Increasing the quantum UNSAT penalty of the circuit-to-Hamiltonian construction

Johannes Bausch*, Elizabeth Crosson†

September 28, 2016

The Feynman-Kitaev Hamiltonian used in the proof of QMA-completeness of the local Hamiltonian problem has a ground state energy which scales as $\Omega((1-\sqrt{\epsilon})T^{-3})$ when it is applied to a circuit of size T and maximum acceptance probability ϵ. We refer to this quantity as the quantum UNSAT penalty, and using a modified form of the Feynman Hamiltonian with a non-uniform history state as its ground state we improve its scaling to $\Omega((1-\sqrt{\epsilon})T^{-2})$, without increasing the number of local terms or their operator norms. As part of the proof we show how to construct a circuit Hamiltonian for any desired probability distribution on the time steps of the quantum circuit (which, for example, can be used to increase the probability of measuring a history state in the final step of the computation). Next we show a tight $\mathcal{O}(T^{-2})$ upper bound on the product of the spectral gap and ground state overlap with the endpoints of the computation for any clock Hamiltonian that is tridiagonal in the time register basis, which shows that the scaling of the quantum UNSAT penalty achieved by our construction cannot be further improved within this framework. Our proof of the upper bound applies a quantum-to-classical mapping for arbitrary tridiagonal Hermitian matrices combined with a sharp bound on the spectral gap of birth-and-death Markov chains. In the context of universal adiabatic computation we show how to reduce the number of qubits required to represent the clock by a constant factor over the standard construction, but show that it is otherwise already optimal in the sense we consider and cannot be further improved with tridiagonal clock Hamiltonians, which agrees with a similar upper bound from a previous study.

*DAMTP, CQIF, University of Cambridge. jkrb2@cam.ac.uk
†IQIM, California Institute of Technology. crosson@caltech.edu

1 Introduction

The initial demonstration of QMA-completeness of the local Hamiltonian problem [1] was followed by a period of development during which the main goal was to broaden the class of interaction terms which suffice to make the local Hamiltonian problem QMA-complete [2, 3]. These results were motivated in part by a desire to understand the hardness of approximating physical systems that resemble those found in nature, and also by the goal of making the closely related universal adiabatic computation construction [4] more suitable for eventual physical implementation [5]. The success of these efforts have resulted in QMA-complete local Hamiltonian problems with restricted properties such as 2-local interactions [2], low dimensional geometric lattices [3, 6], and translational invariance, as well as a complete classification of the complexity of the 2-local Hamiltonian problem for any set of interaction couplings [7].

This great success in classifying the hardness of physically realistic interactions stands in contrast with the relative lack of progress in resolving questions related to the robustness of quantum ground state computation, such as whether fault-tolerant universal adiabatic computing is possible, or to prove or disprove the quantum PCP conjecture [8]. Such questions motivate us to seek (or to limit the possibility of) improvements to the circuit-to-Hamiltonian construction itself, which serves a foundational role in all of the results listed above. Based on ideas by Feynman [9] and cast into its current form by Kitaev [1], the construction remains relatively little changed but has undergone some gradual evolutions throughout its long history [6, 10, 11, 12, 13].

To be robust a circuit-to-Hamiltonian construction should not only have a ground space representing valid computations, but intuitively it should penalize invalid computations with as high of an energy as possible. One way of formalizing this condition is to add constraints on the input and the output of the circuit that cannot be simultaneously satisfied under the valid operation of the circuit. If the Hamiltonian enforces the correct operation of the circuit gates, then the input and output constraints that contradict each other should not be satisfiable by any state, and so the ground state energy should increase. This explains why the higher ground state energy associated with non-accepting circuits can be regarded as an energy penalty against invalid computations.

The specific role of the $\mathcal{O}(T^{-3})$ scaling of the quantum UNSAT penalty in Kitaev's proof is to show that the local Hamiltonian problem is QMA-hard with a promise gap that scales inverse polynomially in the system size. While there exists a well-defined relation between runtime T and the corresponding Hamiltonian's system size n for any *specific* set of constructions—e.g. Kitaev's 5-local one—the explicit scaling of this gap with T is not meaningful to the local Hamiltonian problem beyond the fact that it is polynomial, since the local Hamiltonian problem promise gap is parameterized by the number of qubits n, i.e. $1/\operatorname{poly} n$. Nevertheless, the scaling of the quantum UNSAT penalty with T is a well defined feature of any particular circuit-to-Hamiltonian construction, and therefore we take the view that it is a reasonable metric for exploring the space of possible improvements to this construction.

Results and Overview

We analyze circuit Hamiltonians with history state ground states consisting of an arbitrary complex superposition of the time steps of the computation,

$$|\psi\rangle = \sum_{t=0}^{T} \psi_t |t\rangle \otimes (U_t \cdots U_1)\,|\xi\rangle, \tag{1}$$

where as usual $U_T, \ldots, U_1$ are quantum gates, $|\xi\rangle$ is an arbitrary input to the computation, and $|\psi\rangle$ is a normalized state, so that in particular $\pi_t := \psi_t^* \psi_t$ is a probability distribution on $\{0, \ldots, T\}$. Ground states of the form as in eq. (1) arise from modifications to the usual terms of the Feynman circuit Hamiltonian,

$$H_{\text{circuit}} := \sum_{t=0}^{T} a_t |t\rangle\langle t| \otimes \mathbb{1} + \sum_{t=0}^{T-1} \left(b_t |t+1\rangle\langle t| \otimes U_t + b_t^* |t\rangle\langle t+1| \otimes U_t^\dagger \right), \tag{2}$$

where $|a_t|, |b_t| \leq 1$ for $t = 0, \ldots, T$. Note that most if not all of the constructions that implement the $\mathcal{O}(\log n)$-local interactions with the time register using a k-local Hamiltonian with constant k, such as the domain wall clock which leads to a 5-local circuit Hamiltonian, can be directly applied to the modified form (2).

In addition to the part of the Hamiltonian which checks the propagation of the circuit, projectors $H_{\text{in}} := |0\rangle\langle 0| \otimes \Pi_{\text{in}}$ and $H_{\text{out}} := |T\rangle\langle T| \otimes \Pi_{\text{out}}$ can be added to H_{circuit} to validate specific inputs and the outputs of the computation.

