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THE LOCAL HAMILTONIAN PROBLEM ON A LINE WITH EIGHT STATES IS QMA-COMPLETE

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The Local Hamiltonian problem is the problem of estimating the least eigenvalue of a local Hamiltonian, and is complete for the class QMA. The 1D problem on a chain of qubits has heuristics which work well, while the 13-state qudit case has been shown to be QMA-complete. We show that this problem remains QMA-complete when the dimensionality of the qudits is brought down to 8.

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1 Introduction

The Local Hamiltonian problem – estimating the ground state energy of a local Hamiltonian – is a natural problem in physics, and belongs to the complexity class QMA. QMA is the quantum analogue of NP. Languages in QMA have a quantum verifier: a polynomial-time quantum algorithm that takes (poly-sized) quantum states as witnesses.

In quantum mechanics, the Hamiltonian of a system is the Hermitian operator corresponding to the energy of the system: its eigenvalues are the set of energies that a system can be measured to have. It also determines the time-evolution of the system and defines the interactions between its subsystems. The least eigenvalue (ground state energy) and the corresponding eigenvector (the ground state) are key to understanding the properties of a

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quantum system. Hamiltonians in nature are usually local, in that they can be written as a sum $H = \sum_{i=1}^{M} H_i$ where each term H_i acts only on a small (constant) number of subsystems. Estimating the ground state energy of such an H is therefore a very fundamental question.

The input to the k-Local Hamiltonian problem is a set of Hermitian matrices $\{H_i\}$, each H_i acting on a set of k qubits (out of a total of n), and the problem is to estimate the lowest eigenvalue of the sum $H = \sum_{i=1}^{M} H_i$. Note that even though each H_i acts nontrivially on a constant number k of qubits and is constant-dimensional, H itself acts on the whole space of n qubits and is therefore exponential in size. The Local Hamiltonian problem can be thought of as a generalization of SAT [1]. In particular, MAX2SAT is a special case of the 2-Local Hamiltonian problem. Therefore, 2-Local Hamiltonian is NP-hard.

The 5-Local Hamiltonian problem was the first to be shown to be QMA-complete, in [2]. It is also a very natural complete problem, given that it is a generalization of SAT. Moreover, physicists have worked on similar problems, developing a number of heuristic tools for approximating ground states and ground state energies. However, the Hamiltonian constructed in [2] does not have any constrain the spatial arrangement of the qubits, making it unrealistic. In physical (e.g. spin) systems, the Hamiltonians are often spatially local: the interacting systems (qubits or qudits) may be arranged on a grid, or the interactions are (at least approximately) short-ranged (e.g. nearest-neighbor). Simulation of local Hamiltonians on one- or two-dimensional grids is an important problem in physics, and it is natural to try to understand the complexity in the different cases obtained by changing the locality and the dimensionality of the qudits. Since it is also much easier to realize and manipulate lower-dimensional qudits in the lab, these cases are particularly important.

There have been improvements on this result and its unfrustrated variant Quantum k-SAT [3, 4, 5]. The locality was brought down to 3 [6] and then to 2 [7]. The 2-local problem remains QMA-complete when the Hamiltonians are restricted to be nearest-neighbor interactions on a 2D grid [8]. The 1D case was not expected to be so hard: its classical counterpart, the 1D constraint satisfaction problem, has efficient algorithms. Moreover, there are good heuristic methods that are effective on many instances of the problem. Therefore, it was a somewhat surprising result when [9] showed a hardness proof for the Local Hamiltonian problem on a chain (with nearest-neighbor interactions) of 13-state[c] qudits. In this paper, we bring the number of states down from 13 to 8. For a recent review of QMA-complete problems, see [10].

