COMPLEXITY OF STOQUASTIC FRUSTRATION-FREE HAMILTONIANS

SERGEY BRAVYI∗ AND BARBARA TERHAL†

Abstract. We study several problems related to properties of non-negative matrices that arise at the boundary between quantum and classical probabilistic computation. Our results are twofold. First, we identify a large class of quantum Hamiltonians describing systems of qubits for which the adiabatic evolution can be efficiently simulated on a classical probabilistic computer. These are stoquastic local Hamiltonians with a “frustration free” ground-state. A Hamiltonian belongs to this class iff it can be represented as $H = \sum H_a$ where (1) every term $H_a$ acts non-trivially on a constant number of qubits, (2) every term $H_a$ has real non-positive off-diagonal matrix elements in the standard basis, and (3) the ground-state of $H$ is a ground-state of every term $H_a$. Secondly, we generalize the Cook-Levin theorem proving NP-completeness of the satisfiability problem to the complexity class MA — a probabilistic analogue of NP. Specifically, we construct a quantum version of the $k$-SAT problem which we call “stoquastic $k$-SAT” such that stoquastic $k$-SAT is contained in MA for any constant $k$, and any promise problem in MA is Karp-reducible to stoquastic 6-SAT. This result provides the first non-trivial example of a MA-complete promise problem.

Key words. Adiabatic Quantum Computing, Non-Negative Matrices, Randomized Algorithms, Merlin-Arthur Games

AMS subject classifications. 68Q15, 68Q17, 68W20

1. Introduction. Recent years have seen the first steps in the development of a quantum or a matrix-valued complexity theory. Such complexity theory is interesting for a variety of reasons. Firstly, it increases our understanding of fundamental limitations imposed on computational devices by the laws of physics. Secondly, since quantum computation is an extension of classical computation, quantum complexity theory provides a framework and a new angle to attack major problems in classical complexity theory, see for instance [1].

The problems for which a solution can be efficiently found on a quantum computer constitute the class BQP — the quantum analogue of the classical class BPP. On the other hand, the problems for which a solution can be efficiently verified on a quantum computer constitute the class QMA — the quantum analogue of the class MA. It was realized recently that one can learn a lot about the classes BQP and QMA by studying ground-state properties of local Hamiltonians. Firstly, Aharonov et al. [2] proved that any quantum algorithm can be executed via quantum adiabatic evolution in which parameters of a local Hamiltonian are changed adiabatically while the state of the quantum computer is encoded into the instantaneous ground-state. Secondly, it was shown by Kitaev [3] that determining the ground-state energy of a local Hamiltonian is a problem complete for the class QMA, see [4] 5 6 for some recent progress.

In this paper we present a large family of local Hamiltonians for which quantum adiabatic evolution can be efficiently simulated by a classical probabilistic algorithm while determining the ground-state energy is a problem complete for the class MA (considered as a class of promise problems). To introduce this family of Hamiltonians let us start from setting up some terminology. The Hilbert space of $n$ qubits equipped with the standard basis $\{|x\rangle, x \in \Sigma^n\}$, will be denoted as $Q^n$. Here and below we denote as $\Sigma^n = \{0,1\}^n$ the set of $n$-bit binary strings.

Definition 1.1. A $k$-local Hamiltonian acting on $n$ qubits is a Hermitian oper-
ator $H$ on a Hilbert space $\mathbb{C}^n$ representable as $H = \sum_{a=1}^{M} H_a$, where every term $H_a$ acts non-trivially only on some subset of $k$ or less qubits. We shall consider families of $k$-local Hamiltonians in which $k = O(1), M \leq \text{poly}(n)$, and $\|H_a\| \leq \text{poly}(n)$.

We shall often use the terms $k$-local Hamiltonian and local Hamiltonian interchangeably.

**Definition 1.2.** A local Hamiltonian $H = \sum_{a} H_a$ is called frustration-free if $H_a$ are positive semi-definite operators and the ground-state of $H$ is a zero eigenvector of all operators $H_a$.

**Definition 1.3.** A local Hamiltonian $H = \sum_{a} H_a$ is called stoquastic with respect to a basis $\mathcal{B}$ iff all $H_a$ have real non-positive off-diagonal matrix elements in the basis $\mathcal{B}$.

Throughout this paper we shall consider Hamiltonians that are stoquastic with respect to the standard basis of $n$ qubits formed by tensor products of $|0\rangle$ and $|1\rangle$ states. The term “stoquastic” was introduced in [7] to emphasize a connection with both stochastic matrices and quantum Hamiltonians. The problem of determining the ground-state energy of a stoquastic local Hamiltonian is contained in the complexity class AM (Arthur-Merlin games), see [7] for details.

In the present paper we shall focus on stoquastic frustration-free (SFF) Hamiltonians. Some examples of SFF Hamiltonians will be given in Section 3. These examples demonstrate that SFF Hamiltonians arise naturally at the boundary between quantum computation and classical probabilistic computation or, in physics, at the boundary between classical statistical mechanics and quantum mechanics.

**1.1. Summary of results.** Our first result concerns the computational power of adiabatic quantum evolution with SFF Hamiltonians. Let $H_{in}$ and $H_f$ be SFF Hamiltonians acting on $n$ qubits. We assume that $H_{in}$ and $H_f$ can be connected by an adiabatic path $H(s)$, $0 \leq s \leq 1$, such that $H_{in} = H(0), H_f = H(1)$. In addition the following conditions should be met

(A0) Hamiltonians $H(s)$ are stoquastic and frustration-free for all $s$.

(A1) The path is sufficiently smooth; $J = \max_s \|dH(s)/ds\| \leq \text{poly}(n)$.

(A2) The Hamiltonian $H(s)$ has a non-degenerate ground-state for all $s$. The spectral gap $\Delta(s)$ between the smallest and the second smallest eigenvalues of $H(s)$ is sufficiently large: $\Delta = \min_s \Delta(s) \geq 1/\text{poly}(n)$.

(A3) The initial Hamiltonian is sufficiently simple so there exists a $\text{poly}(n)$ algorithm that finds a basis vector $|x\rangle$ such that the overlap between $|x\rangle$ and the ground-state of $H_{in}$ is at least $2^{-\text{poly}(n)}$.

In contrast to the standard paradigm of adiabatic quantum computation or quantum annealing we do not require the adiabatic path to be a linear interpolation between $H_{in}$ and $H_f$ (since otherwise it may be impossible to fulfill the frustration-free condition). The goal of the simulation is to sample $x \in \{0,1\}^n$ from the probability distribution $\pi(x)$ associated with the ground-state $|\psi\rangle$ of $H_f$, that is, $\pi(x) = |\langle x|\psi\rangle|^2$ (assuming that $\langle \psi|\psi\rangle = 1$). Our first result is as follows.

**Theorem 1.4.** Let $|\psi\rangle$ be the ground-state of $H_f$ and $\pi(x) = |\langle x|\psi\rangle|^2$. Suppose the adiabatic evolution conditions (A0)-(A3) are met. Then for any precision $\delta > 0$ there exists a classical probabilistic algorithm that generates a random variable $x \in \{0,1\}^n$ with a probability distribution $\tilde{\pi}(x)$ such that $\|\tilde{\pi} - \pi\|_1 \leq \delta$. The running time of the algorithm is $\text{poly}(n, \delta^{-1})$.

It should be mentioned that the property of being frustration-free alone cannot render the adiabatic evolution efficiently simulatable on a classical computer. The following proposition is a simple extension of [2].
Proposition 1.5. Let $U$ be a quantum circuit with $n$ input qubits initialized in the state $|0\rangle$ and $L = \text{poly}(n)$ two-qubit gates. Let $|\psi_L\rangle$ be the $n$-qubit output state of $U$. For any precision $\delta > 0$ one can construct a family of frustration-free Hamiltonians $H(s)$, $0 \leq s \leq 1$ acting on $\text{poly}(n,\delta^{-1})$ qubits and satisfying conditions (A1),(A2),(A3) such that the ground-state of $H(1)$ approximates $|\psi_L\rangle$ with precision $\delta$ (after discarding some ancillary qubits).

For the sake of completeness we outline the proof in Appendix B. Proposition 1.5 implies that simulating the adiabatic evolution with frustration-free Hamiltonians is as hard as simulating a universal quantum computer. On the other hand, our technique does not permit an efficient simulation of an adiabatic evolution with stoquastic Hamiltonians which are not necessarily frustration-free. In fact, adiabatic evolution with stoquastic Hamiltonians includes a variety of the quantum annealing algorithms, see [8]. It is an interesting open question whether adiabatic evolution with general stoquastic Hamiltonians can be simulated classically in polynomial (or at least sub-exponential) time. Our result raises a question: how hard is it to verify that a given Hamiltonian is frustration-free requires evaluating the smallest eigenvalue of $H$.

This problem is known to be QMA-hard for general local Hamiltonians, see [3]. For stoquastic Hamiltonians the smallest eigenvalue problem is known to be contained in QMA $\cap$ AM, where AM (Arthur-Merlin games) is a probabilistic analogue of NP in which the prover and the verifier can exchange a constant number of messages, see [7]. One can expect that verifying whether a stoquastic Hamiltonian is frustration-free must be easier than evaluating the smallest eigenvalue because for a positive instance we have the additional information that the ground-state minimizes the expectation of every local term in a Hamiltonian. Let us start from stating the problem more formally.

Definition 1.6. A system of $(n,k)$-constraints is a family of $n$-qubit positive semidefinite Hermitian operators $\{H_a\}$, $a = 1,\ldots,M$, such that every $H_a$ acts non-trivially only on some subset of $k$ or less qubits. A system $C = \{H_a\}$ is satisfiable iff there exists a state $|\psi\rangle$ such that $H_a |\psi\rangle = 0$ for all $H_a$. Such a state is called a satisfying assignment. We shall consider systems in which $k = O(1)$, $M \leq \text{poly}(n)$ and $\|H_a\| \leq \text{poly}(n)$.

If a system $C = \{H_a\}$ is not satisfiable, any state $|\psi\rangle$ violates at least one constraint, i.e., $\langle \psi | H_a | \psi \rangle > 0$ for some $H_a$. Let us define the unsat-value of a system $C$ as the smallest eigenvalue of a Hamiltonian $H_C = \sum_a H_a$.

$$\text{unsat}(C) = \min_{\psi : \langle \psi | \psi \rangle = 1} \langle \psi | H_C | \psi \rangle, \quad H_C = \sum_a H_a.$$ 

By definition, a system $C$ is satisfiable iff the corresponding Hamiltonian $H_C$ is frustration-free. The quantum $k$-SAT problem is to distinguish the case when a system of $(n,k)$-constraints is satisfiable from the case when it has a non-negligible (i.e. polynomial in $1/n$) unsat-value. The quantum version of the Cook-Levin theorem proved by Kitaev [3] and developed further in [9] [10] asserts that quantum $k$-SAT belongs to QMA for any constant $k$ and the quantum 4-SAT is complete for the class QMA$_1$ (the analogue of QMA with zero completeness error). Let us now define a stoquastic systems of constraints and the problem stoquastic $k$-SAT.

Definition 1.7. A system of $(n,k)$-constraints $C = \{H_a\}$ is called stoquastic iff every $H_a$ has real non-positive off-diagonal matrix elements in the standard basis.