More specifically, the ground space of $H_{\text{circuit}} + H_{\text{in}}$ will be spanned by computations starting from a valid input computation (i.e. those for which $|\xi\rangle \in \ker \Pi_{\text{in}}$ in eq. (1)), and H_{out} will raise the energy of the state $|\psi\rangle$ in (1) when $U_T \cdots U_1 |\xi\rangle \notin \ker \Pi_{\text{out}}$. The magnitude of this frustration between the incompatible ground spaces of $H_{\text{in}} + H_{\text{circuit}}$ and H_{out} will depend on the circuit encoded by H_{FK} and the specific in- and output energy penalties, i.e. the acceptance probability of the circuit $\epsilon = \min_{|\xi\rangle, |\eta\rangle} = \langle \eta|\, U_T \cdots U_1 \,|\xi\rangle$. In the following definition we take the Π_{in} and Π_{out} that are used in the standard construction: $\Pi_{\text{out}} := |1\rangle\langle 1|$ measures a single qubit, and Π_{in} constrains a fraction of the input qubits to the $|+\rangle$ state and leaves the rest of the input qubits unconstrained.

For a specific set of in- and output constraints and runtime length T, we want to identify the circuit Hamiltonian best suitable to discriminate accepting and rejecting circuit paths, independent of the particular circuits used. Therefore, we let $C(\epsilon, T)$ be the set of circuits of size T for which the maximum acceptance probability is ϵ for any state obeying the in- and output constraints Π_{in} and Π_{out}, i.e.

$$C(\epsilon, T) := \{U_1, \ldots, U_T : \max_{\substack{|\xi\rangle \in \ker \Pi_{\text{in}} \\ |\eta\rangle \in \ker \Pi_{\text{out}}}} |\langle \xi | U_1 \cdots U_T | \eta \rangle|^2 = \epsilon\}.$$

This leads to our definition of the quantum UNSAT penalty of a circuit-to-Hamiltonian construction, which captures how well a Hamiltonian as in eq. (2) can enforce the input and output penalties described above for an arbitrary circuit.

Definition 1. *Let the $E(H_{\mathrm{FK}})$ and $E(H_{\mathrm{circuit}})$ be the ground state energies of H_{FK} and H_{circuit} respectively and define the quantum UNSAT penalty $E_p(\epsilon, T)$*

$$E_p(\epsilon, T) := \min_{U_1,\ldots,U_T \in C(\epsilon,T)} E(H_{\mathrm{FK}}) - E(H_{\mathrm{circuit}}). \tag{3}$$

Note that the quantum UNSAT penalty has a closely-related quantity, the average energy of any local Hamiltonian constraints $\mathrm{QUNSAT}_\psi = \sum_{e\in E} \langle\psi| h_e |\psi\rangle / |E|$ for some set of interactions $E = \{h_0, \ldots, h_{|E|}\}$ and a specific state ψ, as defined in the context of the detectability lemma [14]. We use the term UNSAT *penalty* to emphasize that it is the energy difference between accepting and non-accepting computations.

Our first step in analyzing the UNSAT penalty of modified Feynman Hamiltonians is to apply the same argument used in the standard construction (cf. [1, sec. 14.4]) to "undo" the computation and show that H_{circuit} is unitarily equivalent to a Hamiltonian which acts trivially on the computational register.

Lemma 1. *If $W := \sum_{t=0}^{T} |t\rangle\langle t| \otimes (U_t \cdots U_1)$, then W is unitary and $W^\dagger H_{\mathrm{circuit}} W = H \otimes \mathbb{1}$, where the clock Hamiltonian H_{clock} is given by*

$$H_{\mathrm{clock}} := \sum_{t=0}^{T} a_t |t\rangle\langle t| + \sum_{t=0}^{T-1} \left(b_t |t+1\rangle\langle t| + b_t^* |t\rangle\langle t+1|\right). \tag{4}$$

Next we apply the same geometrical lemma used in Kitaev's proof to lower bound the UNSAT penalty of modified Feynman Hamiltonians.

Lemma 2. *If the spectral gap $\Delta_H(T)$ of the corresponding clock Hamiltonian $H_{\mathrm{clock}}(T)$ is less than the (constant) spectral gap of $H_{\mathrm{in}} + H_{\mathrm{out}}$, then*

$$\frac{\Delta_H(T)}{4}(1-\sqrt{\epsilon}) \times \min\{\pi_0, \pi_T\} \le E_p(\epsilon, T) \le E\left(H_{\mathrm{clock}}(T) + |0\rangle\langle 0| + |T\rangle\langle T|\right). \tag{5}$$

The upper bound follows immediately by an operator inequality, and says that the increase in the ground state energy due to the penalty terms is at most bounded by the case when all of the frustration is in the system's time register. The lower bound states that the UNSAT penalty can be increased either by boosting the spectral gap of the clock Hamiltonian, or by amplifying the overlap of the ground state with the beginning and ending time steps of the computation. To see that the overlap with the endpoints of the computation can be made arbitrarily close to one, we prove that it is in fact possible to construct a clock Hamiltonian with an arbitrary distribution as its ground state.

Lemma 3. *For any probability distribution μ with support everywhere on its domain $\{0, \ldots, T\}$ there is a choice of coefficients $\{a_t, b_t\}_{t=0}^{T}$ in eq. (4) such that H_{clock} is frustration-free and has a ground space spanned by states of the form eq. (1) with weights $\psi_t = \sqrt{\mu_t}$.*

Using lemma 3 we exhibit a modified Hamiltonian for a target ground state distribution with $\pi_0, \pi_T \geq 1/4$, and show that it has a spectral gap that is $\Omega(T^{-2})$ to establish our first main result.

Theorem 1. *There is a frustration-free modified Feynman circuit Hamiltonian as in eq. (2) with a quantum UNSAT penalty $E_p(\epsilon, T)$ that is $\Omega((1-\sqrt{\epsilon})T^{-2})$.*

Finally, we show that the scaling of the UNSAT penalty achieved in theorem 1 is the optimal scaling that can be achieved by applying the lower bound in lemma 2 to modified Feynman Hamiltonians of the form in eq. (2).