The hardness of the 1D problem (with nearest-neighbor interactions only) for the cases with 2-7 state qudits remains an interesting open question. It is not clear if the QMA-completeness result will continue to hold as we further decrease the dimensionality of the qudits down towards 2. It may happen that below a particular dimensionality, we could find that the problem has an efficient quantum or classical algorithm, e.g. if the ground state entanglement could be shown to be low. Recently, an interesting qutrit chain with a unique unfrustrated ground state with lots of entanglement was analyzed in [11]. Finally, these QMA-completeness results also bear a close relationship to adiabatic quantum computing: the

[c] The paper states hardness for $d = 12$. However, there are two illegal configurations that are not penalized: ⊗ ⊗ ⋐ ○ ○ and ⊗ ⊗ ◎ ○ ○ turn into each other under the action of the Hamiltonian. The superposition of these two configurations forms a zero energy state of the Hamiltonian, which means that the Hamiltonian no longer has the promised $\frac{1}{poly}$ gap. This can be fixed by adding a 13th state, as discussed in footnote 4 in [9].

computation models in these results, and the Hamiltonians that check these computations, can be used to perform universal adiabatic quantum computing. It will be interesting to see if restricted local Hamiltonian systems (e.g., low-dimensional qudits on a line) that most likely do not encode a QMA-complete problem can still be used to perform universal adiabatic QC.

To show QMA completeness for our version of Local Hamiltonian, we reduce an arbitrary QMA language L to a Local Hamiltonian in 1D with $d = 8$ particles, outputting a Hamiltonian that either has a ground state energy below some value a, or whether this energy is at least $1/poly$ larger than a. We base our proof on three ideas.

First, we use Kitaev's Hamiltonian [2]: a Hamiltonian that has as its ground state a *history state* of the verification circuit[d] V_x for the language L. A history state is a state of the form $\sum_t |\phi_t\rangle|t\rangle$, where $|\phi_t\rangle$ is the state after applying the first t gates of V_x to $|\phi_0\rangle$. Kitaev's Hamiltonian induces forward and backward transitions between consecutive time-steps, i.e., $|\phi_t\rangle\,|t\rangle \longleftrightarrow |\phi_{t+1}\rangle\,|t+1\rangle$. In addition, the Hamiltonian serves to ensure that no illegal (i.e., not corresponding to an encoding of the time-step) states occur in the clock register, that the input to the circuit is correct, and that the computation ultimately accepts.

Second, the encoding of a computation in the ground state of a nearest-neighbor 1D Hamiltonian is based on the construction of [9]. The n computational qubits are encoded in subspaces of n of the qudits (of which there are polynomially many) on the line. The line is divided into blocks, and in each block a set of nearest-neighbor gates is performed on the encoded qubits before the qubits are transferred to the next block where the next set of gates can be performed. The gate applications and the qubit transfers occur via two-local (nearest-neighbor) operations. The construction in [9] uses a 2-dimensional "gate" subspace of the qudits to mark the position along the line where a gate is being performed. The qudits storing the qubits on which gates have already been performed are indicated by a two-dimensional space $\boxed{L}$, and the ones on which a gate is yet to be performed are labeled $\boxed{R}$. There are also one-dimensional states $\circlearrowright$ and $\circlearrowleft$: the former marks the transition between the gate-performing steps and the qubit-transferring steps of the computation, and the latter shifts the qubits to the right. A two-dimensional state $\boxed{\triangleright}$ serves to move the active spot back to the right after $\circlearrowleft$ has moved the qubits over one site.

Third, our main contribution is reducing the dimensionality of the qudits to 8. This "leaner" qudit construction comes at a price – allowing the forward/backward transitions in our Hamiltonian to be non-unique, possibly resulting in "illegal" configurations of the qudit chain. However, we can work around this problem and suppress those by adding penalty terms. Raising the energy of states away from the allowed subspace allows us to use the projection lemma from [7], showing that even despite the illegal transitions, the ground state must have a substantial overlap with the legal subspace. Restricted to that subspace, the illegal transitions in the Hamiltonian do not contribute to the expectation value of the energy for a correct history state. Therefore, the history state of a computation that accepts with high probability can be close to the ground state of the entire Hamiltonian, and results in a low ground-state energy. Of course, we also need to show a lower bound on the ground state energy for Hamiltonians corresponding to quantum circuits without easily-accepted witnesses.