Definition 1.8. An instance of stoquastic $k$-SAT is a tuple $(n,C,\epsilon)$, where $C$
is a stoquastic system of \((n, k)\)-constraints and \(\epsilon = n^{-O(1)}\) is a positive number. For yes-instances \(\text{unsat}(C) = 0\). For no-instances \(\text{unsat}(C) \geq \epsilon\).

It should be emphasized that stoquastic \(k\)-SAT is a promise problem. It can be represented by a pair of languages \((L_{\text{yes}}, L_{\text{no}})\) such that

\[
L_{\text{yes}} = \{(n, C, \epsilon) : \text{unsat}(C) = 0\}, \quad L_{\text{no}} = \{(n, C, \epsilon) : \text{unsat}(C) \geq \epsilon\}.
\]

Note that classical \(k\)-SAT can be obtained as a special case of stoquastic \(k\)-SAT when all the constraints \(H_a\) are diagonal in the standard basis with matrix elements 0, 1 on the diagonal. It follows that stoquastic \(k\)-SAT is NP-hard for \(k \geq 3\). Our second result is that stoquastic \(k\)-SAT can be placed in the complexity class MA — a probabilistic analogue of NP with only one message sent from the prover to the verifier. For the sake of completeness we present a formal definition of MA and Promise-MA in Appendix A. In addition, we proved in [7] that stoquastic \(k\)-SAT is complete for the class Promise-MA for sufficiently large \(k\). Putting these results together gives

**Theorem 1.9.** The promise problem stoquastic \(k\)-SAT is contained in MA for any constant \(k\). Any promise problem in MA is Karp-reducible to stoquastic 6-SAT with constraints \(\{H_a = I - \Pi_a\}\) where \(\Pi_a\) are projectors with matrix elements from a set \(\{0, \frac{1}{2}, 1\}\).

This result can be regarded as a generalization of the Cook-Levin theorem proving NP-completeness of the classical satisfiability problem.

The rest of the paper is organized as follows. In Section 1.2 we briefly review the previous work on the subject. Section 2 sketches the main ideas and techniques used in the proof of Theorem 1.4 and Theorem 1.9. Section 3 provides some interesting examples of SFF Hamiltonians. Basic properties of non-negative matrices required for understanding of our simulation algorithms are presented in Section 4. A proof of Theorem 1.4 can be found in Section 5. Theorem 1.9 is proved in Section 6. In Section 7 we discuss some open problems and directions for future work. A formal definition of the classes MA and Promise-MA is given in Appendix A. Finally, Appendix B contains a proof of Proposition 1.5 and a proof of MA-hardness of stoquastic 6-SAT.

### 1.2. Previous work.

Stoquastic Hamiltonians are well known in computational physics as Hamiltonians avoiding the “sign problem”. It was realized decades ago that ground-state properties of such Hamiltonians can be simulated using classical Monte Carlo algorithms, see [11, 12], for systems as large as several hundred qubits. The general limitations of such algorithms which are likely to make them inefficient in the complexity-theoretic sense were also well understood, see e.g. [12, 13]. The first rigorous attempt to analyze the complexity of the smallest eigenvalue problem for stoquastic Hamiltonians was made in [7]. It was shown that this problem belongs to the complexity class AM (Arthur-Merlin games). Using the same ideas the smallest eigenvalue problem was shown in the unpublished [14] to be contained in a smaller class SBP \(\subseteq\) AM, where SBP stands for Small Bounded-Error Probability, see [15].

The complexity of the smallest eigenvalue problem for \(k\)-local stoquastic Hamiltonians was shown to be the same for all \(k \geq 2\), see [7]. A related problem called “Stoquastic Local Consistency” which involves verifying certain consistency conditions for a collection of local density matrices was studied by Liu [16].

A connection between stoquastic Hamiltonians and classical probabilistic computation was studied by Aharonov and Ta-Shma in [17]. Using the technique of adiabatic state generation these authors constructed quantum algorithms for q-sampling from the stationary distribution of a reversible Markov chain satisfying certain additional
properties. An analogous connection between stoquastic Hamiltonians and classical statistical mechanics was obtained by Verstraete et al. [18] and Somma et al. [19]. These authors proved that a coherent version of the Gibbs thermal state associated with any local classical Hamiltonian can be represented as the unique ground-state of stoquastic frustration-free Hamiltonian.

2. Techniques. This section highlights the main ideas and techniques used in the rigorous proofs in Sections 5 and 6.

2.1. A random walk associated with a SFF Hamiltonian. The main technical tool used throughout the paper is a novel random walk algorithm that allows one to simulate some ground-state properties of SFF Hamiltonians. This algorithm is similar in spirit to the Green Function Monte Carlo method (GFMC) — a probabilistic heuristic for the simulation of quantum spin systems, see [11, 12]. However, in contrast to GFMC our algorithm offers rigorous upper bounds on the running time and the error probability.

Let $H = \sum_a H_a$ be some SFF Hamiltonian and $|\psi\rangle$ be a ground-state of $H$, i.e., $H_a |\psi\rangle = 0$ for all $a$. Using the Perron-Frobenius theorem we will show in Section 4 that a ground-state of any SFF Hamiltonian can be chosen as a vector with real non-negative amplitudes in the standard basis (if the smallest eigenvalue has multiplicity $q$, one can choose $q$ orthonormal ground-states such that each state has non-negative amplitudes). For that reason we can assume that $\langle x | \psi \rangle \geq 0$ for all $x \in \Sigma^n$. A set of binary strings that appear in $|\psi\rangle$ with a non-zero amplitude will be called a support of $|\psi\rangle$ and denoted as

$$S(\psi) = \{ x \in \Sigma^n : \langle x | \psi \rangle > 0 \}.$$

A random walk associated with a Hamiltonian $H$ and a ground-state $|\psi\rangle$ is a random walk on the set $S(\psi)$ with transition matrix

$$P_{x \rightarrow y} = \frac{\langle y | \psi \rangle}{\langle x | \psi \rangle} \langle y | G | x \rangle, \quad G = I - \beta H, \quad \text{for any } x \in S(\psi).$$

Here $\beta > 0$ is a real parameter that is chosen sufficiently small in order to make $G$ a matrix with non-negative entries, so that $P_{x \rightarrow y} \geq 0$. One can infer directly from the definition that $P_{x \rightarrow y} = 0$ unless $y \in S(\psi)$. Besides, the eigenvalue equation $G |\psi\rangle = |\psi\rangle$ implies $\sum_{y \in S(\psi)} P_{x \rightarrow y} = 1$ for any $x \in S(\psi)$. Therefore Eq. (2.2) indeed defines a random walk on the set $S(\psi)$. Direct inspection shows that the stationary distribution of the random walk is

$$\pi(x) = \langle x | \psi \rangle^2.$$

Here we assumed that $|\psi\rangle$ is a normalized state, i.e., $\langle \psi | \psi \rangle = 1$. Note that for a given Hamiltonian $H$ one may have several stationary distributions supported on mutually disjoint sets of basis vectors such that each distribution is associated with some non-negative ground-state of $H$.

Let us now argue that the random walk defined in Eq. (2.2) can be efficiently simulated on a classical probabilistic computer. Indeed, let $\Pi_a$ be the spectral projector corresponding to the zero eigenvalue of $H_a$. By definition, $\Pi_a |\psi\rangle = |\psi\rangle$ for all $a$. The crucial property of the projectors $\Pi_a$ is that they have real non-negative matrix elements in the standard basis. This property can be proved using elementary algebra, see Section 4. Moreover, we will show that any projector with non-negative
entries can be decomposed into a direct sum of rank-one projectors with non-negative entries. Using this decomposition we shall be able to show that if \( x \in \mathcal{S}(\psi) \) and \( \langle y | H_a | x \rangle < 0 \) for some \( a \) and some \( y \in \Sigma^n \) then \( y \in \mathcal{S}(\psi) \) and

\[
\frac{\langle y | \psi \rangle}{\langle x | \psi \rangle} = \sqrt{\frac{\langle y | \Pi_a | y \rangle}{\langle x | \Pi_a | x \rangle}}.
\]

Note that \( P_{x \rightarrow y} = 0 \) unless \( \langle y | G | x \rangle > 0 \), that is, \( \langle y | H_a | x \rangle < 0 \) for some \( a \). Since every \( H_a \) acts non-trivially on \( O(1) \) qubits, the number of strings \( y \) such that \( P_{x \rightarrow y} > 0 \) is at most \( \text{poly}(n) \). Therefore, given a current position of the walk \( x \in \mathcal{S}(\psi) \) one can efficiently simulate one step of the walk by first finding all strings \( y \) such that \( \langle y | H_a | x \rangle < 0 \) for some \( a \) and then using Eq. (2.4) and Eq. (2.2) to compute the transition probabilities.

2.2. Simulation of the adiabatic evolution. When we discretize the adiabatic evolution we get a family of SFF Hamiltonians \( H^{(j)} = \sum_{a=1}^{M} H_a(j/T) \), where \( j = 0, \ldots, T \) is a discrete time step. The Hamiltonian \( H^{(j)} \) has a unique non-negative ground-state \( | \psi^{(j)} \rangle \) with support \( \mathcal{S}(\psi^{(j)}) \). Using definition Eq. (2.2) gives us a family of efficiently simulatable random walks \( P^{(0)}, P^{(1)}, \ldots, P^{(T)} \) such that \( P^{(j)} \) is a random walk on the set \( \mathcal{S}(\psi^{(j)}) \). The walk \( P^{(j)} \) has a stationary distribution \( \pi^{(j)} \) such that \( \pi^{(j)} = \langle x | \psi^{(j)} \rangle^2 \). Note that the spectrum of \( P^{(j)} \) coincides with the spectrum of \( G^{(j)} = I - \beta H^{(j)} \) restricted to a subspace spanned by basis vectors from \( \mathcal{S}(\psi^{(j)}) \). Since the largest eigenvector of \( G^{(j)} \) belongs to this subspace, the spectral gap of \( P^{(j)} \) (i.e. the gap between the largest and the second largest eigenvalues) is at least the spectral gap of \( G^{(j)} \). Condition (A2) implies that the spectral gap of \( G^{(j)} \) is at least \( \beta \Delta \). Therefore the spectral gap of \( P^{(j)} \) is at least \( \beta \Delta \) which is polynomial in \( 1/n \).

Recall that the goal of the simulation is to sample \( x \) from the final distribution \( \pi^{(T)}_x \). Since the spectral gap of the walk \( P^{(T)} \) is polynomial in \( 1/n \), all we need is a warm start for \( P^{(T)} \), that is a string \( x \in \mathcal{S}(\psi^{(T)}) \) such that the stationary distribution \( \pi^{(T)} \) has a non-negligible probability at \( x \). Here non-negligible means \( \pi^{(T)}_x \geq 2^{-\text{poly}(n)} \).

