle$ for which the function $f$ is computable in PP may be prepared by a single quantum query to a PP oracle.

2. Any state $|\tau\rangle$, after applying a random unitary $U$, looks like a phase state: in particular, with high probability over the choice of $U$, the state $U|\tau\rangle$ has constant overlap with some phase state.

Our results heavily rely on the preliminaries defined in Section A.1 and A.2.

2.1 One-query search-to-decision for QMA

We now consider the QMA search problem with respect to phase oracles. In general, the statement of the QMA search problem is to construct, given a verification circuit for some QMA language, and an input $\chi$ in the language, a state $|\psi_\chi\rangle$ that is accepted by the verification circuit with high probability. Rather than working with general verifiers, we will restrict to verifiers that measure the energy of a local Hamiltonian on the witness state up to inverse-polynomial precision. This restriction is almost without loss of generality, for two reasons. First, the local Hamiltonian problem with this precision is QMA-complete, so any QMA language has a verifier of this form. And secondly, the reduction to local Hamiltonian can be performed so that every low-energy state is very close to an accepting witness $|\psi\rangle$ for the original verifier. More precisely, given a general QMA verification circuit $V$, we can apply the padding trick of Nirkhe, Vazirani and Yuen [NVY18] to generate a local Hamiltonian instance $H$ such that any ground-state $\rho$ of $H$, $\|\rho - \sigma \otimes \Phi\| \leq \delta$ where $\sigma$ is an accepting witness of $V$ and $\Phi$ is a fixed state independent of the instance. The size of the Hamiltonian instance $H$ scales as $\text{poly}(1/\delta)$ and therefore the approximation can be chosen as any inverse polynomial function of the system size.

Assume the input to the problem is an instance $\chi = (H, a, b)$ of the Local Hamiltonian problem with Hamiltonian $H$ on $n$ qubits and two thresholds $a < b$ such that $b - a = 1/\text{poly}(n)$. Moreover, we assume that $\chi$ is a YES instance, so the minimum eigenvalue of $H$ is at most $a$: $\lambda_{\min}(H) \leq a$. The goal is to construct a state $|\phi\rangle$ such that

$$\langle \phi | H | \phi \rangle \leq \frac{a + b}{2}.$$  \hfill (2.1)

While it would be ideal to construct a state for which the energy is at most $a$ (since one exists), this may drastically increase the computational complexity of the function $f : \{0,1\}^n \rightarrow \{0,1\}$ defining the oracle. Instead, due to the promise gap in the problem, it suffices to construct a

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4The improvement over the algorithm of Aaronson [Aar16] is in the number of oracle queries.
witness state which proves that the Hamiltonian has a state with energy at most \( < b \). A state \( |\phi\rangle \) satisfying eq. (2.1) is a proof that \( \chi \) is a yes instance. We now prove the formal version of Theorem 1.1.

**Theorem 2.1 (QMA-search to PP-decision reduction)** There exists a probabilistic polynomial time quantum algorithm with access to a single PP phase oracle query that, given as input an instance \((H, a, b)\) of the local Hamiltonian problem on \( n \) qubits, either aborts or outputs a witness \( |\phi\rangle \) with \( \langle \phi | H | \phi \rangle \leq (a + b)/2 \) for \( b - a = 1/poly(n) \). The algorithm will succeed in outputting a witness (i.e. not abort) with probability

\[
\geq 1/1024.
\]

**Remark** In fact, we shall see that the algorithm achieves something stronger: if the algorithm does not abort, then the output state is almost entirely supported on states of energy less than \( a + (b - a)/4 + \epsilon \), where \( \epsilon = 1/poly(n) \) is a precision parameter much smaller than \( b - a \). This is performed by using phase estimation to “check” the outcome of the query algorithm by measuring the energy.

At this point, it is useful to remember that in general, the notion of a QMA witness is defined only with reference to a specific verifier. The guarantee we achieve ensures that the “standard” verifier, which measures the energy of the local Hamiltonian \( H \), has a high chance of accepting the given state. If one is willing to use a more sophisticated verifier, e.g. a verifier that performs the Marriott-Watrous amplification procedure [MW04], a witness of considerably worse quality could still be acceptable. Our theorem also sidesteps the issue of unique witnesses: we only guarantee that the energy of our state is low, not that it is the unique such state.

One can easily boost probability that our algorithm does not abort to \( 1 - \exp(-n) \) by repeating the construction in parallel with independent randomness and selecting any witness which did not cause the algorithm to abort. Furthermore, from the design of the algorithm, one can merge the oracle queries into a single larger PP query\(^6\), so the query complexity does not increase.

**Proof:** Assume, without loss of generality, that problem is stated for a normalized Hamiltonian: \( 0 \leq H \leq 1 \). We will use \([C]\) to denote the classical description of the quantum circuit \( C \). Likewise \( \chi = (H, a, b) \) describes an encoding of the problem.

**Algorithm.** The following quantum circuit describes the algorithm:

\[
\begin{array}{c}
[\chi] \\
Samp \\
|0\rangle \otimes n \\
H \otimes n \\
O_f \\
C \dagger \\
\text{Phase Estimation} \\
\end{array}
\]

\[^5\text{We will later argue that this probability can be amplified through a variation of parallel repetition to improve to any function } 1 - \exp(-n).\]

\[^6\text{One way to see that the merged oracle is also definable in PP is through the connection } PP = \text{PostBQP}. \text{ The merged oracle can be seen as the logical exclusive-or (XOR) of multiple PP functions, and it is easy to create a new PostBQP function equal to the logical XOR of multiple PostBQP functions.}\]
Here, the collection of random coins $$$ are $O(\text{poly}(n))$ bits of uniform randomness and the gate Samp use the input randomness to sample the descriptions $|C\rangle$ and $|D\rangle$ of two independent random Clifford unitaries described as circuits. $H^{\otimes n}$ is the tensor-product of the Hadamard gate. The controlled gate $C^\dagger$ denotes the application of the inverse circuit $C^\dagger$ according to the classical description $|C\rangle$. The oracle gate $O_f$ applies a phase oracle

$$
|\chi\rangle, C, D, x \mapsto (-1)^{f(|\chi\rangle, C, D, x)}|\chi\rangle, C, D, x
$$

in superposition for a function $f$ specified in eq. (2.3). The phase estimation unitary applies the energy estimation algorithm algorithm of [Ral21] which writes the energy of the third register state in superposition for a function $f$ (equivalently, over the random choice of $|C\rangle$ and $|D\rangle$). To show that the algorithm succeeds with constant probability over the random coins, we must show the following.

**Correctness** Let $|\tau\rangle = (1 - H)^pD|0^n\rangle$ be an unnormalized state, where $p$ is a parameter that will be chosen later, satisfying $p = \Omega(n/(b - a))$. Let $|\overline{\tau}\rangle = |\tau\rangle/\||\tau\rangle\|$ be the normalization of this state. We will choose our oracle function $f$ such that the state after the oracle is applied yields a phase-state approximation to $C|\overline{\tau}\rangle$ for the sampled random Clifford unitary $C$. Specifically, we define the oracle function $f$ as

$$
f(H, C, D, x) \overset{\text{def}}{=} \text{sgn} \left( \text{Re} \left( \langle x|C(1 - H)^pD|0^n\rangle \right) \right).
$$

(2.3)

For a fixed $H, C, D$, we write $f_{H,C,D}(x) = f(H, C, D, x)$, and denote the corresponding phase state by $|p_{f_{H,C,D}}\rangle$. Observe that the state of the algorithm immediately after the call to $O_f$ is proportional to

$$
|\chi\rangle \otimes \left( \sum_{\text{$$$}} C(\text{$$$}), D(\text{$$$}) \otimes |p_{f_{H,C,D}}\rangle \otimes |0\rangle \otimes O(\log(1/(b-a)))\right).
$$

(2.4)

At this point, we may imagine that the register containing the random coins $$$ has been measured. To show that the algorithm succeeds with constant probability over the random coins (equivalently, over the random choice of $C$ and $D$), we must show the following:

1. The state $|\overline{\tau}\rangle$ has almost all its mass in the low-energy subspace, with respect to $H$.
2. For a random choice of $C$ and $D$, $C^\dagger|p_{f_{H,C,D}}\rangle$ is close to $|\overline{\tau}\rangle$.
3. That the phase estimation algorithm accepts $C^\dagger|p_{f_{H,C,D}}\rangle$ with sufficiently high probability, and the post-measurement state upon a successful measurement has low energy with respect to $H$. The post-measurement state is the state $|\phi\rangle$ in the theorem statement.

We formulate Item 1 precisely as a separate lemma:

**Lemma 2.2** Let $\Pi_<$ be the projector onto the eigenspaces of $H$ with eigenvalue at most $a + (b - a)/4$ (see eq. (2.18) for formal definition). Then, with probability $\geq 1/2$ over the choice of $D$, it holds that $\langle \overline{\tau}|\Pi_<|\overline{\tau}\rangle \geq 1 - (b - a)/2$.

---

7This can be done, for example, with the algorithm of van den Berg [vdB20].
This lemma is proven directly after the end of this proof.

To show Item 2, we will use Lemma A.5 which we state here for convenience:

**Lemma A.5 (Random states have good overlap)** Let \(|\tau\rangle \in (\mathbb{C}^2)^n\) be a unit vector. Let \(C\) be any 2-design (e.g. \(C = \text{Cliff}\)). Sample a random \(C \in C\) and set \(|\psi\rangle = C |\tau\rangle\). Then with constant probability, it has good overlap with the phase state defined by the function \(f(x) = \text{sgn}(\text{Re}(\langle x |\psi\rangle))\). Formally for \(0 \leq \gamma \leq \frac{1}{4}\),

\[
\Pr_{C \in \mathbb{C}} \left( |\langle \psi | p_f \rangle|^2 \geq \gamma \right) \geq \frac{1}{2} - 2\gamma. \tag{A.21}
\]

We prove Lemma A.5 in the Appendix. Let \(\gamma \in (0, 1)\) be a constant to be chosen later. Then, by Lemma A.5 we have that

\[
\Pr_{C \in \text{Cliff}} \left( |\langle p_{f\mu,C,D} | C |\bar{\tau}\rangle|^2 \geq \gamma \right) \geq \frac{1}{2} - 2\gamma. \tag{2.5}
\]

Let us fix a “good” choice of \(C\), such that the event in eq. (2.5) occurs, and write

\[
|\psi\rangle = C^T | p_{f\mu,C,D} \rangle = a |\bar{\tau}\rangle + \beta |\bar{\tau}^\perp\rangle, \tag{2.6}
\]

where \(|a|^2 \geq \gamma\). Combining eq. (2.5) with Lemma 2.2 we obtain that \(|\psi\rangle\) has high overlap with \(\Pi_\leq\).

\[
\eta \overset{\text{def}}{=} \langle \psi | \Pi_\leq |\psi\rangle \tag{2.7}
\]

\[
= |a|^2 \langle \bar{\tau} | \Pi_\leq |\bar{\tau}\rangle + |\beta|^2 \langle \bar{\tau}^\perp | \Pi_\leq |\bar{\tau}^\perp\rangle + a^* \beta \langle \bar{\tau} | \Pi_\leq |\bar{\tau}^\perp\rangle + a \beta^* \langle \bar{\tau}^\perp | \Pi_\leq |\bar{\tau}\rangle \tag{2.8}
\]

\[
\geq |a|^2 \left( 1 - \frac{b - a}{2} \right) - 2|a\beta| \sqrt{b - a} \tag{2.9}
\]

\[
\geq \gamma \left( 1 - \frac{b - a}{2} \right) - 2\sqrt{\gamma(1 - \gamma)(b - a)}. \tag{2.10}
\]

Now in order to prove Item 3, let \(\epsilon = \log \left( \frac{1}{100(b - a)} \right)\) and \(\delta = \frac{1}{(b - a)100}\). By Lemma A.7, the energy estimation succeeds with probability at least \(\eta - \delta\), and the post-measurement state has overlap \(1 - 2\delta/\eta\) with the subspace of energy at most \(a + (b - a)/4 + \eta\). A straightforward calculation shows that this implies that the post-measurement state has expected energy at most \(a + (b - a)/2\), as desired.

It remains to set the parameter \(\gamma\) so that the overall probability of not aborting is at least a constant, and so that \(\eta\) is at least a constant for good \(C,D\). We choose \(\gamma = 1/8\), yielding \(\eta \geq 1/16\) and \(\eta - \delta \geq 1/32\) for all sufficiently large \(n\) such that \((b - a)\) is sufficiently small. This yields a probability of not aborting

\[
\Pr[\text{not abort}] = \sum_{C,D} \Pr[C] \cdot \Pr[D] \cdot \Pr[\text{not abort} | C, D] \tag{2.11}
\]

\[
\geq \sum_{C,D \text{ good}} \Pr[C] \cdot \Pr[D] \cdot \Pr[\text{not abort} | C, D] \tag{2.12}
\]

\[
\geq \left( \frac{1}{2} - 2\gamma \right) \cdot \frac{1}{8} \cdot (\eta - \delta) \tag{2.13}
\]

\[
\geq \frac{1}{1024}. \tag{2.14}
\]
(We note that this bound is extremely loose; our only goal here is to show a some constant lower bound on the non-abort probability as we can amplify with parallel repetition.)

**Complexity of** $O_f$ **To show that the function** $f$ **can be calculated in PP, it suffices to give a counting algorithm for calculating** $f(H, C, x)$. Let us assume that $H = \sum_{i=1}^{m} H_i$ **where each** $H_i$ **is a local Hamiltonian term and** $C = g_1 \cdots g_n$ **where each** $g_j$ **is a 2-qubit Clifford gate. Expanding the Feynman path integral gives**

$$\langle x | C (1 - H)^n C^\dagger | 0^n \rangle$$

$$= \sum_{i_1, \ldots, i_p \in [m]} \langle x | g_1 \cdots g_1 (1 - H_i) \cdots (1 - H_{i_p}) g_1^\dagger \cdots g_i^\dagger | 0^n \rangle$$

$$\leq \sum_{i_1, \ldots, i_p \in [m]} \sum_{y_1, \ldots, y_{2t+1} \in [2^n]} \langle x | g_1 | y_1 \rangle \langle y_1 | \cdots | y_{2t+p-1} \rangle \langle y_{2t+p-1} | g_i^\dagger | 0^n \rangle$$

Note that we only need to calculate the sign of the real component of eq. (2.17). Each quantity of the form $\langle y | g_j | y' \rangle$ or $\langle y | (1 - H_{i_j}) | y' \rangle$ is known to exact precision (in the first case since $g_j$ is a Clifford gate, and in the second since it is an input to the problem). This also implies that each element of the sum can be efficiently calculated as $\langle y | g_j | y' \rangle$ and $\langle y | (1 - H_{i_j}) | y' \rangle$ are efficiently calculable. Since its length is at most poly($n$) bits, the aforementioned computation can be calculated by a #P or PP oracle since it is a counting problem involving terms of size $\exp(n)$. □

**Proof of Lemma 2.2** To prove that $\langle \bar{\tau} | \Pi_\leq | \bar{\tau} \rangle \leq 1 - (a + b)/2$ occurs with constant probability, let us first introduce some notation. Let $\Delta = b - a$, and $m = a + \Delta/4$. Let $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_2^n$ be a sorted list of the eigenvalues of $H$ with corresponding eigenvectors $|\lambda_1\rangle, |\lambda_2\rangle, \ldots, |\lambda_2^n\rangle$ and let $j$ be the first $j$ such that $\lambda_j \geq m \overset{\text{def}}{=} a + \Delta/4$. Then, the projector $\Pi_\leq$ from the statement of the lemma is given by

$$\Pi_\leq \overset{\text{def}}{=} \sum_{j=1}^{j-1} |\lambda_j\rangle \langle \lambda_j|.$$  

(2.18)

We define a complementary projector $\Pi_\geq = I - \Pi_\leq$ as the projector onto the “high”-energy subspace.

Using these projectors, we now write the (unnormalized) state $|\bar{\tau}\rangle$ as a sum of a “low-energy” part and a “high-energy” part:

$$|\bar{\tau}\rangle = |\tau_\leq\rangle + |\tau_\geq\rangle \text{ where } |\tau_\leq\rangle \overset{\text{def}}{=} \Pi_\leq |\tau\rangle \text{ and } |\tau_\geq\rangle \overset{\text{def}}{=} \Pi_\geq |\tau\rangle.$$  

(2.19)

Our goal is to show that

$$q \overset{\text{def}}{=} \frac{\langle \tau_\leq | \tau_\leq \rangle}{\langle \tau_\leq | \tau_\leq \rangle + \langle \tau_\geq | \tau_\geq \rangle} \geq 1 - \Delta/2$$

(2.20)

This event will always occur when

$$\| |\tau_\geq\| \leq \frac{\Delta}{2}.$$  

(2.21)
Now we show that this event occurs with probability $\geq \frac{1}{8}$. It follows from Fact A.3 that

$$\Pr_D \left( \| \Pi_- D | 0^n \rangle \|^2 \geq \frac{1}{2 \cdot 2^n} \right) \geq \frac{1}{8}. \quad (2.22)$$

To see this, apply Fact A.3 with the unitary design $C$ in Fact A.3 taken to be $U \cdot D$, where $U$ is a unitary such that $H = U \cdot \text{diag}(\lambda_1, \lambda_2, \ldots) \cdot U^\dagger$, and $x = 0^n$, and $\theta = 1/2$. This yields a lower bound of $1/2 \cdot 2^n$ on $\| \langle \lambda_1 \rangle D | 0^n \rangle \|_2^2$ with probability at least $1/4$. Therefore, since $\Pi_- \geq | \lambda_1 \rangle \langle \lambda_1 |$, eq. (2.22) follows. Henceforth, we will condition on this event. Since $\Pi_- \commutes (1 - H)^p$,

$$\| \tau_- \|_2^2 = \| \Pi_- (1 - H)^p D | 0^n \rangle \|_2^2 \geq (1 - \lambda_1)^2p \cdot \frac{1}{2 \cdot 2^n}. \quad (2.23)$$

On the other hand,

$$\| \tau_+ \|_2^2 = \| \Pi_+ (1 - H)^p D | 0^n \rangle \|_2^2 \leq (1 - m)^2p \quad (2.24)$$

since $\Pi_+$ projects onto the low-energy subspace of $(1 - H)^p$. Therefore, in order to satisfy eq. (2.21), it suffices to pick $p$ such that

$$(1 - m)^2p \leq \frac{\Lambda}{2} \cdot (1 - \lambda_1)^2p \cdot \frac{1}{2 \cdot 2^n}. \quad (2.25)$$

Since $\lambda_1 \leq a$,

$$\frac{1 - m}{1 - \lambda_1} \leq \frac{1 - m}{1 - a} \leq 1 - (m - a) = 1 - \Delta/4. \quad (2.26)$$

Therefore our threshold for $p$ simplifies to

$$\left( \frac{1 - \Delta}{4} \right)^{2p} \leq \frac{\Lambda}{2 \cdot 2^n} \quad (2.27)$$

which is satisfied for a choice of

$$p = \Omega \left( \frac{n \log \frac{1}{\Delta}}{\Delta} \right). \quad (2.28)$$

(To see this, observe that the left-hand side of eq. (2.27) can be made less than $1/2$ with $p = \Omega(\Delta^{-1})$. The bound of $\Delta/(2 \cdot 2^n)$ can be achieved by multiplying $p$ by $\Omega(n \log(1/\Delta))$. Therefore, with probability $\geq \frac{1}{8}$, we have that $\langle \tau | \Pi_- | \tau \rangle \leq 1 - \Delta/2 = 1 - (b - a)/2$.)