In more detail, our dimension reduction comes from getting rid of the distinction between the two two-dimensional qudit states – the $\boxed{L}$ (done: qubits in a block that have already

[d] The subscript x in the verifier circuit V_x stands for the instance x of the problem.

participated in gate applications) and $\boxed{R}$ (ready: qubits that are yet to have a gate applied to them) qubit types – using instead just one type of qubit $\square$ combined with a 1-dimensional state $\circledcirc$, using parity of the qubit position to distinguish between "done"/"ready". We use the mapping $\boxed{L} \to |\circledcirc\square|$ and $\boxed{R} \to |\square\circledcirc|$, doubling the number of particles on the line. Furthermore, we get rid of the $\boxed{\triangleright}$ qubit type – we instead use the boundary between "done" and "ready" sequences of qubits as the active spot. We also will not need the $\textcircled{\textcircled{}}$ state (used in [9]) anymore.

2 Background

Let us begin by a general definition of the Local Hamiltonian problem:

Definition 1 (The d-state k-Local Hamiltonian Problem) *We are given a Hamiltonian $H = H_1 + H_2 + \ldots + H_s$ on n d-state qudits, with the matrix elements of each H_i specified by poly(n) bits. H is k-local: each H_i acts nontrivially on only k of the n qudits. We are also given two constants $a, b \in \mathbb{R}$ such that $b - a \geq 1/poly(n)$, with the promise that the smallest eigenvalue of H, $\lambda(H)$, is either at most a or greater than b. We must decide if $\lambda(H) \leq a$ or $\lambda(H) > b$.*

As mentioned in the Introduction and shown by Kitaev [2], this problem lies in (and is complete for) the class QMA.

Definition 2 (QMA) *A language L is in the class QMA iff for each instance x there exists a uniform polynomial-size quantum circuit V_x such that*

- *if $x \in L$, $\exists|\xi\rangle$, a polynomial-size quantum state (a witness) such that* $\Pr(accept(V_x, |\xi\rangle)) \geq 2/3$,
- *if $x \notin L$, $\forall|\xi\rangle$* $\Pr(accept(V_x, |\xi\rangle)) \leq 1/3$.

Previous proofs for QMA-completeness rely on a special state encoding a computation (a history state) for showing QMA-hardness of Local Hamiltonian. A circuit is transformed into an appropriate Hamiltonian such that a history state is a zero-eigenvector when there is a witness to make the circuit accept.

Definition 3 (History state) *Let $V = U_K \cdots U_2 U_1$ be a circuit of K gates on n qubits. Consider a Hilbert space with $K+1$ orthogonal subspaces $\{S_t\}_{t=0}^{K}$, each with basis $\{|j_t\rangle\}_{j=0}^{2^n-1}$ of dimension 2^n. We define the* history state *corresponding to the action of V on an initial n-qubit state $|\varphi\rangle$ as a superposition over states coming from orthogonal spaces:*

$$|\eta^{\varphi}\rangle = \frac{1}{\sqrt{K+1}} \sum_{t=0}^{K} |\gamma_t^{\varphi}\rangle \tag{1}$$

where $|\gamma_t^{\varphi}\rangle = \sum_{j=0}^{2^n-1} |j_t\rangle \langle j| U_t \cdots U_2 U_1 |\varphi\rangle$ is a vector in the subspace S_t.

Note that the Hilbert space as a whole can be bigger than the union of S_t's, and we can write it as an orthogonal direct sum of subspaces $\left(\bigoplus_{i=0}^{K} S_t\right) \oplus \mathcal{H}_{rest}$, with the rest of the Hilbert space denoted $\mathcal{H}_{rest}$.