Our strategy is to generate a warm start for the walk \( P^{(j+1)} \) using a warm start for \( P^{(j)} \) by making sufficiently many steps of the walk \( P^{(j)} \) such that the endpoint of \( P^{(j)} \) is a string sampled from the stationary distribution \( \pi^{(j)} \) (with an exponentially small error). As far as the initial walk \( P^{(0)} \) is concerned, a warm start can be efficiently generated due to condition (A3). The main technical challenge is to bound the probability of failure, i.e., the probability that for some \( j \) the end-point of the walk \( P^{(j)} \) is not a warm start for the next walk \( P^{(j+1)} \).

In order to achieve this we introduce the notion of \( t \)-balanced strings. Namely, given probability distributions \( \pi \) and \( \rho \) on the set \( \Sigma^n \), a string \( x \in \Sigma^n \) is \( t \)-balanced with respect to \( \pi \) and \( \rho \) iff \( \pi_x, \rho_x > 0 \) and \( t^{-1} \leq \pi_x/\rho_x \leq t \). We show that for sufficiently large (but constant) \( t \) the probability for a string \( x \) drawn from \( \pi \) to be \( t \)-balanced is at least \( 1 - O(1 - F(\pi, \rho)) \), where \( F(\pi, \rho) = \sum_x \sqrt{\pi_x \rho_x} \) is the fidelity between \( \pi \) and \( \rho \). Using conditions (A1) and (A2) we shall bound the fidelity between \( \pi^{(j)} \) and \( \pi^{(j+1)} \) as

\[
F(\pi^{(j)}, \pi^{(j+1)}) \geq 1 - \frac{J^2}{T^2 \Delta^2}.
\]

It follows that a string drawn from \( \pi^{(j)} \) is \( t \)-balanced (for some \( t = O(1) \)) with respect to \( \pi^{(j)} \) and \( \pi^{(j+1)} \) with probability at least \( 1 - O(J^2 T^{-2} \Delta^{-2}) \). Choosing \( T \gg J^2 \Delta^{-2} \)
and choosing the number of steps in each walk much larger than the inverse spectral gap we shall prove that the end-point of the walk $P^{(j)}$ is a warm start for the walk $P^{(j+1)}$ for all $j = 0, \ldots, T - 1$ with probability at least $1 - O(J^2T^{-1} \Delta^{-2}) \approx 1$.

2.3. Stoquastic k-SAT is contained in MA. Let $(n, C, \epsilon)$ be an instance of the stoquastic k-SAT problem. Here $C = \{H_a\}_{a=1,\ldots,M}$ is a system of stoquastic constraints. Define a Hamiltonian $H = \sum_{a=1}^M H_a$. By definition,

\begin{align*}
(n, C, \epsilon) \text{ is yes-instance} & \implies H \text{ is a SFF Hamiltonian}, \\
(n, C, \epsilon) \text{ is no-instance} & \implies \text{The smallest eigenvalue of } H \text{ is at least } \epsilon.
\end{align*}

Let $\Pi_a$ be the spectral projector corresponding to the zero eigenvalue of $H_a$. We shall partition the set of all binary strings $\Sigma^n$ into good and bad strings, such that

\begin{equation}
S_{\text{good}} = \{x \in \Sigma^n : \langle x | \Pi_a | x \rangle > 0 \text{ for all } a = 1, \ldots, M\}
\end{equation}

and $S_{\text{bad}} = \Sigma^n \setminus S_{\text{good}}$. For any instance $(n, C, \epsilon)$ and any $x \in S_{\text{good}}$ define the transition probabilities

\begin{equation}
P_{x \rightarrow y} = \frac{1}{M} \sum_{a=1}^M \sqrt{\frac{\langle y | \Pi_a | y \rangle}{\langle x | \Pi_a | x \rangle}} \langle y | G_a | x \rangle, \quad G_a = I - \beta H_a,
\end{equation}

where $\beta > 0$ is a real parameter chosen sufficiently small so that all matrices $G_a$ are non-negative. One can infer directly from the definition that $P_{x \rightarrow y} = 0$ unless $\langle y | \Pi_a | y \rangle > 0$ for some $a$. Therefore, for any given $x$ the number of strings $y$ such that $P_{x \rightarrow y} > 0$ is at most $\text{poly}(n)$. The property that $\Pi_a$ is a direct sum of rank-one projectors with non-negative entries implies that the transition probabilities are normalized, that is, $\sum_{y \in \Sigma^n} P_{x \rightarrow y} = 1$ for any $x \in S_{\text{good}}$, see Section 4 for details. However, the transition probabilities Eq. (2.7) do not automatically define a random walk on the set of good strings because one may have transitions from a good string to a bad string. In other words, Eq. (2.7) permits transitions $S_{\text{good}} \rightarrow S_{\text{good}}$ as well as $S_{\text{good}} \rightarrow S_{\text{bad}}$.

It turns out that if $(n, C, \epsilon)$ is a positive instance then Eq. (2.7) does define a random walk on some subset of good strings. Indeed, let $|\psi\rangle$ be a satisfying assignment, i.e., a state satisfying $H_a |\psi\rangle = 0$ for all $a$. As was mentioned above, we can assume that $|\psi\rangle$ has real non-negative amplitudes. Using the eigenvalue equations $\Pi_a |\psi\rangle = |\psi\rangle$ one can easily show that $|\psi\rangle$ is supported only on good strings, $S(\psi) \subseteq S_{\text{good}}$, and for any $x \in S(\psi)$ the transition probabilities Eq. (2.7) can be expressed as

\begin{equation}
P_{x \rightarrow y} = \frac{\langle y | \psi \rangle \langle \psi | x \rangle}{\langle x | \psi \rangle} \langle y | G | x \rangle, \quad G = \frac{1}{M} \sum_{a=1}^M G_a.
\end{equation}

Repeating the same arguments as in Section 2.2 we conclude that Eq. (2.8) is a transition matrix of a random walk on the set $S(\psi)$. For any given starting string $x \in S(\psi)$ the walk stays in $S(\psi)$ forever. The walk can be efficiently simulated on a classical probabilistic computer. (In contrast to Section 2.2 the mixing time of the walk is not a matter of concern.)

Suppose now that $(n, C, \epsilon)$ is a negative instance. One can still use Eq. (2.7) to simulate a random walk starting from a good string until the first time the walk hits a bad string. It will be shown in Section 6 that the probability for the walk starting
from a good string to stay in \( S_{\text{good}} \) for \( L \) steps (and satisfy some extra tests which are always passed for positive instances) decays approximately as \((1 - \beta \epsilon / M)^L\). Given the polynomial bounds on \( \beta, \epsilon, \) and \( M \) we can make this probability exponentially small with \( L = \text{poly}(n) \).

In order to prove that \((n,C,\epsilon)\) is a positive instance, the prover can send the verifier a binary string \( w \in \Sigma^n \) such that some satisfying assignment \(|\psi\rangle\) has a non-negligible amplitude on \( w \) (for a negative instance \( w \) can be arbitrary string). The verifier checks whether \( w \in S_{\text{good}} \) and simulates \( L = \text{poly}(n) \) steps of the random walk defined above starting from \( w \). Whenever the walk hits a bad string, the verifier aborts the simulation and outputs ‘no’. If the walk stays in \( S_{\text{good}} \) for \( L \) steps, the verifier outputs ‘yes’ (conditioned on the outcome of some extra tests described in Section 6).

2.4. MA-hardness. MA-hardness of the stoquastic 6-SAT problem with the constraints satisfying conditions of Theorem 1.9 follows directly from from MA-hardness of the stoquastic 6-local Hamiltonian problem, see Lemma 3 in [7]. In order to make the paper self-contained we repeat the proof of [7] with some minor modifications in Appendix B.

3. Examples of stoquastic frustration-free Hamiltonians. In this section we give some examples of SFF Hamiltonians. Firstly, the results obtained by Verstraete et al. [18] and Somma et al. [19] imply that a coherent version of the thermal Gibbs state associated with any classical local Hamiltonian can be represented as the unique ground-state of a SFF Hamiltonian. Secondly, we use the clock Hamiltonian construction from [3] to show that a coherent version of a probability distribution generated by any polynomial-size classical reversible circuit can be approximated by the ground-state of a SFF Hamiltonian.

3.1. Coherent thermal states of classical Hamiltonians. Let \( H \) be any classical Hamiltonian acting on \( n \) qubits (\( H \) has a diagonal matrix in the standard basis). Denote \( H(x) = \langle x|H|x\rangle \). Choose any \( \beta > 0 \) and consider a coherent version of the thermal Gibbs state

\[
|\pi\rangle = Z^{-1/2} \sum_{x \in \Sigma^n} e^{-\beta H(x)/2} |x\rangle, \quad Z = \text{Tr} e^{-\beta H}.
\]

(3.1)

Given a state \(|\pi\rangle\) one can sample \( x \) from the Gibbs distribution \( \pi_x = Z^{-1} e^{-\beta H(x)} \) by measuring the state in the standard basis. More interestingly, given coherent Gibbs states \(|\pi\rangle\) and \(|\pi'\rangle\) corresponding to some classical Hamiltonians \( H \) and \( H' \), one can perform the swap test on the two states thus evaluating the statistical difference between the two Gibbs distributions, see [17].

Suppose that \( H \) is a local Hamiltonian, \( H = \sum_a H_a \), and each qubit is acted on by a constant number of terms \( H_a \). The analysis performed in [18] [19] shows that the state Eq. (3.1) is the unique ground-state of some SFF Hamiltonian \( H_\beta \). Indeed, one can represent \(|\pi\rangle\) as follows (ignoring the normalization)

\[
|\pi\rangle = e^{-\beta H/2} |+\rangle, \quad |+\rangle = \sum_{x \in \Sigma^n} |x\rangle.
\]

Let \( X_j \) be the Pauli X-matrix, \( X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \), acting on qubit \( j \). Using the representation above one can easily check that

\[
X_j |\pi\rangle = \Gamma_j |\pi\rangle, \quad \Gamma_j = X_j e^{-\beta H/2} X_j e^{\beta H/2}
\]
for all \( j = 1, \ldots, n \). Note that the operator \( \Gamma_j \) is diagonal in the standard basis. Since all matrix elements of \( \Gamma_j \) are real, we conclude that \( \Gamma_j \) is Hermitian. Since we assumed that any qubit is acted on by a constant number of local terms in \( H \), we conclude that \( \Gamma_j \) acts non-trivially on a constant number of qubits. Define a Hamiltonian

\[
H_\beta = \sum_{j=1}^{n} \Gamma_j - X_j
\]

such that \( H_\beta |\pi\rangle = 0 \). The Perron-Frobenius theorem implies that \(|\pi\rangle\) is the unique ground-state of \( H_\beta \) (indeed, \( G = I - \gamma H \) is a non-negative irreducible matrix for sufficiently small \( \gamma > 0 \) and \(|\psi\rangle\) is a positive eigenvector of \( G \)). The same argument shows that \(|\pi\rangle\) is a ground-state of every local term \( \Gamma_j - X_j \). It follows that \( \Gamma_j - X_j \) is a positive semi-definite operator and thus \( H_\beta \) is a SFF Hamiltonian with unique ground-state \(|\pi\rangle\).

