# Quantum Supremacy through the Quantum Approximate Optimization Algorithm

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October 22, 2019

#### Abstract

The Quantum Approximate Optimization Algorithm (QAOA) is designed to run on a gate model quantum computer and has shallow depth. It takes as input a combinatorial optimization problem and outputs a string that satisfies a high fraction of the maximum number of clauses that can be satisfied. For certain problems the lowest depth version of the QAOA has provable performance guarantees although there exist classical algorithms that have better guarantees. Here we argue that beyond its possible computational value the QAOA can exhibit a form of "Quantum Supremacy" in that, based on reasonable complexity theoretic assumptions, the output distribution of even the lowest depth version cannot be efficiently simulated on any classical device. We contrast this with the case of sampling from the output of a quantum computer running the Quantum Adiabatic Algorithm (QADI) with the restriction that the Hamiltonian that governs the evolution is gapped and stoquastic. Here we show that there is an oracle that would allow sampling from the QADI but even with this oracle, if one could efficiently classically sample from the output of the QAOA, the Polynomial Hierarchy would collapse. This suggests that the QAOA is an excellent candidate to run on near term quantum computers not only because it may be of use for optimization but also because of its potential as a route to establishing Quantum Supremacy.

### 1 Introduction

Feynman's original motivation for exploring quantum computing was that quantum mechanics is hard to simulate on a classical computer. In particular, writing down all the amplitudes of a generic n-qubit state requires  $2^n$  complex numbers, which is far too large for any possible classical computer say when  $n \gtrsim 100$ . But what if you only want to calculate a single amplitude of a large quantum state? Or to sample on a classical computer (with a random number generator) from the distribution that would result from performing a quantum measurement? The tasks of computing amplitudes or sampling can be viewed as forms of simulation which might be feasible on classical computers. These tasks can sometimes be accomplished efficiently, using problem-specific techniques. For example, with the known Hydrogen atom eigenstates, we can calculate matrix elements of operators of interest to arbitrary accuracy.

But there are no known methods for computing amplitudes or sampling which run in less than exponential time on a classical computer and work for all quantum systems. As small-scale quantum

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computers come online, we want to understand how difficult it is to simulate their behavior on classical computers. For a such a device to be computationally useful—that is, able to outperform a classical computer for a given task—it had better be hard to classically simulate.

Complexity theoretic assumptions can be used to show that the tasks of classically computing matrix elements of a general quantum circuit [22] or classically sampling from the output of a general quantum circuit [32] cannot be done efficiently. In this paper we will review these arguments. We do not reproduce all of the details needed to establish these results but give what we hope is a faithful outline of the arguments. Related hardness results are known for particular families of quantum circuits such as Boson Sampling, small depth quantum circuits and IQP or Instantaneous Quantum Polytime circuits [3, 11–13, 29, 32].

The Quantum Approximate Optimization Algorithm [18,19] or QAOA is a family of quantum circuits designed to find "good" solutions to optimization problems. Here we will show, using methods that are similar to those used in the IQP case, that classically sampling from even the shallowest depth version of the QAOA can be argued to be difficult for complexity theoretic reasons. In this sense the QAOA can exhibit a form of "Quantum Supremacy" [30], that is be a quantum process whose output distribution cannot be efficiently reproduced on a classical device. It is also possible that versions of the QAOA can find approximate solutions to combinatorial search problems faster than classical algorithms. This may be established by running the algorithms on actual devices or by theoretical analysis. This possible algorithm advantage, together with our non-simulatability results, suggests that the QAOA is a good choice of algorithm to run on a near-term quantum computer.

We also discuss the prospects of sampling from the evolving state of a system running the Quantum Adiabatic Algorithm [20, 27] which we call QADI (so as to not use an acronym which is a subset of QAOA). Here practitioners use numerical simulations of QADI which rely on the assumption that the Hamiltonian governing the evolution is stoquastic (see Section 8 for definitions). We will show that this assumption rules out using the same arguments for Quantum Supremacy that worked for QAOA.

Our paper is organized as follows. First we review the basic ingredients of the QAOA. Since we are going to use complexity theory arguments to argue that it is difficult to simulate this algorithm, we review some of the needed complexity theory. We explain what the Polynomial Hierarchy (PH) is and what it means for it to collapse. In Section 3, we show why the ability to compute on a classical computer the matrix elements of the QAOA would collapse the PH. But to discuss why sampling the output distribution of the QAOA is also hard for complexity theory reasons we need to discuss Post-Selected Quantum Computing which we do in Section 4. Using Post-Selected Quantum Computing as a tool, in Section 5 we show that the efficient sampling of the output of an arbitrary quantum circuit implies the collapse of the PH. This leads up to our new result (in Sections 6 and 7) that efficient sampling from the output of the QAOA also collapses the PH. In Section 8 we turn to a discussion of sampling from the output of the Quantum Adiabatic Algorithm being run in optimization mode. We review the assumptions needed to enable efficient sampling from this type of quantum circuit. Here we argue that this may in fact be easier than sampling from the output of the QAOA. We conclude with a discussion of what these results mean for near-term quantum computers.

# 2 Background

### 2.1 Constraint satisfaction problems

A constraint satisfaction problem (CSP) is specified by n bits and a collection of m constraints (or clauses), each of which involves a small subset of the bits. The computational task is to find a string which maximizes or approximately maximizes the number of satisfied constraints. For each constraint  $a \in [m]$  and each string  $z \in \{0,1\}^n$ , define

$$C_a(z) = \begin{cases} 1 & \text{if } z \text{ satisfies the constraint } a \\ 0 & \text{if } z \text{ does not } . \end{cases}$$
 (1)

Equivalently, the goal is to maximize

$$C(z) = \sum_{a=1}^{m} C_a(z),$$
 (2)

which counts the number of satisfied constraints. One example of a CSP is MAX-CUT, where the constraints are indexed by edges  $\langle i, j \rangle$  in a graph and are satisfied when  $z_i$  and  $z_j$  disagree; i.e.

$$C_{\langle i,j\rangle}(z) = (z_i - z_j)^2. \tag{3}$$

Thus maximizing the sum of these clauses is equivalent to finding the minimum energy of a Ising antiferromagnet where the spins sit on the vertices of a graph.

In this paper we consider two quantum algorithms for CSPs: the Quantum Approximate Optimization Algorithm and the Quantum Adiabatic Algorithm. We will come back to the second one later in the paper. Both operate in the  $2^n$ -dimensional Hilbert space with basis vectors  $|z\rangle$  and accordingly we define the operator C by

$$C|z\rangle := C(z)|z\rangle.$$
 (4)

We will also define the operator

$$B := \sum_{i=1}^{n} \sigma_x^{(i)},\tag{5}$$

where  $\sigma_{\alpha}^{(i)}$  denotes the Pauli operator  $\sigma_{\alpha}$  acting on the  $i^{\text{th}}$  qubit. Both algorithms also start with the same initial state

$$|s\rangle := \frac{1}{\sqrt{2^n}} \sum_{z \in \{0,1\}^n} |z\rangle. \tag{6}$$

# 2.2 Quantum Approximate Optimization Algorithm (QAOA)

This algorithm is designed to find a string z that approximately maximizes C. Let

$$C_{\max} := \max_{z \in \{0,1\}^n} C(z). \tag{7}$$

Then we seek a z such that the approximation ratio defined as  $C(z)/C_{\text{max}}$  is large. The algorithm depends on an integer  $p \geq 1$  and we begin by describing the p = 1 version. Here we start with two angles  $\gamma$  and  $\beta$  and use the quantum computer to construct the state

$$|\gamma, \beta\rangle = \exp(-i\beta B) \exp(-i\gamma C)|s\rangle.$$
 (8)

The goal now is to make

$$\langle \gamma, \beta | C | \gamma, \beta \rangle \tag{9}$$

as big as possible. One way to do this is to search for the  $\gamma$  and  $\beta$  which make (9) big. For a fixed  $\gamma$  and  $\beta$ , use the quantum computer to make the state  $|\gamma,\beta\rangle$  and then measure in the computational basis to get a string z and evaluate C(z). Using an enveloping classical search routine, hunt for the  $\gamma$  and  $\beta$  that maximize (9) using the quantum computer as part of the subroutine that produces values of C.