A propagation Hamiltonian can be defined to ensure that a low-energy candidate state has the form (1), when the state evolution satisfies a certain orthogonality condition. Note that

for any initial n-qubit state $|\varphi\rangle$ and any $t \in \{0, \ldots, K\}$, we have $|\gamma_t^\varphi\rangle \in S_t$. The *propagation Hamiltonian* associated with the circuit V is $H_{\text{prop}} := \sum_{t=0}^{K-1} H_t$ where

$$H_t := \sum_{j=0}^{2^n-1} \left(|j_t\rangle\langle j_t| + |j_{t+1}\rangle\langle j_{t+1}| - U'_{t+1}|j_{t+1}\rangle\langle j_t| - |j_t\rangle\langle j_{t+1}| {U'_{t+1}}^\dagger \right), \tag{2}$$

with $U'_{t+1} = \sum_{k,j=0}^{2^n-1} |k_{t+1}\rangle\langle k| U_{t+1} |j\rangle\langle j_{t+1}|$ acting as the unitary U_{t+1} on the subspace S_{t+1}.

Observe that the action of H_t on $|\gamma_t^\varphi\rangle$ and $|\gamma_{t+1}^\varphi\rangle$ is (not summing over t)

$$\begin{aligned} H_t |\gamma_t^\varphi\rangle &= |\gamma_t^\varphi\rangle - \left|\gamma_{t+1}^\varphi\right\rangle, \\ H_t |\gamma_{t+1}^\varphi\rangle &= |\gamma_{t+1}^\varphi\rangle - |\gamma_t^\varphi\rangle, \end{aligned} \tag{3}$$

since $\left|\gamma_{t+1}^\varphi\right\rangle = U'_{t+1} \sum_{j=0}^{2^n-1} |j_{t+1}\rangle\langle j_t|\gamma_t^\varphi\rangle$. It is then straightforward to verify that $|\gamma_t^\varphi\rangle + \left|\gamma_{t+1}^\varphi\right\rangle$ is a zero-energy eigenvector of H_t. A history state is then also a zero eigenvector of each H_t, and so a zero eigenvector of H_{prop}. The propagation Hamiltonian thus serves to "check" the progress of the computation, by giving an energy penalty to all non-history states. For a specific construction of a QMA-complete k-Local Hamiltonian problem, it will have to be shown that H_{prop} can be built from operators that obey the chosen locality restrictions.

Let V_x be a verifying circuit for an instance $x \overset{?}{\in} L \in QMA$, taking as input $n - m$ ancilla qubits in the state $|0\rangle$ and an m-qubit state $|\xi\rangle$, and it has squared amplitude $2/3$ on some designated output qubit if $x \in L$, and less than $1/3$ otherwise. Kitaev's proof used a history state of the following form. The unitaries U_i are the ones from the original verifier circuit $V_x = U_K \ldots U_1$ and are 2-local. An extra unary clock register is used to build the structure of orthogonal subspaces S_t, requiring a 2-local clock checking Hamiltonian H_{clock} in the Hamiltonian for distinguishing the subspaces S_t from $\mathcal{H}_{rest}$ spanned by states with illegal clock configurations. The history state for verifying a valid witness $|\xi\rangle$ using V_x is

$$|\eta\rangle = \frac{1}{\sqrt{K+1}} \sum_{t=0}^{K} \left(U_t \ldots U_1 \left(|0\rangle^{n-m} \otimes |\xi\rangle \right) \right) \otimes |t\rangle_{\text{clock}}.$$

This history-state structure for low-energy state candidates is enforced by H_{prop} imposing energy penalties for deviating from the indicated form. With the unary clock construction, the required locality of the terms in H_{prop} is 5. In addition, Kitaev adds two more Hamiltonian terms: H_{in} penalizing states with improperly initialized ancillae (not of the form $|\gamma_0\rangle = |0\rangle^{n-m} \otimes |\xi\rangle$), and H_{out} verifying whether the computation accepts. This turns out to be enough to ensure that $x \notin L$ instances of the 5-Local Hamiltonian have no low-energy eigenvector.