### 3.2. Coherent probabilistic computation

Let \( U \) be a classical polynomial-size circuit with reversible gates (e.g. Toffoli gates) with \( n \) input and \( n \) output bits. Assume that the first \( k \) input bits are drawn from the uniform distribution and the last \( n - k \) input bits are initialized to 0. Let \( \pi \) be the corresponding probability distribution of the output bits. Consider a coherent version of \( \pi \),

\[
|\pi\rangle = \sum_{x \in \Sigma^n} \sqrt{\pi_x} |x\rangle.
\]

We claim that \(|\pi\rangle\) can be represented as the unique ground-state of some SFF Hamiltonian. More strictly, for any precision \( \delta > 0 \) there exists a SFF Hamiltonian \( H \) acting on \( \text{poly}(n, \delta^{-1}) \) qubits such that \( H \) has an unique ground-state \(|\psi\rangle\) satisfying \( \langle \psi | \pi \otimes \phi_a \rangle \geq 1 - \delta \) for some simple ancillary state \(|\phi_a\rangle\). Such a Hamiltonian \( H \) can be constructed by transforming \( U \) into a quantum circuit \( \tilde{U} \) taking as input a state \(|+\rangle^\otimes k |0\rangle^\otimes (n-k)\), where \(|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2} \). The circuit \( \tilde{U} \) first applies the gates of \( U \) in a coherent fashion and then applies \( \delta^{-1} L \) identity gates, where \( L \) is the number of gates in \( U \). Note that the output state of \( \tilde{U} \) is \(|\pi\rangle\). Applying the clock Hamiltonian construction of \( \tilde{U} \) to \( U \) we get the desired Hamiltonian \( H \). The details of this construction are presented in Appendix B.

### 4. Non-negative matrices: basic properties

This section summarizes some basic properties of non-negative matrices that are needed in understanding our simulation algorithms. Let us start from setting up some terminology and notations. A matrix is called non-negative iff all its entries are real and non-negative. A term non-negative projector will refer to a Hermitian projector acting on \( Q^n \) which has a non-negative matrix in the standard basis. Analogously, a term non-negative state will refer to a normalized vector \(|\psi\rangle \in Q^n \) such that all amplitudes of \(|\psi\rangle\) in the standard basis are real and non-negative. Let us start from a simple observation.

**Proposition 4.1.** Let \( H \) be a Hermitian operator with non-positive off-diagonal matrix elements in the standard basis. Then the spectral projector \( \Pi \) corresponding to the smallest eigenvalue of \( H \) is non-negative.

**Proof.** Indeed, \( \Pi = q \cdot \lim_{\beta \to -\infty} e^{-\beta H} / Z(\beta) \), where \( Z(\beta) = \text{Tr}(e^{-\beta H}) \) and \( q \) is the multiplicity of the smallest eigenvalue. Since \( e^{-\beta H} \) is a non-negative matrix for any \( \beta \geq 0 \), the limit \( \Pi \) is a non-negative matrix.

Next we shall give a simple characterization of non-negative projectors.

**Lemma 4.2.** For any non-negative projector \( \Pi \) of rank \( q \) there exist non-negative states \(|\psi_1\rangle, \ldots, |\psi_q\rangle\) such that \( \langle \psi_a | \psi_b \rangle = \delta_{a,b} \) for all \( a, b \) and \( \Pi = \sum_{a=1}^{q} |\psi_a\rangle \langle \psi_a| \).
Note that non-negative states are pairwise orthogonal iff they have support on non-overlapping subsets of basis vectors, that is, $\mathcal{S}(\psi_a) \cap \mathcal{S}(\psi_b) = 0$ for $a \neq b$. Thus the lemma asserts that a non-negative projector is always block-diagonal (up to a permutation of basis vectors) with each block being a projector onto a non-negative state. Combining Lemma 4.2 and Proposition 4.1 one concludes that

**Corollary 4.3.** The ground-subspace of any stoquastic Hamiltonian has an orthonormal basis of non-negative ground-states.

Let us proceed with the proof of Lemma 4.2.

**Proof.** For any basis vector $|x\rangle$ define a “connected component”

$$T_x = \{ y \in \Sigma^n : \langle x|\Pi|y \rangle > 0 \}.$$

(Some of the sets $T_x$ may be empty.) For any triple $x, y, z$ the inequalities $\langle x|\Pi|y \rangle > 0$, $\langle y|\Pi|z \rangle > 0$ imply $\langle x|\Pi|z \rangle > 0$ since

$$\langle x|\Pi|z \rangle = \langle x|\Pi^2|z \rangle = \sum_{u \in \Sigma^n} \langle x|\Pi|u \rangle \langle u|\Pi|z \rangle \geq \langle x|\Pi|y \rangle \langle y|\Pi|z \rangle > 0.$$

A similar argument shows that if $T_x$ is non-empty then $\langle x|\Pi|x \rangle > 0$, that is, $x \in T_x$. Therefore the property $\langle x|\Pi|y \rangle > 0$ defines a symmetric transitive relation on $\Sigma^n$ and we have

- $y \in T_x$ implies $T_y = T_x$,
- $y \notin T_x$ implies $T_y \cap T_x = \emptyset$.

Consider a subspace $\mathcal{H}(T_x) \subseteq \mathcal{Q}^n$ spanned by the basis vectors from $T_x$. Clearly $\mathcal{H}(T_x)$ is $\Pi$-invariant. Thus $\Pi$ is block diagonal w.r.t. decomposition of the whole Hilbert space into the direct sum of spaces $\mathcal{H}(T_x)$ and the orthogonal complement where $\Pi$ is zero. Moreover, the restriction of $\Pi$ onto any non-zero subspace $\mathcal{H}(T_x)$ is a projector with strictly positive entries. According to the Perron-Frobenius theorem, the largest eigenvalue of a Hermitian operator with positive entries is non-degenerate. Thus each block of $\Pi$ has rank 1, since a projector has eigenvalues 0 and 1 only. □

We shall use this characterization of non-negative projectors to derive the following lemma that plays a key role in the definition of a random walk in Section 6.

**Lemma 4.4.** Let $\Pi$ be a non-negative projector. Suppose $\Pi|\psi\rangle = |\psi\rangle$ for some non-negative state $|\psi\rangle$. Then for any $x \in \mathcal{S}(\psi)$ one has

1. $\langle x|\Pi|x \rangle > 0$,
2. If $\langle x|\Pi|y \rangle > 0$ for some $y \in \Sigma^n$ then $y \in \mathcal{S}(\psi)$ and

$$\langle y|\psi \rangle = \sqrt{\frac{\langle y|\Pi|y \rangle}{\langle x|\Pi|x \rangle}}.$$

**Proof.** Statement (1) can be proved by contradiction. Assume $x \in \mathcal{S}(\psi)$ and $\langle x|\Pi|x \rangle = 0$. Then $\Pi|x\rangle = 0$ and thus $\langle x|\psi \rangle = \langle x|\Pi|\psi \rangle = 0$ which contradicts the definition of $\mathcal{S}(\psi)$. To prove the first part of statement (2) note that $\langle x|\Pi|y \rangle > 0$ implies

$$\langle y|\psi \rangle = \langle y|\Pi|\psi \rangle \geq \langle y|\Pi|x \rangle \langle x|\psi \rangle > 0,$$
Computing the ratio (5.1) follows from Lemma 4.3. Indeed, consider a decomposition of \( \Pi \) into non-negative pairwise orthogonal rank-one projectors:

\[
\Pi = \sum_{a=1}^{q} |\psi_a\rangle \langle \psi_a|, \quad q = \text{rank}(\Pi).
\]

The condition \( \langle x|\Pi|y \rangle > 0 \) implies that \( x \) and \( y \) belong to the same rank-one block of \( \Pi \), that is

\[
\Pi |y \rangle = \langle \psi_a| |y \rangle = \sqrt{\langle x|\Pi|y \rangle} |\psi_a\rangle,
\]

\[
\Pi |y \rangle = \langle \psi_a| |y \rangle = \sqrt{\langle y|\Pi|y \rangle} |\psi_a\rangle
\]

for some block \( a \). Now we have

\[
\langle x|\psi \rangle = \langle x|\Pi|\psi \rangle = \sqrt{\langle x|\Pi|x \rangle} \langle \psi_a|\psi \rangle,
\]

\[
\langle y|\psi \rangle = \langle y|\Pi|\psi \rangle = \sqrt{\langle y|\Pi|y \rangle} \langle \psi_a|\psi \rangle.
\]

Computing the ratio \( \langle y|\psi \rangle / \langle x|\psi \rangle \) we get Eq. (5.1). \( \Box \)

Now we are ready to prove Eq. (2.4).

**Lemma 4.5.** Let \( H = \sum_{a=1}^{M} H_a \) be some SFF Hamiltonian and \( \Pi_a \) be the spectral projector corresponding to the zero eigenvalue of \( H_a \). Suppose \( H |\psi \rangle = 0 \) for some non-negative state \( |\psi \rangle \). If for some \( x \in S(\psi) \), \( y \in \Sigma^n \), and \( a \in \{1, \ldots, M\} \) one has \( \langle y|H_a|x \rangle < 0 \) then \( y \in S(\psi) \) and

\[
\frac{\langle y|\psi \rangle}{\langle x|\psi \rangle} = \sqrt{\frac{\langle y|\Pi_a|y \rangle}{\langle x|\Pi_a|x \rangle}}.
\]

**Proof.** Without loss of generality \( x \neq y \). Let us show that \( \langle y|H_a|x \rangle < 0 \) implies \( \langle y|\Pi_a|x \rangle > 0 \). Indeed, let \( \delta > 0 \) be the second smallest eigenvalue of \( H_a \). Then

\[
0 \leq \delta(I - \Pi_a) \leq H_a.
\]

Define a Hermitian operator \( O = |y\rangle \langle x| + |x\rangle \langle y| \). It follows that

\[
-\delta \text{Tr}(\Pi_a) = \delta \text{Tr}(O(I - \Pi_a)) \leq \text{Tr}(OH_a) = 2\langle x|H_a|y \rangle.
\]

Since we already know that \( \Pi_a \) has real matrix elements, see Proposition 4.1, we get

\[
\delta \langle x|\Pi_a|y \rangle \geq -\langle x|H_a|y \rangle \geq 0
\]

and thus \( \langle x|\Pi_a|y \rangle > 0 \). Now the lemma follows from Lemma 4.3. \( \Box \)

**5. Simulation of the adiabatic evolution.** In this section we prove Theorem 4.3. Let us start with discretizing the adiabatic evolution. Define \( H^{(j)} = H(j/T) \), \( j = 0, \ldots, T \) where \( T \) is a large integer that will be chosen later. Using the bound \( \|dH(s)/d(s)\| \leq J \) we get

\[
\|H^{(j+1)} - H^{(j)}\| \leq \frac{J}{T}.
\]

The next step is to bound the overlap (inner product) between the instantaneous ground-states at time \( j \) and \( j + 1 \). Let \( |\psi^{(j)}\rangle \) be the ground-state of \( H^{(j)} \), that is, \( H^{(j)} |\psi^{(j)}\rangle = 0 \). We can assume that \( |\psi^{(j)}\rangle \) are non-negative states, see Corollary 4.3.

**Lemma 5.1.** Let \( \Delta \) be the smallest spectral gap of \( H^{(j)} \), \( j = 0, \ldots, T \). Then for any \( j \) one has

\[
\langle \psi^{(j+1)}|\psi^{(j)}\rangle \geq 1 - \frac{J^2}{T^2\Delta^2}.
\]
A more general version of this lemma was proved in [17]. For the sake of completeness we prove the lemma below.