**Difficulty in improving the oracle complexity.** In the previous section, we detail a proof that a witness to any QMA problem can be constructed with access to a single PP oracle query. This does not satisfy our desire to understand search-to-decision for QMA since it is widely suspected that $\text{QMA} \neq \text{PP}$. We also note that without any additional assumptions, we cannot simplify that search-to-decision algorithm (Theorem 2.1) to utilize a QMA oracle. Consider the class of local Hamiltonians problems for which the gap between the completeness ($c$) and soundness ($s$) thresholds is inverse exponentially small, i.e. $c - s = 2^{-\text{poly}(n)}$ but we are promised that the
satisfactory gap of $H$ is at least $1/poly(n)$. The complexity of deciding this class of problems (called PGQMA) is PP-complete by a result of Deshpande, Gorshkov, and Fefferman [DGJF20]. We refer to their work for more details and precise definitions. We note that there is a simple modification\(^8\) of Theorem 2.1 that can be applied to this class of PP-complete Hamiltonians which provides a search-to-decision algorithm. Therefore, we cannot reduce the complexity of the oracle from PP without critically assuming that we are only interested in finding witnesses for a promise gap precision of $1/poly(n)$.

### 2.2 Search-to-decision for QMA\(_{\text{exp}}\)

Instead, we note that our proof can be adjusted slightly to construct a search-to-decision reduction for the class QMA\(_{\text{exp}}\) which is the class of quantum Merlin-Arthur promise problems for which the gap between the completeness ($c$) and soundness ($s$) thresholds is inverse exponentially small, i.e. $c - s = 2^{-poly(n)}$ but there is no promise on the spectral gap of the Hamiltonian. The canonical complete problem for this class is, unsurprisingly\(^9\), the local Hamiltonian problem for a promise gap of $2^{-poly(n)}$. An earlier work of Fefferman and Lin [FL16] showed that QMA\(_{\text{exp}} = \text{PSPACE}\).

**Theorem 2.3 ([FL16])** The problem of deciding, for a local Hamiltonian $H$ on $n$ qubits, if $\lambda_{\text{min}}(H) \leq a$ or $> b$ with a promise gap of $b - a = 2^{-poly(n)}$ is PSPACE-complete.

Using this interesting connection between complexity classes, we can actually create a 1 query search-to-decision algorithm for QMA\(_{\text{exp}}\).

**Theorem 2.4** Pick a constant $0 < \gamma < 1/4$. There exists a probabilistic polynomial time quantum algorithm with access to a single QMA\(_{\text{exp}}\) phase oracle query that given an instance $(H, a, b)$ of the local Hamiltonian problem on $n$ qubits for $b - a = 1/\text{exp}(n)$, outputs a state $|\psi\rangle$ with the following property. With probability $\gamma/8$, there exists a state $|\bar{\tau}\rangle$ such that $\langle \bar{\tau}|H|\bar{\tau}\rangle \leq (a + b)/2$ and $|\langle \bar{\tau}|\psi\rangle|^2 \geq 1/2 - 2\gamma$.

**Proof:** The proof follows almost identically to that of Theorem 2.1 except for two critical variations. First, we remove the phase estimation step from the procedure and use the quantum register as the output without any possibility of aborting. This is because running phase estimation to the $2^{-poly(n)}$ precision necessary for determining if the quantum register is a witness would require an exponentially long runtime [AA17]. By eschewing the phase estimation step, the protocol will run in polynomial time but at the cost that it cannot detect if it has produced a witness. This is not surprising because unless QMA = PSPACE, the quantum witness should not be verifiable in polynomial time and, in effect, the phase estimation routine is verifying if the witness is valid.

And second, we need to prove that the complexity of the oracle function $f$ is now solvable in PSPACE (instead of PP). The function $f$ is the same as in the previous proof (see eq. (2.3)). But now

\[^{8}\text{More specifically, the previous algorithm ignores the differences between spectral and promise gap and conflates the two notions. We notice that whenever the spectral gap is } 1/poly(n), (1 - H)^p \text{ is still a "good" approximate projector onto the ground-space and for a choice of } p = poly(n), \text{ it projects onto the ground-space up to exponentially small error. One can derive that for PGQMA local Hamiltonians, the equivalent lower bound on } p \text{ as that in eq. (2.25) is }
\]

\[^{9}\text{This follows directly from Kitaev' s proof [KKR06] of QMA-completeness for local Hamiltonians.}\]
the exponent of \((1 - H)\) is \(p = \Omega(n / (b - a)) = 2^{\text{poly}(n)}\). Therefore, the Feynman path integral used in eq. \((2.17)\) is over an exponential number of variables. To solve this issue, we simply rewrite the Feynman path integral to not include \((1 - H)^p\).

\[
\langle x | C(1 - H)^p C^\dagger | 0^p \rangle = \sum_{y_1, \ldots, y_{2^p} \in \{0, 1\}^p} \langle x | y_1 \rangle \ldots \langle x | (1 - H)^p | y_{t+1} \rangle \ldots \langle x | y_{2^p} \rangle S_{y_1}^\dagger | 0^p \rangle. \quad (2.30)
\]

We now only need to show that \(\langle y_t | (1 - H)^p | y_{t+1} \rangle\) is computable in \(\text{PSPACE}\). We proceed by induction. Notice

\[
\langle y_t | (1 - H) | y_{t+1} \rangle = \mathbb{E}_{z \in \{0, 1\}^n} \langle y_t | (1 - H_z) | y_{t+1} \rangle \quad (2.31)
\]

which is easily computable in polynomial space. For the induction step, notice

\[
\langle y_t | (1 - H)^{2k} | y_{t+1} \rangle = \sum_{z \in \{0, 1\}^n} \langle y_t | (1 - H)^k | z \rangle \cdot \langle z | (1 - H)^k | y_{t+1} \rangle. \quad (2.32)
\]

By reusing the space for both parts of the sub-computation, the computation for exponent \(2k\) only uses \(\text{poly}(n)\) additive additional step over the computation for exponent \(k\). Since, we only need to calculate the result for \(p = 2^{\text{poly}(n)}\), it follows that \(\langle y_t | (1 - H)^p | y_{t+1} \rangle\) is computable in \(\text{PSPACE}\) and the overall function \(f\) is computable in \(\text{PSPACE}\). Since \(\text{QMA}_{\text{exp}} = \text{PSPACE}\), the proof is complete. \(\square\)

### 2.3 Search-to-decision for QCMA with one oracle query

With a completely different procedure, we can show a one oracle query search-to-decision procedure for QCMA. More specifically, we show that a polynomial time quantum algorithm can produce a classical witness for any QCMA problem with a single query. Note that since the witness is classical, as intuition suggests, one can also show that a polynomial time randomized classical algorithm can produce, with high probability, a classical witness for any QCMA problem with \(\text{poly}(n)\) classical queries to a QCMA oracle based on the binary-search algorithm\(^{10}\). We show that a variation of the Bernstein-Vazirani algorithm \([BV97]\) allows us to reduce the query complexity to a single query which succeeds with probability \(\Omega(m^{-1})\), where \(m\) is the size of the witness. This is particularly pertinent because if QCMA = QMA, then there exists a single query search-to-decision reduction for QMA, albeit with sub-constant probability.

Recall the Bernstein-Vazirani algorithm \([BV97]\) for learning a hidden string \(d \in \{0, 1\}^m\) given quantum access to a specific \(m\)-bit oracle. If the oracle \(f : \{0, 1\}^m \rightarrow \{0, 1\}\) is defined by \(f(x) = x^\top d\) (over \(\mathbb{F}_2\)), then

\[
H^{\otimes m} O_f H^{\otimes m} | 0^m \rangle = H^{\otimes m} O_f \frac{1}{\sqrt{2^m}} \sum_x | x \rangle
\]

\[
= H^{\otimes m} \frac{1}{\sqrt{2^m}} \sum_x (-1)^{x^\top d} | x \rangle \quad (2.34)
\]

\[
= \frac{1}{2^m} \sum_{x, y} (-1)^{x^\top (y + d)} | y \rangle \quad (2.35)
\]

\[
= | d \rangle. \quad (2.36)
\]

\(^{10}\)The reduction involves a randomized mapping the QCMA instance to a UQCMA instance and then applying binary-search for the witness to the UQCMA problem.
Therefore, a polynomial time quantum algorithm with a single oracle query can produce a $m = \text{poly}(n)$ output string. To show that QCMA search has a single query algorithm, it suffices to show that the function $f(x) = x^T d$ is QCMA-computable when $d$ is the classical QCMA witness to the instance $\chi$.

Let us notice that the witness $d$ needs to be made explicit if we are to define such a function $f$. In particular, $f(x)$ should only depend on $x$ and $\chi$. For example, consider defining $f(x) = 1$ iff there exists a witness $d$ such that $x^T d = 1$. Since there can be many witnesses $d$, it is even possible that $f = 1$ everywhere. One idea is to define the description $d$ as that of the lexicographically first witness. However, calculating the lexicographically first witness is not known to be contained in QCMA and the best upper bound on the complexity of calculating $d$ is $\text{P}^{\text{QCMA}}$. This gives us one search-to-decision result.

**Theorem 2.5** Consider any QCMA problem optimizing over witnesses of length $m$. There exists a probabilistic polynomial time quantum algorithm with access to a single $\text{P}^{\text{QCMA}}$ phase oracle that outputs a satisfying witness $d \in \{0, 1\}^m$ with probability 1.

In order to consider an oracle of only QCMA complexity, however, we will need to isolate a specific witness $d$ through a different manner. To achieve this we recall the randomized reduction from QCMA to UQCMA formalized in [ABOBS08]. Here UQCMA is the class of QCMA problems for which there holds an additional promise that in the case of yes instances, there exists a unique accepting classical witness $d \in \{0, 1\}^{\text{poly}(n)}$.

**Theorem 2.6** ([ABOBS08, Corollary 40]) $\text{UQCMA} \subseteq \text{RP}^{\text{QCMA}}$.

When presented with a UQCMA instance, the question of $f(x) = 1$ iff there exists a witness with description $d$ such that $x^T d = 1$ is equivalent to $f(x) = x^T d_0$ where $d_0$ is the unique satisfying witness.

The reduction from QCMA to UQCMA follows a standard technique originating from the Valiant-Vazirani theorem and can be used to reduce NP and MA to their unique counterparts. By adding additional constraints to the QCMA problem, we can reduce the number of accepting witnesses until a unique witness remains. More formally, we can pose a constraint of the form $Ad = 0$ where $A \in F_2^{k \times m}$ is a uniformly random matrix and arithmetic is over the field $F_2$. Each row of $A$ is an additional constraint which roughly halves the number of accepting witnesses. Therefore, is known that when $2^k$ is approximately the number of accepting witnesses, with high probability there will only be one witness which satisfies the original QCMA problem as well as the constraint $Ad = 0$. A critical difficulty in this approach is that the verifier does know how many accepting witnesses the original QCMA instance has; they need this to select an appropriate $k$.

What we instead do is uniformly randomly guess a choice of $k \in \{1, \ldots, n\}$. Notice that if the verifier were to make a guess for $k$ that is too large, then with high probability, the new instance will be unsatisfied. On the other hand, if the guess is too small, then the new instance will have many solutions and the algorithm will not necessarily output a valid witness. However, note that whatever purported witness results from applying the Bernstein-Vazirani algorithm [BV97] to the quantum oracle (eq. (2.33)) and then measuring the register, one can easily verify the validity of said witness.

Therefore, we have all the ingredients for a one-query search-to-decision algorithm for QCMA. Let $V$ be the original instance and $m$ the witness length. Namely, one chooses a uniformly random
\( k \in \{1, \ldots, n\} \) and then a uniformly random matrix \( A \in \mathbb{F}_2^{k \times m} \). Let \( V' \) be the instance \( V \) appended with the additional test that \( Ad = 0 \) for witness \( d \). The oracle function \( f(x) \) is defined as

\[
f(x) = 1 \iff \exists \text{ witness } d \text{ for } V' \text{ and } x^\top d = 1. \tag{2.37}
\]

Then, the algorithm computes the left-hand side of eq. (2.33) and measures in the standard basis to obtain a witness \( d \). Then, the algorithm checks that \( d \) is a solution to \( V \) and accordingly answers with \( d \) or aborts.

**Theorem 2.7** Consider any QCMA problem optimizing over witnesses of length \( m \). There exists a probabilistic polynomial time quantum algorithm with access to a single QCMA phase oracle query that either aborts or outputs a satisfying witness \( d \in \{0, 1\}^m \). The algorithm will output a witness with probability \( \geq \Omega(1/m) \).

Likewise there is a probabilistic polynomial time quantum algorithm with access to a single NP (MA, respectively) phase oracle query that either aborts or outputs a satisfying witness \( d \in \{0, 1\}^m \). The algorithm will output a witness with probability \( \geq \Omega(1/m) \).

**Remarks.** One could also perform a similar classical query algorithm to generate a witness for QCMA using the search-to-decision paradigm for UNP, UMA, UQCMA of learning the witness bit-by-bit with \( O(m) \) queries. However, to extend this algorithm to NP, MA, QCMA, this protocol requires an expected \( O(m^2) \) classical queries due to the guessing required to apply the reduction from QCMA to UQCMA.

Secondly, one can improve the success probability of this algorithm to any \( 1 - 2^{-t} \), by running the algorithm independently in parallel \( k = O(n + t) \) times. Ideally, one would like to be able to merge the oracle queries into a singular, albeit larger, oracle query. This would involve defining a function

\[
f(x_1, \ldots, x_k) = \prod_{i=1}^{k} \left[ \exists \text{ witness } d_i \text{ for } V_i \text{ and } x_i^\top d_i = 1 \right] \tag{2.38}
\]

where \( V_1, \ldots, V_k \) are the \( k \) independent instances that the reduction outputs. However, it is not necessarily the case that \( f \) is a QCMA decidable function since it is a product of QCMA problems. Instead, the complexity upper-bound we can place on \( f \) is at most \( P^{QCMA} \). However, this results in an algorithm strictly worse than Theorem 2.5 Thus, without increasing the complexity of the oracle, we do not know of a method of probability amplification without multiple queries.

**Corollary 2.8** Theorem 2.7 can be amplified to a success probability of \( 1 - 2^{-t} \) with \( O(n + t) \) parallel queries to a QCMA phase oracle.

### 3 Impossibility of search-to-decision for QMA in oracle model

In this section we show that efficient search-to-decision reductions for QMA do not exist in general in the oracle setting, perhaps providing some evidence that QMA does not have efficient search-to-decision reductions “in the real world.” More precisely, we show that there exists a quantum oracle \( O \) relative to which all polynomial-time quantum query algorithms fail to be a good search-to-decision reduction for \( QMA^O \), the relativization of QMA. Equivalently, \( QMA^O \)-search problems are...
not reducible to QMA$^O$-decision problems. We contrast this impossibility result with the fact that complexity classes like NP, MA and QCMA all have efficient search-to-decision reductions, relative to any oracle (i.e. the reductions relativize)! For example, it is not hard to verify that the search-to-decision procedure for QCMA described in Section 2.3 relativizes. Thus, Theorem 3.1 illustrates that, at least in the relativized setting, changing the proof model from classical to quantum nullifies the possibility of search-to-decision reductions.

We first define QMA$^O$ by way of a complete problem. Fix a small constant $\delta < \frac{1}{100}$. Define an $O$-verifier circuit $C$ to be a quantum circuit that can make queries to $O$ (which can be viewed as applying a unitary gate for $O$), and also takes as input a quantum proof state $|\phi\rangle$, as well as some ancilla qubits set to $|0\rangle$. Define the promise problem $O$-QCIRCUITSAT whose YES instances consist of $O$-verifier circuits $C$ for which there is a quantum proof state $|\phi\rangle$ such that $C(|\phi\rangle)$ accepts with probability at least $1 - \delta$, and the NO instances are those circuits such that on all quantum witness states, $C$ accepts with probability at most $\delta$. Without access to $O$, this is simply the canonical QMA-complete problem QCIRCUITSAT. The class QMA$^O$ is then the set of all promise decision problems that are polynomial-time reducible to $O$-QCIRCUITSAT.

Now we formalize the notion of search-to-decision reductions for QMA$^O$. Consider quantum circuits that can make queries in superposition to both the quantum oracle $O$ and a classical oracle $A^O$ that decides the promise problem $O$-QCIRCUITSAT as well as the controlled-versions of these oracles. Alternatively, we can consider a standard quantum circuit with special oracle “gates” implementing $O$ and $A^O$ unitary transformations. Specifically, the oracle $A^O$ implements the unitary transformation

$$|C\rangle|b\rangle \mapsto |C\rangle|b \oplus A^O(C)\rangle$$

(3.1)

where $C$ is supposed to be a description of an $O$-oracle circuit, $b \in \{0, 1\}$, $A^O(C) \in \{0, 1\}$ with $A^O(C) = 1$ if $C$ is a YES instance of $O$-QCIRCUITSAT, $A^O(C) = 0$ if $C$ is a NO instance, and otherwise $A^O(C)$ is defined arbitrarily. This is sufficiently general as we previously remarked that all QMA$^O$ problems can be expressed as $O$-oracle circuits $C$.

To recap, let $S$ be a quantum circuit describing such a search-to-decision reduction. This means that $S$ consists of standard 2-qubit unitary gates, gates for the oracle $O$ as well as gates for implementing $A^O$ as described previously. The input to $S$ is the description of a $O$-oracle circuit $C$ which is, again, the description of a collection of 2-qubit unitary gates and gates for the oracle $O$. The output of $S$ is a quantum state. In the following analysis, it will be useful to separate the description of $S$ from the oracles $O$ and $A^O$ being used in them. In our analysis, we will consider the circuit $S$ with access to different oracles $O'$ and $A'O'$. To visualize this, it may be helpful to think of $S$ as a circuit with “holes” for $O$ and $A^O$ gates that could be later filled in and swapped out with different oracle gates.

We then say that such a quantum circuit $S$ is an $\epsilon$-good search-to-decision reduction for the problem $O$-QCIRCUITSAT – or, alternatively, $\epsilon$-solves the search version of $O$-QCIRCUITSAT – if when given a YES instance $C$ of $O$-QCIRCUITSAT, it outputs a state that is accepted by $C$ with probability at least $1 - \delta - \epsilon$.

We now state the main result of this section (the technical version of Theorem 1.2).

**Theorem 3.1** There exists a constant $\epsilon > 0$ and a quantum oracle $O$ relative to which there is no poly$(n)$-sized $\epsilon$-good search-to-decision reduction for $O$-QCIRCUITSAT

---

11Technically, we should be considering an infinite family of oracles $O$ and $A^O$ where each oracle is parameterized
The quantum oracle we use to prove Theorem 3.1 is a reflection unitary $I - 2 |\psi\rangle\langle\psi|$ where $|\psi\rangle$ is some $n$-qubit state\textsuperscript{12}. The existence of a separating oracle $O$ is established via the probabilistic method; we show that by picking $|\psi\rangle$ from the Haar measure, with high probability all polynomial-size search-to-decision reduction algorithms fail to solve $O$-$\text{QCIRCUITSAT}$. The challenging part is to deal with the fact that $O$-$\text{QCIRCUITSAT}$ is a promise problem, and that a candidate search-to-decision algorithm may attempt to query the classical oracle $A^O$ on an input $C$ that does not satisfy the promise. However, note that we have some freedom in defining $A^O$ outside of the promise of $O$-$\text{QCIRCUITSAT}$ since any search-to-decision procedure should behave correctly regardless of the responses on invalid queries. We will make careful use of the freedom in defining the oracle $A^O$ on inputs outside of the promise in order to prove the result.

This choice of oracle is inspired by the quantum oracle separation between QMA and QCMA obtained by Aaronson and Kuperberg [AK07]. In fact, one can view Theorem 3.1, in some sense, as a strengthening of their oracle separation, since the impossibility of search-to-decision for QMA (essentially) implies that QMA is different from QCMA.