However it was shown in [18] that for a given  $\gamma$  and  $\beta$  the value of (9) can be efficiently classically calculated. Once the best  $\gamma$  and  $\beta$  are chosen, the quantum computer would only be used to find a string z where C(z) is equal to (9) (or larger). It was shown in [18, 19] that for certain combinatorial optimization problems this algorithm can give approximation ratios that are better than what can be achieved by randomly picking a string z. The importance here is that this is a quantum approximation algorithm with a provable worst-case guarantee, something which had not been previously achieved by any quantum algorithm for combinatorial optimization. However in these cases the p=1 QAOA is outperformed by certain classical algorithms that go beyond random guessing [7,23].

Note that the circuit depth of the p=1 algorithm is low. If the cost function C is a sum of m terms each of which say involves 2 qubits as in (3) then the first unitary hitting  $|s\rangle$  in (8) can be written as the product of m commuting two-qubit unitaries. The instance-independent B term is a sum of n commuting one-qubit operators. The low circuit depth and simple form make the p=1 QAOA an attractive candidate to run on a near-term gate-model computer.

For p > 1 we select 2p angles  $\vec{\gamma} := (\gamma_1, \dots, \gamma_p)$  and  $\vec{\beta} := (\beta_1, \dots, \beta_p)$  and construct the state

$$|\vec{\gamma}, \vec{\beta}\rangle = \exp(-i\beta_p B) \exp(-i\gamma_p C) \cdots \exp(-i\beta_1 B) \exp(-i\gamma_1 C) |s\rangle.$$
 (10)

The goal is now to find the 2p angles  $\vec{\gamma}$  and  $\vec{\beta}$  that make

$$\langle \vec{\gamma}, \vec{\beta} | C | \vec{\gamma}, \vec{\beta} \rangle \tag{11}$$

as big as possible. For a given  $\vec{\gamma}, \vec{\beta}$ , we can use a quantum computer to evaluate (11). This can be used as a subroutine in an enveloping classical algorithm to find the best angles  $\vec{\gamma}, \vec{\beta}$ . Note that performance can only improve as p increases because the maximization over angles at level p-1 is a constrained version of the maximization at level p where the last two angles are set to 0. In fact it was shown in [18] that as p goes to infinity,  $C_{\text{max}}$  can be achieved.

As in the p=1 case, classical computers could be used to calculate (11), but now with a run-time that grows doubly exponentially in p [18]. Even for small p this classical calculation can be impractical. By contrast, the quantum circuit depth is p times the circuit depth of the p=1 circuit. For small p it might be possible to run this algorithm on a near-term gate-model quantum computer and explore its performance empirically.

#### 2.3 The Polynomial Hierarchy

Here we offer a review of a few concepts from complexity theory needed to understand the results of this paper. We will discuss the polynomial hierarchy (PH) and what it means to say the PH collapses. We will also discuss the relationship between counting problems and the PH. For a fuller account see [6].

We begin by reviewing what the complexity class NP is by starting with the familiar case of 3SAT. 3SAT is an example of a clause-based decision problem over n-bit strings with each clause acting only on a subset of the bits of size  $\leq 3$ . The input is a string c that encodes the clauses and we ask if there exists an n-bit string z that satisfies all of the clauses. The key feature of being in NP is that if there is a satisfying assignment z and you have z in hand then you can quickly check that all of the clauses are True on the string z. The satisfying string is called a "proof" or a "witness" because it can be used to establish that the instance is indeed satisfiable. On the other hand, if an instance has no satisfying assignment then there is no known witness that can in general convince you of that in short order.

We can think of NP as the set of problems specified by an input c (encoding clauses in the case of 3SAT) which acts on strings z through an easily computable function Check(c, z), defined by

$$\operatorname{Check}(c, z) = \begin{cases} 1 & z \text{ satisfies } c \\ 0 & z \text{ does not satisfy } c \end{cases}$$
 (12)

The function  $\operatorname{Check}(c, z)$  depends on the problem at hand whose clauses are encoded as c. For a general combinatorial combinatorial search problem with cost function (2) we have that  $\operatorname{Check}(c, z) = 1$  iff C(z) = m, where C(z) is the number of clauses in c satisfied by z. Then the decision question becomes "Given an input c, is the following statement true?":

There exists 
$$z$$
 such that  $\operatorname{Check}(c, z) = 1$ . (13)

One way to solve the decision problem is to look through all  $2^n$  strings z to see if one or more satisfies the clauses. It is generally believed that there is no efficient (that is, polynomial in n) algorithm which can answer the decision question for all problems in NP. Equivalently it is believed that no efficient algorithm exists for 3SAT. This belief is written as  $P \neq NP$  where P is the class of decision problems that can be solved in polynomial time.

The polynomial hierarchy is a tower of classes of problems which seemingly require more and more resources to solve. At level 0 we have the class P and at level 1 we have the class NP. At level 2 we have problems specified by clauses encoded as c which act on two n-bit strings  $z_1$  and  $z_2$ . Again there is an efficiently computable function  $\operatorname{Check}(c, z_1, z_2)$  such that

$$\operatorname{Check}(c, z_1, z_2) = \begin{cases} 1 & z_1, z_2 \text{ satisfies } c \\ 0 & z_1, z_2 \text{ does not satisfy } c \end{cases}$$
 (14)

Now the decision question becomes "Given an input c, is the following statement true?"

For all 
$$z_1$$
, there exists  $z_2$  such that  $\operatorname{Check}(c, z_1, z_2) = 1$ . (15)

We can see that this is (apparently) exponentially harder than NP as follows. Suppose we have a magical machine or "oracle" that can solve NP in a single step. For a fixed  $c, z_1$  we can view Check $(c, z_1, z_2)$  as an efficiently computable function with clauses  $c, z_1$  acting on strings  $z_2$ . For fixed  $c, z_1$  we give this function to the oracle which can quickly say if there is a satisfying string  $z_2$ . However to answer the decision question at level 2 we may need to cycle through all  $2^n$  values of  $z_1$ . So here the ability to solve quickly the level-1 problem does not give rise to an efficient solver at level 2. The argument here is similar to the argument that P is unlikely to equal NP since brute-force enumeration of witnesses takes exponential time. It is only a conjecture that level 2 of

the polynomial hierarchy is exponentially harder than level 1, but this conjecture is widely believed for the same reasons that  $P \neq NP$  is widely believed.

At the next level of the hierarchy, level 3, we have clauses which act on strings  $z_1, z_2, z_3$  and the decision question becomes "Given c, is the following statement true?"