Theorem 2. *Let $|\psi\rangle$ be the ground state of a Hamiltonian H with eigenvalues $E := E_0 \leq E_1 \leq \ldots \leq E_T$. If H is tridiagonal in the basis $\{|0\rangle, \ldots, |T\rangle\}$,*

$$H := \sum_{t=0}^{T} a_t |t\rangle\langle t| + \sum_{t=0}^{T-1} \left(b_t |t+1\rangle\langle t| + b_t^* |t\rangle\langle t+1|\right),$$

with $|a_t|, |b_t| \leq 1$ for $t = 0, \ldots, T$ then the product $\Delta_H \cdot \min\{|\psi|_0^2, |\psi_T|^2\}$ of the spectral gap $\Delta_H = E_1 - E$ and the minimum endpoint overlap is $\mathcal{O}(T^{-2})$.

The rest of the paper is organized as follows. The proofs of lemma 1 and lemma 3 can be found in section 2.1. The construction used for lemma 3 is given in section 2.2 along with some necessary background on Markov chains that will be used in the proof of theorem 1 in section 2.3. In section 3.1 we develop the quantum-to-classical mapping for arbitrary tridiagonal matrices and use it to prove theorem 2. In section 4 we describe the implications of our work for universal adiabatic computation. Finally, in section 5 we discuss the open problem of further increasing the quantum UNSAT penalty and relate it to some of the longstanding goals in the subject of quantum ground state computation.

2 Non-uniform circuit histories for improving the UNSAT penalty

2.1 Analysis of modified Feynman Hamiltonians

Proof of lemma 1. Since W is a linear operator the calculations we need to check for lemma 1 are the same as in the standard unweighted case [1, ch. 14.4]. As a reminder,

$$W^\dagger W = \sum_{t,t'=0}^{T} \Big(|t\rangle\langle t| \otimes (U_1^\dagger \cdots U_t^\dagger)\Big)\Big(|t'\rangle\langle t'| \otimes (U_1 \cdots U_{t'})\Big) = \sum_{t=0}^{T} |t\rangle\langle t| \otimes \mathbb{1} = \mathbb{1}, \tag{6}$$

$$W^\dagger(|t+1\rangle\langle t| \otimes U_{t+1})W = |t+1\rangle\langle t| \otimes (U_1^\dagger \cdots U_{t+1}^\dagger)U_{t+1}(U_t \cdots U_1) = |t+1\rangle\langle t| \otimes \mathbb{1}, \tag{7}$$

and so the claim of lemma 1 follows by linearity.

Proof of lemma 2. Kitaev's geometrical lemma provides the starting point for the lower bound (5).

Lemma (Kitaev's geometrical lemma)**.** *Let $A, B \geq 0$ be positive semi-definite operators, both with a zero eigenspace, and such that* $\ker A \cap \ker B = \{0\}$*. Denote with $\lambda_{\neq 0}(A), \lambda_{\neq 0}(B)$ the minimal non-zero eigenvalue of A and B, respectively. Then*

$$A + B \geq \min\{\lambda_{\neq 0}(A), \lambda_{\neq 0}(B)\} \times 2\sin^2\frac{\theta}{2}, \tag{8}$$

where θ is the angle between the kernels of A and B.

For us, $A = H_{\text{in}} + H_{\text{out}}$, and $B = H_{\text{circuit}}$, and in this section we use the freedom to shift the energy in *eq.* (2) to set $E(H_{\text{circuit}}) = 0$ (since the system can be frustrated this means the local terms may no longer be positive semi-definite, but this will not present a problem in applying the geometrical lemma above because H_{circuit} itself is positive semi-definite). Denote the projector onto the kernel of the penalty terms A with $\Pi_{\text{pen}} := |0\rangle\langle 0| \otimes \Pi_{\text{in}}^{\perp} + |T\rangle\langle T| \otimes \Pi_{\text{out}}^{\perp} + \sum_{t=2}^{T-1} |t\rangle\langle t| \otimes \mathbb{1}$. Denote with $U = U_T \cdots U_1$ the entire encoded quantum circuit. We first want to bound the angle θ between the kernels of the propagation and penalty Hamiltonians.

$$\begin{aligned}
\cos^2\theta &= \max_{\substack{|\xi\rangle \in \ker A \\ |\eta\rangle \in \ker B}} |\langle \xi | \eta\rangle|^2 \\
&= \max_{\substack{|\xi\rangle \\ |\eta\rangle \in \ker B}} |\langle \eta| \Pi_{\text{pen}} |\xi\rangle|^2 \\
&\overset{*}{=} \max_{|\eta\rangle \in \ker B} \langle \eta| \Pi_{\text{pen}} |\eta\rangle \\
&= \max_{|\eta\rangle \in \ker B} \langle \eta| W^\dagger (W \Pi_{\text{pen}} U^\dagger) W |\eta\rangle \\
&= \max_{|\eta'\rangle \in \ker WBW^\dagger} \langle \eta'| \, |0\rangle\langle 0| \otimes \Pi_{\text{in}}^{\perp} + |T\rangle\langle T| \otimes U\Pi_{\text{out}}^{\perp}U^\dagger + \sum_{t=2}^{T-1} |t\rangle\langle t| \otimes \mathbb{1} \, |\eta'\rangle \\
&= \max_{|\phi\rangle} \sum_{s=1}^{T} \psi_s^* \psi_s \langle s| \langle \phi| \left(|0\rangle\langle 0| \otimes \Pi_{\text{in}}^{\perp} + |T\rangle\langle T| \otimes U\Pi_{\text{out}}^{\perp}U^\dagger + \sum_{t=2}^{T-1} |t\rangle\langle t| \otimes \mathbb{1} \right) |t\rangle |\phi\rangle \\
&= \max_{|\phi\rangle} \langle \phi| (\operatorname{abs}\psi_0^2 \Pi_{\text{in}}^{\perp} + \operatorname{abs}\psi_T^2 U\Pi_{\text{out}}^{\perp}U^\dagger) |\phi\rangle + 1 - \operatorname{abs}\psi_0^2 - \operatorname{abs}\psi_T^2,
\end{aligned}$$