Proof of Theorem 3.1: We use a combination of the probabilistic method and a diagonalization argument. Let $S_1, \ldots, S_M$ be an enumeration of all search-to-decision circuits of size at most $T$ for some $T$ to be determined later. Note that $M \leq \exp(\text{poly}(n))$. We will assume each search-to-decision circuit $S_i$ is to take as input the description of a circuit with oracle gates. Pick $M + 1$ Haar-random $n$-qubit states $|\psi_1\rangle, \ldots, |\psi_{M+1}\rangle$, and define $O_j \overset{\text{def}}{=} I - 2 |\psi_j\rangle\langle\psi_j|$. We aim to show that there exists a choice of quantum oracle $O_j$ such that each $S_i$ fails to be a good search-to-decision reduction for $O_j$-$\text{QCIRCUITSAT}$. To do this, we have to define the behavior of the oracles $A^O_j$ on inputs $C$ that lie outside of the promise of the problem $O_j$-$\text{QCIRCUITSAT}$.

Let $\text{acc}_O(C)$ denote the maximum acceptance probability of an $O$-verifier circuit $C$, over the choice of quantum proof state. If we treat $C$ as a unitary operator that maps $\mathcal{H}_{\text{proof}} \otimes \mathcal{H}_{\text{anc}}$ (proof and ancilla registers, respectively) to $\mathcal{H}_{\text{out}} \otimes \mathcal{H}_{\text{junk}}$ (output qubit and junk registers, respectively), then $\text{acc}_O(C)$ is equivalently defined as

$$\text{acc}_O(C) = \left\| \left( |1^\text{out}\rangle \otimes I \right) C (I \otimes |0 \cdots 0\rangle_{\text{anc}}) \right\|^2$$

(3.2)

where the $|1^\text{out}\rangle$ vector acts on the output qubit of the circuit $C$, and $|0 \cdots 0\rangle_{\text{anc}}$ acts on the ancillary qubits of $C$. The norm $\| \cdot \|$ denotes the operator norm (i.e. maximum singular value).

Defining the first oracle $A^{O_1}$. We now define the first classical oracle $A^{O_1}$: for every valid circuit description $C$, we set $A^{O_1}(C) = 1$ if and only if $\text{acc}_O(C) > 1/2$, otherwise we set it to 0. For strings $C$ that don’t correspond to valid circuits, we define $A^{O_1}(C) = 0$.

Defining the rest of the oracles $A^O_j$ for $j > 1$. The other oracles $A^{O_j}$ are defined exactly in the same fashion, except for circuits $C$ such that $\delta < \text{acc}_O(C) < 1 - \delta$ (i.e. the $C$ lie outside of the promise of $O_j$-$\text{QCIRCUITSAT}$), we define $A^{O_j}(C) = A^{O_1}(C)$.

by some input length $n$. However for simplicity we shall just deal with one input length; we will forgo the trouble of spelling out the details of stating our results for asymptotic $n$. To that end, let $O$ be a unitary that acts on $n$ qubits, and we only consider $O$-verifier circuits who accept $n$-qubit quantum proof states; the verifier circuits themselves will be of size $\text{poly}(n)$.

\textsuperscript{12}We conjecture that it may, in fact, be possible to relax this condition to reflection unitaries about only phase states (See Definition A.1). The only ingredient one would need is a ”discrete” version of Levy’s lemma.
Draw a table $\mathcal{T}$ whose columns are indexed by the circuits $S_1, \ldots, S_M$, and the rows are indexed by $O_1, \ldots, O_{M+1}$. Place a $\checkmark$ in the entry $(S_i, O_j)$ if $S_i$ $\epsilon$-solves the search version of $O_j$-$\text{QCIRCUITSAT}$ when given access to $O_j$ and $A_{O_j}^T$, and put an $\times$ otherwise.

**Lemma 3.2 (Main Lemma)** With high probability over the choice of oracles $O_1, \ldots, O_{M+1}$, there is at most one $\checkmark$ in every column of $\mathcal{T}$.

Theorem 3.1 follows from the Main Lemma, because it implies that with high probability there exists an oracle $O_j^*$ for which there is no $\checkmark$ in its row (because there is one more row than there are columns of $\mathcal{T}$) – implying that there is no search-to-decision reduction for $O_j$-$\text{QCIRCUITSAT}$.

We now prove the Main Lemma: Fix a candidate search-to-reduction circuit $S_i$ (i.e., the $i$’th column of table $\mathcal{T}$). Fix two distinct row indices $j < k \in [M + 1]$. We calculate the probability that $(S_i, O_j)$ and $(S_i, O_k)$ both have $\checkmark$’s in them.

Consider the following verifier circuit $C^*$: given a supposed proof state $|\phi\rangle$, it applies the unitary oracle $O_j$ conditioned on a control qubit $|\rangle$. Then it projects the control qubit on the state $|\rangle$, and accepts if the projection succeeds. It is easy to see that it accepts with probability $\langle \phi | H_j | \phi \rangle^2$. Thus for all oracles $O_j$, the circuit $C^*$ is a YES instance of $O_j$-$\text{QCIRCUITSAT}$ because there is always a proof that $C^*$, equipped with oracle $O_j$, accepts with probability 1 (namely, the proof is $|\psi_j\rangle$).

We first show that with very high probability, the circuit $S_i$ cannot tell the difference when given access to the oracle pair $O_j, A_{O_j}^T$ versus the oracle pair $O_k, A_{O_k}^T$. Let $|\phi_j\rangle$ (resp. $|\phi_k\rangle$) denote the output of $S_i$ on input $C^*$ given query access to $O_j$ and $A_{O_j}^T$ (resp. $O_k$ and $A_{O_k}^T$).

**Lemma 3.3**

$$\Pr \left[ \left\| |\phi_j\rangle - |\phi_k\rangle \right\|^2 \geq O(\exp(-\Theta(2^{n/4}))) \right] \leq O(\exp(-\Theta(2^{n/4}))) \tag{3.3}$$

where the probability is over the choice of states $|\psi_j\rangle$ and $|\psi_k\rangle$.

Given the lemma, we then have that, with high probability, it cannot be that $S_i$ simultaneously $\epsilon$-solves the search versions of $O_j$-$\text{QCIRCUITSAT}$ and $O_k$-$\text{QCIRCUITSAT}$:

$$\Pr \left[ S_i \text{ $\epsilon$-solves } O_j \text{-QCIRCUITSAT and } O_k \text{-QCIRCUITSAT} \right] \leq \Pr \left[ \left\| \langle \phi_j | \psi_j \rangle \right\|^2 \geq 1 - \delta - \epsilon \text{ and } \left\| \langle \phi_k | \psi_k \rangle \right\|^2 \geq 1 - \delta - \epsilon \right] \tag{3.4}$$

$$\leq \Pr \left[ \left\| \langle \phi_j | \psi_j \rangle \right\|^2 \geq 1 - \delta - \epsilon \text{ and } \left\| \langle \phi_k | \psi_k \rangle \right\|^2 \geq 1 - \delta - \epsilon \text{ and } \left\| |\phi_j\rangle - |\phi_k\rangle \right\|^2 \leq O(\exp(-\Theta(2^{n/4}))) \right]$$

$$+ \Pr \left[ \left\| |\phi_j\rangle - |\phi_k\rangle \right\|^2 \geq O(\exp(-\Theta(2^{n/4}))) \right] \tag{3.5}$$

$$\leq \Pr \left[ \left\| \langle \psi_j | \psi_k \rangle \right\|^2 \geq 1 - O(\delta + \epsilon) \right] + \Pr \left[ \left\| |\phi_j\rangle - |\phi_k\rangle \right\|^2 \geq O(\exp(-\Theta(2^{n/4}))) \right] \tag{3.6}$$

Eq. (3.5) follows because $\epsilon$-solving the search versions of both $O_j$- and $O_k$-$\text{QCIRCUITSAT}$ implies that $S_i$ can solve those problems on input $C^*$, which means that the output states $|\phi_j\rangle, |\phi_k\rangle$ are
close to the states $|\psi_j\rangle$, $|\psi_k\rangle$, respectively. Eq. (3.6) follows from the union bound, and eq. (3.7) follows from the triangle inequality.

On the other hand, with high probability over the choice of $O_j, O_k$, we have that $|\psi_j\rangle$ is far from $|\psi_k\rangle$. This follows from Levy’s Lemma (Lemma A.8):

$$\Pr \left( |\langle \psi_j | \psi_k \rangle|^2 \geq \frac{1}{2} \right) \leq \exp \left( -\Omega(2^n) \right). \quad (3.8)$$

This, combined with Lemma 3.3, implies that eq. (3.7) is at most $O(\exp(-\Omega(2^{n/4})))$. Union bounding over all pairs $j < k$ of rows and all columns $i$, we have that the probability there is a column with more than a single $\checkmark$ is at most $O(M^3) \cdot O(\exp(-\Omega(2^{n/4}))) \leq O(\exp(-\Omega(2^{n/4})))$, which proves the Main Lemma.

Thus it just remains to show Lemma 3.3. The circuit $S_i$ can be expressed as a product of $R \leq T$ unitary operations for

$$S_i = U_R U_{R-1} \cdots U_1 \quad (3.9)$$

where $U_i$ is either a unitary that’s independent of the choice of $O$, a (controlled) call to $O$, or a (controlled) call to $A^O$. The oracles may act on different subsets of qubits each time.

Fix a $U = U_t$ for some $t \in [R]$. We argue that, when $U$ is either a controlled call to $O$ or $A^O$, for a fixed input state $|\alpha\rangle$, the state $U |\alpha\rangle$ is very close to a fixed vector that is independent of the oracle $O$, with high probability over $O = I - 2 |\psi\rangle\langle\psi|$. (This is also trivially true when $U$ is independent of $O$.)

Suppose $U$ is a query to $O = I - 2 |\psi\rangle\langle\psi|$. Suppose for now that $O$ is applied to the first $n$ qubits of $|\alpha\rangle$. Then

$$\langle \alpha | O | \alpha \rangle = 1 - 2 \Tr \left( |\alpha\rangle\langle\alpha| |\psi\rangle\langle\psi| \right). \quad (3.10)$$

Note that $|\psi\rangle$ is an $n$-qubit state, while $|\alpha\rangle$ is a state on potentially more qubits, because it is supposed to represent the intermediate state the circuit $S_i$. Define the function $f : (\mathbb{C}^2)^\otimes n \to \mathbb{R}$ be defined as

$$f(|\psi\rangle) \stackrel{\text{def}}{=} \Tr \left( |\alpha\rangle\langle\alpha| |\psi\rangle\langle\psi| \right). \quad (3.11)$$

The expectation of $f$ over a Haar-random $|\psi\rangle$ is simply $2^{-n}$. By Levy’s Lemma, this implies that

$$\Pr \left[ |f(|\psi\rangle) - 2^{-n}| > \eta \right] \leq 2\exp(-\Omega(2^n \eta^2)). \quad (3.12)$$

Set $\eta = 2^{-n/3}$. Translating from inner products to squared Euclidean distance and taking a union bound we have

$$\Pr \left[ \max \left\{ \| |\alpha\rangle - O_j |\alpha\rangle \|^2, \| |\alpha\rangle - O_k |\alpha\rangle \|^2 \right\} \geq \Omega(\eta) \right] \leq 2 \Pr \left[ \| |\alpha\rangle - O |\alpha\rangle \|^2 \geq O\eta \right] \quad (3.13)$$

$$= 2 \Pr \left[ 2 - 2 \langle \alpha | O | \alpha \rangle \geq O(\eta) \right] \quad (3.14)$$

$$= 2 \Pr \left[ f(|\psi\rangle) \geq O(\eta) \right] \quad (3.15)$$

$$\leq 2 \Pr \left[ f(|\psi\rangle) \geq O(\eta) \right] \quad (3.16)$$

$$\leq O(\exp(-\Omega(2^{n/3}))) \quad (3.17)$$
where the probability is over the choice of $O_j, O_k$.

Now suppose $U$ is a query to $A^O$. Consider an input state
\[
|\alpha\rangle = \sum_{C,b} \alpha_{C,b} |C,b\rangle |\varphi_{C,b}\rangle
\]
(3.18)
where the registers $|C,b\rangle$ correspond to the query registers for $A^O$, and the $\{|\varphi_{C,b}\rangle\}$ are arbitrary states that depend on $C$ and $b$, but are not acted upon by $A^O$. The sum runs over all verifier circuit instances $C$ of size at most $T$ (many of which are not proper encodings of circuits), and $|b\rangle$ is a qubit register.

Let $|\beta_j\rangle = A^{O_j} |\alpha\rangle$ and $|\beta_k\rangle = A^{O_k} |\alpha\rangle$ be the result of running $A^{O_j}$ or $A^{O_k}$ on the fixed input state $|\alpha\rangle$. We have that
\[
|\beta_j\rangle = \sum_{C,b} \alpha_{C,b} |C,b\rangle + A^{O_j}(C) \rangle |\varphi_{C,b}\rangle
\]
(3.19)
\[
|\beta_k\rangle = \sum_{C,b} \alpha_{C,b} |C,b\rangle + A^{O_k}(C) \rangle |\varphi_{C,b}\rangle.
\]
(3.20)
Therefore
\[
E \| |\beta_j\rangle - |\beta_k\rangle \|^2 = 2 \sum_{C} |\alpha_{C,b} - \alpha_{C,1}|^2 \cdot \mathbf{1}\{A^{O_j}(C) \neq A^{O_k}(C)\} \leq 4 \sum_{C} (|\alpha_{C,b}|^2 + |\alpha_{C,1}|^2) \cdot \mathbf{1}\{A^{O_j}(C) \neq A^{O_k}(C)\}
\]
(3.21)
\[
= 4 \sum_{C} (|\alpha_{C,b}|^2 + |\alpha_{C,1}|^2) \cdot \Pr \left[ A^{O_j}(C) \neq A^{O_k}(C) \right]
\]
(3.22)
Here, the expectation is over the choice $O_j, O_k$. Now we argue that for any fixed circuit $C$ of size at most $T$, the probability $\Pr \left[ A^{O_j}(C) \neq A^{O_k}(C) \right]$ is small. If $C$ is not a valid verifier circuit, then this probability is 0 (since both $A^{O_j}$ and $A^{O_k}$ by construction give answer 0).

Now suppose that $C$ is a properly encoded verifier circuit. Let us define $\text{acc}_\varphi(C)$ as $\text{acc}_O(C)$ for $O = I - 2 |\psi\rangle \langle \psi|$ and $\text{acc}_O(C)$ defined in equation eq. (3.2); we abbreviate this as $\text{acc}_\varphi(C) = \| \langle 1 |C_\varphi |0\rangle \|^2$ where $C_\varphi$ denotes the unitary operator corresponding to circuit $C$ that makes calls to oracles $O$ and $A^O$ that depend on $|\psi\rangle$. Define $\text{avg}_\varphi(C) \equiv E \text{acc}_\varphi(C)$, where the expectation is over a Haar-random $|\psi\rangle$. Define the function $f(|\psi\rangle) = \text{acc}_\varphi(C)$. We calculate its Lipschitz constant. We have for all $|\psi\rangle, |\theta\rangle$,
\[
|f(|\psi\rangle) - f(|\theta\rangle)| = \| \langle 1 |C_\varphi |0\rangle \|^2 - \| \langle 1 |C_\theta |0\rangle \|^2 \]
\[
\leq 2 \| \langle 1 |C_\varphi |0\rangle - \langle 1 |C_\theta |0\rangle \| ^2 \]
\[
\leq 2 \| C_\varphi - C_\theta \|^2.
\]
(3.24)
(3.25)
(3.26)
The second line follows from the triangle inequality for the operator norm. The third line follows from the fact that $\| AB \| \leq \| A \| \cdot \| B \|$ for operators $A, B$. Next, suppose we write $C$ as $V_T V_{T-1} \cdots V_1$ where $V_t$ are unitary operators that are either independent of the oracle $O$, or $V_t = O$. We can then write
\[
C_\varphi = V_R^\varphi V_{R-1}^\varphi \cdots V_1^\varphi \quad \text{and} \quad C_\theta = V_R^\theta V_{R-1}^\theta \cdots V_1^\theta.
\]
(3.27)
By a hybrid argument we have
\[ \|C_{\psi} - C_{\theta}\| \leq \sum_{t=1}^{R} \|V_{t}^{\psi} - V_{t}^{\theta}\|. \] (3.28)

If \( V_{t}^{\psi} \) and \( V_{t}^{\theta} \) are independent of \( \psi, \theta \), respectively, then the \( t \)'th term is 0. If \( V_{t}^{\psi} = I - 2|\psi\rangle\langle\psi| \) and \( V_{t}^{\theta} = I - 2|\theta\rangle\langle\theta| \), then we have
\[ \|V_{t}^{\psi} - V_{t}^{\theta}\| \leq 2\|\psi\rangle\langle\psi| - |\theta\rangle\langle\theta|\|. \] (3.29)

Thus, we have
\[ |f(|\psi|) - f(|\theta|)| \leq O\left(T^2 \|\psi\rangle\langle\psi| - |\theta\rangle\langle\theta|\|\|^2\right) \leq O\left(T^2 \|\psi\rangle - |\theta\rangle\|\right) \] (3.30)
where we used that \( \|\psi\rangle\langle\psi| - |\theta\rangle\langle\theta|\|^2 \leq 4\|\psi\rangle - |\theta\rangle\|^2 \leq 16\|\psi\rangle - |\theta\rangle\|. \) This implies that the Lipschitz constant for \( f \) is at most \( O(T^2) \). Hence by Levy’s Lemma,
\[ \Pr[|f(|\psi|) - \text{avg}(C)| \geq \eta] \leq 2\exp\left(-\Omega(2^\eta T^2 / 16 T^4)\right). \] (3.31)

Define \( \gamma \overset{\text{def}}{=} 2\exp\left(-O(2^\eta T^2 / 16 T^4)\right) \).

We can now evaluate the probability that \( A^{O_1}(C) \neq A^{O_k}(C) \). We consider two cases. The first is that \( \text{avg}(C) \) is in the “grey zone”, meaning that \( \delta + \eta < \text{avg}(C) < 1 - \delta - \eta \). This means that, on average, the acceptance probability of \( C \) is outside of the promise of \( O\)-QCIRCUIT-SAT. Then with probability at least \( 1 - 2\gamma \), the acceptance probabilities \( \text{acc}_{\psi_1}(C) \) and \( \text{acc}_{\psi_k}(C) \) are going to remain strictly between \( \delta \) and \( 1 - \delta \). By construction, this means that \( A^{O_1}(C) = A^{O_k}(C) = A^{O_1}(C) \), so in this case \( \Pr\left[A^{O_1}(C) \neq A^{O_k}(C)\right] \leq 2\gamma \).

The second case is that \( \text{avg}(C) \) is not in the grey zone. Consider the case that \( \text{avg}(C) \leq \delta + \eta \). With probability at least \( 1 - 3\gamma \), all of \( \text{acc}_{\psi_1}(C), \text{acc}_{\psi_j}(C), \text{acc}_{\psi_k}(C) \) are at most \( \delta + 2\eta \ll \frac{1}{2} \). This means that \( A^{O_1}(C) = 0 \), and thus regardless of whether \( C \) lies outside the promise of \( O_j\)-QCIRCUIT-SAT or \( O_k\)-QCIRCUIT-SAT, we have that \( A^{O_1}(C) = A^{O_k}(C) = A^{O_1}(C) = 0 \) by construction. A similar argument goes for for when \( \text{avg}(C) > 1 - \delta - \eta \).

Therefore in all cases \( \Pr\left[A^{O_1}(C) \neq A^{O_k}(C)\right] \leq 3\gamma \). This implies that \( \mathbb{E} \|\beta_j - |\beta_k\|^2 \leq 12\gamma \).

By Markov’s inequality with probability at least \( 1 - O(\sqrt{\gamma}) \), we have \( \|\beta_j - |\beta_k\|^2 \leq O(\sqrt{\gamma}) \).