There exists 
$$z_1$$
, such that for all  $z_2$ , there exists  $z_3$  such that  $\operatorname{Check}(c, z_1, z_2, z_3) = 1$ . (16)

Again we can see that an oracle at level 2 may need to be called an exponential number of times to solve the decision question at level 3, so in that sense level 3 is harder than level 2. Hopefully it is now straightforward to see how higher levels of the hierarchy are defined and that each level is exponentially harder than the level below. The PH is the union of these decision problems at all levels.

One way to understand the levels of the hierarchy is to consider the game of chess where we can consider an analogous hierarchy where we see the alternating quantifiers (but not the scaling with n). Suppose we ask "For a board in position c, does White have a guaranteed mate in k moves?". For example at level 3 of the chess hierarchy we are asking if there exists a move for White,  $z_1$ , such that all of Black's moves  $z_2$  can be countered with a move  $z_3$  with which White mates Black.

In this paper we are going to say that "something" implies the collapse of the PH so we now want to say what the collapse of the PH means. The ultimate collapse of the PH would come about if P=NP which would automatically imply that all levels of the hierarchy are equal to P. However we are only going to be able to show that something implies the collapse of the hierarchy at level 3. What this collapse means is that given an oracle for the level-3 decision problem, that oracle can be called only a polynomial number of times to solve the level-4 decision problem. This would imply that all levels of the hierarchy above 3 are equal to level 3 but it would not imply that P=NP. Still it seems very implausible that the hierarchy collapses at any level. One could object here and say that presuming the existence of an oracle at level 3 is unreasonable so we shouldn't care what it would imply. Aren't we saying that if dogs could talk then pigs could fly? No. We are saying that no matter what the computational resources are of the level-3 oracle, that is unreasonable to suppose that a polynomial number of calls to that oracle would solve the level-4 problem.

#### 2.4 Counting

Return to our example of 3SAT and now ask the question: how many strings z satisfy an instance with clauses c? This is not a decision problem so it does not sit in the class NP. But if we had an oracle which could solve this problem, in other words an efficient function of c which counts the number of satisfying assignments then we could solve the decision problem by simply seeing if the answer is 0 or not. In this sense the counting problem is harder than the decision problem. The class of counting problems of this nature is called #P. This class includes problems such as finding the permanent of a matrix whose entries are 0's and 1's. In fact the #P class can be viewed (somewhat imprecisely) as containing the whole PH. More precisely, any problem in PH can be solved with a poly-time classical computer that can make a polynomial number of calls to a #P oracle.

# 3 Efficient Classical Computation of Matrix Elements of Quantum Circuits Implies that P = NP

Here we give an argument for why exactly computing matrix elements of quantum circuits is hard based on beliefs from complexity theory that we just reviewed. Our argument will then be slightly modified to show that even computing the matrix elements of a p = 1 QAOA circuit is hard.

We consider a quantum computer that can implement gates of the form  $\exp(-i\gamma C)$ , where C(z) arises from a CSP with m clauses as described in (2). The quantum computer can also implement the Hadamard gate on each qubit, meaning the gate

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

For each  $r \in \{0, 1, \dots, m\}$ , consider the matrix element

$$\langle 0^n | H^{\otimes n} \exp\left(-\frac{2\pi i r}{m+1} C\right) H^{\otimes n} | 0^n \rangle, \tag{17}$$

which is equivalently (using the definition of  $|s\rangle$  from (6))

$$= \langle s | \exp\left(-\frac{2\pi i r}{m+1}C\right) | s \rangle \tag{18}$$

$$= \frac{1}{2^n} \sum_{z \in \{0,1\}^n} \exp\left(-\frac{2\pi i r}{m+1} C(z)\right). \tag{19}$$

If we define  $p_v$  to be the fraction of z for which C(z) = v, then (17) is

$$= \sum_{v} p_v \exp\left(-\frac{2\pi i r}{m+1}v\right). \tag{20}$$

This is equal to the Fourier transform of  $p_v$ . Thus if we can compute the matrix element (17) for each value of r then we can reconstruct the distribution  $p_v$  by performing the inverse Fourier transform on the m+1 amplitudes. Note that we can assume that m+1 is of order n so that this operation can be done efficiently in n. Now knowing the exact value of  $p_m$  would let us compute how many strings satisfy all of the clauses, a #P-hard problem. As we discussed in the last section if this could be calculated efficiently then we would have P = NP. Since we believe that  $P \neq NP$  we conclude that the matrix elements (17) can not be efficiently calculated on a classical computer. We view this argument as a concrete version of Feynman's intuition.

We now specialize to the case of the QAOA. The p=1 QAOA with  $\beta=0$  produces the state

$$\exp\left(-\frac{2\pi i r}{m+1}C\right)|s\rangle. \tag{21}$$

and if we take the  $|s\rangle$  component we get (18) which is (17). This means that an efficient classical algorithm for computing this particular matrix element of the output of the QAOA would imply that P = NP.

We have just argued that a classical computer cannot (under reasonable assumptions) exactly compute matrix elements of general quantum circuits, or even of the lowest depth QAOA. But

quantum computers do not output matrix elements. Rather a quantum circuit produces a state which is then measured in some basis. The outcome of the measurement will follow the probability distribution arising from the amplitudes squared but you cannot decide in advance which outcome will be obtained. So a question that we can ask is "Can a classical computer which uses random bits, produce outcomes which follow the same probability distribution that a quantum circuit would give?" Later we will show that under reasonable assumptions the distribution of outcomes of even the p=1 QAOA cannot be faithfully reproduced by a classical computer.

# 4 Post-Selected Quantum Computing

In this section we will describe a model of quantum computing that allows one to decide in advance what the outcome of a measurement will be. This model does not correspond to anything we imagine being able to do with a real quantum computer but it will serve as a stepping stone to establishing other results. First we see that with this model we can solve the Grover problem with one call. The search space has size N and there are M marked items. The function f(z) is equal to 1 if z is a marked item and 0 otherwise. Start with the uniform superposition of N basis vectors with an additional one-qubit register set to 0:

$$\sum_{z=1}^{N} \frac{1}{\sqrt{N}} |z\rangle |0\rangle, \tag{22}$$

and then compute f(z) into the second register so we have

$$\sum_{z=1}^{N} \frac{1}{\sqrt{N}} |z\rangle |f(z)\rangle. \tag{23}$$

Now if we post-select on discovering upon measurement that the second register is a 1 we get

$$\sum_{z \text{ such that } f(z)=1} \frac{1}{\sqrt{M}} |z\rangle, \tag{24}$$

where M is the number of marked items. So we see that with post-selected quantum computing we could solve the Grover problem with one call. This means that with a polynomial-time post-selected quantum computer we could also solve an NP-complete problem such as 3SAT.

Post-selected quantum computing has even more computational power in that it allows one to solve counting problems. There is a result due to Aaronson [1] that says that the ability to do post-selected quantum computing allows one to solve problems in #P, that is, to perform exact counting. To see why this is so let us use post-selection to count the number of marked items M in the Grover problem. Start with uniform superposition  $|s\rangle$  as we just did and append another register which is in the state  $|+\rangle$ .

$$\sum_{z=1}^{N} \frac{1}{\sqrt{N}} |z\rangle |+\rangle$$

where

$$|+\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}} \,,$$

and act with

$$(-1)^{\left[f\otimes|1\rangle\langle1|\right]},\qquad(25)$$

where f is the operator, acting on the first register, corresponding to the function f(z). The state now, up to normalization, is

$$\sum_{z} |z\rangle|0\rangle + \sum_{z} (-1)^{f(z)}|z\rangle|1\rangle. \tag{26}$$

Now we measure the first register post-selecting on the outcome being  $|s\rangle$ . This resulting state is, up to normalization,

$$|0\rangle + (1 - 2M/N)|1\rangle. \tag{27}$$

Perform a Hadamard on this bit and get a state proportional to

$$(N-M)|0\rangle + M|1\rangle. (28)$$

For illustration suppose we know that M is N/2 or N/2 + 1 and we want to figure out which case we have. Since we imagine that N is exponentially big, the two coefficients in (28) differ from each other only by an exponentially small amount so even multiple copies of this state will not allow us to tell which one of the two coefficients is bigger. But we can use post-selection again.