where we have saturated Cauchy-Schwartz in the third line ($*$). To bound the first inner product, we observe that if $\psi_0^2 \geq \psi_T^2$, picking $|\phi\rangle \in \ker \Pi_{\text{in}}$ gives the bound

$$\max_{|\phi\rangle} \langle \phi| (\pi_0 \Pi_{\text{in}}^{\perp} + \pi_T U\Pi_{\text{out}}^{\perp}U^\dagger) |\phi\rangle \leq \pi_0 + \pi_T \cos\vartheta,$$

where ϑ is the angle between $\operatorname{supp}\Pi_{\text{in}}$ and $\operatorname{supp} U\Pi_{\text{out}}U^\dagger$. This angle can be lower-bounded by the acceptance probability of the circuit:

$$\cos^2\vartheta = \max_{\substack{|\eta\rangle \in \operatorname{supp}\Pi_{\text{in}} \\ |\xi\rangle \in \operatorname{supp} U\Pi_{\text{out}}U^\dagger}} |\langle \eta | \xi\rangle|^2 \leq \max_{\substack{|\eta\rangle \in \operatorname{supp}\Pi_{\text{in}} \\ |\xi\rangle \in \operatorname{supp}\Pi_{\text{out}}}} |\langle \eta| U |\xi\rangle|^2 \leq \epsilon.$$

Similarly, if $\psi_0^2 < \psi_T^2$, one can show an upper bound of $\pi_0 \cos\vartheta + \pi_T$. We thus obtain an overall upper bound

$$\begin{aligned}\cos^2\theta &\leq \max\{\pi_0, \pi_T\} + \min\{\pi_0, \pi_T\}\sqrt{\epsilon} + 1 - \pi_0 - \pi_T \\ &\leq 1 - \min\{\pi_0, \pi_T\}(1 - \sqrt{\epsilon}).\end{aligned}$$

In Kitaev's lemma, we thus obtain a lower bound

$$2\sin^2\frac{\theta}{2} \geq 2 \times \frac{1-\cos^2\theta}{8\cos^2\theta} \geq \frac{1}{4}\min\{\pi_0, \pi_T\}(1 - \sqrt{\epsilon}),$$

and the claim follows.

2.2 Symmetrized Metropolis Hamiltonians with target GS distributions

In this section we describe our construction which fulfills lemma 3. We review most concepts as needed but assume the reader has some familiarity with Markov chain transition matrices as can be found in any textbook on the subject, such as [15].

Proof of lemma 3. Given a probability distribution π with support everywhere on its domain $\mathcal{S} = \{0, \ldots, T\}$ we can construct an irreducible Markov chain P with state space $\mathcal{S}$ and by taking the Metropolis chain with transition probabilities given by

$$P_{t,t+1} = \frac{1}{4}\min\left\{1, \frac{\pi_{t+1}}{\pi_t}\right\} \quad , \quad P_{t,t-1} = \frac{1}{4}\min\left\{1, \frac{\pi_{t-1}}{\pi_t}\right\} \quad P_{t,t} = 1 - P_{t,t+1} - P_{t,t-1} \qquad (9)$$

for all $i \in \mathcal{S}$ (setting the expressions $P_{0,-1}$ and $P_{T,T+1}$ to zero) and $P(i,i') = 0$ for all $i, i' \in \mathcal{S}$ with $|i - i'| > 1$. The transition matrix $P := \sum_{i,i' \in \mathcal{S}} P_{i,i'}|i\rangle\langle i|$ is not a symmetric matrix, but a well established technique in the analysis of Markov chains is to relate P to a symmetric matrix,

$$A := \sum_{i,i' \in \mathcal{S}} \pi_i^{1/2}\pi_{i'}^{-1/2} P_{i,i'}|i\rangle\langle i'|. \qquad (10)$$

The two matrices are related by the fact that if $\langle v_0|, \cdots, \langle v_T|$ are the left eigenvectors of P with eigenvalues $\lambda_0 = 1 \geq \lambda_1 \geq, \ldots, \geq \lambda_T \geq 0$ then $|w_i\rangle := \sum_{t\in\mathcal{S}}\langle v_i|t\rangle\langle t|v_0\rangle^{-1/2}\ |t\rangle$ satisfies $A|w_i\rangle = \lambda_i|w_i\rangle$. Therefore A has the same eigenvalues as P, and in particular it has largest eigenvalue 1 corresponding to the eigenvector $|w_0\rangle$ with components satisfying $\langle t|w_0\rangle = \langle t|v_0\rangle^{1/2} = \sqrt{\pi_t}$. Therefore $H = I - A$ is a non-negative Hermitian matrix with ground state that has energy zero and components $\sqrt{\pi_t}$ in the time register basis, as claimed.

Markov chain spectral gaps. Substantial efforts been devoted to characterizing spectral gaps of Markov chains. A particularly fruitful characterization procedes by defining a quantity called the conductance,

$$\Phi := \min_{S\subseteq\Omega} \frac{Q(S,S^c)}{\min\{\pi(S), \pi(S^c)\}} \quad , \quad Q(S,S^c) := \sum_{x,y\in\Omega} \pi(x)P(x,y) \qquad (11)$$

which determines the spectral gap within a quadratic factor,

$$\frac{\Phi^2}{2} \leq \Delta_P \leq 2\Phi. \tag{12}$$

The lower bound in eq. (12) is usually called Cheeger's inequality, and it was initially discovered in the analysis of manifolds [16] before being adapted to the setting of Markov chains [17]. In the next section we will use this method to lower bound the spectral gap of the Symmetrized Metropolis Hamiltonian corresponding to a particular non-uniform stationary distribution.