To summarize, we have showed that for any \( t \in [R] \), for any fixed state \( |\alpha\rangle \), with probability at least \( 1 - \exp(-\Omega(2^{n/3} / T^4)) \), we have that
\[ \|U_t^{\psi}|\alpha\rangle - U_t^{\psi_k}|\alpha\rangle \| \leq O(\exp(-\Omega(2^{n/3} / T^4))) \] (3.32)

where \( U_t^{\psi} \) and \( U_t^{\psi_k} \) denote the \( t \)'th unitary operation of the candidate search-to-decision circuit \( S_t \) when querying oracles \( O_j, A^{O_j} \) and \( O_k, A^{O_k} \), respectively. Summing over all \( R \) time steps of the circuit \( R \), we get that with probability at least
\[ 1 - O(R \exp(-\Omega(2^{n/3} / T^4))) \] (3.33)
the outputs of \( S_t \) with either oracle \( O_j \) or \( O_k \) are going to be at most \( O(R \exp(-\Omega(2^{n/3} / T^4))) \)-far from each other. Plugging in \( R \leq T = \text{poly}(n) \), we obtain Lemma 3.3.

\[ \square \]
4 1-query state synthesis algorithm with polynomially small error

We describe here a 1-query, polynomial-space algorithm that achieves polynomially small error. The state synthesis algorithm will not be efficient. We will start with a first attempt, which has exponential space complexity and then fix it so that it has polynomial space complexity. The algorithm makes use of the Swap Test Distillation algorithm described in Section 5 that takes as input a polynomial number of states, each with at least constant overlap with the target state, and uses successive applications of the Swap Test to produce a final state whose overlap with the target state is at least $1 - 1/\text{poly}(n)$.

4.1 A space-inefficient algorithm

Let $d = 2^n$, $n' = n^2$, and $d' = 2^{n'}$. The $m$ applications of the 1-query algorithm along with the Swap Test Distillation algorithm will be applied to $n'$-qubit registers with target state $|\tau\rangle = |\tau\rangle \otimes |0\rangle^{(n'-n)}$. The expansion of the space is important for derandomizing the algorithm later on. In particular, we will show that there is a fixed sequence of unitaries that works for all $|\tau\rangle$ of the form $|\tau\rangle \otimes |0\rangle^{(n'-n)}$. This will allow us to hard-code the unitaries into the oracle function. The resulting algorithm will still require exponential time to implement the unitaries, but the derandomized algorithm will require only polynomial space.

We will define a function $f_{\tau} : U(d') \times \{0, 1\}^{n'} \rightarrow \{0, 1\}$, where $U(d')$ is the space of all unitaries on a $d'$-dimensional Hilbert space, and

$$f_{\tau}(U, x) \overset{\text{def}}{=} \text{sgn} \left( \text{Re} \left( \langle x | U | \tau \rangle \right) \right)$$

(4.1)

The corresponding phase state is

$$|p_U\rangle = \sum_{x \in \{0, 1\}^{n'}} (-1)^{f_{\tau}(U, x)} |x\rangle$$

(4.2)

---

**ONEQUERYSTATESYNTHESIS (space inefficient version)**

(1) for $j = 1, \ldots, m$ in parallel:

(2) Sample Haar-random $n'$-qubit unitary $U_j$.

(3) In the $j$th $n'$-qubit register, prepare the equal superposition $\sum_{x \in \{0, 1\}^{n'}} |x\rangle$.

(3) Controlled on basis state $|x\rangle$, query the oracle on input $(U_j, x)$ to apply $f_{\tau}(U_j, x)$ and produce phase state $|p_{U_j}\rangle$ on $n'$ qubits.

(4) Apply $U_j^\dagger$ to the phase state.

(5) Apply the SWAPTESTDISTILLATION Algorithm (Figure 2) to the $m$ resulting states $|\psi_1\rangle, \ldots, |\psi_m\rangle$.

(6) Output the first $n$ qubits of any surviving register.

---

Figure 1: Pseudo-code for the ONEQUERYSTATESYNTHESIS query algorithm that uses exponential space complexity.

The algorithm will output $m$ expanded registers on $n'$ qubits. We will apply the Swap Test Distillation algorithm to $m$ states on $n'$ qubits generated by $m$ parallel (and independent) applications of the 1-query algorithm and analyze the probability that the resulting state has at least
1 − 1/poly(n) overlap with |τ′⟩. The mixed state ρ in the first n-qubits will also have Tr{ρ |τ⟩⟨τ|} ≥ 1 − 1/poly(n).

The following lemma establishes that with high probability after step (4) of the algorithm, the conditions for the Swap Test Distillation Algorithm are met.

Lemma 4.1 (Probability Conditions Satisfied for Swap Test Distillation) Let |ψ₁⟩ ⊗ · · · ⊗ |ψₘ⟩ be the states in the m registers after Step (4). There is a constant C such that

1. \( \Pr_{U₁,...,Uₘ} \left[ \min_j \{ |⟨ψ_j|τ′⟩|^2 \} ≤ \frac{1}{8} \right] ≤ m \cdot \exp(-Cd′) \)

2. \( \Pr_{U₁,...,Uₘ} \left[ \max_{i \neq j} \{ |⟨ψ_i| (I − |τ′⟩⟨τ′|) |ψ_j⟩|^2 \} ≥ (d′)^{-1/4} \right] ≤ m² \cdot \exp(-C(d′)^{1/2}) \)

Proof: For the first part, consider a single application of the 1-query protocol with Haar random unitary U. Let |p_U⟩ be the phase state corresponding to U |τ⟩. The output state is \( U^† |p_U⟩ \) and we would like to upper bound the probability that |⟨p_U| U |τ′⟩|^2 is less than 1/8:

\[
\Pr \left[ |⟨p_U| U |τ′⟩|^2 ≤ \frac{1}{8} \right] = \Pr \left[ |⟨p_U| U |τ′⟩| ≤ \sqrt{\frac{1}{2}} \right] ≤ \Pr \left[ |⟨p_U| \text{Re}(Uτ′)⟩| ≤ \sqrt{\frac{1}{2}} \right].
\]

Using Fact A.2

\[
\Pr \left[ |⟨p_U| \text{Re}(Uτ′)⟩| ≤ \sqrt{\frac{1}{2}} \right] = \Pr \left[ ||\text{Re}(Uτ′)||_1 ≤ \sqrt{d′}/\sqrt{2} \right].
\]

Since U |τ′⟩ is a Haar-random state, the expected \( L_1 \) norm of |Re(Uτ′)⟩ is \( \sqrt{d′}/2 \). We can now use Levy’s Lemma (A.8) with the dimension \( N = d′ \) and \( δ = \sqrt{d′}/2 \). If the function \( f \) in Levy’s Lemma is the \( L_1 \) norm, then the value of \( K \) is \( \sqrt{d′} \). Thus,

\[
\Pr \left[ ||\text{Re}(Uτ′)||_1 ≤ \sqrt{d′}/\sqrt{2} \right] ≤ \Pr \left[ ||\text{Re}(Uτ′)||_1 − \sqrt{d′}/2 ≤ \sqrt{d′}/2 \right] \leq \exp(-C₁d′),
\]

for some constant \( C₁ \). The probability that the protocol fails to produce a state with overlap at least 1/8 with the target state in a single run is at most \( \exp(-C₁d′) \). Since the 1-protocol is run \( m \) times in parallel, the probability that any of the resulting states fails to have overlap at least 1/8 is at most \( m \cdot \exp(-C₁d′) \).

For the second part, define |φ_j⟩ to be the normalized component of |ψ_j⟩ that is orthogonal to |τ′⟩ and |r_j⟩ the component of |p_U⟩ that is orthogonal to U |τ′⟩. Equivalently,

\[
|φ_j⟩ = \frac{(I − |τ′⟩⟨τ′|) |ψ_j⟩}{\| (I − |τ′⟩⟨τ′|) |ψ_j⟩ \|}, \quad \text{and} \quad |r_j⟩ = \frac{|p_u⟩ − ⟨τ′| U^† |p_u⟩ U |τ′⟩}{\| |p_u⟩ − ⟨τ′| U^† |p_u⟩ U |τ′⟩ \|}.
\]

We will bound \( |⟨φ_j|φ_j⟩|^2 \) which is in turn an upper bound for \( |⟨ψ_j| (I − |τ′⟩⟨τ′|) |φ_j⟩|^2 \). Note that \( U^† |r_j⟩ = |φ_j⟩ \).

Now fix |φ_j⟩ from the \( i^{th} \) run of the 1-query algorithm and consider the selection of U_j on the \( j^{th} \) run. We can think of selecting U_j in two stages:

1. First select the target of state |τ⟩ under U_j, which we will call |s_j⟩ \( \overset{def}{=} U_j |τ⟩ \).
2. Then select a Haar-random isometry \( V_j \) that maps \( |s_j⟩\perp \) to \( |τ⟩\perp \), where \( |s_j⟩\perp \) is the subspace perpendicular to \( |s_j⟩ \) and \( |τ⟩\perp \) is the subspace perpendicular to \( |τ⟩ \).

Then \( U_j = |s_j⟩⟨τ| + V_j \). The state \( |φ_j⟩ \) is a fixed state (independent of the choice of \( U_j \)) that lies in \( |τ⟩\perp \). The selection of \( |s_j⟩ \) in Step 1 determines \( |r_j⟩ \). Then, the unitary \( V \) maps \( |s_j⟩ \) to a random state in \( |τ⟩\perp \). We can apply Levy’s Lemma again with \( f(V \ | s_j⟩) = |⟨φ_j| V |s_j⟩|^2 \). The value of \( K \) is \( O(1) \), and the expectation of \( f \) over the choice of \( V_j \) is then \( 1/(d' - 1) \). Setting \( δ = (d')^{-1/4} \), we have that

\[
\Pr \left[ |⟨φ_i| V |s_j⟩|^2 \geq (d')^{-1/4} \right] \leq \exp(-C_2(d')^{1/2}).
\]  

(4.9)

There are at most \( m^2 \) pairs of states. The probability that any of them have \( |⟨φ_i| φ_j⟩|^2 \geq (d')^{-1/4} \) is at most \( m^2 \exp(-C_2(d')^{1/2}) \). The final constant \( C \) in the statement of the theorem can be taken to be \( \min\{C_1, C_2\} \).

\[\square\]

### 4.2 A space-efficient algorithm

The algorithm described above suffers from needing exponential space complexity; this is because specifying a Haar-random unitary on \( n' \) qubits requires \( \exp(Ω(n')) \) space, and thus the oracle \( f(U, x) \) needs to act on exponentially many input bits. We derandomize this construction, and show via the probabilistic method that there exists a single choice of unitaries \( U_1, \ldots, U_m \) that works for all \( n \)-qubit states — this is why we expanded the space to dimension \( d' \).

Let \( |v_1⟩, \ldots, |v_D⟩ \) denote an \( ε \)-net for the space of \( n \)-qubit quantum states where \( ε = d^{-1} \). Then there at most \( D = ε^{-d} = d^d \) states in this enumeration. Fix an index \( 1 \leq i \leq D \). Imagine running the 1-query protocol in Figure 1 in parallel \( m \) times with target state \( |φ_i⟩ \otimes |0⟩ \). The probability that the protocol fails to satisfy the conditions for the Swap Test Distillation algorithm from Lemma 4.1 is at most \( m^2 \exp(-Ω((d')^{3/4})) \) over the choice of \( U_1, \ldots, U_m \). By a union bound, the probability that a random choice of \( U_1, \ldots, U_m \) fails to satisfy the conditions from Lemma 4.1 for a single one of the \( |v_1⟩, \ldots, |v_D⟩ \) is at most

\[
d^d \cdot m^2 \exp(-Ω((d')^{1/2})) \leq 2^{n2^n} \cdot m^2 \exp(-Ω(2^n/2)).
\]  

Since \( m \) is polynomial in \( n \), for sufficiently large \( n \), this probability is less than 1. Thus there exists a choice of unitaries \( U_1, \ldots, U_m \) that results in a set of \( m \) states that satisfy the conditions for the Swap Test Distillation algorithm for all the \( |v_1⟩, \ldots, |v_D⟩ \). Hardcode these unitaries into the algorithm and oracles: \( f_{τ,j}(x) = f_τ(U_τ, x) \). Now the oracles only take \( n' \) bits as input each, and the resulting query algorithm now only requires \( \text{poly}(n) \) space. Note that the implementation of the unitaries \( U_1, \ldots, U_m \) will not be time-efficient in general, but they are still fixed unitary operators that act on \( n' \) qubits.

Thus for an arbitrary target state \( |τ⟩ \), use the oracles \( f_{τ,1}(U_{s,1}, x), \ldots, f_{τ,m}(U_{s,m}, x) \) corresponding to the nearest state \( |v_j⟩ \) in the \( ε \)-net, which is within \( d^{-1} \) of \( |τ⟩ \). Therefore, the one-query algorithm using unitaries \( U_1, \ldots, U_m \), followed by the Swap Distillation Algorithm will incur an additional \( O(d^{-1}) \) error.

**Theorem 4.2** (One Query State Synthesis Performance) *For every polynomial \( q \), there is a polynomial \( p \) and constant \( C' \) such that if the ONEQUERYSTATESYNTHESIS is run with \( m \geq p(n) \) registers, then*
with probability at least $1 - \exp(-C/n)$, the algorithm produces a state $\rho$ such that $\text{Tr}\{\rho |\tau\rangle\langle\tau|\} \geq 1 - 1/q(n)$. The oracle queried by the algorithm will depend on the closest state to $|\tau\rangle$ in the $\epsilon$-net.

**Proof:** Those choice of $U_{\ast,1}, \ldots, U_{\ast,m}$ guarantees that the conditions from Lemma 4.1 hold for the nearest state to the target state $|\tau\rangle$ from the $\epsilon$-net. The overlap between the $|\phi_i\rangle$'s will be $\delta = C(d')^{-1/4} = C2^{-n^2/4}$. The overlap $a$ between each $|\phi_i\rangle$ and the target state will be at least $1/8$.

From Theorem 5.10, we can select $\ell = c\log_{5/4}(2n) + 1/2a^2$ and $m \geq n\ell$ to obtain overlap to the nearest state in the $\epsilon$-net that is at least $1 - 1/n^{c} - 8m\sqrt{\delta}$ with probability at least $1 - 2\exp(-n/12) - 4m\sqrt{\delta}$. The overlap with the desired target state is then at least $1 - 1/n^{c} - 8m\sqrt{\delta} - 2^{-n}$. Select a constant $c$ so that the overlap is at least $1 - 1/q(n)$ which then determines $\ell$ and the polynomial $p(n) \geq n\ell$.

## 5 Swap test distillation procedure

If a synthesis protocol is able to produce a state with at least constant overlap with the target state and the target state is a witness for a QMA verifier, then phase estimation can be used to boost the overlap and the probability of success. If the target state is an arbitrary state, we may not have the means to directly measure whether the output state is close to the target. In this section we describe a procedure that can take the output of $m$ parallel applications of a state synthesis protocol, each of which has a constant overlap with the target state and apply a procedure to increase the overlap. The algorithm begins with $m$ states, $|\psi_1\rangle, \ldots, |\psi_m\rangle$, each of which is stored in an $n$-qubit register. We show that if the number of states $m$ is a sufficiently large polynomial in $n$, then the overlap of the final output state will be at least $1 - 1/n^c - 8m\sqrt{\delta} - 2^{-n}$. Select a constant $c$ so that the overlap is at least $1 - 1/q(n)$ which then determines $\ell$ and the polynomial $p(n) \geq n\ell$.

The second condition is satisfied if the portion of each state $|\psi_i\rangle$ that is perpendicular to the target state $|\tau\rangle$ is essentially random. If the $|\psi_i\rangle$'s are generated according to some independent randomness, one might expect that the overlap between these perpendicular components to be (exponentially) small. In this section, we analyze the behavior of the Swap Test distillation procedure subject to these two properties. At the end of the section, we will show that the first condition can be relaxed to a lower bound on the expectation of the overlap as long as the $m$ states are generated according to some independent randomness. In Section 4 we showed how the algorithm can be used in conjunction with a 1-query protocol to produce a state that has $1 - 1/poly(n)$ overlap with the target state.
5.1 The Algorithm

Each round of the algorithm begins with some set of surviving registers. The surviving registers are paired up and the swap test is applied to each pair. An auxiliary qubit is used in each application of the swap test which is measured at the end of the swap test. If the outcome is 0 (a successful outcome), then one of the two registers is selected to survive to the next iteration. If the outcome is 1 (an unsuccessful outcome), neither register survives. Figure 2 shows the pseudocode for the procedure. Figure 3 shows an example of the procedure for one iteration applied to eight input states. Note that the state in a surviving register may be entangled with the other registers. If $\rho$ is the reduced density matrix of the state in one of the surviving registers obtained by tracing out the other registers, we will refer to $\text{Tr}\{\rho \mid \tau \rangle \langle \tau \mid\}$ as the overlap of $\rho$ with $\mid \tau \rangle$. We will show that for $m$ sufficiently large, with high probability the overlap of a surviving register with $\mid \tau \rangle$ is at least $1 - 1/\text{poly}(n)$.

Consider one round of the algorithm applied to a particular pair of registers. We will prove that if the swap test succeeds, then the surviving register has an overlap with $\mid \tau \rangle$ that is at least the average of the overlap of the states in the two registers before the round. Moreover, if each of the two registers at the beginning of a round have overlap at least $\gamma$, then the overlap of a surviving register is strictly larger than $\gamma$ and with enough successful rounds will tend towards 1.

```
SWAPTESTDISTILLATION
Input: m states $|\psi_1\rangle, \ldots, |\psi_m\rangle$ stored in n-qubit registers numbered 1 through m
(1) Initialize $(R_1, \ldots, R_m) \leftarrow (1, \ldots, m)$
(2) $\ell = \lceil \log_6 (m/n) \rceil$
(3) for $k = 1, \ldots, \ell$:
(4) count = 0
(5) for $j = 1, \ldots, [m/2]$:
(6) if SWAPTEST($R_{2j-1}, R_{2j}$) returns 0
(7) count = count + 1
(8) $R_{\text{count}} = R_{2j-1}$
(9) end
(10) $m = \text{count}$
(11) end

SWAPTEST($R, R'$)
Start with auxiliary qubit $b$ initialized to $|0\rangle$
(1) Apply:
(2) $H_b \otimes I_{R,R'}$
(3) Controlled SWAP operation on Registers $R$ and $R'$, controlled by qubit $b$
(4) $H_b \otimes I_{R,R'}$
(5) Measure qubit $b$ and return the result
(6) end
```

Figure 2: Pseudo-code for SWAPTESTDISTILLATION algorithm.
Figure 3: The Swap Test Distillation algorithm applied to eight input registers. The value measured in the auxiliary qubit indicates whether an application of the Swap Test is successful. In the first iteration, the swap tests applied to pairs $|\psi_3\rangle, |\psi_4\rangle$ and $|\psi_5\rangle, |\psi_6\rangle$ are successful. The resulting states in registers 3 and 5 advance to the next round. In each iteration, the sequence $(R_1, R_2, \ldots)$ indicates the indices of the surviving registers from left to right.

5.2 Analysis: no overlap case

We will first analyze the algorithm for the idealized case in which there is no overlap between the portion of each input state that is perpendicular to the target $|\tau\rangle$. That is, for the remainder of this subsection, we assume that $\langle \phi_i | \phi_j \rangle = 0$ for $i \neq j$. We also assume that Condition 1 above is met, namely, for all $j$, $|\langle \psi_j | \tau \rangle|^2 \geq a$, for some constant $a$.