Even without post-selection we can use the old idea of unambiguous state discrimination [14]. This is a method for distinguishing any two distinct quantum states with zero probability of error, but with some probability of outputting "don't know." Suppose the states are  $|\psi_1\rangle$ ,  $|\psi_2\rangle \in \mathbb{C}^2$ . Let  $|\psi_2^{\perp}\rangle$  be the unique vector (up to phase) that is orthogonal to  $|\psi_2\rangle$ , and similarly for  $|\psi_1^{\perp}\rangle$ . One way to perform unambiguous state discrimination is randomly either measure in the  $\{|\psi_1\rangle, |\psi_1^{\perp}\rangle\}$  basis or the  $\{|\psi_2\rangle, |\psi_2^{\perp}\rangle\}$  basis. If the outcome is  $|\psi_1^{\perp}\rangle$  then we know that the original state must have been  $|\psi_2\rangle$  and likewise if the outcome is  $|\psi_2^{\perp}\rangle$  then we know that the original state must have been  $|\psi_2\rangle$  and likewise if the outcome is  $|\psi_1\rangle$  then we cannot definitively determine the original state and so we output "don't know". The probability of the "don't know" outcome is  $\frac{1}{2} + \frac{1}{2} |\langle \psi_1 | \psi_2 \rangle|^2$ . This is always < 1 unless  $|\psi_1\rangle$  and  $|\psi_2\rangle$  are identical up to phase. (While the "don't know" probability can be made lower [14], this will not be necessary for our argument.) If the states are very close but not equal, say if they correspond to M = N/2 and M = N/2+1, then the probability of "don't know" will be very close, but not equal to, 1. In this case, we can post-select on getting an answer other than "don't know" and the result will be correct with probability 1.

This idea can be generalized to distinguish between the cases  $M \leq N/2$  and M > N/2, as described by Aaronson in [1]. The new complication is that we don't know how far M is from N/2. If, say,  $M > \frac{3}{4}N$  or  $M < \frac{1}{4}N$  then we can distinguish these cases even without the help of postselection. Otherwise it is possible to use postselection to amplify the difference between these two possibilities. We can unitarily map the state (27) to

$$|0\rangle \otimes \frac{|0\rangle + \sqrt{3}|1\rangle}{2} + (1 - 2M/N)|1\rangle \otimes |0\rangle.$$
 (29)

If we then postselect on the second qubit being in the  $|0\rangle$  state we will be left with a state proportional to

$$|0\rangle + 2(1 - 2M/N)|1\rangle.$$
 (30)

Now performing a Hadamard yields a state proportional to

$$(N - M')|0\rangle + M'|1\rangle, \tag{31}$$

where M' - N/2 = 2(M - N/2). In other words we have doubled the difference between M and N/2. If now  $M' > \frac{3}{4}N$  or  $M' < \frac{1}{4}N$  then states can be easily distinguished, or if not then we can continue amplifying. This whole process requires only  $O(\log N)$  time and copies of the original state, and so can be done efficiently by a quantum computer with post-selection.

Now we further extend the algorithm. The same argument that worked for N/2 could work for any threshold. Repeatedly calling this subroutine can then allow a postselected quantum computers to determine the exact value of M, i.e. the number of satisfying assignments for a combinatorial search problem such as 3SAT.

The complexity class BQP, Bounded-error Quantum Polynomial time, is what we generally think of as conventional quantum computing with a polynomial number of qubits and a polynomial number of unitary gates. Technically it is a class of decision problems which means that we are using the quantum computer to answer Yes-No questions. But sometimes people say that the Shor factoring algorithm is in BQP because we could turn factoring into a decision problem ("is there a factor less than F?") and we will not bother too much with this kind of distinction. What we mean by PostBQP is what we have running a quantum computer with a polynomial number of qubits and a polynomial number of gates with the additional magical power of being able to post-select on the outcome when a subset of the qubits are measured. We have seen that PostBQP allows one to solve #P problems and in fact (loosely speaking) it contains the whole PH.

The classical analog of BQP is called BPP and it is the class of decision problems that can be answered with bounded error in polynomial time allowing for randomness as part of the algorithm. So BPP is what we think of as what can be achieved with conventional classical computers. Now PostBPP allows us to post-select on some subset of the bits after the circuit is run. For example, consider the Grover problem where the conventional computer has two registers, z for the input and second register where f(z) is stored. Now if we pick z at random and post-select on the second register being 1, we find a marked item. This means that PostBPP has even more power than NP. Even though PostBPP is very powerful, it is not believed to be powerful enough to solve counting problems. In fact PostBPP is known to be contained in the third level of the PH [24]. (We are not going to try to explain this as it would take us too far afield.) As a result, if PostBPP were to equal PostBQP then the PH would collapse to the third level; meaning that level 3 of the PH would equal level k for all  $k \geq 3$ . This statement is a key fact from complexity theory that we need for what follows.

In our proof that PostBQP can exactly compute M, there is only one step that could not be performed in PostBPP. This is the Hadamard mapping (27) to (28). In this way quantum computers with postselection can amplify the distance of M from N/2, while classical computers with postselection could only amplify the distance of M from 0 or N. This is enough for postselected classical computers to perform approximate counting but (apparently) not exact counting.

# 5 Efficient Classical Sampling of the Output of an Arbitrary Quantum Circuit Implies the Collapse of the Polynomial Hierarchy

Suppose you have a polynomial-size quantum circuit which produces the state  $U|0\rangle$  and you measure in the z basis. The probability of getting z is

$$q(z) = \left| \langle z | U | 0 \rangle \right|^2. \tag{32}$$

The quantum computer will naturally produce strings z with this probability. Now suppose that you had a classical device that uses random bits and produces strings z with probability p(z). What we argue in this section is that if p(z) is close to q(z) for all poly-size quantum circuits U and all inputs z then PostBPP = PostBQP. But this would imply the collapse of the PH as we just explained at the end of the last section. For this reason it is believed that classical computers cannot simulate the outputs of general quantum computers. This is all known and our goal here is to familiarize the reader with these arguments since they are necessary background for our statements below about sampling from the output of the QAOA.

Since classical computation is a subset of quantum computation we have that BPP  $\subseteq$  BQP. Suppose that with a classical computer using random bits we could efficiently produce strings with probability p(z) with p(z) very close to q(z). This means that the classical device would have the same power as BQP so in this case we would have that BPP = BQP.

We now show that if we could classically efficiently sample from the output of a quantum computer, then PostBPP = PostBQP. First note that  $PostBPP \subseteq PostBQP$  for the same reason that  $BPP \subseteq BQP$ . Now we need to show that if a decision problem can be solved with a post-selection on a quantum computer and quantum computer outputs can be classically sampled then the same decision problem can be solved with a classical computer that uses post-selection; in other words, that  $PostBQP \subseteq PostBPP$ .