2.3 Proof of Theorem 1

Set $\pi_0 = \pi_T = 1/2$ and $\pi_t = (2T-2)^{-1}$ for $t = 1, \ldots, T-1$, and define H_{circuit} as the Symmetrized Metropolis Hamiltonian corresponding to this probability distribution. Keeping with tradition [18, 4, 6], we exhibit H as a $T+1$ by $T+1$ matrix in the time register basis,

$$H = \begin{pmatrix} \frac{1}{2T-2} & -\frac{1}{2\sqrt{2T-2}} & 0 & & \cdots & & 0 \\ -\frac{1}{2\sqrt{2T-2}} & \frac{1}{2} & -\frac{1}{4} & 0 & \ddots & & \vdots \\ 0 & -\frac{1}{4} & \frac{1}{2} & -\frac{1}{4} & 0 & \ddots & \vdots \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \\ \vdots & & 0 & -\frac{1}{4} & \frac{1}{2} & -\frac{1}{4} & 0 \\ & & & 0 & -\frac{1}{4} & \frac{1}{2} & -\frac{1}{2\sqrt{2T-2}} \\ 0 & & \cdots & & 0 & -\frac{1}{2\sqrt{2T-2}} & \frac{1}{2T-2} \end{pmatrix} \tag{13}$$

A few low energy eigenstates of this Hamiltonian are illustrated in figure 1. Since π_0 and π_T are $\Omega(1)$ it only remains to check that the spectral gap Δ_H of the clock Hamiltonian is $\Omega(T^{-2})$, which since this spectral gap is equal to the spectral gap of the Metropolis transition matrix P that is reversible with respect to π we can apply Cheeger's inequality (12).

The goal is to show that every subset S of $\mathcal{S}$ has large conductance, so we divide the proof into cases corresponding to the different possibilities for the subset S. First if $S = \{0\}$ then since $P_{0,1} = (8T-8)^{-1}$ so $\Phi(S)$ is $\Omega(T^{-1})$, with similar statements holding for $S = \{T\}$ and $S = \{0, T\}$. Now if $S = \{1, \ldots, T-1\}$ is non-empty there must be at least one $t \in \{1, \ldots, T-1\}$ such that there is a $t \in S^c$ with $P_{t,t'} \geq 1/4$, and since $\pi_t = (2T-2)^{-1}$ this shows that $\Phi(S)$ is $\Omega(T^{-1})$ in this case as well. Therefore Δ_P is $\Omega(T^{-2})$ by (12) and since $\Delta_H = \Delta_P$ this concludes the proof of theorem 1.

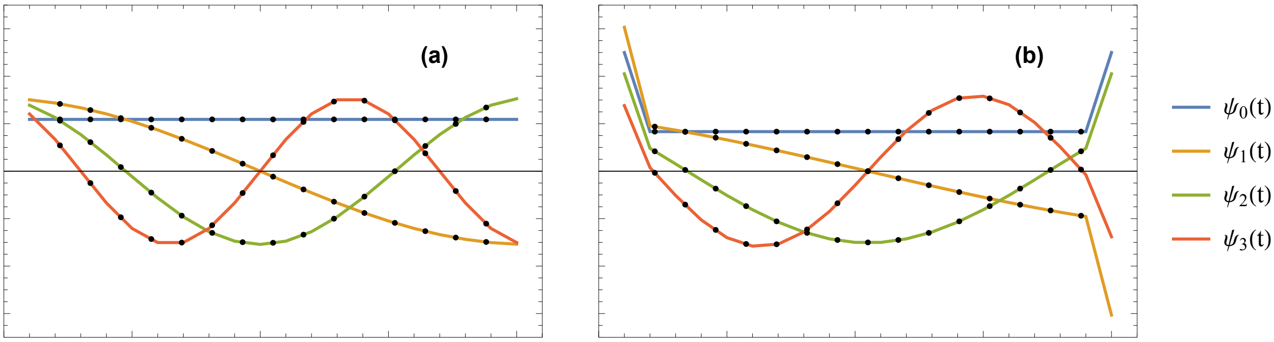

Figure 1: Low energy eigenstates of **(a)** the path graph Laplacian used in the standard circuit-to-Hamiltonian construction and **(b)** the symmetrized Metropolis Hamiltonian corresponding to the distribution with $\pi_0, \pi_T = 1/4$ that is used in this section.

3 Limitations on further improvement

3.1 Proof of Theorem 2

The proof of Theorem 2 is based on applying a sharp spectral gap bound for birth-and-death Markov chains to a quantum-to-classical mapping that has been studied previously in the closely related context of universal adiabatic computation [4] and the complexity of stoquastic Hamiltonians [19, 20]. A new feature of our application is the realization that this quantum-to-classical mapping defines a Markov chain even for tridiagonal Hamiltonian matrices with arbitrary complex entries, while previous applications have been restricted to cases for which H has all non-positive off-diagonal matrix entries in the time register basis.

In this section we continue with the notation of (2), but now we use the freedom to shift the energy to set $a_t \geq 0$ for all t, and so the ground state energy E will in general satisfy $0 \leq E < 1$. Define $G := (\mathbb{1} - H)/(1 - E)$ to be a shifted and rescaled version of H which is designed to satisfy $G|\psi\rangle = |\psi\rangle$, where $|\psi\rangle$ labels the ground state of H. For all $t, t' \in \{0, \ldots, T\}$, define

$$P_{t,t'} := \begin{cases} \psi_{t'} G_{t,t'} \psi_t^{-1} & \text{if } \psi_t \neq 0 \text{ and } \psi_{t'} \neq 0, \\ 0 & \text{otherwise.} \end{cases} \tag{14}$$

In the following lemma we will show that the $P_{t,t'}$ are transition probabilities for an irreducible Markov chain on $\{0, \ldots, T\}$, i.e. in particular that they are all non-negative. First, observe that if H is stoquastic as in previous applications, then G is a non-negative matrix in the time register basis, ψ has non-negative amplitudes in this basis by the Perron-Frobenius theorem and so $P_{t,t'}$ is explicitly non-negative. Here we show that even when G contains arbitrary complex matrix entries (while being tridiagonal) we still have $P_{t,t'} \geq 0$, because of cancellations that occur between the matrix elements of G and the amplitudes of the ground state wave function in the time register basis. Continuing with the same notation used in (4),

Lemma 4. *If $\psi_0 \neq 0$, $\psi_T \neq 0$, and $b_t \neq 0$ for $t = 0, \ldots, T$, then $\psi_t \neq 0$ for $t = 1, \ldots, T-1$ and $P_{t,t+1} = \psi_{t+1} G_{t,t+1} \psi_t^{-1} \geq 0$ for all $t \in \{0, \ldots, T-1\}$.*

Before proving the lemma, note that the conditions may be taken to hold without loss of generality, since $\psi_0 = 0$ or $\psi_T = 0$ immediately implies Theorem 2, or similarly if $b_{t'} = 0$ for some t' then $|\psi^\perp\rangle := \sum_{t=0}^{T} \psi_t^\perp |t\rangle$ defined by

$$\psi_t^\perp := \begin{cases} \frac{\psi_t}{\psi^2([0,t'])} & 0 \leq t \leq t' \\ -\frac{\psi_t}{\psi^2([t'+1,T])} & t' < t \leq T-1 \end{cases} \tag{15}$$

satisfies $\langle \psi^\perp | \psi \rangle = 0$ and $H|\psi^\perp\rangle = E|\psi^\perp\rangle$, which implies $\Delta_H = 0$ and so again Theorem 2 holds in this case[1].