Proof. Consider a decomposition \(|\psi^{(j+1)}⟩ = a|\psi^{(j)}⟩ + b|\psi^{(j)}⟩\), where \(|\psi^{(j)}⟩\) is a normalized vector orthogonal to \(|\psi^{(j)}⟩\), so that \(|a|^2 + |b|^2 = 1\). Then

\[
\|H^{(j)}|\psi^{(j+1)}⟩\| = |b| \cdot \|H^{(j)}|\psi^{(j)}⟩\| \geq |b| \Delta.
\]

On the other hand,

\[
\|H^{(j)}|\psi^{(j+1)}⟩\| = \| (H^{(j)} - H^{(j+1)})|\psi^{(j+1)}⟩\| \leq \|H^{(j)} - H^{(j+1)}\|.
\]

Taking into account the bound Eq. (5.1) we arrive at \(|b| \leq J \Delta^{-1} T^{-1}\). Therefore

\[
⟨\psi^{(j+1)}|\psi^{(j)}⟩ = a \geq a^2 = 1 - |b|^2 \geq 1 - J^2 \Delta^{-2} T^{-2}.
\]

\[\square\]

For every \(j = 0, \ldots, T\) define an operator

\[
G^{(j)} = I - \beta H^{(j)}, \quad \text{where} \quad \beta = \max_{0 \leq s \leq T} \sum_{a=1}^{M} \|H_a(s)\|.
\]

By definition of a local Hamiltonian \(\|H_a(s)\| \leq poly(n), M \leq poly(n)\) and thus \(\beta \geq poly(1/n)\). The following properties of \(G^{(j)}\) follow directly from the definition.

Proposition 5.2. The operator \(G^{(j)}\) has a non-negative matrix in the standard basis. The spectrum of \(G^{(j)}\) belongs to the interval \([0, 1]\) and \(|\psi^{(j)}⟩\) is the only eigenvector of \(G^{(j)}\) with eigenvalue 1. The eigenvalue 1 is separated from the rest of the spectrum by a gap which is at least \(\beta \Delta\).

For any \(x, y \in S(\psi^{(j)})\) define the transition probability

\[
P_{x \rightarrow y}^{(j)} = \frac{⟨y|G^{(j)}|x⟩}{⟨x|G^{(j)}|x⟩} ⟨y|G^{(j)}|x⟩.
\]

As was explained in Section 2.2 \(P^{(j)}\) defines a random walk on the set \(S(\psi^{(j)})\) with the stationary distribution

\[
\pi^{(j)}_x = ⟨x|ψ^{(j)}⟩^2.
\]

Since \(P^{(j)}\) is obtained from \(G^{(j)}\) by a similarity transformation, the spectrum of the matrix \(P^{(j)}\) coincides with the spectrum of \(G^{(j)}\) restricted to the subspace spanned by basis vectors from \(S(\psi^{(j)})\). Since the largest eigenvector of \(G^{(j)}\) belongs to this subspace, we conclude that \(P^{(j)}\) has a spectral gap at least \(\beta \Delta\). Lemma 5.1 allows one to bound the fidelity between the stationary distributions \(π^{(j)}\) and \(π^{(j+1)}\),

\[
F(π^{(j)}, π^{(j+1)}) = \sum_{x \in Σ^n} \sqrt{π_x^{(j)} π_x^{(j+1)}} = ⟨ψ^{(j)}|ψ^{(j+1)}⟩ \geq 1 - J^2 T^{-1} \Delta^2.
\]

In order to simulate the adiabatic evolution we shall generate a sequence of strings \(x^{(0)}, x^{(1)}, \ldots, x^{(T+1)} \in Σ^n\) such that \(x^{(0)}\) is an arbitrary string satisfying \(⟨x^{(0)}|ψ^{(0)}⟩ \geq 2^{-n}\), and \(x^{(j+1)}\) is generated from \(x^{(j)}\) by making \(L\) steps of the random walk \(P^{(j)}\) starting from \(x^{(j)}\). We shall try to choose the number of steps \(L\) such that for all \(j\) the
distribution $\pi^{(j)}$ has a non-negligible probability at $x^{(j)}$. More specifically, we want the following inequality to be satisfied with high probability for all $j = 0, 1, \ldots , T$:

\begin{equation}
(5.5) \quad \langle x^{(j)}|\psi^{(j)}\rangle \geq 2^{-n-2}.
\end{equation}

A string $x^{(j)}$ satisfying Eq. (5.5) will be referred to as a warm start (for the random walk $P^{(j)}$). Let $\tilde{\pi}^{(j)}$ be the probability distribution of a string $x$ obtained by making $L$ steps of $P^{(j)}$ with a fixed warm start $x^{(j)}$. Using the definition of the random walk $P^{(j)}$ one can express the statistical difference between the distributions $\tilde{\pi}^{(j)}$ and $\pi^{(j)}$ as

$$
\|\tilde{\pi}^{(j)} - \pi^{(j)}\|_1 = \frac{1}{2\langle x^{(j)}|\psi^{(j)}\rangle} \sum_{x \in \Sigma^n} \langle x|\psi^{(j)}\rangle \left| \langle x|\tilde{G}^{(j)}L|x^{(j)}\rangle \right|
$$

where $\tilde{G}^{(j)} = G^{(j)} - |\psi^{(j)}\rangle\langle\psi^{(j)}|$. Applying the Cauchy-Schwartz inequality and taking into account that the largest eigenvalue of $\tilde{G}^{(j)}$ is at most $1 - \beta\Delta$, we arrive at

$$
\|\tilde{\pi}^{(j)} - \pi^{(j)}\|_1 \leq \frac{1}{2\langle x^{(j)}|\psi^{(j)}\rangle} \| \langle \tilde{G}^{(j)}L|x^{(j)}\rangle \| \leq 2^{n+1}(1 - \beta\Delta)^L.
$$

Clearly the statistical difference can be made exponentially small with $L = \text{poly}(n)$. Neglecting exponentially small errors, we shall assume for simplicity that $\tilde{\pi}^{(j)} = \pi^{(j)}$, that is, given the warm start condition at step $j$, the endpoint $x^{(j+1)}$ of the walk $P^{(j)}$ is drawn from the stationary distribution $\pi^{(j)}$. All that remains is to evaluate the probability for the warm start condition to be violated. In order to achieve this, let us introduce the notion of $t$-balanced strings.

**Definition 5.3.** Let $\pi$, $\rho$ be probability distributions on $\Sigma^n$ and $t \geq 1$ be a real number. A string $x \in \Sigma^n$ is called $t$-balanced with respect to $\pi$ and $\rho$ iff $\pi_x > 0$, $\rho_x > 0$ and $t^{-1} \leq \pi_x/\rho_x \leq t$. We shall denote a set of all $t$-balanced strings as $M_t(\pi, \rho)$, that is

\begin{equation}
(5.6) \quad M_t(\pi, \rho) = \{ x \in \Sigma^n : \pi_x > 0, \quad \rho_x > 0, \quad t^{-1} \leq \pi_x/\rho_x \leq t \}.
\end{equation}

Let $F(\pi, \rho) = \sum_{x \in \Sigma^n} \sqrt{\pi_x \rho_x}$ be the fidelity between $\pi$ and $\rho$.

**Lemma 5.4.** Suppose $F(\pi, \rho) \geq 1 - \delta$ and $t \geq 4$. Then the probability for a string $x$ drawn from the distribution $\pi$ to be $t$-balanced is

\begin{equation}
(5.7) \quad \sum_{x \in M_t(\pi, \rho)} \pi_x \geq 1 - \frac{2\delta}{1 - 2^{-t-1/2}}.
\end{equation}

**Proof.** Indeed, if $x$ is not $t$-balanced then

$$
\sqrt{\pi_x \rho_x} \leq t^{-1/2} \max \{ \pi_x, \rho_x \} \leq t^{-1/2}(\pi_x + \rho_x).
$$

Thus

$$
1 - \delta \leq \sum_{x \in M_t(\pi, \rho)} \sqrt{\pi_x \rho_x} + t^{-1/2} \sum_{x \notin M_t(\pi, \rho)} (\pi_x + \rho_x).
$$

Taking into account that $\sqrt{\pi_x \rho_x} \leq (1/2)(\pi_x + \rho_x)$ we get

$$
1 - \delta \leq \frac{1}{2} \sum_{x \in M_t(\pi, \rho)} (\pi_x + \rho_x) + t^{-1/2} \sum_{x \notin M_t(\pi, \rho)} (\pi_x + \rho_x) = 1 - (1/2-t^{-1/2}) \sum_{x \notin M_t(\pi, \rho)} (\pi_x + \rho_x).
$$

It follows that
\[
\delta \geq (1/2 - t^{-1/2}) \sum_{x \notin M_t(\pi, \rho)} (\pi_x + \rho_x)
\]
which yields Eq. (5.7).

Using Lemma 5.1 we can bound the probability for \(x^{(j+1)}\) to be \(t\)-balanced with respect to \(\pi^{(j)}\) and \(\pi^{(j+1)}\) for \(t = 16\) as
\[
\Pr[x^{(j+1)} \in M_{16}(\pi^{(j)}, \pi^{(j+1)})] \geq 1 - \frac{4J^2}{\Delta^2T^2}.
\]

Thus in order to prove that \(x^{(j+1)}\) is a warm start for \(P^{(j+1)}\) it suffices to show that \(\pi^{(j)}\) has large enough probability at \(x^{(j+1)}\). Recall that \(x^{(j+1)}\) is random string drawn from the stationary distribution \(\pi^{(j)}\) (with exponentially small error).

**Proposition 5.5.** Let \(\pi\) be a probability distribution on \(\Sigma^n\). The probability for a string \(x\) drawn from \(\pi\) to satisfy \(\pi_x \geq 2^{-2n}\) is at least \(1 - 2^{-n}\).

**Proof.** Indeed,
\[
\sum_{x : \pi_x \leq 2^{n-2n}} \pi_x \leq 2^n 2^{-2n} = 2^{-n}.
\]

Again ignoring, for simplicity, events that occur with exponentially small probability, we assume that \(\pi_x^{(j+1)} \geq 2^{-2n}\) and thus Eq. (5.8) implies
\[
\Pr[\langle x^{(j+1)} \psi^{(j+1)} \rangle \geq 2^{-n-2}] \geq 1 - \frac{4J^2}{\Delta^2T^2}.
\]

Thus the conditional probability for \(x^{(j+1)}\) to be a warm start provided that \(x^{(j)}\) is a warm start is at least \(1 - 4J^2 \Delta^{-2}T^{-2}\). Therefore the probability for \(x^{(j)}\) to be a warm start for all \(j = 1, 2, \ldots, T\) is at least \((1 - 4J^2 \Delta^{-2}T^{-2})^T \approx 1 - 4J^2 \Delta^{-2}T^{-1}\) for \(T \gg \Delta^{-2}J^2\). If the warm start condition has been violated at some step, we can not guarantee that \(x^{(T+1)}\) is drawn from the distribution \(\pi^{(T)}\) (in fact, the final distribution might not be defined in this case because the endpoint of some walk \(P^{(j)}\) may be outside of \(S(\psi^{(j+1)})\)). Therefore, our simulation scheme fails with probability at most \(\delta \sim J^2 \Delta^{-2}T^{-1}\). It follows that \(T = poly(n, \delta^{-1})\).