Consider a general quantum circuit U acting on a tensor product Hilbert space where the first factor is a single qubit and the second is an n-qubit space. Let

$$q(z_1, z_2) = \left| \langle z_1, z_2 | U | 0, 0^n \rangle \right|^2.$$
(33)

We are going to post select on  $z_2 = 0^n$  so we define

$$q_{\text{post}}(z_1) = \frac{q(z_1, 0^n)}{q(0, 0^n) + q(1, 0^n)},$$
(34)

which is our normalized post-selected probability distribution over the outcomes  $z_1 = 0, 1$ . A decision problem (one with a YES/NO answer) specified by some input is said to be in PostBQP if there is a quantum circuit U depending on the input such that  $q_{\text{post}}(1) \geq 2/3$  in the YES case and  $q_{\text{post}}(1) \leq 1/3$  in the NO case.

Now suppose that we have a classical computer that using coin flips can output strings  $z_1, z_2$  with a probability  $p(z_1, z_2)$  that is very close to  $q(z_1, z_2)$ . If we post-select on the second string being  $0^n$  then we have

$$p_{\text{post}}(z_1) = \frac{p(z_1, 0^n)}{p(0, 0^n) + p(1, 0^n)},$$
(35)

where again  $z_1 \in \{0, 1\}$ .

Let us now describe more precisely our hypothesis that p is close to q. Suppose that

$$|p(z_1, z_2) - q(z_1, z_2)| \le 0.1 \, q(z_1, z_2). \tag{36}$$

These bounds on p and q immediately imply that  $p_{post}$  and  $q_{post}$  can be related as

$$\frac{0.9}{1.1}q_{\text{post}}(z_1) \le p_{\text{post}}(z_1) \le \frac{1.1}{0.9}q_{\text{post}}(z_1). \tag{37}$$

This means that  $p_{\text{post}}(1) \ge 0.54$  in the YES case and  $p_{\text{post}}(1) \le 0.41$  in the NO case, so the post-selected classical computer can solve the decision problem; i.e. the problem is in PostBPP. We then

see that under the assumption of an efficient classical simulation of the output of a general quantum computer we have that  $PostBQP \subseteq PostBPP$ . This would then imply PostBPP = PostBQP.

As we said at the end of the last section, if PostBPP = PostBQP. then the PH collapses at the third level. Since we believe this does not happen we conclude that no classical device can efficiently produce samples that match those output by a general quantum computer. We now argue that no classical device can efficiently produce samples that match those output by the p=1 QAOA. To this end we first show that PostQAOA = PostBQP.

## 6 PostQAOA = PostBQP

It was shown by Bremner, Josza and Shephard [11] that if a classical computer could efficiently sample from the output of an IQP circuit then the PH would collapse. In fact IQP or "Instantaneous Quantum Polytime" is rather similar in structure to the p=1 QAOA. For IQP there are two unitaries used to construct a circuit. The first is the Hadamard

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

which acts on each individual qubit. The second is a unitary diagonal in the z basis of the form

$$U_D = \exp(iD) \tag{38}$$

where D is a quadratic function of the  $\sigma_z$  operators:

$$D = \sum_{k,l} J_{kl} \sigma_z^k \sigma_z^l + \sum_k M_k \sigma_z^k \,, \tag{39}$$

with  $J_{kl}, M_k$  arbitrary coefficients. The circuit is of the form

$$H^{\otimes n}U_DH^{\otimes n}|0^n\rangle \tag{40}$$

and measurement is made in the computational basis. So we have

$$q^{\text{IQP}}(z) = \left| \langle z | H^{\otimes n} U_D H^{\otimes n} | 0^n \rangle \right|^2. \tag{41}$$

What was shown in [11] is that if there exists an efficient classical algorithm that can produce strings z with a distribution close to  $q^{IQP}(z)$  then the PH collapses at the third level.

We will now essentially copy the argument of [11] with the p=1 QAOA replacing the IQP circuit. To show the similarities between IQP and QAOA, let  $\beta = \pi/4$  and define for a single qubit

$$\tilde{H} = \exp(-i\frac{\pi}{4}\sigma_x) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix},$$

so we see that a special case of the p = 1 QAOA circuit (8) is

$$\tilde{H}^{\otimes n} e^{-i\gamma C} H^{\otimes n} |0^n\rangle. \tag{42}$$

which is to be compared with (40). Furthermore if the cost function C is a sum of two-bit clauses then  $e^{-i\gamma C}$  is of the form (38) with D of the form (39).

QAOA is a special case of BQP so we have that PostQAOA  $\subseteq$  PostBQP. We now show the reverse inclusion, that PostBQP is contained in PostQAOA by showing that any PostBQP circuit can be rewritten as a PostQAOA circuit. The tricky part is that BQP circuits can have polynomial depth and we are going to use post selection to collapse a general PostBQP circuit to the very shallow PostQAOA.

Any BQP circuit can be rewritten in terms of a few basic unitary gates. One such universal gate set consists of H,  $e^{i\frac{\pi}{8}\sigma_z}$  and the controlled-phase gate  $e^{-i\frac{\pi}{4}(I-\sigma_z^1)(I-\sigma_z^2)}$  [4]. If we set  $\gamma = \pi/4$ , then these latter two gates can be written (up to an overall phase) in the form  $e^{-i\gamma C_a}$  for 0/1-valued clauses  $C_a$ :

$$e^{i\frac{\pi}{8}\sigma_z} = e^{i\frac{\pi}{8}}e^{-i\frac{\pi}{4}|1\rangle\langle 1|} \tag{43a}$$

$$e^{-i\frac{\pi}{4}(I-\sigma_z^1)(I-\sigma_z^2)} = e^{-i\frac{\pi}{4}4|11\rangle\langle 11|}$$
 (43b)

Eq. (43a) comes from a single one-bit clause whereas (43b) requires repeating the same two-bit clause four times.

The crucial difference between a general quantum circuit and (42) is that in (42) all the diagonal gates are performed consecutively without any H's interspersed, while in a general circuit these noncommuting gates are interspersed without restriction. But if we introduce post selection we can replace each internal H gate with a gadget that involves an auxiliary qubit and a post-selected measurement involving a circuit of the form (42). To see how this works consider a general circuit that consists of a sequence of one- and two-qubit gates of the form (43) interspersed with H gates acting on individual qubits. Consider one internal H acting say on qubit j when the state of the system is

$$|\alpha\rangle_{j,\text{rest}} = |0\rangle_j |a\rangle_{\text{rest}} + |1\rangle_j |b\rangle_{\text{rest}},$$

where  $|a\rangle_{\rm rest}$ ,  $|b\rangle_{\rm rest}$  represent all qubits of the system other than j. Now in our post-selected QAOA circuit we add an auxiliary qubit which is in the state  $H|0\rangle_{\rm aux}=|+\rangle_{\rm aux}$  since all qubits are initialized in this state. Act on the auxiliary qubit and qubit j with the diagonal unitary

$$\begin{pmatrix} 1 & & & \\ & i & & \\ & & 1 & \\ & & & -i \end{pmatrix}. \tag{44}$$

This gate can also be written as

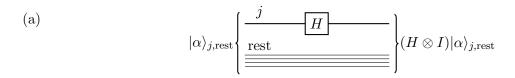
$$e^{-i\frac{\pi}{4}6|01\rangle\langle01|} e^{-i\frac{\pi}{4}2|11\rangle\langle11|} \tag{45}$$

so we can see explicitly that it is of the form  $e^{-i\frac{\pi}{4}C}$  with C containing repeated clauses. Next we act with  $\tilde{H}$  on qubit j, measure qubit j, and post select on the outcome being 0. It is straightforward to see that the remaining state is  $(H \otimes I)|\alpha\rangle_{\text{aux.rest}}$  where

$$|\alpha\rangle_{\text{aux,rest}} = |0\rangle_{\text{aux}}|a\rangle_{\text{rest}} + |1\rangle_{\text{aux}}|b\rangle_{\text{rest}}.$$

In this sense we have teleported the operation from the qubit j to the auxiliary qubit but using post selection we guarantee that the measurement step gives the desired outcome.