Now turning to the proof of Lemma 4. From $H|\psi\rangle = E|\psi\rangle$ we have that

$$a_0\psi_0 + b_0\psi_1 = E\psi_0 \tag{16}$$

$$b_{i-1}^*\psi_{i-1} + a_i\psi_i + b_i\psi_{i+1} = E\psi_i \quad , \quad \text{for } i = 1, \ldots, T-1 \tag{17}$$

$$a_T\psi_T + b_{T-1}^*\psi_{T-1} = E\psi_T \tag{18}$$

Since $P_{t,t'} = 0$ when $|t - t'| > 1$, our goal is to show $P_{t,t+1} > 0$ for $t \in \{0, \ldots, T-1\}$, and $P_{t,t-1} > 0$ for $t \in \{1, \ldots, T\}$. The first claim $P_{t,t+1} > 0$ will follow by showing that E is minimized when $\psi_t \neq 0$ and $\psi_{t+1} b_t \psi_t^{-1} < 0$ for all $t = 0, \ldots, T-1$. The second claim $P_{t-1,t} > 0$ is then implied immediately since

$$\psi_t b_t^* \psi_{t+1}^{-1} = \left(\frac{|\psi_t|}{|\psi_{t+1}|}\right)^2 \frac{\psi_{t+1}^*}{\psi_t^*} b_t^* = \left(\frac{|\psi_t|}{|\psi_{t+1}|}\right)^2 \left(\psi_{t+1} b_t \psi_t^{-1}\right)^*. \tag{19}$$

Rearranging eq. (16) yields $\psi_1 b_0 \psi_0^{-1} = E - a_0$, and since $E - a_0$ is real the value of E implied by this equation alone is minimized when the LHS is negative. This observation will be taken as the base case for an argument by mathematical induction on the finite set $\{1, \ldots, T-1\}$. The inductive hypothesis is that the value of E implied by considering only equations 0 through i in the list eq. (17) is minimized when $\psi_t b_{t-1} \psi_{t-1}^{-1}$ is negative for $1, \ldots, t$, and this will be used to show that the minimum value of E that satisfies equations 0 through $t+1$ in eq. (17) will be achieved when $\psi_{t+1} b_t \psi_t^{-1}$ is negative as well. Using the fact that $\psi_t \neq 0$ from the inductive hypothesis we may express eq. (17) as

$$b_{t-1}^* \frac{\psi_{t-1}}{\psi_t} + b_t \frac{\psi_{t+1}}{\psi_i} = E - a_t \quad , \quad \text{for } t = 1, \ldots, T-1. \tag{20}$$

Since $E - a_t$ is real and $\psi_{t-1} b_{t-1}^* \psi_t^{-1} = (|\psi_{t-1}|/|\psi_t|)^2 (\psi_t b_{t-1} \psi_{t-1}^{-1})^*$ is negative by the inductive hypothesis, the value of E implied by equations 0 through $t+1$ in the list eq. (17)

[1] Note that the same idea behind (15) can be used to upper bound the spectral gap by the minimum of $\pi_t \pi_{t+1}$ over all $t \in \{0, ..., T-1\}$ such that $\psi^2([0, t'])$ and $\psi^2([t'+1, T])$ are both $\Omega(1)$.

will indeed be minimized by taking $\psi_{t+1} b_t \psi_t^{-1}$ to be negative. This establishes the inductive claim and completes the proof of Lemma 4.

Having established that $P_{t,t'} \geq 0$ we now list several standard facts which have been previously applied to P when G is non-negative, which can also be seen in the present case by direct computation:

1. P is a stochastic matrix, i.e. $\sum_{t'=0}^{T} P_{t,t'} = 1$ for all $t \in \{0, \ldots, T\}$, and therefore it can be regarded as the transition matrix of a discrete time Markov chain.

2. The largest eigenvalue of P is equal to 1 and it corresponds to the unique principal eigenvector $|\pi\rangle = \sum_{t=0}^{T} |\psi_t|^2 |t\rangle$. The probability distribution $\pi_t := \langle t|\pi\rangle$ is the stationary distribution of the corresponding Markov chain.

3. The Markov chain defined by P is reversible with respect to its stationary distribution,
$$\pi_t P_{t,t'} = \langle t'|\psi\rangle\langle\psi|t\rangle G_{t,t'} = \left(\langle t|\psi\rangle\langle\psi|t'\rangle G^*_{t,t'}\right)^* = \pi'_t P_{t',t}.$$

4. If $|\psi_0\rangle, |\psi_1\rangle, \ldots, |\psi_T\rangle$ are the eigenvectors of H with corresponding eigenvalues $E_0 < E_1 \leq \ldots \leq E_T$, then $|\phi_k\rangle = \sum_{x\in\Omega} \langle\psi_0|x\rangle\langle x|\psi_k\rangle|x\rangle$ is an eigenvector of P with eigenvalue $(1-E_k)/(1-E_0)$. Since this is the complete list of eigenvectors of P we have shown that the spectral gaps of H and P satisfy
$$\Delta_P = (1-E)\Delta_H. \tag{21}$$

The relation eq. (21) means that we can apply techniques developed for upper bounding the spectral gap of Markov chains to the problem of upper bounding the spectral gap of H. A non-trivial example of such an upper bound is eq. (12): if the overlap of the stationary distribution with the end points $|0\rangle$ and $|T\rangle$ is constant then we can immediately see that the conductance Φ is $\mathcal{O}(T^{-1})$ by the fact that the stationary distribution is normalized, and this implies that Δ_H is $\mathcal{O}(T^{-1})$. It turns out we can obtain an even tighter bound by using a characterization of spectral gaps that applies specifically to birth-and-death chains [21], which we state here as a lemma.