**6. Stoquastic \(k\)-SAT is contained in MA.** Recall that we consider an instance of stoquastic \(k\)-SAT \((n, C, \epsilon)\), where \(\epsilon = n^{-O(1)}\) is a precision parameter and \(C = \{H_a\}_{a=1, \ldots, M}\) is a stoquastic system of \((n, k)\)-constraints.

A formal description of the prover’s strategy is the following. Consider first a yes-instance. Let \(|\psi\rangle \in Q^n\) be any satisfying assignment (which can always be chosen as a non-negative vector). The prover sends the verifier a string \(w \in \Sigma^n\) corresponding to the largest amplitude of \(|\psi\rangle\), that is, \(\langle w | \psi \rangle \geq \langle x | \psi \rangle\) for all \(x \in \Sigma^n\). In case of a no-instance the prover may send the verifier an arbitrary string \(w \in \Sigma^n\).

The verifier starts by choosing \(\beta > 0\) such that \(\beta \|H_a\| \leq 1\) for all \(a\) and an integer \(L\) such that
\[
2^{\Phi} (1 - \epsilon \beta M^{-1})^L \leq \frac{1}{3}.
\]

Note that this inequality can be satisfied with \(L = poly(n)\). Then the verifier performs a random walk with \(L\) steps as prescribed below.
**Step 1:** Receive a string $w \in \Sigma^n$ from the prover. Set $x_0 = w$.

**Step 2:** Suppose the current state of the walk is $x_j$. Verify that $x_j \in S_{\text{good}}$, see Eq. (2.6). Otherwise, output 'no'.

**Step 3:** If $j = L$ goto Step 8.

**Step 4:** Generate a random uniform $a \in \{1, \ldots, m\}$.

**Step 5:** Find the set $N_a(x_j) = \{y \in \Sigma^n : \langle x_j | \Pi_a | y \rangle > 0\}$.

**Step 6:** Generate a random $x_{j+1} \in N_a(x_j)$ from the distribution

$$P^a_{x_j \rightarrow x_{j+1}} = \sqrt{\frac{\langle x_{j+1} | \Pi_a | x_{j+1} \rangle}{\langle x_j | \Pi_a | x_j \rangle}} \langle x_{j+1} | G_a | x_j \rangle, \quad G_a = I - \beta H_a. \quad (6.2)$$

**Step 7:** Compute and store the number

$$r_{j+1} = \frac{P^a_{x_j \rightarrow x_{j+1}}}{\langle x_{j+1} | G_a | x_j \rangle}. \quad (6.3)$$

Set $j \rightarrow j + 1$ and goto Step 2.

**Step 8:** Verify that $\prod_{j=1}^L r_j \leq 1$. Otherwise output 'no'.

**Step 9:** Output 'yes'.

### 6.1. Completeness of the protocol

In this subsection we prove that for yes-instances the verifier outputs 'yes' with probability 1. Let $|\psi\rangle$ be a satisfying assignment chosen by the prover. We can assume that $|\psi\rangle$ is a non-negative vector, see Corollary 4.3. Lemma 4.5 implies that for any choice of $a$ at Step 4 one has

$$P^a_{x_j \rightarrow x_{j+1}} = \frac{\langle x_{j+1} | \Pi_a | x_j \rangle}{\langle x_j | \Pi_a | x_j \rangle} \langle x_{j+1} | G_a | x_j \rangle$$

and thus the overall probability of a transition from $x_j$ to $x_{j+1}$ at Steps 4,5,6 is

$$P_{x_j \rightarrow x_{j+1}} = \frac{\langle x_{j+1} | \psi \rangle}{\langle x_j | \psi \rangle} \langle x_{j+1} | G | x_j \rangle, \quad G = \frac{1}{M} \sum_{a=1}^{M} G_a. \quad (6.4)$$

It follows from Lemma 4.5 that the walk never leaves the set $S(\psi)$. Using the above expression for $P^a_{x_j \rightarrow x_{j+1}}$ one has

$$r_j = \frac{\langle x_{j+1} | \psi \rangle}{\langle x_j | \psi \rangle}$$

Therefore,

$$\prod_{j=1}^L r_j = \frac{\langle x_L | \psi \rangle}{\langle x_0 | \psi \rangle} = \frac{\langle x_L | \psi \rangle}{\langle w | \psi \rangle}.$$
Taking into account that \( w \) is a string with the largest amplitude one can see that \( \prod_{j=1}^{L} r_j \leq 1 \) for all possible \( x_L \in S(\psi) \) and thus the test at Step 8 will always be passed. Thus the verifier outputs ‘yes’ with probability 1.

Let us remark that the completeness of the protocol is not affected by the precision up to which the verifier approximates the probability distribution \( P_{x_j \rightarrow x_{j+1}} \) at Step 6 as long as \( x_{j+1} \in N_0(x_j) \) with probability 1 and the coefficients \( r_j \) are computed using exact formulas Eqs. (6.2,6.3). The precision will be important for the soundness of the protocol, see the next section.

### 6.2. Soundness of the protocol.

In this subsection we shall prove that for no-instances the verifier outputs ‘yes’ with probability at most \( 1/3 \). Without loss of generality the witness \( w = x_0 \) is a good string (otherwise the verifier outputs ‘no’ at the very first step of the walk). The probability for the walk starting from \( x_0 \in S_{\text{good}} \) to stay in \( S_{\text{good}} \) at every step \( j = 1, 2, \ldots, L \) is

\[
p_{\text{good}}(L) = \frac{1}{ML} \sum_{a_1, \ldots, a_L = 1, \ldots, M} \prod_{j=1}^{L} P_{x_0 \rightarrow x_1}^{a_1} P_{x_1 \rightarrow x_2}^{a_2} \cdots P_{x_{L-1} \rightarrow x_L}^{a_L}.
\]

Taking into account Eq. (6.3) one gets

\[
p_{\text{good}}(L) = \frac{1}{ML} \sum_{x_1, \ldots, x_L \in S_{\text{good}}} \prod_{j=1}^{L} r_j \langle x_0 | G_{a_1} | x_1 \rangle \langle x_1 | G_{a_2} | x_2 \rangle \cdots \langle x_{L-1} | G_{a_L} | x_L \rangle.
\]

Here the coefficients \( r_j \) are functions of the “trajectory” \( x_0, \ldots, x_L \) and \( a_1, \ldots, a_L \) of the walk. At this point we invoke the test at Step 8. The verifier outputs ‘yes’ iff the walk stays in \( S_{\text{good}} \) at every step \( j = 1, 2, \ldots, L \) and \( \prod_{j=1}^{L} r_j \leq 1 \). Thus the probability \( p_{\text{yes}}(x_0) \) for the verifier to output ‘yes’ for a fixed starting string \( x_0 = w \in S_{\text{good}} \) can be bounded from above as

\[
p_{\text{yes}}(x_0) \leq \frac{1}{ML} \sum_{x_1, \ldots, x_L \in S_{\text{good}}} \langle x_0 | G_{a_1} | x_1 \rangle \langle x_1 | G_{a_2} | x_2 \rangle \cdots \langle x_{L-1} | G_{a_L} | x_L \rangle.
\]

Using the operator \( G = M^{-1} \sum_{a=1}^{M} G_a = I - \beta M^{-1} H \) we have

\[
p_{\text{yes}}(x_0) \leq \frac{1}{ML} \sum_{x_1, \ldots, x_L \in S_{\text{good}}} \langle x_0 | G | x_1 \rangle \langle x_1 | G | x_2 \rangle \cdots \langle x_{L-1} | G | x_L \rangle.
\]

Taking into account that all matrix elements of \( G \) are non-negative, we get

\[
p_{\text{yes}}(x_0) \leq 2^\frac{n}{2} \langle x_0 | G^L | + \rangle,
\]

where \( |+\rangle = 2^{-n/2} \sum_{x \in \Sigma^n} |x \rangle \) is the uniform superposition of all \( 2^n \) basis vectors. Let \( \lambda \) be the largest eigenvalue of \( G \). The promise for a no-instance implies that \( \lambda \leq 1 - \epsilon \beta M^{-1} \) and thus

\[
\langle x_0 | G^L | + \rangle \leq \lambda^L \leq (1 - \epsilon \beta M^{-1})^L.
\]

Therefore

\[
p_{\text{yes}}(x_0) \leq 2^\frac{n}{2} (1 - \epsilon \beta M^{-1})^L \leq \frac{1}{3}.
\]
for any starting string $x_0$. It proves that the verifier outputs 'yes' with probability at most $1/3$. Now suppose that Step 6 is implemented with some finite precision using a probability distribution $\tilde{P}_{x_j \rightarrow y}$ such that

$$(6.5) \sum_{y \in \mathcal{N}_a(x_j)} |\tilde{P}_{x_j \rightarrow y} - P_{x_j \rightarrow y}| \leq \delta \quad \text{for any} \quad x_j \in S_{\text{good}}, \quad \text{for any} \quad a = 1, \ldots, m.$$\

One can easily verify that Eq. (6.5) implies

$$\left| \sum_{x_1, \ldots, x_L \in S_{\text{good}}} P_{x_0 \rightarrow x_1}^{a_1} P_{x_1 \rightarrow x_2}^{a_2} \cdots P_{x_{L-1} \rightarrow x_L}^{a_L} - \tilde{P}_{x_0 \rightarrow x_1}^{a_1} \tilde{P}_{x_1 \rightarrow x_2}^{a_2} \cdots \tilde{P}_{x_{L-1} \rightarrow x_L}^{a_L} \right| \leq \delta,$$

Thus using an approximate probability distribution at Step 6 leads to corrections of order $L\delta$ to the overall acceptance probability. Choosing $\delta \ll L^{-1}$ we can get an acceptance probability smaller than 1/2 which can be amplified to 1/3 using standard majority voting.

### 6.3. Simplified stoquastic $k$-SAT.

Let $C = \{H_a = I - \Pi_a\}_{a=1,\ldots,M}$ be a system of $(n, k)$-constraints where each $\Pi_a$ is a projector with matrix elements 0, 1/2, 1. Recall that verifying satisfiability of $C$ is a problem complete for Promise-MA if $k \geq 6$, see Theorem 1.9. It is of interest to consider in more detail how the random walk algorithm described above works for this simplified version of stoquastic $k$-SAT.

The identity $\Pi_a = \Pi_a^2$ implies that $\Pi_a$ is a block-diagonal matrix (up to a permutation of basis vectors) such that every one-dimensional block is either 0 or 1, every two-dimensional block is a matrix

$$\frac{1}{2} \left( \begin{array}{cc} 1 & 1 \\ 1 & 1 \end{array} \right),$$

and there are no blocks with dimension higher than two. Let us define a graph $G = (V, E)$ such that vertices of $G$ are $n$-bit strings and a pair of strings $(x, y)$ is connected by an edge if there is at least one projector $\Pi_a$ such that $\langle x | \Pi_a | y \rangle = 1/2$.