We have just shown how to replace a Hadamard gate acting on a qubit inside a general quantum circuit with a piece of a post-selected circuit of the form (42). But we need to ensure that the whole circuit is of the form (42), meaning in addition that all the qubits in the post-selected circuit start



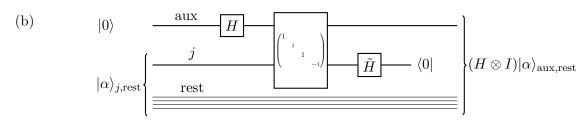


Figure 1: (a) Somewhere inside of a big quantum circuit consisting of Hadamards and diagonal unitaries, a Hadamard acts on qubit j. The quantum state before the Hadamard acts is  $|\alpha\rangle$  which we denote as  $|\alpha\rangle_{j,\text{rest}}$  to keep track of how it can be decomposed into qubit j and the rest. This circuit element can be replaced by the post-selected circuit in (b). Qubit j has been replaced by an auxiliary qubit and the new circuit is of the form (42) with qubit j post-selected to be  $|0\rangle$ .

in the state  $|0\rangle$  and are then acted on by a Hadamard and the last gate that any qubit is hit by is an  $\tilde{H}$ . We can ensure this as follows. Suppose that in the original circuit, some qubit is first acted on by a diagonal operator. Then before the diagonal acts, insert  $H \cdot H$  which of course is the identity. The first H which acts maintains the form (42). The second will need to be replaced by the construction in Fig. 1. Now suppose that the last operator that hits some qubit is anything other than  $\tilde{H}$ . Then insert the gates  $\tilde{H} \cdot \tilde{H}^{\dagger}$  so the last operator that acts on the qubit is indeed an  $\tilde{H}$ . Now

$$\tilde{H}^{\dagger} = H \exp(i\frac{\pi}{4}\sigma_z)H$$

which explicitly is made from elements of our universal gate set. Both H's can be replaced by the construction of the previous paragraph. Thus, after all of these replacements the post-selected circuit will be of the form (42).

The construction just outlined allows us to rewrite any BQP circuit as a post selected QAOA circuit. So we have shown that BQP is contained in PostQAOA. But what about PostBQP? We wanted to show that this is contained in PostQAOA. A PostBQP circuit will look like a BQP circuit except that at the end some qubits will be post-selected onto the 0 state. To incorporate this into our PostQAOA simulation, we post-select two batches of qubits into the 0 state: the ones that were post-selected in the original PostBQP circuit and the new ones that we used in our Hadamard gadgets. The overall circuit still only uses resources that are in PostQAOA.

We have just shown that PostBQP  $\subseteq$  PostQAOA and along with the reverse inclusion we have that PostBQP = PostQAOA. In fact our reduction does not introduce any error. Suppose we have an arbitrary quantum circuit built from Hadamards,  $e^{i\frac{\pi}{8}Z}$  and controlled-phase gates whose post-selected output distribution is  $q_{\text{post}}(z)$ . We have shown that there exists a C of the form (2) for which the corresponding p=1 QAOA circuit satisfies

$$q_{\text{post}}^{\text{QAOA}}(z) = q_{\text{post}}(z).$$
 (46)

# 7 Efficient Classical Sampling of the Output of the p = 1 QAOA Implies the Collapse of the Polynomial Hierarchy

Given an arbitrary QAOA circuit of the form (42) the probability distribution over measurement outcomes z is

 $q^{\text{QAOA}}(z) = \left| \langle z | \tilde{H}^{\otimes n} e^{-i\frac{\pi}{4}C} H^{\otimes n} | 0^n \rangle \right|^2, \tag{47}$ 

where C is of the form (2). If we have a poly-time randomized classical algorithm that takes as input C of the form (2) and outputs a string z with probability p(z) satisfying the bound

$$\left| p(z) - q^{\text{QAOA}}(z) \right| \le 0.1 \, q^{\text{QAOA}}(z) \tag{48}$$

then PH collapses. We now prove this by making use of the results in the previous section.

Our strategy is to show that using the assumption of a classical simulator for QAOA satisfying (48) we have PostBQP  $\subseteq$  PostBPP. The only difference with Section 5 is that we have replaced general quantum circuits with QAOA.

Consider a problem in PostBQP. By definition there exists a quantum circuit U with output distribution  $q(z_1, z_2)$  such that  $q_{\text{post}}(1) \geq 2/3$  if the answer is YES and  $q_{\text{post}}(1) \leq 1/3$  if not. This circuit can be assumed to be comprised of Hadamards and two-qubit diagonal unitaries, since these are a universal gate set. From the final result of the last section, there exists a p = 1 QAOA circuit with output distribution  $q^{\text{QAOA}}(z)$  such that  $q_{\text{post}}^{\text{QAOA}}(1) \geq 2/3$  in the YES case and  $q_{\text{post}}^{\text{QAOA}}(1) \leq 1/3$  in the NO case. Now using assumption (48) and repeating the error analysis of Section 5 we see that  $p_{\text{post}}(1) \geq 0.54$  in the YES case and  $p_{\text{post}}(1) \leq 0.41$  in the NO case. This means that a post-selected classical algorithm could solve a problem in PostBQP, proving that PostBQP  $\subseteq$  PostBPP. As we argued in Section 5 this implies the collapse of the polynomial hierarchy since PostBPP is contained in the third level of the PH. In other words, if we could efficiently classically sample from a distribution p(z) close to  $q^{\text{QAOA}}$  of (47) with tolerance (48) then the PH collapses.

**Sampling vs estimating.** The QAOA circuit, for general p, produces states of the form (10). For fixed p, if we specify 2p angles  $\vec{\gamma}$  and  $\vec{\beta}$  and measure the state in the computational basis we find string z with probability

$$|\langle z|\vec{\gamma}, \vec{\beta}\rangle|^2$$
.

It is this distribution that we claim (at least in worst case) cannot be sampled from efficiently with a classical device.

What if we only want to estimate  $\langle \vec{\gamma}, \vec{\beta} | C | \vec{\gamma}, \vec{\beta} \rangle$ ? It was shown in [18] that this expected value can be determined on a classical computer using resources that grow only polynomially in n and m but doubly exponentially in p. The situation is unusual in that we can classically determine the expected value of the cost function, but we use the quantum computer to produce strings with this value of the cost function. The distribution of the output is what cannot be reproduced classically. (See also [2].)

From the optimization point of view, at least for low p, we can classically determine the angles that maximize (11) but we use a quantum computer to find a string achieving roughly that value. Even if the QAOA has worse performance guarantees than certain classical algorithms, it can exhibit Quantum Supremacy because its output distribution cannot be efficiently classically sampled from. If for p > 1 or for some problem at p = 1, the QAOA outperforms all known classical algorithms then it will achieve Quantum Supremacy in an algorithmic sense.