Lemma 5. *If P is a birth and death chain with stationary distribution π, then the spectral gap Δ_P satisfies*
$$\frac{1}{2\ell} \leq \Delta_P \leq \frac{4}{\ell} \tag{22}$$
where
$$\ell := \max\left\{\max_{j:j\leq i'} \sum_{k=j}^{i'-1} \frac{\pi([0,j]}{\pi(k)P_{k,k+1}}, \max_{j:j>i'} \sum_{k=i'+1}^{j} \frac{\pi([j,T])}{\pi(k)P_{k,k-1}}\right\} \tag{23}$$
where i' satisfies $\pi([0,i']) \geq 1/2$ and $\pi([i',n]) \geq 1/2$.

In the present case we are seeking a lower bound on ℓ in order to have an upper bound on the gap. To simplify the formulas we assume that the stationary distribution of the weighted history state is symmetric around $t = T/2$ (otherwise the problem divides into two similar cases). Since we are seeking a lower bound on ℓ we can ignore the factor of $P_{k,k+1} \leq 1$ in the denominator, and we are also free to replace the maximization over j with any fixed choice of j.

With these simplifications and the choice of $j = 1$ eq. (23) becomes

$$\ell \geq \psi_0^2 \sum_{t=1}^{T/2-1} \frac{1}{\psi_t^2}.$$

Applying the inequality of the arithmetic and geometric means yields,

$$\sum_{t=1}^{\frac{T}{2}-1} \frac{1}{\psi_t^2} \geq \left(\frac{T}{2} - 1\right) \left(\psi_1^2 \cdots \psi_{\frac{T}{2}-1}^2\right)^{-1/k} \tag{24}$$

$$\geq \left(\frac{T}{2} - 1\right)^2 \left(\sum_{t=1}^{T/2-1} \psi_t\right)^{-1} \tag{25}$$

and so ℓ is $\Omega(\psi_0^2 T^2)$, and from eq. (22) we have that the spectral gap Δ_P is $\mathcal{O}(\ell^{-1})$ and so $\Delta_H \cdot \psi_0^2$ is $\mathcal{O}(T^{-2})$ as claimed.

4 Relation to universal adiabatic computation

First we point out that modified Feynman Hamiltonians, together with the symmetrized Metropolis Hamiltonian construction of section 2.2, open up a new set of trade-offs in universal adiabatic computation that may be relevant for practical implementations. Specifically, the Hamiltonian used in section 2.3 with $\Omega(1)$ probability on the endpoints can be used to increase the probability that measuring the time register will collapse the computational register of the system into the final time step of the computation. This provides an alternative to the theoretical solution of "padding the end of the computation with identity gates" that is normally used to raise the probability of sampling from the final time step of the computation. Padding the length of the computation with identity gates is relatively expensive in practical terms when the time register is encoded using local interactions (such as the domain wall clock) because the clock must be represented in unary, meaning the number of clock qubits scales linearly with the total length of the (padded) computation.

Achieving an overlap of $\delta \approx 1$ with the final step of the computation by padding the system with identity gates requires a total of $\mathcal{O}(T/(1-\delta))$ clock qubits, however one can instead prepare the weighted history state with $\pi_T = \delta$ using only T clock qubits. The price that one has to pay for this improvement is in an increase in the precision of the couplings needed to implement eq. (2) now must scale like $\mathcal{O}(T^{-1})$, as seen in (13). This is a reasonable trade off, however, since the total number of qubits is generally the limiting factor in most experiments.

Furthermore, theorem 2 can be interpreted as proving that the standard universal adiabatic construction plus the weighted endpoint modification made above is in a sense optimal for Hamiltonians of the form (2). First, the problem of upper bounding the spectral gap of universal adiabatic constructions was addressed before [22] by combining the quantum lower bound for unstructured search with the technique of spectral gap amplification. This previous work found a general $\tilde{\mathcal{O}}(T^{-1})$ bound on the spectral gap of *any* adiabatic Hamiltonian, a $\tilde{\mathcal{O}}(T^{-2})$ gap for any frustration-free adiabatic Hamiltonian, and finally an $\tilde{\mathcal{O}}(T^{-2})$ bound on the spectral gap of modified Feynman Hamiltonians of the form (2) when the weights near the endpoints satisfy a reasonable assumption for any adiabatic computation. Our theorem 2 corroborates this last result by showing a tight $\mathcal{O}(T^{-2})$ upper bound on the spectral gap and the minimum overlap of the weighted history state with either endpoint of the computation.

5 Outlook

One of the main aims of the present work is to motivate new ideas in quantum ground state computation by focusing on the quantum UNSAT penalty as a metric for the improvement of circuit Hamiltonians. In this section we discuss a range of open problems related to the UNSAT penalty, in case that they are more tractable or lead to a different perspective on some of the open challenges facing this field. One difficulty is that there is at present no general abstract formulation of what it means for a Hamiltonian to have a ground space of circuit histories, as further improvement could involve alterations to the tridiagonal form of the clock Hamiltonian (one such construction allowing for computational paths that include branching, concurrency, and loops is given in [13]). Therefore we describe these open problems without specifying a precise form for future circuit-to-Hamiltonian constructions e.g. how the number of local terms might scale, and so we are implicitly discussing *relative* energy penalties that are not simply made larger by e.g. increasing the overall norm of the Hamiltonian.

The classical baseline. The classical Cook-Levin theorem encodes the history of a classical circuit into the satisfying assignment of a 3-SAT formula. If the computation has T time steps, then the associated constraint satisfaction problem has $\mathcal{O}(T)$ local terms and if each has a constant norm than the classical UNSAT penalty is immediately $\Omega(1)$. Therefore we ask: is it possible for a circuit Hamiltonian containing $\mathcal{O}(T)$ local terms of bounded norm, which may be of a form more general than (2), to achieve an UNSAT penalty that is independent of the length of the computation?