Note that $G$ has degree at most $M$, the number of projectors $\Pi_a$. The vertices of $G$ can be partitioned into good and bad vertices, see Eq. (2.6). In other words,

$$S_{\text{good}} = \{ x \in \Sigma^n : \langle x | \Pi_a | x \rangle \in \{ 1, \frac{1}{2} \} \quad \text{for all} \quad a \},$$

and $S_{\text{bad}} = \{ x \in \Sigma^n : \langle x | \Pi_a | x \rangle = 0 \quad \text{for some} \quad a \}$.

The random walk described by Steps 4, 5 and 6 of the verifier’s protocol can now be simplified as follows (we shall assume that $\beta = 1$ so that $G_a = \Pi_a$). Suppose at some step $j$ the walk was at some good vertex $x_j$. Then at the next step the walker moves to one of the nearest neighbors of $x_j$ with probability $1/(2M)$ and stays at the vertex $x_j$ with probability $1 - \deg(x_j)/2M$, where $\deg(x_j)$ is the number of edges incident to $x_j$.

One can easily observe that the system $C$ is satisfiable, unsat($C$) = 0, if the graph $G$ has a connected component $G' = (V', E')$ that contains only good vertices, $V' \subseteq S_{\text{good}}$. Given such a connected component, a state $|\psi\rangle = \sum_{u \in V'} |u\rangle$ is a satisfying assignment, that is, $\Pi_a |\psi\rangle = |\psi\rangle$ for all $a$. Hence for a ‘yes’-instance the prover can simply give any string in $V'$. Note also that the test at Step 8 of the protocol is not needed now since $r_j = 1$ for any realization of the walk.
The promise on the unsat-value for ‘no’-instances can be translated into a promise that for any starting vertex the random walk will hit a bad vertex after polynomially number of steps. Note that the classical SAT problem corresponds to the special case in which the projectors have no 1/2 matrix-elements and hence there are no edges in the associated graph (and hence also no walk).

7. Discussion. We hope that the stoquastic $k$-SAT problem may potentially lead to new insights into the question whether $\text{MA} \subseteq \text{NP}$. Note that it is widely believed that $\text{MA} = \text{NP}$, see e.g. [20]. Indeed, the simplified stoquastic $k$-SAT problem described in Section 6.3 is the problem of deciding whether the associated graph $G$ with $2^n$ vertices has a connected component $G'$ that contains only good vertices (the verifier can efficiently check whether a vertex is good). If the size of $G'$ were polynomial, then a NP proof-system would suffice, since a prover can simply list all vertices in $G'$. However in general the size of $G'$ could be exponentially large and there is no time or space to explore or list the whole subgraph $G'$, hence the need for randomness. For ‘yes’-instances the prover simply gives the verifier a vertex $v \in G'$ and a random walk on $G$ starting from $v$ will always stay in $G'$. For ‘no’-instances, the promise guarantees that no matter where one starts the random walk, with a polynomial number of steps one will always hit a bad vertex with high probability.

The derandomization question is the question whether a pseudo-random walk from any starting vertex using a random bit string of length $O(\log n)$ will also hit a bad vertex with sufficiently high probability.

Another open question is the simulatability of stoquastic adiabatic computation in general. Given a stoquastic Hamiltonian $H$ and its ground state $|\psi\rangle$ satisfying $H|\psi\rangle = 0$ (which can be always achieved by an energy shift) one can still use Eq. (2.2) to define a random walk on the set $S(\psi)$. However, in order to simulate this random walk on a classical computer one must be able to compute the ratio of the amplitudes $\langle y|\psi\rangle/\langle x|\psi\rangle$ for which no efficient algorithm is known. Another possibility to define a random walk is to modify the verifier’s protocol in Section 6. It suffices to modify Step 6 such that the walk stays at $x_j$ with probability 1 whenever $\langle x_j|\Pi_a|x_j\rangle = 0$. An open question is whether the stationary distribution of this modified walk is anyhow related to the distribution $\pi(x) = \langle x|\psi\rangle^2$ associated with a ground-state $|\psi\rangle$ of the stoquastic Hamiltonian.

Acknowledgments. We would like to thank David DiVincenzo for useful comments and discussions. This work was supported by NSA and ARDA through ARO contract number W911NF-04-C-0098.

Appendix A. The complexity class $\text{MA}$ (Merlin-Arthur games) was introduced by Babai in [22]. A language $L$ is in $\text{MA}$ iff there exists a probabilistic polynomial-time machine $V$ (a verifier) that takes as input a pair $(x,w)$ where $x$ is string representing an instance of the problem, $w$ is a witness string, and such that

- $x \in L \Rightarrow V$ accepts $(x,w)$ with probability 1 for some witness $w$.
- $x \notin L \Rightarrow V$ accepts $(x,w)$ with probability at most 1/3 for any witness $w$.

One gets an equivalent definition if the acceptance probabilities 1 and 1/3 are replaced by $p_{\text{yes}}$ and $p_{\text{no}}$ such that $p_{\text{yes}} - p_{\text{no}} \geq 1/\text{poly}(n)$, see [23]. To better understand the relationship between $\text{MA}$ and other complexity classes it is desirable to have some $\text{MA}$-complete problems, or at least, some problems in $\text{MA}$ that are not known to be in $\text{NP}$. Unfortunately, no such problems are currently known. This
lack of interesting problems in MA is not very surprising though because probabilistic algorithms are usually allowed to give an inconclusive answer for some inputs (the acceptance probability is close to 1/2) while the definition above does not allow that. From this perspective it is more natural to define MA as a class of promise problems. Recall that a promise problem is a pair of non-intersecting sets \( L_{\text{yes}}, L_{\text{no}} \subseteq \{0,1\}^* \) that represent yes-instances and no-instances respectively.

**Definition 7.1.** A promise problem \( (L_{\text{yes}}, L_{\text{no}}) \) belongs to MA iff there exists a probabilistic polynomial-time machine \( V \) taking as input a pair of strings \( (x,w) \) such that

\[
x \in L_{\text{yes}} \Rightarrow V \text{ accepts } (x,w) \text{ with probability } 1 \text{ for some witness } w.
\]

\[
x \in L_{\text{no}} \Rightarrow V \text{ accepts } (x,w) \text{ with probability at most } 1/3 \text{ for any witness } w.
\]

A promise problem \( (L_{\text{yes}}, L_{\text{no}}) \) is MA-complete iff for any promise problem \( (L'_{\text{yes}}, L'_{\text{no}}) \) in MA there exists a function \( f : \{0,1\}^* \rightarrow \{0,1\}^* \) computable by a deterministic polynomial-time machine such that \( f(L'_{\text{yes}}) \subseteq L_{\text{yes}} \) and \( f(L'_{\text{no}}) \subseteq L_{\text{no}} \).

Note that the behavior of \( V \) on instances \( x \notin L_{\text{yes}} \cup L_{\text{no}} \) may be completely arbitrary. Throughout this paper MA refers to the class of promise problems rather than the class of languages. It should be mentioned that many important results concerning NP are formulated in terms of promise problems, for example, the inapproximability version of the PCP theorem [24], or the complexity of \( k \)-SAT with a unique solution [25] (see the survey [26] for other examples). Thus one can also expect to get more insight in the complexity of MA by studying promise problems.

**Appendix B.** This section serves three purposes. First, we prove Proposition 1.5. Secondly, we prove the second part of Theorem 1.9, that is, MA-hardness of stoquastic 6-SAT. Thirdly, we explain in more details the connection between SFF Hamiltonians and classical probabilistic computation mentioned in Section 3.2. All these results follow directly from the clock Hamiltonian construction of [9] and the analysis performed in [2][17].

We start form reviewing the clock Hamiltonian construction. Let \( U = U_L \cdots U_2 U_1 \) be a quantum circuit acting on \( N \) data qubits with \( L = \text{poly}(N) \) gates. We assume that the \( N \) data qubits are partitioned into two groups: \( N_a \) ancillary qubits and \( N_w \) witness qubits (one may have \( N_w = 0 \)). Each ancillary qubit \( k \) is initialized by some pure state \( |\phi_k\rangle \). The witness qubits may be initialized by an arbitrary pure state \( |\psi^{\text{wit}}\rangle \in \mathbb{Q}^{N_w} \). Accordingly, the input state of the circuit is \( |\psi_{in}\rangle = |\psi^{\text{anc}}\rangle \otimes |\psi^{\text{wit}}\rangle \), where \( |\psi^{\text{anc}}\rangle \) is a tensor product of the ancillary states \( |\phi_k\rangle \). Let \( |\psi_j\rangle = U_j \cdots U_1 |\psi^{\text{anc}}\rangle \otimes |\psi^{\text{wit}}\rangle \), \( j = 0, \ldots, L \), be a state obtained by terminating the circuit after the \( j \)-th gate. We adopt a convention that \( |\psi_0\rangle = |\psi_{in}\rangle \) is the input state. The output state of the circuit is \( |\psi_L\rangle \).

Consider a composite system that consists of \( N \) data qubits and \( L+1 \) clock qubits. Let \( |j\rangle_u = |j+1 0^{L-j}\rangle \in \mathbb{Q}^{L+1} \) be the unary encoding of the time steps \( j = 0, \ldots, L \). Define a linear subspace \( \mathcal{H} \subseteq \mathbb{Q}^{N+L+1} \) as

\[
\mathcal{H} = \left\{ |\phi\rangle = \sum_{j=0}^{L} |\psi_j\rangle \otimes |j\rangle_u, \quad |\psi_j\rangle = U_j \cdots U_1 |\psi^{\text{anc}}\rangle \otimes |\psi^{\text{wit}}\rangle, \quad |\psi^{\text{wit}}\rangle \in \mathbb{Q}^{N_w} \right\}
\]

(7.1)

States from \( \mathcal{H} \) represent computational paths of the verifier’s quantum computer starting from an arbitrary witness state \( |\psi^{\text{wit}}\rangle \). We shall label the \( j \)-th clock qubit
as \( cl(j), j = 0, \ldots, L \). Note that the clock qubit \( cl(0) \) is always set to 1. For any \( j = 1, \ldots, L \), the clock qubit \( cl(j) \) is a flag telling whether the gate \( U_j \) has or has not been applied. The \( k \)-th ancillary qubit will be labeled \( a(k), k = 1, \ldots, N_a \). Let us show that \( \mathcal{H} \) is spanned by ground states of some SFF Hamiltonian. Indeed, introduce 3-qubit constraints

\[
H_k^{\text{init}} = (I - |\phi_k\rangle \langle \phi_k|) a(k) \otimes |10\rangle \langle 10|_{cl(0),cl(1)}, \quad j = k, \ldots, N_a,
\]

States satisfying these constraints (i.e. zero eigenvectors of \( H_k^{\text{init}} \)) satisfy correct initial conditions. Introduce also constraints

\[
H_j^{\text{prop}} = \frac{1}{2} |1\rangle \langle 1|_{cl(j-1)} \otimes \left(|1\rangle \langle 1|_{cl(j)} + |0\rangle \langle 0|_{cl(j)} - |1\rangle \langle 1|_{cl(j)} \otimes U_j + |0\rangle \langle 0|_{cl(j)} \otimes U_j^\dagger \right) \otimes |0\rangle \langle 0|_{cl(j+1)},
\]

where \( j = 1, \ldots, L \). States satisfying these constraints obey the correct propagation rules relating computational states at different time steps. Finally, introduce 2-qubit constraints

\[
H_0^{\text{clock}} = |0\rangle \langle 0|_{cl(0)}, \quad H_l^{\text{clock}} = |01\rangle \langle 01|_{cl(l-1),cl(l)}, \quad l = 1, \ldots, L.
\]

States satisfying these constraints belong to the subspace spanned by “legal” clock states, i.e., \( Q_N \otimes |j\rangle_c, j = 0, \ldots, L \). Therefore we arrive at

\[
\mathcal{H} = \{ |\phi\rangle \in Q^{N+L+1} : H_k^{\text{init}} |\phi\rangle = H_j^{\text{prop}} |\phi\rangle = H_l^{\text{clock}} |\phi\rangle = 0 \quad \text{for all} \; j, k, l \}.
\]

Define a clock Hamiltonian

\[
H = \sum_{k=1}^{N_a} H_k^{\text{init}} + \sum_{j=1}^{L} H_j^{\text{prop}} + \sum_{l=0}^{L} H_l^{\text{clock}}.
\]

It follows that \( \mathcal{H} \) is the ground-subspace of \( H \). Note that all terms in \( H \) are positive semi-definite and any vector from \( \mathcal{H} \) is a zero eigenvector of \( H \). Thus \( H \) is a frustration-free Hamiltonian.