Sampling with additive error. Our results rule out efficient classical sampling algorithm with low multiplicative error, as specified in (48). This requirement on the error is rather stringent. Alternatively, one might consider "additive error" meaning that  $\sum_{z} |p(z) - q(z)|$  is upper bounded by a small constant. It is more challenging to rule out efficient classical simulation with additive error. This can be done for certain models of quantum computing [3,12] but subject to additional conjectures from complexity theory and/or probability theory. We believe that these results (especially [12]) could be extended to cover the p=1 QAOA, but we leave this question to future work.

# 8 Quantum Adiabatic Algorithm

We now discuss the prospects of sampling from the output of the QADI. We are thinking here of the QADI as being used to solve optimization problems and not as a universal quantum computer. We will place restrictions on the form of the Hamiltonian that governs the evolution and see that these may make it more likely that classical simulation is available. To begin we review the basic idea of the algorithm and set the notation.

### 8.1 Definition and background

With the Quantum Adiabatic Algorithm in optimization mode, we are seeking the maximum of the cost function C given by (2). The basic building blocks are given by (4), (5), and (6). This algorithm is designed to find the maximum of C, which is of course the same as finding the minimum of -C, and we do this by ground-state computation. Note that  $|s\rangle$  is the ground state of -B and we are seeking the ground state of -C. Introduce a parameter-dependent Hamiltonian

$$H(s) = (1-s)(-B) + s(-C)$$
 with  $0 \le s \le 1$ , (49)

a run time T, and a time-dependent Hamiltonian (which also depends on T):

$$\tilde{H}(t) = H(t/T). \tag{50}$$

Then we evolve according to the Schrödinger equation

$$i\frac{d}{dt}|\psi(t)\rangle = \tilde{H}(t)|\psi(t)\rangle$$
 with  $|\psi(0)\rangle = |s\rangle$ 

which is the ground state of  $\tilde{H}(0)$ . Run for time T to get the state  $|\psi(T)\rangle$ . Note that the ground state of  $\tilde{H}(T)$  is the ground state of -C, so by the adiabatic theorem, in the  $T \to \infty$  limit the state  $|\psi(T)\rangle$  is the ground state of -C.

Actually for this to be true we need that the gap is not zero throughout the evolution but this is guaranteed because with our choice of driving Hamiltonian, -B, (see (5)), the off-diagonal entries of H(s) are non-positive and the Perron-Frobenius theorem then guarantees a non-vanishing gap. Hamiltonians with real non-positive off-diagonal elements are called "stoquastic" and this restriction is key to the ability to simulate ground-state properties of these Hamiltonians.

Note that the QADI will work perfectly if the run time is infinite but we are interested in performance in realistic situations. The required run time for good performance scales inversely with a power of the minimum gap. Here the community has struggled to analytically derive useful

bounds on the gaps of classes of instances. Much numerical work has been done, enabled by the stoquastic nature of the Hamiltonian; for example, see [21]. The D-Wave device [9, 17, 26, 28] is designed to run the QADI and its performance has been contrasted with simulations of the QADI as well as as with simulated annealing algorithms [8, 16, 31]. Here again the ultimate proof of performance may come from running the algorithm on physical devices.

### 8.2 Classical simulation of the Quantum Adiabatic Algorithm

For the QADI, classical simulation may be easier than it is for universal quantum computers. To argue this, we will need to restrict what we mean by adiabatic quantum computation by assuming the following three conditions:

- 1. H(s) is stoquastic. For simplicity we could assume that H(s) is of the form in (49).
- 2. The gap between the bottom two eigenvalues of H(s) is  $> 1/\operatorname{poly}(n)$  for all values of s.
- 3. The total time T is large enough that the adiabatic condition holds and the evolving state  $|\psi(t)\rangle$  is approximately equal to the instantaneous ground state  $|g;s\rangle$  (up to a phase) with s=t/T. Because of our second assumption this means that T=poly(n) suffices.

We call QADI subject to conditions 1-3 stoquastic gapped adiabatic evolution, or QADI-SG for short. When conditions 2 and 3 hold, they guarantee that the QADI-SG run on a quantum computer will efficiently find the string minimizing the cost function -C. Condition 1 is not necessary for the success of the quantum algorithm but it will be needed for the classical simulation. We discuss later the prospect of relaxing these conditions.

Since we are working with T large enough that the evolving state is very close to the instantaneous ground state, we will approximate the evolving state by the instantaneous ground state  $|g;s\rangle$  where again s=t/T. Now we are interested in sampling in the computational basis  $|z\rangle$  from the ground state  $|g;s\rangle$  and so the string z will be found with probability  $|\langle z|g;s\rangle|^2$ . The question now becomes: how hard is it to sample from this distribution?

The first thing to try is Quantum Monte Carlo, which is a family of classical algorithms that can be used to sample from the ground states of stoquastic Hamiltonians. (Please try not to be confused by the terminology and remember that QMC is a classical algorithm used to find properties of quantum systems.) If we choose an inverse temperature  $\beta$  that is sufficiently larger than the inverse gap of H(s) (meaning  $\geq \text{poly}(n)$ , due to assumption 2 above) then

$$\frac{e^{-\beta H(s)}}{\operatorname{tr} e^{-\beta H(s)}}$$

will have high overlap with  $|g;s\rangle\,\langle g;s|.$  In this case  $|\langle z|g;s\rangle\,|^2$  is approximately equal to

$$\frac{\langle z|e^{-\beta H(s)}|z\rangle}{\operatorname{tr} e^{-\beta H(s)}}.$$
 (51)

Here we will use our stoquastic assumption which states that the off-diagonal elements are non-positive. In fact, let us also replace H(s) with H(s) - cI for some  $c \ge 0$  so that all entries of H(s) are non-positive and accordingly all entries of -H(s) are non-negative. This change will not affect the physics, nor will it change (51). Now the numerator of (51) can be written as a sum of an exponential number of nonnegative numbers. There are various ways to do this but we will focus

specifically on an approach known as Path-Integral Monte Carlo. For brevity, write H = H(s) and note

$$\langle z|e^{-\beta H}|z\rangle = \langle z|(e^{-\frac{\beta H}{L}})^L|z\rangle \tag{52}$$

$$= \sum_{x_1 \in \{0,1\}^n} \sum_{x_2 \in \{0,1\}^n} \cdots \sum_{x_L \in \{0,1\}^n} \langle z | e^{-\frac{\beta H}{L}} | x_1 \rangle \langle x_1 | e^{-\frac{\beta H}{L}} | x_2 \rangle \cdots \langle x_L | e^{-\frac{\beta H}{L}} | z \rangle.$$
 (53)

Each term  $\langle x_i|e^{-\frac{\beta H}{L}}|x_{i+1}\rangle$  is nonnegative and, if L is sufficiently large, can be approximated by expanding the exponential, although (53) as written is exact.