We can track which original states are used to create the state in each surviving register after every iteration of the while loop. Originally, $S_i = \{i\}$. Whenever a swap test succeeds in Line (6), we can update the set associated with $R_{\text{count}}$ to be $S_{\text{count}} \leftarrow S_{2j-1} \cup S_{2j}$. Thus, at the end of each iteration of the while loop, the collection of sets $\{S_j\}$ is pairwise disjoint. Moreover, the reduced density matrix of the state $\rho_j$ in register $R_j$ has support contained in the space spanned by $\{|\tau\rangle\} \cup \{|\phi_i\rangle \mid j \in S_j\}$. Define $\Pi = \mathbb{I} - |\tau\rangle\langle\tau|$ to be the projector onto the perpendicular space to $|\tau\rangle$. Then $\text{Tr}(\rho_j \Pi \rho_j \Pi) = 0$ for any two surviving registers $R_i$ and $R_j$. Also, the combined state is a tensor product state: $\rho_i \otimes \rho_j$. The lemma below gives an expression for the resulting state in two registers after a successful swap test is applied.

Lemma 5.1 (Result of a Successful Swap Test) Suppose that the SWAP TEST is performed on $|0\rangle\langle0| \otimes \rho_1 \otimes \rho_2$. Let $S$ be the Swap operation for the second and third registers that contain $\rho_1$ and $\rho_2$, respectively. If the measurement outcome is 0, then the resulting state is $|0\rangle\langle0| \otimes \tilde{\rho} / \text{Tr}(-\tilde{\rho})$, where

$$\tilde{\rho} = (\rho_1 \otimes \rho_2) + S(\rho_1 \otimes \rho_2)S + S(\rho_1 \otimes \rho_2)S + (\rho_1 \otimes \rho_2)S.$$  

Proof: After step (2) the state is $|+\rangle\langle+| \otimes \rho_1 \otimes \rho_2$. The controlled swap operation is $|0\rangle\langle0| \otimes I + |1\rangle\langle1| \otimes S$. After the controlled swap is applied in Step (3), the state equals

$$|0\rangle\langle0| \otimes (\rho_1 \otimes \rho_2) + |1\rangle\langle1| \otimes S(\rho_1 \otimes \rho_2)S + |0\rangle\langle0| \otimes (\rho_1 \otimes \rho_2)S + |1\rangle\langle0| \otimes S(\rho_1 \otimes \rho_2).$$  

(5.3)
After the Hadamard gate, $H_i$ is applied again to the first qubit, the component of the state corresponding to the $|0\rangle|0\rangle$ term (which is the result after a 0 is measured) will equal

$$\frac{|0\rangle|0\rangle \otimes (\rho_1 \otimes \rho_2) + |0\rangle|0\rangle \otimes S(\rho_1 \otimes \rho_2)S + |0\rangle|0\rangle \otimes (\rho_1 \otimes \rho_2)S + |0\rangle|0\rangle \otimes S(\rho_1 \otimes \rho_2)}{4}.$$  

(5.4)

The following lemma will be useful in understanding the contribution of the $S(\rho_1 \otimes \rho_2)$ and $(\rho_1 \otimes \rho_2)S$ terms from Lemma 5.1.

**Lemma 5.2** Consider a tensor product state $\rho_i \otimes \rho_j$. Let $S$ be the swap operator on the registers holding $\rho_i$ and $\rho_j$. Suppose also that $\text{Tr}(\rho_i(1 - |\tau\rangle\langle \tau|)\rho_j(1 - |\tau\rangle\langle \tau|)) = 0$. Then

$$\text{Tr}\{S(\rho_i \otimes \rho_j)(1 - |\tau\rangle\langle \tau|, \tau\rangle\langle \tau|)\} = \text{Tr}\{(\rho_i \otimes \rho_j)S(1 - |\tau\rangle\langle \tau|, \tau\rangle\langle \tau|)\} = 0$$

and

$$\text{Tr}\{S(\rho_i \otimes \rho_j)|\tau\rangle\langle \tau|, \tau\rangle\langle \tau|\} = \text{Tr}\{(\rho_i \otimes \rho_j)S|\tau\rangle\langle \tau|, \tau\rangle\langle \tau|\} = \text{Tr}\{\rho_i |\tau\rangle\langle \tau|\} \cdot \text{Tr}\{\rho_j |\tau\rangle\langle \tau|\}.\quad (5.5)$$

**Proof**: Since $\text{Tr}\{\rho_i(1 - |\tau\rangle\langle \tau|)\rho_j(1 - |\tau\rangle\langle \tau|)\} = 0$, there is an orthonormal basis of the Hilbert space of a single register $B = \{|\tau\rangle\} \cup \{|1\rangle, \ldots, |D - 1\rangle\}$ where the support of $\rho_i$ is contained in the space spanned by $\{|\tau\rangle\} \cup \{|1\rangle, \ldots, |r\rangle\}$ for some $r$ and the support of $\rho_j$ is contained in the space spanned by $\{|\tau\rangle\} \cup \{|r + 1\rangle, \ldots, |D - 1\rangle\}$. When $\rho_i$ and $\rho_j$ are expressed in the basis $B$, row and column 0 correspond to $|\tau\rangle$, so $\rho_i[0, 0] = \text{Tr}\{\rho_i |\tau\rangle\langle \tau|\}$ and $\rho_j[0, 0] = \text{Tr}\{\rho_j |\tau\rangle\langle \tau|\}$. The figure below shows the matrices $\rho_i$ and $\rho_j$. The non-zero entries are contained within the shaded regions in each matrix.

Now express $\rho_i \otimes \rho_j$ in the $B \otimes B$ basis. This matrix consists of $D^2$ submatrices of size $D \times D$. A row is indexed by a pair $(a, b) \in [D] \times [D]$, where $a$ denotes the row of submatrices and $b$ denotes the row within the row of submatrices. Similarly a column is indexed by a pair $(c, d) \in [D] \times [D]$, where $c$ denotes the column of submatrices and $d$ denotes the column within the column of submatrices. The entry corresponding to row $(a, b)$ and column $(c, d)$ is $\rho_i[a, c] \cdot \rho_j[b, d]$. When the Swap operator, $S$, is applied to the left ($S(\rho_i \otimes \rho_j)$), the rows, but not the columns, of the matrix are permuted. Thus, the entry corresponding to row $(a, b)$ and column $(c, d)$ becomes $\rho_i[b, c] \cdot \rho_j[a, d]$. A diagonal entry has $(a, b) = (c, d)$ which is $\rho_i[b, a] \cdot \rho_j[a, b]$. If $a = b = 0$, then the entry corresponding to row $(0, 0)$ and column $(0, 0)$ is

$$\rho_i[0, 0] \cdot \rho_j[0, 0] = \text{Tr}(\rho_i |\tau\rangle\langle \tau|) \cdot \text{Tr}(\rho_j |\tau\rangle\langle \tau|).$$

(5.7)

Now consider the case where $a \neq 0$ or $b \neq 0$. Assume, without loss of generality, that $a \neq 0$. If $a \in \{1, \ldots, r\}$ then $\rho_j[a, b] = 0$ because the support of $\rho_j$ is contained in the space spanned by
\{|\tau\} \cup \{|r+1, \ldots, |D-1\}\). Similarly, if \(a \in \{r+1, \ldots, D-1\}\) then \(\rho_i[b,a] = 0\) because the support of \(\rho_i\) is contained in the space spanned by \(\{|\tau\}\} \cup \{|1, \ldots, |r\}\). In either case \(\rho_i[b,a] \cdot \rho_j[a,b] = 0\). A similar argument holds for \((\rho_i \otimes \rho_j)S\) where the columns are permuted instead of the rows. \(\square\)

**Lemma 5.3 (Change in Overlap After One Iteration)** Suppose that the Swap Test is performed on \(|0\rangle\langle 0| \otimes \rho_1 \otimes \rho_2\). The first register holds the control qubit, and the second and third registers are \(n\)-qubit registers that hold \(\rho_1\) and \(\rho_2\), respectively. Suppose also that \(\text{Tr}(\rho_1 \mid \tau\rangle\langle \tau\mid) = a_1\) and \(\text{Tr}(\rho_2 \mid \tau\rangle\langle \tau\mid) = a_2\). If the measurement outcome is 0, and \(\rho\) is the result of tracing out the first and third registers, then

1. \(\text{Tr}(\rho \mid \tau\rangle\langle \tau\mid) \geq (a_1 + a_2)/2\)

2. If \(a_1 \geq a\) and \(a_2 \geq a\) for some constant \(a\), then \(\text{Tr}(\rho \mid \tau\rangle\langle \tau\mid) \geq \frac{a(1+a)}{1+a^2}\).

**Proof:** According to Lemma 5.1, the contents of the second and third registers after the 0 is measured in the first register is \(|0\rangle\langle 0| \otimes \bar{\rho} / \text{Tr}(\bar{\rho})\), where \(\bar{\rho}\) is given by eq. (5.2). We will first calculate \(\text{Tr}(\bar{\rho})\). Since \(\text{Tr}(\rho_1) = \text{Tr}(\rho_2) = 1\), we have that \(\text{Tr}(\rho_1 \otimes \rho_2) = 1\) and \(\text{Tr}(S(\rho_1 \otimes \rho_2)S) = \text{Tr}(\rho_2 \otimes \rho_1) = 1\). Lemma 5.2 implies that \(\text{Tr}(S(\rho_1 \otimes \rho_2)) = \text{Tr}(S(\rho_1 \otimes \rho_2)S) = a_1a_2\). Therefore \(\text{Tr}(\bar{\rho}) = 2(1 + a_1a_2)\).

Now consider the state \(\bar{\rho} / \text{Tr}(\bar{\rho})\) in registers 2 and 3. Let \(\{|\tau\} \cup \{|1, \ldots, |D-1\}\}\) be a basis for the Hilbert space of each register. We can express the state \(\bar{\rho} / \text{Tr}(\bar{\rho})\) as a \(D^2 \times D^2\) matrix, which can be divided into \(D \times D\) submatrices of dimension \(D \times D\). When we trace out the third register, the result is \(\rho\), which is a \(D \times D\) matrix, where each entry is the trace of the corresponding submatrix in \(\bar{\rho} / \text{Tr}(\bar{\rho})\). The value of \(\text{Tr}(\rho \mid \tau\rangle\langle \tau\mid)\) is the trace of the submatrix in the upper left corner. We will consider the four terms in \(\rho\) separately. The contribution from \(\rho_1 \otimes \rho_2\) is \(\rho_1[0,0]\). \(\text{Tr}(\rho_2) = a_1\). The contribution from \(S(\rho_1 \otimes \rho_2)\) is \(\rho_2[0,0] \cdot \text{Tr}(\rho_1) = a_2\). From Lemma 5.2 \(S(\rho_1 \otimes \rho_2)\) and \((\rho_1 \otimes \rho_2)\) have the same diagonal, which consists of \(a_1a_2\) in the upper left corner and 0 elsewhere. Therefore the contribution from each of these matrices is \(a_1a_2\). The result is that

\[
\text{Tr}(\rho \mid \tau\rangle\langle \tau\mid) = \frac{a_1 + a_2 + 2a_1a_2}{2(1 + a_1a_2)} = \frac{a_1 + a_2}{1 + a_1a_2}. \tag{5.8}
\]

To establish the first fact in the lemma, since \((a_1 + a_2)/2 \in [0,1]\),

\[
\text{Tr}(\rho \mid \tau\rangle\langle \tau\mid) = \frac{a_1 + a_2}{1 + a_1a_2} \geq \frac{a_1 + a_2}{2}. \tag{5.9}
\]

Now for the second fact, note that

\[
\text{Tr}(\rho \mid \tau\rangle\langle \tau\mid) = \frac{a_1 + a_2}{1 + a_1a_2} \geq \frac{\sqrt{a_1a_2} + a_1a_2}{1 + a_1a_2}, \tag{5.10}
\]

where the inequality follows from the fact that the arithmetic mean/geometric mean inequality. Define \(\gamma \overset{\text{def}}{=} \sqrt{a_1a_2}\), so \(\text{Tr}(\rho \mid \tau\rangle\langle \tau\mid) \geq (\gamma + \gamma^2)/(1 + \gamma^2)\). Since \(a_1 \geq a\) and \(a_2 \geq a\), we have that \(1 \geq \gamma \geq a \geq 0\) and we would like to show that

\[
\frac{\gamma + \gamma^2}{1 + \gamma^2} \geq \frac{a + a^2}{1 + a^2}. \tag{5.11}
\]
After some rearranging, this inequality is equivalent to
\[ \gamma^2 + (\gamma - a) \geq a^2 + \gamma a (\gamma - a). \]  
(5.12)

Since \( \gamma \geq a \) and \( \gamma a \leq 1 \), it follows that \( (\gamma - a) \geq \gamma a (\gamma - a) \). The fact that \( \gamma \geq a \) also implies that \( \gamma^2 \geq a^2 \). The sum of the two inequalities implies the inequality in eq. (5.12). \( \Box \)

We are now ready to analyze the result of the entire SwapTestDistillation algorithm. First we need some definitions to describe the state of the algorithm after each iteration.

**Definition 5.4** Let \( m_k \) be the number of surviving registers after the \( k^{th} \) iteration of the algorithm. Initially \( m_0 = m \), the number of states at the beginning of the algorithm. We will denote the state in the \( j^{th} \) surviving register after \( k \) iterations as \( \rho_{j,k} \), for \( 1 \leq j \leq m_k \).

**Lemma 5.5 (Overlap After \( \ell \) Rounds)** Suppose that the SwapTestDistillation algorithm lasts for \( \ell \) rounds, then for every \( 1 \leq j \leq m_{\ell} \),

\[ 1 - \text{Tr}(\rho_{j,\ell} | \tau \rangle \langle \tau |) \leq \frac{1}{2} \cdot \left( \frac{4}{5} \right)^{\ell - 2/a^2}. \]  
(5.13)

where \( a \) is a lower bound on the overlap of every input state with the target state.

**Proof:** Let \( \gamma_i \) be the smallest overlap of any of the surviving registers after \( i \) rounds. We start with \( \gamma_0 \geq a \). Using Lemma 5.3, we have by induction that

\[ \gamma_{i+1} \geq \gamma_i \cdot \frac{1 + \gamma_i}{1 + (\gamma_i)^2}. \]  
(5.14)

Since \( \gamma_i \leq 1 \), this recurrence implies that the \( \gamma_i \)'s are strictly increasing. We start by analyzing the number of iterations to reach \( \gamma \geq 1/2 \). If \( \gamma_i \leq 1/2 \), then

\[ \frac{\gamma_i + (\gamma_i)^2}{1 + (\gamma_i)^2} = (\gamma_i + (\gamma_i)^2) \left( 1 - \frac{(\gamma_i)^2}{1 + (\gamma_i)^2} \right) \geq (\gamma_i + (\gamma_i)^2)(1 - (\gamma_i)^2) \geq \gamma_i + (\gamma_i)^2 - (\gamma_i)^3 - (\gamma_i)^4 \geq \gamma_i + (\gamma_i)^2 - (\gamma_i)^2(1/2 + 1/4) \geq \gamma_i + (\gamma_i)^2/4. \]  
(5.15)

(5.16)

(5.17)

(5.18)

(5.19)

Since \( \gamma_{i+1} \geq \gamma_i + (\gamma_i)^2/4 \), we know that \( \gamma_{i+1} - \gamma_i \geq (\gamma_0)^2/4 \). Therefore, the number of iterations to reach \( 1/2 \) from \( \gamma_0 \) is at most \( 4(1/2 - \gamma_0)/(\gamma_0)^2 \leq 2/a^2 \). Next we show that once \( \gamma_i \) reaches \( 1/2 \), then \( 1 - \gamma_i \) decreases by a constant factor in each iteration.

\[ 1 - \gamma_{i+1} \leq 1 - \gamma_i \cdot \frac{1 + \gamma_i}{1 + (\gamma_i)^2} \leq \frac{1 - \gamma_i}{1 + (\gamma_i)^2} \leq \frac{4}{5}(1 - \gamma_i), \]  
(5.20)

where the last inequality uses the assumption that \( \gamma_i \geq 1/2 \).

After the next \( 2/a^2 \) iterations, \( 1 - \gamma_k \leq 1/2 \). After every successive iteration, \( 1 - \gamma_k \) decreases by a factor of \( 4/5 \). The lemma follows. \( \Box \)

Finally, \( \ell \) the number of rounds must be chosen so that given the number of input states, with high probability, the algorithm lasts for \( \ell \) rounds.
Lemma 5.6 (Probability of a Surviving Register After $\ell$ Rounds) For $m \geq n \cdot 6^\ell$ and $n \geq 12$, the probability that there are no surviving registers after $\ell$ rounds is at most $2\exp(-n/12)$.

Proof: First we analyze the probability that $m_k \geq n \cdot 6^{\ell-k}$ conditioned on the event that $m_{k-1} \geq n6^{\ell-k+1}$. There will be $m_{k-1}/2$ pairs in round $k$ to which the Swap Test is applied. Each pair succeeds with probability at least $1/2$. The number of registers surviving to round $k$ is the number of pairs that succeed the swap test. Thus, the expected number of surviving registers is $m_{k-1}/4$. Using Chernoff’s Inequality, the probability that there are fewer than $m_{k-1}/6$ is at most $\exp[-(m_{k-1}(1/3)^2(1/2))] = \exp(-m_{k-1}/72)$ (5.21)

The probability that any of the iterations fails to keep $1/6$ of their registers is at most $\sum_{k=0}^{\ell-1} \exp(-n \cdot 6^{\ell-k}/72) \leq 2\exp(-n/12)$. (5.22)

Theorem 5.7 (Swap Test Distillation Performance: No Overlap) For every pair of constants $c$ and $a \in [0,1]$, there is a polynomial $p$ such that if the DISTILLATION\textsc{SwapTest} algorithm starts with $m$ states $|\psi_1\rangle, \ldots, |\psi_m\rangle$ such that $m \geq p(n)$ and

1. for all $j$, $|\langle \psi_j | \tau \rangle|^2 \geq a$
2. for all $i \neq j$, $\langle \psi_j | (I - |\tau\rangle\langle\tau|) |\psi_i\rangle = 0$,

then the algorithm succeeds with probability at least $1 - \exp(-n/12)$ in producing a state $\rho$ such that $\text{Tr}\{|\tau\rangle\langle\tau| \rho\} \geq 1 - 1/n^c$.

Proof: The proof follows directly from Lemmas 5.5 and 5.6 and selecting the polynomial $p(n) \geq n \cdot 6^\ell$, where $\ell = c \log_{5/4}(2n) + 2/a^2$. The probability of success is at least $1 - 2\exp(-n/12)$. □

Relaxing the Conditions for Swap Test Distillation. We can relax the requirements for Theorem 5.7 so that the expected overlap (instead of the actual overlap) of each input state is at least some constant $a$ as long as the input states are orthogonal outside the $|\tau\rangle$ component. The algorithm will require some additional rounds in this case, which in turn requires a larger number of input states. The analysis for small overlap in the next section applies to both versions.

Theorem 5.8 (Swap Test Distillation Performance: Relaxed Conditions, No Overlap) For every pair of constants $c$ and $a \in [0,1]$, there is a polynomial $p$ such that if the DISTILLATION\textsc{SwapTest} algorithm starts with $m$ states $|\psi_0\rangle, \ldots, |\psi_m\rangle$ generated according to some independent randomness such that $m \geq p(n)$ and

1. for all $j$, $\mathbb{E}[|\langle \psi_j | \tau \rangle|^2] \geq a$
2. for all $i \neq j$, $\langle \psi_j | (I - |\tau\rangle\langle\tau|) |\psi_i\rangle = 0$,

then the algorithm succeeds with probability at least $1 - 2\exp(-n/12) - m2^{-n}$ in producing a state $\rho$ such that $\text{Tr}\{|\tau\rangle\langle\tau| \rho\} \geq 1 - 1/n^c$.}

33
Proof: A state $\rho$ in a register that survives after $\ell$ rounds depends on exactly $2^\ell$ input states. After $\ell'$ rounds, there are $2^{\ell-\ell'}$ surviving registers that will be used to create the final surviving state $\rho$. Consider an arbitrary $\rho'$ in one of these registers after $\ell'$ rounds. $L'$ input states are used to create $\rho'$, where $L' = 2^{\ell'}$. Let $a_1, \ldots, a_{L'}$ be the overlap of each of those input states with the target state. Then by Lemma 5.3, $\text{Tr} \{ \rho | \tau \langle \tau | \} = a_1, \ldots, a_{L'}$. Note that the event that the register containing $\rho$ survives is not independent from the $a_1, \ldots, a_{L'}$, but the probability of a successful swap test increases with the average of the overlaps of the pair of registers to which it is applied. Therefore, the probability that an arbitrary $L'$ registers have an average overlap of $a/2$ is a lower bound on the probability when we condition on the register surviving to a particular round.