**Proof of Proposition 1.6.** In the case of the adiabatic evolution there are no witness qubits, \( N_w = 0 \). Accordingly, the clock Hamiltonian has a unique ground-state

\[
|\psi\rangle = (L + 1)^{-1/2} \sum_{j=0}^{L} |\psi_j\rangle \otimes |j\rangle_u.
\]

It was shown by many researchers, see for instance Lemma 3.11 in [2] and the improved estimates in [21], that the spectral gap of the clock Hamiltonian can be bounded as \( \Delta = \Omega(1/L^2) = 1/poly(N) \) regardless of the choice of the gates \( U_1, \ldots, U_L \). Let us define a family of quantum circuits \( U(s) = U_L(s) \cdots U_1(s) \) where \( 0 \leq s \leq 1 \) and \( U_j(s) \) interpolates smoothly between \( U_j(0) = I \) and \( U_j(1) = U_j \) (without loss of generality \( \det(U_j) = 1 \) in which case the possibility of such a smooth interpolation follows from the connectivity of the special unitary group). Applying definition Eq. (7.4) we get a family of frustration-free clock Hamiltonians \( H(s), 0 \leq s \leq 1 \) satisfying conditions (A1)-(A2),(A3). Without loss of generality the last \( (1-\delta)L \) gates of the circuit \( U \) are identity gates. Therefore the ground-state of \( H \) satisfies \( \langle \psi|\psi_L \otimes A \rangle \geq 1 - \delta, \) where
|A⟩ = (L + 1)^{-1/2} \sum_{j=0}^{L} |j⟩u is an ancillary state. Thus |ψ⟩ approximates the output state |ψ_L⟩ with precision δ (after discarding the ancilla |A⟩).

**Stoquastic 6-SAT is MA-hard.** It was shown in [7] (see Lemma 2 in [7]) that any classical MA verifier V can be transformed into a quantum verifier V' which uses a quantum circuit U involving only classical reversible gates (for example, the 3-qubit Toffoli gates) together with ancillary states |0⟩, |+⟩, and measures one of the output qubits in the |0⟩, |1⟩ basis. This transformation has a property that the maximum acceptance probability of V (over all classical witnesses) is equal to the maximum acceptance probability of V' (over all quantum witnesses). In order to apply the clock Hamiltonian construction to V' we shall treat part of the ancillary qubits as the qubits encoding an instance of the problem, that is, we shall allow ancillas |φ_k⟩ = |0⟩, |1⟩, |+⟩.

In addition, we shall add one more term into H representing the final measurement. Define a 3-qubit constraint

\[ H_{meas} = (I - \Pi_{out}) \otimes |1⟩⟨1|_{cl(L)}. \]

Here \( \Pi_{out} \) is the projector used by V' to decide whether he accepts the witness (say, \( \Pi_{out} \) projects the first data qubit onto the state |0⟩). Note that H contains a vector satisfying \( \Pi_{meas} \) iff the verifier V' accepts some witness state |ψ_wit⟩ with probability 1. Define a system of constraints

\[ \mathcal{C} = \{H_{init}^k, H_{prop}^j, H_{clock}^l, H_{meas}\} \]

(7.5)

i.e. the system including all the constraints defined above. Since all ancillary states |φ_k⟩ are either |0⟩ or |+⟩, the off-diagonal matrix elements of the operators \( H_{init}^k \) are either 0 or \(-1/2\), see Eq. (7.2). Furthermore, since all gates \( U_j \) are classical Toffoli gates, the off-diagonal matrix elements of the operators \( H_{prop}^j \) are either 0 or \(-1/2\), see Eq. (7.3). Finally, the operators \( H_{clock} \) and \( H_{meas} \) are diagonal. Thus \( \mathcal{C} \) is a stoquastic system of \((n, 6)\)-constraints where \( n = N + L + 1 \). By definition, the unsat-value of \( \mathcal{C} \) coincides with the smallest eigenvalue of a clock Hamiltonian

\[ H' = H + H_{meas}, \]

where H is defined in Eq. (7.4). If V' accepts some witness state |ψ_wit⟩ with probability 1 then unsat(\( \mathcal{C} \)) = 0. On the other hand, if V' accepts any witness state with probability at most \( 1 - \epsilon \), the derivation of [3] implies that the smallest eigenvalue of the Hamiltonian Eq. (7.6) can be bounded as

\[ \lambda_{min}(H') \geq c(1 - \sqrt{1-\epsilon})L^{-3} \geq 1/poly(N). \]

where c is some positive constant. Thus in the latter case unsat(\( \mathcal{C} \)) \( \geq 1/poly(N) \). It follows that any problem in MA is reducible to the stoquastic 6-SAT problem.

Finally, we remark that any constraint from the system \( \mathcal{C} \) can be represented as \( I - \Pi \) where \( \Pi \) is a non-negative projector with matrix elements belonging to the set \{0, 1/2\}.

**Coherent probabilistic computation.** The Hamiltonian mentioned in Section 3.2 is the clock Hamiltonian defined in Eq. (7.4). The proof that the ground-state of H has the desired properties is completely analogous to the proof of Proposition 1.5.

REFERENCES
[1] S. Aaronson, “Quantum Computing, Postselection, and Probabilistic Polynomial-Time”, Proc. Roy. Soc. A 461(2063), pp. 3473-3482 (2005). arXiv:quant-ph/0412187

[2] D. Aharonov, W. van Dam, Z. Landau, S. Lloyd, J. Kempe, and O. Regev, “Adiabatic Quantum Computation is Equivalent to Standard Quantum Computation”, SIAM Journal of Computing, Vol. 37, Issue 1, pp. 166-194 (2007).

[3] A. Kitaev, A. Shen, and M. Vyalyi, “Classical and Quantum Computation”, Vol. 47 of Graduate Studies in Mathematics (AMS, Providence, RI) (2002).

[4] J. Kempe, A. Kitaev, and O. Regev, “The Complexity of the Local Hamiltonian Problem”, SIAM Journal of Computing, 35, p. 1070 (2006).

[5] R. Oliveira and B.M. Terhal, “The complexity of quantum spin systems on a two-dimensional square lattice”, arXiv:quant-ph/0504050. To appear in Quant. Inf. Comp.

[6] D. Aharonov, D. Gottesman, S. Irani, and J. Kempe, “The power of quantum systems on a line”, In Proceedings of 48th FOCS, pp. 373–383 (2007), arXiv.org:0705.4077 and arXiv:0705.4067.

[7] S. Bravyi, D. DiVincenzo, R. Oliveira, and B.M. Terhal, “The Complexity of Stoquastic Local Hamiltonian Problems”, Quant. Inf. Comp. 8, No.5, pp. 0361-0385 (2008).

[8] A.M. Childs, E. Farhi, J. Goldstone and S. Gutmann, “Finding cliques by quantum adiabatic evolution”, Quant. Inf. Comp. 2, p. 181 (2002).

[9] S. Bravyi, “Efficient algorithm for a quantum analogue of 2-SAT”, arXiv:quant-ph/0611021.

[10] D. Nagaj and S. Mozes, “A new construction for a QMA-complete 3-local Hamiltonian”, J. Math. Phys. 48, 072104 (2007), arXiv:quant-ph/0612113.

[11] N. Trivedi and D. Ceperley, “Green-function Monte-Carlo study of quantum antiferromagnets”, Phys. Rev. B40, p. 2737 (1989).

[12] M. Buonaura and S. Sorella, “Numerical study of the two-dimensional Heisenberg model using a Green’s function Monte-Carlo technique with a fixed number of walkers”, Phys. Rev. B57, p. 11446 (1998).

[13] J. Hetherington, “Observations on the statistical iteration of matrices”, Phys. Rev. A30, No. 5, p. 2713 (1984).

[14] S. Bravyi, A.J. Bessen, and B.M. Terhal, “Merlin-Arthur Games and Stoquastic Complexity”, arXiv:quant-ph/0611021.

[15] E. Böhlter, C. Glaßer, and D. Meister, “Error-bounded probabilistic computations between MA and AM”, In Proceedings of 28th MFCS, pp. 249-258 (2003).

[16] D. Aharonov and A. Ta-Shma, “Adiabatic Quantum State Generation and Statistical Zero Knowledge”, Proc. of 35th STOC, pp. 20-29 (2003), arXiv:quant-ph/0301023.

[17] F. Verstraete, M. Wolf, D. Perez-Garcia, and J.I. Cirac, “Criticality, the area law, and the computational power of PEPS”, Phys. Rev. Lett. 96, 220601 (2006).

[18] R.D. Somma, C.D. Batista, and G. Ortiz, “A Quantum Approach to Classical Statistical Mechanics”, Phys. Rev. Lett. 99, 030603 (2007), arXiv:quant-ph/0609216.

[19] R. Santhanam, “Circuit lower bounds for Merlin-Arthur classes”, Proc. of 39th STOC, p. 275 (2007).

[20] P. Deift, M. Ruskai, W. Spitzer, “Improved Gap Estimates for Simulating Quantum Circuits by Adiabatic Evolution”, arXiv:quant-ph/0605156.

[21] L. Babai, “Trading group theory for randomness”, Proc. of 17th STOC, pp. 421-429 (1985).

[22] M. Furer, O. Goldreich, Y. Mansour, S. Sipser, S. Zachos, “On completeness and soundness in Interactive Proof Systems”, Advances in Computing Research, 5, pp. 429-442 (1989).

[23] I. Dinur, “The PCP Theorem by gap amplification”, Proc. of 38th STOC, pp. 241-250 (2006).

[24] L. Valiant and V. Vazirani, “NP is as easy as detecting unique solutions”, Proc. of 17th STOC, p. 458 (1985).

[25] O. Goldreich, “On Promise Problems”, ECCC Report TR05-018.