Our goal now is to sample z from a distribution proportional to (53). Let

$$w(z,x) := \langle z|e^{-\frac{\beta H}{L}}|x_1\rangle\langle x_1|e^{-\frac{\beta H}{L}}|x_2\rangle\cdots\langle x_L|e^{-\frac{\beta H}{L}}|z\rangle$$
(54)

where x denotes the tuple  $(x_1, \ldots, x_L)$ . Since  $w(z, x) \ge 0$  we can define a normalized probability distribution

$$p(z,x) := \frac{w(z,x)}{\sum_{z',x'} w(z',x')} = \frac{w(z,x)}{\text{tr}[e^{-\beta H}]}.$$
 (55)

If we can sample from strings (z, x) according to p then the marginal distribution on z (that is for fixed z sum over x) will be equal to (51) and with  $\beta$  large enough this will be close to  $|\langle z|g;s\rangle|^2$ . So the task now is to sample from p. To this end we use the Metropolis method. This method will produce a Markov chain which settles down to following the distribution p. Suppose that at some point in the process the configuration is (z,x). The method requires some rule for selecting possible next values of the configuration (z',x'). For example it might be to flip a bit (or some bits) at random. The new value (z',x') is accepted according to a rule which only involves the ratio

$$\frac{p(z',x')}{p(z,x)} = \frac{w(z',x')}{w(z,x)}.$$
 (56)

For the problem at hand, using say single-bit flips on (z,x) we can easily compute the ratio of probabilities knowing only w which has the explicit formula (54). This means it is possible to sample from p and then find out how frequently the string z would be measured in the ground state of H(s).

What we just described will work in principle but it may take exponentially long for the Markov chain to settle down to the desired distribution. To see that the process can take exponentially long to settle consider a cost function C for an NP-complete problem with only one string satisfying all the clauses. Then the ground state of -C corresponds to this assignment and the gap of -C is at least 1. If s=1 and  $\beta$  is large, then  $e^{-\beta H(s)}$  has most of its weight on the ground state, and so sampling from (51) will have a high chance of revealing the satisfying assignment. It should not be possible for any algorithm, whether QMC or anything else, to efficiently achieve this, unless NP-complete problems could be solved in polynomial time. One might object that the s=1 case is too degenerate, since H(s=1) has no off-diagonal entries. But the s=1 argument can be extended to s near 1, say  $s=1-1/\operatorname{poly}(n)$ , to see that efficient sampling from the ground state of this H(s) would allow one to solve NP-complete problems.

One approach to attempt to sample from the ground state of H(1) is for the classical algorithm to track the adiabatic path. We start with s=0, where the ground state is the uniform superposition which we can easily sample from. Then incrementally increase s and for each value of s run the

Metropolis procedure hopefully long enough to achieve the desired distribution. In this way we have "warm starts" for successive values of s. In fact this procedure can be viewed as a classical algorithm for finding the minimum of -C and is sometimes referred to as SQA for Simulated Quantum Annealing [8,15,21,31].

Despite the fact that there are cases (see the above discussion as well as Ref. [25]) where we know that QMC takes exponentially long to equilibrate, QMC works well in practice in many cases. In fact numerical simulations of QADI-SG out to 100's of qubits have been achieved. More generally QMC is a standard tool in many-body quantum physics and has been successfully used to simulate quantum systems with millions of degrees of freedom by incorporating problem-specific insights.

# 8.3 Formal Evidence that Stoquastic Gapped Adiabatic Evolution is Easier to Simulate than QAOA

We can use QMC to provide formal evidence that QADI-SG is easier to simulate than QAOA. Specifically, QADI-SG can be simulated in PostBPP; that is, by a poly-time classical randomized computer with the ability to postselect. Recall from Section 7 that if QAOA could be simulated in PostBPP then the PH would collapse. So, if the PH does not collapse then QADI-SG can be thought of as easier to simulate then QAOA. Another way to say this is that if we had an oracle for problems in PostBPP, we could call that oracle a polynomial number of times and efficiently sample from the ground state of a gapped stoquastic Hamiltonian, but we have strong reasons to believe that such an oracle would not allow for the efficient sampling of the QAOA.

We now sketch the argument for why QADI-SG is in PostBPP, following [10]. This argument uses QMC but does not rely on a Markov chain or any other method of sampling. Instead post-selection can be used to immediately jump to the right distribution using rejection sampling. We know already that  $w(z,x) \geq 0$ , but from the form (54) we can also bound  $w(z,x) \leq w_{\text{max}}$  for some easily computable bound  $w_{\text{max}}$  which need not be tight. These ingredients are now enough for a post-selected sampling algorithm. Let b be a work bit that we will post-select on. Then the algorithm is:

- 1. Choose (z,x) uniformly at random.
- 2. Set b=1 with probability  $\frac{w(z,x)}{w_{\text{max}}}$  and b=0 with probability  $1-\frac{w(z,x)}{w_{\text{max}}}$ .

Conditioned on b = 1 the resulting probability distribution over (z, x) is exactly proportional to w(z, x). So if we post-select on b = 1 we get (z, x) with probability p(z, x).

As with many algorithms in PostBPP, the probability of rejection (b = 0) can be very high and so this does not give a polynomial time algorithm for actual classical computers. But this argument is still enough to show that simulating QADI-SG can be done in PostBPP.

#### 8.4 Universal adiabatic quantum computing

It is known that adiabatic quantum computing is a universal form of quantum computing [5]. This means that given any quantum circuit with n qubits and  $\mathcal{T}$  unitaries producing a state  $|\psi\rangle$ , one can construct a local Hamiltonian H(s) with gap  $\geq 1/\operatorname{poly}(n,\mathcal{T})$  that can be used in a poly-time adiabatic algorithm to produce a good approximation of the same state  $|\psi\rangle$ . This construction makes use of a non-stoquastic Hamiltonian to drive the evolution.

Suppose that QADI-SG could be used to perform universal quantum computation. We just showed that QADI-SG could be simulated in PostBPP. But this would imply that BQP is in PostBPP. As we showed in Section 5 this would imply that PostBQP is in PostBPP, which in turn would collapse the PH. So here again we see a crucial difference. An oracle for problems in PostBPP would allow the simulation of QADI-SG but the same oracle would not be strong enough to simulate general QADI.

#### 9 Discussion

We are entering an era when small-scale gate-model quantum computers are being built. The natural question is what algorithms should be run on them? Answering this question as the devices are being built will influence the design of hardware architecture and help set performance goals.

Devices exist and are being built to run the Quantum Adiabatic Algorithm in optimization mode. We argue that if the Hamiltonian governing the evolution is stoquastic then simulation is more feasible than it is for the QAOA. We believe that this makes a compelling case that future devices should be governed by Hamiltonians which are not restricted to be stoquastic. This will make simulation more difficult both in practice and for complexity theoretic reasons. It might be the case that a stoquastic system can be of real computational value when compared with all known classical algorithms. But still it would seem prudent to operate quantum computers in a way that makes classical simulation more difficult.

Another candidate quantum algorithm to run on near-term quantum computers is the QAOA. This gate model algorithm is designed to find approximate solutions to combinatorial search problems. Running it may be competitive with or outperform classical computers as the size of quantum computers gets larger. What we show in this paper is that efficient sampling from the output of even the lowest depth version of this algorithm would collapse the PH. This means that, based on plausible conjectures from complexity theory, there are choices of  $\gamma$ ,  $\beta$  and cost function C for which the output of a quantum computer running the p=1 QAOA could not be mimicked with a classical device. This strengthens the case that the QAOA should be run on a near term quantum device.

# Acknowledgments

We are grateful to Michael Bremner, Daniel Brod, David Gosset, Sam Gutmann, Jeffrey Goldstone and Eleanor Rieffel for helpful comments and discussions. Thanks to Alex Dalzell for catching a mistake in the first version of this paper. EF would like to thank the Google Quantum AI team for stimulating discussion. EF was funded by NSF grant CCF-1218176. AWH was funded by NSF grants CCF-1111382 and CCF-1452616 and IARPA via DoI/IBC contract number D15PC00242. Both were funded by ARO contract W911NF-12-1-0486. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of IARPA, DoI/NBC, or the U.S. Government.

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