Let $S_j = \left( \sum_{i=1}^{j} a_i \right) - ja$, where $a$ is the expected overlap of each initial state with the target states. The sequence $S_0, \ldots, S_{L'}$ forms a Martingale with $|S_{j+1} - S_j| \leq 1 - a$. The event that the average of the $a_i$’s is less than $a/2$ is the same as $S_{L'} \leq -aL'/2$. We can apply Azuma’s Inequality (Lemma A.9) to get that the probability $S_{L'} \leq -aL'/2$ is at most $\exp(-L' a^2 / 8(1 - a)^2)$. We will select $L' = 8n(1 - a)^2 / a^2$ so that the probability of a surviving register after $L'$ rounds not having overlap at least $a/2$ is at most $2^{-n}$. Since $\ell' = \log_2(L')$, $\ell' = \log_2 n + \log_2(8(1 - a)^2 / a^2)$. The probability that all of the $2^\ell - \ell'$ registers that are used to create $\rho$ have an overlap of $a/2$ with the target state is at least $1 - 2^{\ell'-\ell-n}$.

Assuming that this condition is true, we can now apply Lemmas 5.5 and 5.6 using a lower bound of $a/2$ on the overlap instead of $a$. By selecting the polynomial $p(n) \geq n \cdot 6^\ell$, where $\ell = c \log_{5/4}(2n) + 8/a^2 + \log_2 n + \log_2(8(1 - a)^2 / a^2)$. The probability of success is at least $1 - 2\exp(-n/12) - 2^{\ell-n} \geq 1 - 2\exp(-n/12) - m2^{-n}$. $\square$

5.3 Analysis: small overlap case

Now we extend the analysis for the DISTILLATIONSWAPTEST algorithm to the situation where there is a small overlap between the portion of each state that is orthogonal to $|\tau\rangle$. We have expressed each state $|\psi_i\rangle$ as $\alpha_j |\tau\rangle + \beta_j |\phi_j\rangle$, where $|\phi_j\rangle$ lies in the space perpendicular to $|\tau\rangle$. Previously, we assumed that for $i \neq j$, $\langle \phi_i | \phi_j \rangle = 0$. Now we will assume that $|\langle \phi_i | \phi_j \rangle|^2 \leq \delta$. Note that this is a weaker assumption that Condition 2: $|\langle \psi_i | (I - |\tau\rangle \langle \tau | \psi_j) \rangle|^2 \leq \delta$.

We will use the Gram-Schmidt procedure to produce a new orthonormal set $\{ |1\rangle, \ldots, |m\rangle \}$, all of which are orthogonal to $|\tau\rangle$, and such that for each $j$, the space spanned by $\{ |\phi_1\rangle, \ldots, |\phi_j\rangle \}$ lies in the space spanned by $\{ |1\rangle, \ldots, |j\rangle \}$. Specifically:

$$|j\rangle = \frac{|\phi_j\rangle - \sum_{i=1}^{j-1} |i\rangle \langle i | \phi_j \rangle}{\| |\phi_j\rangle - \sum_{i=1}^{j-1} |i\rangle \langle i | \phi_j \rangle \|}.$$  (5.23)

We will use $|0\rangle$ to represent the target state $|\tau\rangle$. We can now break up $|\phi_j\rangle$ into components: $|j\rangle$ and $|\tilde{\phi}_j\rangle$, where $|\phi_j\rangle$ is orthogonal to $|j\rangle$:

$$|\phi_j\rangle = \alpha_j |0\rangle + \beta_j |\phi_j\rangle = \alpha_j |0\rangle + \beta_j \left( \langle j | \phi_j \rangle |j\rangle + \tilde{\beta}_j |\phi_j\rangle \right),$$  (5.24)

where

$$|\tilde{\phi}_j\rangle = \frac{\sum_{i=1}^{j-1} |i\rangle \langle i | \phi_j \rangle}{\| \sum_{i=1}^{j-1} |i\rangle \langle i | \phi_j \rangle \|}.$$  (5.25)
First, we would like to show that for all of the states $|\psi_j\rangle$, most of the weight is on $|\tau\rangle$ and $|j\rangle$ so that the initial collection of states closely approximates a tensor product of states with no overlap as assumed in the previous section. Thus we would like to bound $|\tilde{\beta}_j|^2$ for every $j$.

**Lemma 5.9** If $|\langle \phi_j | \psi_i \rangle|^2 \leq \delta$ for all $i \neq j$ and $\sqrt{\delta} \leq 1/8m$, then for all $j$, $|\tilde{\beta}_j|^2 \leq (2j - 1)\delta$.

**Proof:** We will define a parameter $a_i$ that is an upper bound for $|\langle \phi_j | i \rangle|^2$ for any $j > i$ and define

$$b_j \equiv a_1 + \cdots + a_j.$$ 

$b_{i-1}$ is an upper bound for $|\tilde{\beta}_i|^2$.

We will derive a recurrence to upper bound the $b_j$’s and show by induction that $b_j \leq (2j - 1)\delta$. For the base case, $|\phi_1\rangle = |1\rangle$, for all $j > 1$, $|\langle \phi_j | 1 \rangle|^2 \leq \delta$, so $a_1 = b_1 = \delta$. Now we will derive a recurrence relation for the $b_j$’s. For $j > i$, we can express the inner product $\langle \phi_j | \phi_i \rangle$ as

$$\langle \phi_j | \phi_i \rangle = \langle i | \phi_i \rangle \langle \phi_j | i \rangle + \langle i - 1 | \phi_i \rangle \langle \phi_j | i - 1 \rangle + \cdots + \langle 0 | \phi_i \rangle \langle \phi_j | 0 \rangle,$$

and solve for $|\langle \phi_j | i \rangle|^2$:

$$|\langle \phi_j | i \rangle|^2 = \frac{|\langle \phi_j | \phi_i \rangle - \sum_{k=1}^{i-1} |\langle k | \phi_i \rangle ||\langle \phi_j | k \rangle|||^2}{|\langle i | \phi_i \rangle|^2}.$$ 

(5.28)

$$|\langle \phi_j | \phi_i \rangle|^2 \leq \frac{2 \sum_{k=1}^{i-1} |\langle k | \phi_i \rangle||\langle \phi_j | k \rangle||^2}{1 - \sum_{k=1}^{i-1} |\langle k | \phi_i \rangle|^2}.$$ 

(5.29)

$\sqrt{\delta}$ is an upper bound for $|\langle \phi_j | \phi_i \rangle|$ and $\sqrt{a_k}$ is an upper bound for both $|\langle k | \phi_i \rangle|$ and $|\langle \phi_j | k \rangle|$. Therefore,

$$|\langle \phi_j | i \rangle|^2 \leq \frac{\delta + 2\sqrt{\delta} \sum_{k=1}^{i-1} a_k + \left[ \sum_{k=1}^{i-1} a_k \right]^2}{1 - \sum_{k=1}^{i-1} a_k} = \frac{\delta + 2\sqrt{\delta} b_{i-1} + [b_{i-1}]^2}{1 - b_{i-1}}.$$ 

(5.30)

We will use the expression above on the right as $a_i$ to get:

$$b_i = b_{i-1} + a_i = b_{i-1} + \frac{\delta + 2\sqrt{\delta} b_{i-1} + [b_{i-1}]^2}{1 - b_{i-1}}.$$ 

(5.31)

We will show that if $b_{i-1} \leq (2i - 3)\delta$, then $b_i \leq (2i - 1)\delta$. The assumption $\sqrt{\delta} \leq 1/8m$ in the statement of the lemma implies that $\sqrt{\delta} \leq 1/8$. Also since by the inductive hypothesis,
Then the algorithm succeeds with probability at least \( \frac{1}{b} \). The original state is orthogonal to the target state. 

**Proof:** Let \( b = b_{i-1} + \frac{\delta + 2\sqrt{\delta}b_{i-1} + [b_{i-1}]^2}{1 - b_{i-1}} \) (5.32)

\[
\leq (2i - 3)\delta + (\delta + 2\sqrt{\delta}b_{i-1} + [b_{i-1}]^2) \cdot \frac{32}{31}
\]  

(5.33)

\[
\leq (2i - 3)\delta + \left( \delta + \frac{\delta}{2} + \frac{\delta}{16} \right) \cdot \frac{32}{31}
\]  

(5.34)

\[
\leq (2i - 3)\delta + 2\delta = (2i - 1)\delta.
\]  

(5.35)

We are now ready to bound the effect of the small overlap between the components of each state that is orthogonal to the target state.

**Theorem 5.10 (Swap Test Distillation Performance: Small Overlap)** For every pair of constants \( c \) and \( a \in [0, 1] \), there is a polynomial \( p \) such that if the DISTILLATIONSWAPTEST algorithm starts with \( m \) states \( |\psi_1\rangle, \ldots, |\psi_m\rangle \) such that \( m \geq p(n) \) and

1. for all \( j \), \( |\langle \psi_j | \tau \rangle|^2 \geq a \)

2. for all \( i \neq j \), \( |\langle \psi_j | (I - |\tau\rangle\langle\tau|) |\psi_i\rangle|^2 \leq \delta \),

then the algorithm succeeds with probability at least \( 1 - 2\exp(-n/12) - 4m\sqrt{\delta} \) in producing a state \( \rho \) such that \( \text{Tr}\{\rho |\tau\rangle\langle\tau|\} \geq 1 - 1/n^c - 8m^2\sqrt{\delta} \).

**Proof:** Let \( \epsilon = 1 - \prod_{j=1}^{m} (1 - 2j\delta) \). Note that \( \epsilon \leq 2m^2d \). We can define the state

\[
|\Omega\rangle = \frac{1}{\sqrt{1-\epsilon}}(a_1 |\tau\rangle + \beta_1 |1\rangle) \otimes (a_2 |\tau\rangle + \beta_2 |2\rangle) \otimes \cdots \otimes (a_m |\tau\rangle + \beta_m |m\rangle).
\]  

(5.36)

The original state \(|\Psi\rangle = |\psi_1\rangle \otimes \cdots \otimes |\psi_m\rangle\) is equal to

\[
(1 - \epsilon)^{1/2} |\Omega\rangle + \sqrt{\epsilon} |\Phi\rangle.
\]  

(5.37)

for some state \(|\Phi\rangle\) that is orthogonal to \(|\Omega\rangle\). Furthermore, \(|\Omega\rangle\) has the properties assumed in the no-overlap case.

Now imagine a coherent version of the DISTILLATIONSWAPTEST algorithm in which the measurements are deferred to the end. For coherence, we will need to fix the number of iterations to \( \ell \) so that in the no-overlap case, there is at least one surviving register after \( \ell \) iterations with some probability \( p \) that is exponentially close to 1. We will have auxiliary qubits \( b_1, \ldots, b_m \) such that \( b_j = 1 \) if Register \( R_j \) survives the \( \ell \) rounds, and a final qubit \( s \) such that \( s = 1 \) if any of the registers succeed after \( \ell \) rounds. Thus, if qubit \( s = 1 \) when measured then the algorithm succeeds. The result of applying the algorithm (before measurement) is \( A(|\Psi\rangle \otimes |0\rangle) \), where the second register contains the auxiliary qubits initialized to 0. \( A \) is the unitary performed by the DISTILLATIONSWAPTEST algorithm before measurement.

\[
A(|\Psi\rangle \otimes |0\rangle) = (1 - \epsilon)^{1/2} A(|\Omega\rangle \otimes |0\rangle) + \sqrt{\epsilon} A(|\Phi\rangle \otimes |0\rangle)
\]  

(5.38)

\[
= (1 - \epsilon)^{1/2}[a_0 |0\rangle_s |\Omega_0\rangle + \beta_0 |1\rangle_s |\Omega_1\rangle]
\]  

(5.39)

\[
+ \sqrt{\epsilon}[a_1 |0\rangle_s |\Phi_0\rangle + \beta_1 |1\rangle_s |\Phi_1\rangle]
\]  

(5.40)
The probability of success with $|\Omega\rangle$ is at least $p$, so $|\beta_0|^2 \geq p$. The probability of success with $|\Psi\rangle$ is then at least

$$[(1 - \epsilon)^{1/2} \beta_0 - \sqrt{\epsilon}]^2 \geq p - 2\sqrt{\epsilon}. \quad (5.41)$$

In the no-overlap case (Theorem 5.7) if we select $\ell = c \log_{5/4}(2n) + 2/a^2$ and $m \geq n \cdot 6^\ell$, then The probability of success $p$ is at least $1 - 2\exp(-n/12)$. The probability of success with overlap $\delta$ is then

$$1 - 2\exp(-n/12) - 2\sqrt{\epsilon} \geq 1 - 2\exp(-n/12) - 4m\sqrt{\delta}. \quad (5.42)$$

Now suppose that we change the algorithm slightly so that when a pair of registers passes the swap test, the register that survives to the next iteration is selected randomly from the pair. Since the $|\psi_j\rangle$ are all generated according to the same process, the probability of any register surviving the the last stage is the same for every register. There are $m$ registers and the probability of success is at least $p$, so the probability that any particular register survives is at least $p/m$. We are going to analyze the contents of register $R_j$ conditioned on the event that the register survives and shows that the probability that this register contains the target state $|\tau\rangle$ conditioned on survival is roughly the same, regardless if we start with $|\Psi\rangle$ or $|\Omega\rangle$. Qubit $b_j$ contains the information regarding the survival of register $R_j$, so are interested in the probability that $R_j$ contains $|0\rangle$ conditioned on $b_j = 1$. To ease the notation, we will drop the subscript $j$ and just refer to qubit $b$ and register $R$. We can divide $A(|\Omega\rangle \otimes |0\rangle)$ into three components:

$$a \langle 0 |_s |\Psi_0\rangle + \beta_0 \langle 1 |_s |\tau\rangle_R |\Psi_{10}\rangle + \beta_1 \langle 1 |_s |\phi\rangle_R |\Psi_{11}\rangle , \quad (5.43)$$

where $|\phi\rangle$ is an $n$-qubit state in register $R$ that is orthogonal to $|\tau\rangle$. The probability that register $R_j$ survives is $|\beta_0|^2 + |\beta_1|^2 \geq p/m$. The overlap of the state in $R$ with $|\tau\rangle$ conditioned on $R$ surviving is $|\beta_0|^2 / (|\beta_0|^2 + |\beta_1|^2)$. Since $|\Omega\rangle$ satisfied the non-overlapping condition from Theorem 5.7, this quantity is some $q$, which is at least $1 - 1/n^c$. If we start with $A(|\Psi\rangle \otimes |0\rangle)$ instead, this quantity will be at least

$$\frac{|(1 - \epsilon)^{1/2} \beta_0 - \sqrt{\epsilon_1}|^2}{|(1 - \epsilon)^{1/2} \beta_0 - \sqrt{\epsilon_1}|^2 + |\beta_1 + \sqrt{\epsilon_2}|^2} \quad (5.44)$$

where $\epsilon_1 + \epsilon_2 \leq \epsilon$. $\epsilon_1/\epsilon$ is the probability of measuring $|1\rangle_s |\tau\rangle_R$ with state $A(|\Phi\rangle \otimes |0\rangle)$ and $\epsilon_2/\epsilon$ is the probability of measuring $|1\rangle_s |\phi\rangle_R$, where $|\phi\rangle$ is orthogonal to $|\tau\rangle$. This quantity is minimized with $\epsilon_1 = \epsilon$ and $\epsilon_2 = 0$, which gives:

$$\frac{|(1 - \epsilon)^{1/2} \beta_0 - \sqrt{\epsilon}|^2}{|(1 - \epsilon)^{1/2} \beta_0 - \sqrt{\epsilon}|^2 + |\beta_1|^2} \geq \frac{|\beta_0|^2 - 2\sqrt{\epsilon}}{|\beta_0|^2 + |\beta_1|^2 - 2\sqrt{\epsilon}} \geq \frac{|\beta_0|^2 - 2\sqrt{\epsilon}}{|\beta_0|^2 + |\beta_1|^2} \geq q - \frac{2m\sqrt{\epsilon}}{p}. \quad (5.45)$$

Thus if $\rho$ is the state in Register $R$ conditioned on $R$ surviving $\ell$ rounds ($b = 1$), then

$$\text{Tr}\{\rho |\tau\rangle \langle \tau|\} \geq q - \frac{2\sqrt{\epsilon}}{p/m} \geq 1 - \frac{1}{n^c} - 4m\sqrt{\epsilon} \geq 1 - \frac{1}{n^c} - 8m^2 \sqrt{\delta}. \quad (5.48)$$

The first inequality above holds if $n$ is large enough so that the probability of success $p = 1 - 2\exp(-n/12)$ is at least $1/2$. \hfill \Box
6 2-query state synthesis algorithm with exponentially small error

We now describe a 2-query state synthesis algorithm that achieves exponentially small error. Like with the 1-query algorithm from Section 4, it will be space-efficient, but not time-efficient. And also like in Section 4, we first describe a version of the algorithm with exponential space complexity, and then describe how to reduce the space complexity to polynomial.

6.1 A space-inefficient algorithm

Let \( d = 2^n, n' = n^2 \) and \( d' = 2^n \). Let \( \{\sigma_{U,V}\}_{U,V} \) denote a set of permutations on \( \{0,1\}^{n'} \), indexed by unitaries \( U, V \) on \( n' \) qubits. For all unitaries \( U, V \) and \( n' \)-bit strings \( x \), let \( \phi(U, V, x) \) denote a number in \( [0, 2\pi) \), representable using \( (n')^2 \) bits. We will specify \( \{\sigma_{U,V}\} \) and \( \phi \) later. Define the oracles

\[
\begin{align*}
    f(U, V, x) &\equiv (\phi(U, V, x), \sigma_{U,V}(x)) \quad \text{and} \quad g(U, V, y) = (\sigma_{U,V}^{-1}(y), \phi(U, V, \sigma_{U,V}^{-1}(y))) .
\end{align*}
\]

These oracles have the property that if \( f(U, V, x) = (\phi, y) \), then \( g(U, V, y) = (x, \phi) \).

---

**TwoQueryStateSynthesis (space inefficient version)**

1. Sample Haar-random \( n' \)-qubit unitaries \( U, V \).
2. Prepare the state \( |\theta\rangle = U |0\rangle^{\otimes n'} \) in an \( n' \)-qubit register \( A \).
3. Controlled on basis state \( |x\rangle \) in register \( A \), call the oracle \( f \) on input \( (U, V, x) \) to obtain \( \phi \in [0, 2\pi) \) in register \( B \) and \( y \in \{0, 1\}^{n'} \) in register \( C \).
4. Controlled on basis state \( |\phi\rangle \) in register \( B \), apply the phase \( e^{i\phi} \).
5. Controlled on basis state \( |y\rangle \) in register \( C \), call the oracle \( g \) on input \( (U, V, y) \) to uncompute \( |x\rangle \otimes |\phi\rangle \) in registers \( A \) and \( B \).
6. Apply the inverse unitary \( V^\dagger \) on register \( C \).
7. Output the first \( n \) qubits of register \( C \).

---

Figure 4: Pseudo-code for the TwoQueryStateSynthesis query algorithm that uses exponential space complexity.