Macroscopic UNSAT penalty. Building on the previous question which asks whether the UNSAT penalty can be made independent of the length of the computation, we further ask whether the UNSAT penalty can be made to scale macroscopically with the number of qubits n in the computation. Specifically, is there a circuit Hamiltonian with $\mathcal{O}(\mathrm{poly}(n)T)$ local terms that achieves a $\mathrm{poly}(n)$ UNSAT penalty that is independent of T? Such a construction could be a useful step towards fault-tolerant adiabatic computation. An intuition for this connection can be gained by considering a construction for energetically encoded fault-tolerant classical computation, whereby each logical bit could be encoded as an arrangement of spins in a self-correcting model (e.g. the 2D Ising model), so that the UNSAT penalty could have a macroscopic scaling (i.e. with the number of physical spins representing each logical bit) that is independent of T.

Constant relative UNSAT penalty A circuit Hamiltonian with $O(m)$ local terms of bounded norm, where $m = \mathrm{poly}(T)$, with constant relative UNSAT penalty E_p/m would yield a proof of the quantum PCP conjecture by spectral gap amplification. The reduction consists of applying the circuit Hamiltonian with constant relative UNSAT penalty to the circuit verifier that decides the ground state energy of the arbitrary input local Hamiltonian.

It is a testament to Feynman's great legacy that an idea first introduced in 1987 has had such a profound impact for wide scope of research, from condensed matter physics to quantum computation, and that despite the growth of the field of Hamiltonian complexity his original construction continues to remain essentially unchanged to date. We do not know whether or where limitations of improving the circuit-to-Hamiltonian construction will be reached, but hope that our contribution will help to push this boundary a little further.

6 Acknowledgements

J. B. acknowledges support from the German National Academic Foundation and the EPSRC (grant 1600123). E. C. acknowledges support provided by the Institute for Quantum Information and Matter, an NSF Physics Frontiers Center (NSF Grant PHY-1125565) with support of the Gordon and Betty Moore Foundation (GBMF-12500028). J. B. would also like to thank Thomas Vidick and the IQIM for hospitality during spring 2016.

References

[1] Alexei Yu. Kitaev, Alexander Shen, and Mikhail N. Vyalyi. Classical and quantum computing. In *Quantum Information*, pages 203–217. Springer New York, New York, NY, 2002.

[2] Julia Kempe, Alexei Kitaev, and Oded Regev. The Complexity of the Local Hamiltonian Problem. *SIAM Journal on Computing*, 35(5):1070–1097, jan 2006.

[3] Roberto Oliveira and Barbara M. Terhal. The complexity of quantum spin systems on a two-dimensional square lattice. *Quantum Information & Computation*, pages 1–23, apr 2005.

[4] Dorit Aharonov, Wim Van Dam, Julia Kempe, Zeph Landau, Seth Lloyd, and Oded Regev. Adiabatic quantum computation is equivalent to standard quantum computation. *SIAM review*, 50(4):755–787, 2008.

[5] Jacob D Biamonte and Peter J Love. Realizable Hamiltonians for universal adiabatic quantum computers. *Physical Review A*, 78(1):012352, 2008.

[6] Dorit Aharonov, Daniel Gottesman, Sandy Irani, and Julia Kempe. The power of quantum systems on a line. *Communications in Mathematical Physics*, 287(1):41–65, may 2009.

[7] Toby Cubitt and Ashley Montanaro. Complexity classification of local Hamiltonian problems. *SIAM Journal on Computing*, 45(2):268–316, 2016.

[8] Dorit Aharonov, Itai Arad, and Thomas Vidick. Guest column: the quantum PCP conjecture. *Acm sigact news*, 44(2):47–79, 2013.

[9] Richard P. Feynman. Quantum mechanical computers. *Foundations of Physics*, 16(6):507–531, jun 1986.

[10] Daniel Gottesman and Sandy Irani. The Quantum and Classical Complexity of Translationally Invariant Tiling and Hamiltonian Problems. *Theory of Computing*, 9(1):31–116, may 2013.

[11] Nikolas P Breuckmann and Barbara M Terhal. Space-time circuit-to-Hamiltonian construction and its applications. *Journal of Physics A: Mathematical and Theoretical*, 47(19):195304, 2014.

[12] Sean Hallgren, Daniel Nagaj, and Sandeep Narayanaswami. The Local Hamiltonian problem on a line with eight states is QMA-complete. *Quantum Information and Computation*, 13(9&10):28, dec 2013.

[13] Johannes Bausch, Toby Cubitt, and Maris Ozols. The Complexity of Translationally-Invariant Spin Chains with Low Local Dimension. *arXiv:1605.01718*, may 2016.

[14] Dorit Aharonov, Itai Arad, Zeph Landau, and Umesh Vazirani. The detectability lemma and quantum gap amplification. In *Proceedings of the 41st annual ACM symposium on Symposium on theory of computing - STOC '09*, page 417, New York, New York, USA, 2009. ACM Press.

[15] David Asher Levin, Yuval Peres, and Elizabeth Lee Wilmer. *Markov chains and mixing times.* American Mathematical Soc., 2009.

[16] J. Cheeger. A lower bound for the smallest eigenvalue of the Laplacian, problems in analysis. In *Papers dedicated to Salomon Bochner (1969)*, page 195–199. Princeton Univ. Press, Princeton, N. J., 1970.

[17] Alistair Sinclair and Mark Jerrum. Approximate counting, uniform generation and rapidly mixing Markov chains. *Information and Computation*, 82(1):93–133, 1989.

[18] Dorit Aharonov and Tomer Naveh. Quantum NP-a survey. *arXiv preprint quant-ph/0210077*, 2002.

[19] Sergey Bravyi, Arvid J Bessen, and Barbara M Terhal. Merlin-Arthur games and stoquastic complexity. *arXiv preprint quant-ph/0611021*, 2006.

[20] Sergey Bravyi and Barbara Terhal. Complexity of stoquastic frustration-free Hamiltonians. *Siam journal on computing*, 39(4):1462–1485, 2009.

[21] Guan-Yu Chen and Laurent Saloff-Coste. On the mixing time and spectral gap for birth and death chains. *arXiv preprint arXiv:1304.4346*, 2013.

[22] Anand Ganti and Rolando Somma. On the gap of Hamiltonians for the adiabatic simulation of quantum circuits. *International Journal of Quantum Information*, 11(07):1350063, 2013.