The algorithm has the following behavior. Fix unitaries \( U, V \). Let

\[
|\theta\rangle = U |0\rangle^{\otimes n'} = \sum_{x \in \{0,1\}^{n'}} u_x |x\rangle
\]

where \( u_x \in \mathbb{C} \) are amplitudes that depend on the unitary \( U \). After Step 3 of the algorithm, the state of registers ABC is

\[
\sum_x u_x |x\rangle_A \otimes |\phi(U, V, x)\rangle_B \otimes |\sigma_{U,V}(x)\rangle_C .
\]

After Step 4, the state becomes

\[
\sum_x e^{i\phi(U,V,x)} u_x |x\rangle_A \otimes |\phi(U, V, x)\rangle_B \otimes |\sigma_{U,V}(x)\rangle_C .
\]
We now analyze the distance between eq. (6.6) and have that since $k$ is the non-increasing order. Let $u$ close to the same rank of function $\phi$. The state of register $C$ at the end of the algorithm is thus

$$V^* \sum_x e^{i\phi(U,V,x)} u_x |\sigma_{U,V}(x)\rangle_C .$$

We now argue that for every choice of $n$-qubit state $|\psi\rangle$, there exist permutations $\{\sigma_{U,V}\}_{U,V}$ and a function $\phi(U,V,x)$ such that the state in eq. (6.6), with high probability over $U,V$, is exponentially close to $|\psi\rangle \otimes |0\rangle^\otimes n' - n$. Write

$$V(|\psi\rangle \otimes |0\rangle^\otimes n' - n) = \sum_{y \in \{0,1\}^n} v_y |y\rangle .$$

Let $u = (u_x)_{x \in \{0,1\}^{n'}}$ and $v = (v_y)_{y \in \{0,1\}^n}$. Let $|u|$ and $|v|$ denote the entry-wise absolute values of $u$ and $v$, respectively. For a vector $v \in \mathbb{R}^m$, let sort$(v) \in \mathbb{R}^m$ denote the entries of $v$ sorted in non-increasing order.

Define the permutation $\sigma_{U,V}$ on $\{0,1\}^{n'}$ to be such that $\sigma_{U,V}(x) = y$ if and only if $|u_x|$ and $|v_y|$ have the same rank in the sorted $\text{sort}(|u|)$ and $\text{sort}(|v|)$, respectively. In other words, if $|u_x|$ is the $k$'th largest entry in $\text{sort}(|u|)$, then $|v_y|$ must also be the $k$'th largest entry in $\text{sort}(|v|)$.

Define $\phi(U,V,x)$ to be the best $(n')^2$-bit approximation of the phase $\theta(U,V,x) \in [0,2\pi)$ such that $e^{i\theta(U,V,x)} u_x$ has the same phase as $v_y$ where $y = \sigma_{U,V}(x)$. In other words, for all $U,V,x$, we have

$$|\phi(U,V,x) - \theta(U,V,x)| \leq \exp(-\Omega(n'^2)) .$$

Since $|e^{ib} - e^{ia}| \leq |a - b|$ for all $a, b \in \mathbb{R}$, we have

$$|e^{i\phi(U,V,x)} - e^{i\theta(U,V,x)}| \leq \exp(-\Omega(n'^2)) .$$

We now analyze the distance between eq. (6.6) and $|\psi\rangle \otimes |0\rangle^\otimes n' - n$, or equivalently, the distance

$$\left\| \sum_x e^{i\phi(U,V,x)} u_x |\sigma_{U,V}(x)\rangle - V(|\psi\rangle \otimes |0\rangle^\otimes n' - n) \right\|^2$$

$$= \left\| \sum_x \left( e^{i\phi(U,V,x)} u_x - v_{\sigma_{U,V}(x)} \right) |\sigma_{U,V}(x)\rangle \right\|^2$$

$$\sum_x \left| e^{i\phi(U,V,x)} u_x - v_{\sigma_{U,V}(x)} \right|^2$$

$$\sum_x \left| e^{i\theta(U,V,x)} u_x - v_{\sigma_{U,V}(x)} \right|^2$$

$$\leq \sum_x \left( \left| e^{i\theta(U,V,x)} u_x - v_{\sigma_{U,V}(x)} \right|^2 + \left| e^{i\theta(U,V,x)} - e^{i\phi(U,V,x)} \right|^2 \right)$$

$$\leq \sum_x 2 \left| u_x \right|^2 + 2 \left| e^{i\theta(U,V,x)} - e^{i\phi(U,V,x)} \right|^2$$

$$\leq 2 \left\| \text{sort}(|u|) - \text{sort}(|v|) \right\|^2 + 2 n' \exp(-\Omega(n'^2))$$
where Equation (6.13) follows from the definition of $\phi(U, V, x)$, and the last line follows from the definition of the permutation $\sigma_{U, V}$ as well as Equation (6.9).

We now argue that, with overwhelming probability, the distance $\|\text{sort}(|u|) - \text{sort}(|v|)\|^2$ is exponentially small. Notice that the vectors $u, v$ correspond to the amplitudes of two independent Haar-random states on $n'$ qubits; this allows us to use the following Proposition.

**Proposition 6.1.** Let $u, v$ denote two independent Haar-random unit vectors in $\mathbb{C}^d$. There exist universal constants $C, C' > 0$ such that

$$\Pr\left[\|\text{sort}(|u|) - \text{sort}(|v|)\| \geq C d^{-1/4}\right] \leq \exp(-C'd^{1/4})$$

(6.16)

where the probability is over the choice of $u, v$.

Applying Proposition 6.1 shows that with probability at least $1 - \exp(-\Omega((d')^{1/4}))$ over the choice of $U, V$, the output of the algorithm is $O((d')^{-1/4})$-close to $|\psi\rangle$.

### 6.2 A space-efficient algorithm

The algorithm described above suffers from needing exponential space complexity; this is because specifying a Haar-random unitary on $n'$ qubits requires $\exp(\Omega(n'))$ space, and thus the oracles $f, g$ need to act on exponentially many input bits. We derandomize this construction, and show via the probabilistic method that there exists a single choice of unitary $U, V$ that works for all $n$-qubit states — this is why we expanded the space to dimension $d'$.

Let $|\psi_1\rangle, \ldots, |\psi_D\rangle$ denote an $\epsilon$-net for the space of $n$-qubit quantum states. Set $\epsilon = d^{-1}$. Then there at most $D \leq e^{-d} = d^d$ states in this enumeration. Fix an index $1 \leq i \leq D$. Imagine running the aforementioned protocol on state $|\psi_i\rangle$. As discussed, the probability that the protocol fails to synthesize a $(d')^{-1/4}$-approximation to $|\psi_i\rangle$ is at most $\exp(-\Omega((d')^{1/4}))$ over the choice of $U, V$. By a union bound, the probability that a random choice of $U, V$ fails to synthesize a $(d')^{-1/4}$-approximation to a single one of the $|\psi_1\rangle, \ldots, |\psi_D\rangle$ is at most

$$d^d \cdot \exp(-\Omega((d')^{1/4})) \leq 2^{n2^n} \cdot \exp(-\Omega(2^{n^2/4}))$$

(6.17)

which, for sufficiently large $n$, is less than 1. Thus there exists a choice of unitaries $U, V$ that enables successful synthesis of all the $|\psi_1\rangle, \ldots, |\psi_D\rangle$. Hardcode these unitaries into the algorithm and oracles in Figure 4; i.e., the oracles $f$ and $g$ only take $n'$ bits as input. The resulting query algorithm now only requires $\text{poly}(n)$ space. Note that the implementation of the unitaries $U, V$ will not be time-efficient in general, but they are still fixed $n'$-qubit unitary operators that are independent of the state being synthesized.

Thus for an arbitrary state $|\psi\rangle$, by letting the oracles $A, B$ correspond to the nearest state $|\psi_i\rangle$ in the $\epsilon$-net that is within $d^{-1}$ of $|\psi\rangle$, the two-query algorithm synthesizes $|\psi\rangle$ with $O(d^{-1})$ error.

**Theorem 6.2 (Two Query State Synthesis Performance).** For all $n$-qubit states $|\tau\rangle$, the algorithm **TwoQueryStateSynthesis** uses $\text{poly}(n)$ space, makes two queries to a classical oracle depending on $|\tau\rangle$, and outputs a mixed state that is $\exp(-\Omega(n))$-close in trace distance to $|\tau\rangle\langle\tau|$. 

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6.3 Proof of Proposition 6.1

We now prove Proposition 6.1.

Sample a Haar-random unit vector \( u \in \mathbb{C}^d \) by sampling i.i.d. complex Gaussians \( g = (g_1, \ldots, g_d) \) where \( g_i \sim \mathcal{CN}(0, 1) \)\(^{13}\) for all \( i \), and then defining

\[
u = \frac{g}{\|g\|}.
\]

(6.18)

Sample another independent Haar-random unit vector \( v = h / \|h\| \) in the same way. Define \( |u| \) and \( |v| \) to be the entry-wise absolute value of the vectors \( u \) and \( v \), respectively.

We prove Proposition 6.1 by arguing that dividing by the norms of \( u \) and \( v \) respectively does not change the distance by much.

Let \( \hat{g} = |g| \) and \( \hat{h} = |h| \). We prove this Proposition by first observing that the entries of \( \hat{g} \), \( \hat{h} \) are distributed according to a Rayleigh distribution [Wik21]. In other words, since each entry is distributed as the absolute value of a standard complex Gaussian \( z \sim \mathcal{CN}(0, 1) \), we have

\[
\sqrt{zz^*} = \sqrt{(x + iy)(x - iy)} = \sqrt{x^2 + y^2}
\]

(6.19)

where \( x, y \sim \mathcal{N}(0, \frac{1}{2}) \). We now relate \( \|\text{sort}(\hat{g}) - \text{sort}(\hat{h})\| \) to the 2-Wasserstein distance between the empirical distributions on \( \mathbb{R} \) induced by \( \hat{g} \) and \( \hat{h} \).

We explain the 2-Wasserstein distance. Let \( \mu, \nu \) denote two probability measures on the real line \( \mathbb{R} \). Then we define the 2-Wasserstein distance between them as

\[
W_2^2(\mu, \nu) \overset{\text{def}}{=} \inf_{\omega} \int |\mu(x) - \nu(y)|^2 \, d\omega(x, y)
\]

(6.20)

where the infimum is over all probability measures \( \omega \) on \( \mathbb{R} \times \mathbb{R} \) such that the marginal on the first coordinate is \( \mu \), and the marginal on the second coordinate is \( \nu \). This is also known as the “\( \ell_2 \)-Earth Mover Distance”, because it captures the minimum amount of “earth” that has to be moved if we want to morph the distribution \( \mu \) to \( \nu \), viewing the distributions as mounds of dirt. We now list some useful properties of the Wasserstein distances.

Let \( \mu, \nu, \tau \) denote probability distributions on \( \mathbb{R} \). Then

1. (Symmetry) \( W_2(\mu, \nu) = W_2(\nu, \mu) \).
2. (Triangle inequality) \( W_2(\mu, \tau) \leq W_2(\mu, \nu) + W_2(\nu, \tau) \).
3. (Discrete distributions) Suppose that \( \mu \) (resp. \( \nu \)) is a discrete distribution that assigns \( \frac{1}{d} \) mass on distinct points \( x_1, \ldots, x_d \in \mathbb{R} \) (resp. \( y_1, \ldots, y_d \in \mathbb{R} \)). Then

\[
W_2^2(\mu, \nu) = \frac{1}{d} \sum_{i=1}^{d} |\bar{x}_i - \bar{y}_i|^2
\]

(6.21)

where \( (\bar{x}_1, \ldots, \bar{x}_d) = \text{sort}(x_1, \ldots, x_d) \) and similarly \( (\bar{y}_1, \ldots, \bar{y}_d) = \text{sort}(y_1, \ldots, y_d) \). A reference for this can be found in Lemma 4.2 of [BL19].

\(^{13}\)A complex Gaussian \( z \sim \mathcal{CN}(0, 1) \) can be sampled by sampling two independent real Gaussians \( x, y \sim \mathcal{N}(0, \frac{1}{2}) \) and then setting \( z = x + iy \).
Finally, we will use the fact that the empirical distribution of $d$ i.i.d. Rayleigh samples converges to the Rayleigh distribution $\mathcal{R}$ with respect to the Wasserstein distance. The first lemma states that the expected value of the Wasserstein distance between the two distributions is small:

**Lemma 6.3** Let $\mathcal{R}$ denote the Rayleigh distribution. Let $\mu_{\hat{g}}$ denote the discrete distribution that assigns $1/d$ mass to each point $\hat{g}_1, \ldots, \hat{g}_d$. Then

$$\left[ \mathbb{E} W_2(\mu_{\hat{g}}, \mathcal{R}) \right]^2 \leq \mathbb{E} W_2^2(\mu_{\hat{g}}, \mathcal{R}) \leq O\left( \frac{\log d}{d} \right)$$  \hspace{1cm} (6.22)

where the expectation is over the choice of $\hat{g}$.

**Proof:** This is a consequence of Corollary 6.12 of [BL19], which states that for a log-concave density $\nu$ with standard deviation $\sigma$, we have

$$\left[ \mathbb{E} W_2(\nu_d, \nu) \right]^2 \leq \mathbb{E} W_2^2(\nu_d, \nu) \leq C\sigma^2 \log d$$  \hspace{1cm} (6.23)

for some universal constant $C > 0$. Here $\nu_d$ denotes the empirical distribution arising from $d$ independent samples from $\nu$.

The lemma is established by using that the Rayleigh distribution $\mathcal{R}$ is log-concave with standard deviation $\sqrt{\left( \frac{2 - \pi^2}{2} \right) \cdot \frac{1}{\sqrt{2}}}$ [Wik21]. □

The next lemma shows that $W_2(\mu_{\hat{g}}, \mathcal{R})$ concentrates around $\mathbb{E} W_2(\mu_{\hat{g}}, \mathcal{R})$:

**Lemma 6.4 ([Wik21, Theorem 7.1])** For all log-concave densities $\nu$ with standard deviation $\sigma$, for all $\delta > 0$,

$$\Pr \left[ \left| W_2(\nu_d, \nu) - \mathbb{E} W_2(\nu_d, \nu) \right| \geq \delta \right] \leq O\left( \exp\left( -\frac{d^{1/2} \delta}{6\sigma^2} \right) \right).$$  \hspace{1cm} (6.24)

Now we put everything together to prove Proposition 6.1. Let $\mu_{\hat{g}}, \mu_{\hat{h}}$ denote the empirical distributions corresponding to the random vectors $\hat{g}, \hat{h}$. Then

$$\|\text{sort}(\hat{g}) - \text{sort}(\hat{h})\| = \sqrt{d} W_2(\mu_{\hat{g}}, \mu_{\hat{h}}) \leq \sqrt{d} \left( W_2(\mu_{\hat{g}}, \mathcal{R}) + W_2(\mu_{\hat{h}}, \mathcal{R}) \right)$$  \hspace{1cm} (6.25)

where we used the triangle inequality for the Wasserstein distance. Using Lemma 6.3 and Lemma 6.4 with $\delta = d^{-1/4}$ we get that

$$\Pr \left[ \|\text{sort}(\hat{g}) - \text{sort}(\hat{h})\| \geq 2(d^{1/4} + O(\log d)) \right] \leq \Pr \left[ W_2(\mu_{\hat{g}}, \mathcal{R}) + W_2(\mu_{\hat{h}}, \mathcal{R}) \geq 2(d^{-1/4} + O(d^{-1/2} \log d)) \right]$$  \hspace{1cm} (6.26)

$$\leq \Pr \left[ W_2(\mu_{\hat{g}}, \mathcal{R}) \geq d^{-1/4} + O(d^{-1/2} \log d) \right] \hspace{1cm} (6.27)

$$\leq 2 \Pr \left[ W_2(\mu_{\hat{g}}, \mathcal{R}) \geq d^{-1/4} + O(d^{-1/2} \log d) \right] \hspace{1cm} (6.28)

$$\leq O\left( \exp(-\Omega(d^{1/4})) \right).$$  \hspace{1cm} (6.29)
We now relate this to the distance \(\|\text{sort}(|u|) - \text{sort}(|v|)\|^2\):

\[
\|\text{sort}(|u|) - \text{sort}(|v|)\|^2 = \|u\|^2 + \|v\|^2 - 2\langle \text{sort}(|u|), \text{sort}(|v|) \rangle \\
= 2\left(1 - \frac{1}{\|g\| \cdot \|h\|} \langle \text{sort}(\hat{g}), \text{sort}(\hat{h}) \rangle \right)
\]

\[
\leq \frac{\|\text{sort}(\hat{g}) - \text{sort}(\hat{h})\|^2}{\|g\| \cdot \|h\|}
\]

(6.30)

(6.31)

(6.32)

where we used that \(u, v\) are unit vectors, and the last inequality follows from

\[
2\langle \text{sort}(\hat{g}), \text{sort}(\hat{h}) \rangle = \|g\|^2 + \|h\|^2 - \|\text{sort}(\hat{g}) - \text{sort}(\hat{h})\|^2 \geq 2\|g\| \cdot \|h\| - \|\text{sort}(\hat{g}) - \text{sort}(\hat{h})\|^2 .
\]

(6.33)

We now argue that \(\|\hat{g}\|, \|\hat{h}\|\) concentrate around \(\sqrt{d}\). This follows from standard (sub-)Gaussian concentration bounds. We use the following bound:

**Lemma 6.5 (Concentration of sum of squared Gaussians [GM17, Section 1.5.2])** Let \(x_1, \ldots, x_m \sim \mathcal{N}(0, 1)\) denote i.i.d. standard Gaussians. Let \(z = x_1^2 + \cdots + x_m^2\). Then

\[
\Pr[|z - m| \geq \epsilon m] \leq 2\exp\left(-\frac{m \epsilon^2}{8}\right).
\]

(6.34)

The norms \(\|g\|^2, \|h\|^2\) are sums of squared Gaussians; this is because

\[
\|g\|^2 = \sum_j |g_j|^2 = \sum_j g_j g_j^* = \sum_j (x_j + iy_j)(x_j - iy_j) = \sum_j x_j^2 + y_j^2
\]

(6.35)

where \(x_j, y_j\) are independent real Gaussians drawn from \(\mathcal{N}(0, \frac{1}{2})\). Thus \(2\|g\|^2\) is a sum of \(2d\) independent real Gaussians drawn from \(\mathcal{N}(0, 1)\), and thus Lemma 6.5 applies. We get

\[
\Pr[\|g\| \leq \sqrt{d/2}] = \Pr[2\|g\|^2 \leq d] \leq 2\exp\left(-\frac{d}{16}\right).
\]

(6.36)

Thus, by union bound,

\[
\Pr[\|g\| \cdot \|h\| \leq d/2] \leq 4\exp\left(-\frac{d}{16}\right).
\]

(6.37)

Combining this with eq. (6.29) we get

\[
\|\text{sort}(|u|) - \text{sort}(|v|)\| \leq O\left(d^{-1/4} + d^{-1/2} \log d\right) = O(d^{-1/4})
\]

(6.38)

with probability at least \(1 - \exp(-\Omega(d^{1/4}))\).
7 Open Questions

We exhibited state synthesis algorithms for QMA witnesses and arbitrary states that only require a single query to a classical oracle, that generate the target state up to inverse polynomial error. We also presented a two-query state synthesis algorithm that generates the target state up to inverse exponential error. As mentioned, this resolves Open Question 3.3.6 of Aaronson [Aar16]. However, there are several remaining open questions regarding these algorithms.

1. The one- and two-query algorithms for arbitrary states use polynomial space, but they aren’t time efficient (because their existence is argued by sampling a Haar-random unitary and applying the probabilistic method). Can this probabilistic construction be derandomized (and thus be made time efficient) by using (approximate) unitary designs?

2. Is there a one-query algorithm for state synthesis that also achieves inverse exponential error?

7.1 The power of quantum queries to QMA oracles

Our impossibility result in Section 3 combined with our reduction of QMA-search to PP-decision problems leaves an interesting gap as to what exactly is the power of QMA oracle. More specifically, are there interesting computational tasks solvable only with quantum access to a QMA oracle? One question is to understand the collection of problems which have search-to-decision reductions where the oracle is a QMA oracle. Is this class strictly larger than QCMA, a class with known search-to-decision reductions (Theorem 2.7)?

7.2 The Unitary Synthesis Problem

In Aaronson’s lecture notes [Aar16] and his published list of open questions in quantum query complexity [Aar21], he identifies the unitary synthesis problem as one of the major unresolved questions.

**Conjecture 7.1 ([Aar21, Problem 6])** For every n-qubit unitary transformation U, does there exists an oracle \( A : \{0,1\}^n \to \{0,1\} \) such that a BQP\(^A\) machine can implement U?

While, we do not know how to synthesize the unitary \( U \), we do know how to synthesize the Choi-Jamiolkowski state, [Cho75, Jam72]

\[
|g_U\rangle_{LR} \overset{\text{def}}{=} \sqrt{\frac{1}{2^n}} \sum_{x \in \{0,1\}^n} |x\rangle_L U |x\rangle_R, \tag{7.1}
\]

which can also be seen as applying the unitary \( I_L \otimes U_R \) to the maximally entangled state. This comes from the previously constructed state synthesis algorithms or the state synthesis algorithm of Aaronson [Aar16]. While the Choi-Jamiolkowski state contains all the information about \( U \), it is unclear how to use \( |g_U\rangle \) to apply the unitary \( U \). One idea is to use the gate-by-teleportation technique from measurement-based quantum computation to apply \( U \). In this procedure, one measures an \( n \)-qubit input state \( |\psi\rangle \) in register \( A \) and the half of \( |g_U\rangle \) in register \( L \) in the generalized Bell basis, i.e. the POVM with elements \( |g_{x=Z}^a\rangle\langle g_{x=Z}^b|_A \) for \( a, b \in \{0,1\}^n \). It is known that each
outcome \((a, b)\) is equally likely to occur and the resulting state on the \(R\) register is \(UX^aZ^b|\psi\rangle\). Unfortunately, the Pauli twirl, \(X^aZ^b\), has been applied inside of the unitary \(U\).

However, note that whenever the measurement outcome \(a = b = 0^n\) occurs, the resulting state is \(U|\psi\rangle\) as desired. Therefore, there is a post-selection algorithm which generates the output \(U|\psi\rangle\) by post-selecting on the outcome \(a = b = 0^n\). The issue, of course, is that post-selection is a non-unitary operation. However, we note that while post-selection is non-unitary, the classes PostBQP and PostQMA have definitions as classical complexity theory classes \(PP\) and \(PSPACE\), respectively. We previously outlined search-to-decision reductions for both of these classes through their equivalences with \(PGQMA\) and \(QMA_{exp}\), respectively. While not obvious to us at the moment, we suspect that there may be an insight connecting these ideas together to generate a solution to the unitary state synthesis problem.

7.3 Improving the construction of witnesses for \(QMA_{exp}\)

We leave it as an open question as to whether the Swap Test Distillation algorithm can be used to improve the overlap with a \(QMA_{exp}\) witness produced by the protocol described in Section 2.2. The challenge is establishing that the conditions for the distillation algorithm are met when \(t\)-designs (such as Clifford unitaries) are used to randomize the target state instead of Haar-random unitaries. We know that Clifford unitaries will produce a state whose expected overlap with the target state is at least a constant. Theorem 5.8 shows that the Swap Test Distillation algorithm still works under this relaxed condition (instead of requiring that every input state have constant overlap with probability 1). The problem lies in the second condition: showing that with high probability, for two independently generated output states, their components orthogonal to the target state are close to orthogonal to each other. The proof in Lemma 4.1 showing that this holds for the 1-query protocol that uses Haar-random unitaries relies on the following fact: for any two orthogonal states \(|\psi_1\rangle\) and \(|\psi_2\rangle\), even when conditioning on the event that \(U|\psi_1\rangle = |\phi\rangle\) for some specific \(|\phi\rangle\), the state \(U|\psi_2\rangle\) is still distributed in a manner that looks close to random. We leave it as an open question whether a similar fact can be shown when \(U\) is a \(t\)-design or whether there is a different way to establish the second requirement for the Swap Test Distillation algorithm. A proof that \(t\)-designs satisfy the second requirement for the distillation algorithm would also result in an improvement over the 1-query protocol for synthesizing arbitrary states shown in Section 3, by reducing the time complexity of the protocol from exponential to polynomial time.

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A Preliminaries

We assume the reader has a standard knowledge of quantum computation lexicon. The following are definitions important for the results of this paper.
Circuits
Quantum circuits on \( n \) qubits are defined as an ordered lists of unitaries, each acting on 2-qubits, and a specification \((i, j) \in [n]^2\) of the two qubits being acted on. \( O \)-oracle quantum circuits are quantum circuits augmented with list terms corresponding to the multi-qubit unitary \( O \) and a specification of the qubits \( \subseteq [n] \) being acted on. This can be generalized to multiple oracles.

A.1 Proximity of phase states

In this subsection, we define the notion of a phase state and prove results on how they are good approximations for random states. These definitions are pertinent for Section 2 (where we discuss search-to-decision for QMA) as well as Section 4 (where we discuss the 1-query algorithm for general state synthesis).

Definition A.1 A phase state on \( n \) qubits is a state of the form

\[
|p_f\rangle = 2^{-n/2} \sum_{x \in \{0,1\}^n} (-1)^{f(x)} |x\rangle ,
\]

for some boolean function \( f : \{0,1\}^n \to \{0,1\} \).

Phase states are an interesting collection of states as they form good approximations for states of large \( \ell_1 \) norm, i.e. \( \| \cdot \|_1 \approx \Omega(\sqrt{2^n}) \). While basis states do not have this property (their \( \ell_1 \) norm is 1), it is a property of Haar-random states and even outputs of 2-designs. We show this in the following statements.

Fact A.2 (Good overlap with phase states) Let \( |a\rangle \in \mathbb{R}^d \) be a vector. There exists a phase state \( |p_f\rangle \) defined by \( f(x) = \text{sgn}(ax) \) and

\[
\langle a|p_f\rangle = \sum_x \frac{a_x \cdot \text{sgn}(a_x)}{\sqrt{d}} = \frac{||a||_1}{\sqrt{d}} .
\]

Furthermore, the previous phase state is the optimal phase state in terms of overlap (up to a global phase).

Fact A.3 Let \( C \) be a unitary 2-design on \( n \) qubits and \( |\tau\rangle \) be an arbitrary \( n \)-qubit state. Then,

\[
\mathbb{E}_{C \in C} |\langle x|C|\tau\rangle|^2 = \frac{1}{2^n}, \quad \mathbb{E}_{C \in C} |\langle x|C|\tau\rangle|^4 = \frac{2}{2^n(2^n + 1)} .
\]

Furthermore, for any \( x \in [2^n] \),

\[
\Pr_{C \in C} \left( |\langle x|C|\tau\rangle|^2 \geq \frac{\theta}{2^n} \right) \geq \frac{(1-\theta)^2}{2} .
\]
Proof: First suppose that C is a Haar random unitary. For the first two statements, calculations of second and fourth moments for Haar random states in \( \mathbb{C}^d \) are well-known and can be found in [Hia00, Chapter 4.2], which in general gives

\[
\mathbb{E}_{|\psi\rangle \sim H} |\langle x|\psi\rangle|^2 = \frac{1}{d}, \text{ and } \mathbb{E}_{|\psi\rangle \sim H} |\langle x|\psi\rangle|^4 = \frac{2}{d(d+1)}.
\] (A.5)

For the third statement, by the Payley-Zygmund inequality, we have

\[
\Pr_{|\psi\rangle \sim H} \left( |\langle x|\psi\rangle|^2 \geq \frac{\theta}{d} \right) \geq (1-\theta)^2 \cdot \frac{\left( \mathbb{E}_{|\psi\rangle \sim H} |\langle x|\psi\rangle|^2 \right)^2}{\mathbb{E}_{|\psi\rangle \sim H} |\langle x|\psi\rangle|^4} = (1-\theta)^2 \cdot \frac{d^2 + d}{2d^2} \geq \frac{(1-\theta)^2}{2}.
\] (A.6)

The expectations only involve polynomials of degree 2 in the entries of C and \( C^\dagger \), and so have the same value when C is chosen uniformly from \( \mathcal{C} \). We can furthermore translate these results to unitary 2-designs. For example,

\[
\mathbb{E}_{C \in \mathcal{C}} |\langle x|C|\tau\rangle|^4 = \mathbb{E}_{C \in \mathcal{C}} |\langle x|C|\tau\rangle|\langle x|C|\tau\rangle|\langle x|C|\tau\rangle|\langle x|C|\tau\rangle|
\] (A.7)

\[
= \int_{U \sim \mathcal{H}} dU |\langle x|U|\tau\rangle|\langle x|U^\dagger|\tau\rangle|\langle x|U|\tau\rangle|\langle x|U^\dagger|\tau\rangle|
\] (A.8)

\[
= \mathbb{E}_{\psi \in \mathcal{H}} |\langle x|\psi\rangle|\langle x|\psi\rangle|\langle x|\psi\rangle|\langle x|\psi\rangle|
\] (A.9)

\[
= \mathbb{E}_{\psi \in \mathcal{H}} |\langle x|\psi\rangle|^4
\] (A.10)

\[
= \frac{2}{2^n(2^n + 1)}.
\] (A.11)

Here we defined \( |\psi\rangle = U|\tau\rangle \) which is Haar-randomly distributed and used the result for Haar states. Likewise, we can use similar arguments for the second moment and the probability bound. \( \square \)

Then, this can be easily extended to showing that

\[
\mathbb{E}_{C \in \mathcal{C}} \sum_x |\langle x|\psi\rangle|^4 = \frac{2}{2^n + 1}.
\] (A.12)

By a standard Markov’s inequality argument and the following fact, Fact A.4.

\[
\Pr_{C \in \mathcal{C}} \left( \|\psi\|_1 \geq \frac{\sqrt{2^n}}{2\sqrt{\alpha}} \right) \geq \Pr_{C \in \mathcal{C}} \left( \frac{1}{\sqrt{\sum_x |\psi_x|^4}} \geq \sqrt{\frac{2^n + 1}{2\alpha}} \right)
\] (A.13)

\[
= \Pr_{C \in \mathcal{C}} \left( \sum_x |\psi_x|^4 \leq \frac{2\alpha}{2^n + 1} \right)
\] (A.14)

\[
\geq 1 - \frac{1}{\alpha}.
\] (A.15)
**Fact A.4** Let $|a⟩ ∈ \mathbb{C}^d$ be a unit vector. Then,

$$\|a\|_1 \geq \frac{1}{\|a\|_4^2} = \frac{1}{\sqrt{\sum_x |a_x|^4}}.$$  \hfill (A.16)

**Proof:** Let $|b⟩ = \sum_x |a_x|^{4/3} |x⟩$ and $|c⟩ = \sum_x |a_x|^{2/3} |x⟩$. Then by Hölder’s inequality,

$$1 = \sum_x |a_x|^2 = \sum_x |b_x c_x|$$ \hfill (A.17)

$$\leq \left( \sum_x |b_x|^3 \right)^{1/3} \cdot \left( \sum_x |c_x|^{3/2} \right)^{2/3}$$ \hfill (A.18)

$$= \left( \sum_x |a_x|^4 \right)^{1/3} \cdot \left( \sum_x |a_x|^{2/3} \right)^{2/3}$$ \hfill (A.19)

$$= \|a\|_4^{4/3} \cdot \|a\|_1^{2/3}.$$ \hfill (A.20)

The statement follows after rearrangement. \hfill □

Now we can prove our main lemma about the approximability of states by 2-design unitaries. We recall that the collection of Clifford unitaries form a 2-design [DL102]. We denote the Clifford group as Cliff.

**Lemma A.5 (Random states have good overlap)** Let $|τ⟩ ∈ (\mathbb{C}^2)^⊗n$ be a unit vector. Let $C$ be any 2-design (ex. $C = \text{Cliff}$). Sample a random $C ∈ C$ and set $|ψ⟩ = C |τ⟩$. Then with constant probability, it has good overlap with the phase state defined by the function $f(x) = \text{sgn}(\text{Re}(⟨x|ψ⟩))$. Formally for $0 ≤ γ ≤ \frac{1}{4}$,

$$\Pr_{C ∈ C \atop |ψ⟩=C |τ⟩} \left( |⟨ψ|p_f⟩|^2 ≥ γ \right) ≥ \frac{1}{2} - 2γ.$$ \hfill (A.21)

**Proof:** For any state $|ψ⟩ ∈ (\mathbb{C}^2)^⊗n$, we can write $|ψ⟩$ as $|a⟩ + i |b⟩$ where $|a⟩, |b⟩ ∈ \mathbb{R}^{2^n}$. With probability $\frac{1}{2}$, $\|a\|_1 ≥ \|b\|_1$. Combining this with the previous statement eq. (A.15),

$$\Pr_{C ∈ C \atop |a⟩=\text{Re}(C |τ⟩)} \left( \|a\|_1 ≥ \sqrt{γd} \right) ≥ \frac{1}{2} - 2γ.$$ \hfill (A.22)

Therefore, since $|⟨ψ|p_f⟩|^2 ≥ |⟨a|p_f⟩|^2$, we can use Fact A.2 to complete the proof:

$$\Pr_{C ∈ C \atop |ψ⟩=C |τ⟩} \left( |⟨ψ|p_f⟩|^2 ≥ γ \right) ≥ \Pr_{C ∈ C \atop |a⟩=\text{Re}(C |τ⟩)} \left( |⟨a|p_f⟩|^2 ≥ γ \right) \hfill (A.23)$$

$$= \Pr_{C ∈ C \atop |a⟩=\text{Re}(C |τ⟩)} \left( \|a\|_1 ≥ \sqrt{γd} \right).$$ \hfill (A.24)

□
A.2 Phase estimation algorithm results

Our algorithm in Section 2 will rely on a finer analysis of the phase estimation algorithm. We use the following lemmas.

Lemma A.6 ([Ral21, Corollary 16]) Let $H$ be a local Hamiltonian on $n$ qubits and $\delta > 0$. Then the Improved Energy Estimator of [Ral21] has query complexity $O(\log(\delta^{-1}) \cdot 2^n)$ that returns an estimate to the energy that is accurate up to $1/2^m$. That is, on input that is an eigenstate of $H$ with eigenvalue $E_j$, the output state of the algorithm is within trace distance $\delta$ of

$$\rho_j = (p_j \ket{2^m E_j} \bra{2^m E_j} + (1 - p_j) \ket{2^m E_j - 1} \bra{2^m E_j - 1}) \otimes |E_j \rangle \langle E_j|,$$

where the outcome register is interpreted mod $2^n$, and $0 \leq p_j \leq 1$.

Proof: This follows from the cited lemma of [Ral21], applying the case without a rounding promise, and converting the stronger diamond norm bound on the map to a trace distance bound on the output state. □

The following fact describes the use of phase estimation to improve a low-quality QMA witness. This technique was introduced by Abrams and Lloyd [AL99].

Lemma A.7 Let $H$, $m$, and $\delta$ be as in the previous lemma, let $|\psi\rangle$ be an arbitrary $n$-qubit state. Let the eigenvalues of $U$ be $\lambda_i = e^{2\pi i \phi_i}$ where $\phi_i \in [0,1)$. Suppose that $|\psi\rangle$ has overlap at least $C > 0$ on the subspace spanned by eigenvectors corresponding to $\phi_i \in [a,b]$. Then, the Improved Energy Estimator of [Ral21] returns a value $\theta \in [a - \frac{1}{2^m}, b + \frac{1}{2^m}]$ with probability at least $C - \delta$. Moreover, conditioned on phase estimation returning a value $\theta$ in this interval, the residual state has overlap at least $1 - 2\delta/C$ with the subspace spanned by eigenvectors of $U$ corresponding to $\phi_i \in [a - \frac{2}{2^m}, b + \frac{2}{2^m}]$.

Proof: Write the input state as

$$|\psi\rangle = \sum_j c_j |E_j\rangle.$$  \hspace{1cm} (A.26)

Then, by Lemma A.6, the state after the energy estimation algorithm is run is $\delta$-close in trace distance to the following ideal state:

$$\rho_{\text{ideal}} = \sum_j |c_j|^2 (p_j \ket{2^m E_j} \bra{2^m E_j} + (1 - p_j) \ket{2^m E_j - 1} \bra{2^m E_j - 1}) \otimes |E_j \rangle \langle E_j|,$$

where the outcome register is interpreted mod $2^n$. The claim about the probability of returning $\theta$ in the specified range then follows by inspection, and the given bound that the overlap of $|\psi\rangle$ with the $[a, b]$-eigenspace is at least $C$.

Now, for the claim about the residual state conditioned on obtaining $\theta$ in the desired range, consider jointly measuring both registers of the true output state in the computational basis. This yields a probability distribution over outcomes

$$\Pr[\theta, E = E_j] \approx \delta |c_j|^2 (p_j \cdot 1[\theta = 2^m E_j] + (1 - p_j) \cdot 1[\theta = 2^m E_j - 1]),$$

where the $\approx_\delta$ notation means that the distributions on the two sides are $\delta$-close in total variational distance.
Define $E_{good} = [a - \frac{2}{2m}, b + \frac{2}{2m}]$ and $\Theta_{good} = [a - \frac{1}{2m}, b + \frac{1}{2m}]$. The quantity we now wish to bound from below is $\Pr[E_j \in E_{good} | \theta \in \Theta_{good}]$. We may do this using Bayes’ rule:

\[
\Pr[E \in E_{good} | \theta \in \Theta_{good}] = \frac{\Pr[E \in E_{good}, \theta \in \Theta_{good}]}{\Pr[\theta \in \Theta_{good}]}.
\]

(A.29)

\[
= \frac{\Pr[\theta \in \Theta_{good} | E \in E_{good}] \Pr[E \in E_{good}]}{\Pr[\theta \in \Theta_{good}]}
\]

(A.30)

\[
\geq \frac{C - \delta}{C + \delta} \geq 1 - \frac{2\delta}{C}.
\]

(A.31)

\[\square\]

A.3 Concentration Inequalities

**Lemma A.8 (Levy’s Lemma)** Let $S(\mathbb{C}^d)$ denote the set of unit vectors in $\mathbb{C}^d$. Let $K, f : S(\mathbb{C}^d) \to \mathbb{R}$ be such that for all $|\psi\rangle, |\phi\rangle \in S(\mathbb{C}^d)$ we have

\[
|f(|\psi\rangle) - f(|\phi\rangle)| \leq K \cdot |||\psi\rangle - |\phi\rangle ||.
\]

(A.32)

Then there exists a universal constant $C > 0$ where

\[
\Pr[|f(|\psi\rangle) - \mathbb{E} f| \geq \delta] \leq 2\exp\left(-Cd^2/\delta^2\right)
\]

(A.33)

where the probability is over the choice of $|\psi\rangle$ drawn from the Haar measure over $S(\mathbb{C}^d)$, and $\mathbb{E} f$ is the average of $f$ over the Haar measure.

A.4 Azuma’s Inequality

**Lemma A.9 (Azuma’s Inequality)** Suppose that the sequence of random variables $S_0, S_1, S_2, \ldots$ is a Martinagale ($E[S_{j+1} | S_1, \ldots, S_j] = S_j$ for all $j \geq 0$). Suppose also that $|S_j - S_{j-1}| \leq c_j$. Then

\[
\Pr[S_L - S_0 < -\epsilon] \leq \exp\left(\frac{-\epsilon^2}{2 \sum_{j=1}^{L} c_j}\right)
\]
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