3 Encoding a computation in a sequence of orthogonal states of a line of 8-dimensional qudits.

Our goal is to encode a quantum verifier circuit V_x into a 2-Local Hamiltonian instance with nearest-neighbor interactions on a line of qudits, satisfying certain properties. In this section we do the first step, transforming V_x into a modified circuit $\tilde{V}_x$ that does the same computation as V_x, but instead of on n qubits, it acts on a line of $poly(n)$ qudits of dimension $d = 8$. All gates in $\tilde{V}_x$ are nearest-neighbor on this line, and the states occurring during the

computation are pairwise orthogonal. This is the condition given in Section 2. Finding the circuit $\tilde{V}_x$ with these properties allows us to define a Hamiltonian such that, in the case that there exists a witness on which the circuit $\tilde{V}_x$ accepts with high probability, the history state of the computation on the witness is a low-energy state of the Hamiltonian. Otherwise, we will be able to lower bound the ground state energy of this Hamiltonian.

Assume V_x works on a space of n qubits. Choose a way to arrange the qubits on a line. The original circuit can be transformed to a circuit V'_x consisting of R rounds of gates, where each round is composed of $n-1$ nearest-neighbor gates: the first gate in a round acts on qubits 1 and 2, the second on qubits 2 and 3, and so on. Any quantum circuit can be recast in this fashion, by inserting swap gates and identity gates, with a polynomial blowup increase in the number of gates.

We now convert the circuit V'_x to a circuit $\tilde{V}_x$ acting on a line of 8-state qudits arranged in R blocks of $2n$ particles each. The qudits are 8-dimensional, and we will utilize some of the 8 states as data-carriers (holding qubits the computation acts on). The rest will guarantee the orthogonality conditions and the proper progress of the computation. At any time during the computation, we want exactly n of the qudits to be in the "data-holding" states, and we simply call them qubits. Initially, all of the n qubits are located in the first block of particles. After each round of gates from V'_x is carried out, the qubits are transferred to the next block of $2n$ particles where the next set of gates from V'_x can be performed.

Claim 1 *Given a QMA verifier circuit V_x on n qubits, an equivalent QMA verifier circuit $\tilde{V}_x$ can be efficiently computed such that $\tilde{V}_x$ operates on $2nR$ 8-state qudits on a line, only uses nearest neighbor gates, and such that the states occurring during the computation are pairwise orthogonal.*

In the rest of this Section we describe the sequence of orthogonal states that appear in the computation on the qudit line. Later, in Section 4 we present the positive semidefinite 2-local Hamiltonian whose ground state is the uniform superposition over states from this desired sequence.

Let us choose the Hilbert space of each particle as an orthogonal direct sum: $\mathcal{H}_8 = \circledcirc \oplus \circleddash \oplus \bigcirc \oplus \otimes \oplus \square \oplus \blacktriangleright$. The subspaces denoted $\circledcirc, \circleddash, \bigcirc$, and $\otimes$ are 1-dimensional. Then we have 2-dimensional subspaces $\square$ and $\blacktriangleright$, each designed to hold a state of a qubit (specified by two complex numbers a_0 and a_1, with a_0, $a_1 \in \mathbb{C}$ and $|a_0|^2 + |a_1|^2 = 1$). We label the basis vectors of these 2-dimensional subspaces $|\square^{(s)}\rangle$ and $|\blacktriangleright^{(s)}\rangle$ with $s = 0, 1$. A qudit in the state $\sum_{s=0}^{1} a_s |\square^{(s)}\rangle$ or $\sum_{s=0}^{1} a_s |\blacktriangleright^{(s)}\rangle$ is then said to have the *qubit content* $a_0 |0\rangle + a_1 |1\rangle$.

When we label a qudit by one of the symbols $\{\circledcirc, \circleddash, \bigcirc, \otimes, \square, \blacktriangleright\}$, we mean that its state belongs to a particular subspace of $\mathcal{H}_8$. Such labeling of the whole chain defines a *configuration*. The Hilbert space of the qudit chain thus decomposes into orthogonal subspaces indexed by configurations. We can choose a basis for the Hilbert space of the entire system as a tensor product of $2nR$ (one for each site) of the basis vectors $\left\{|\circledcirc\rangle, |\circleddash\rangle, |\bigcirc\rangle, |\otimes\rangle, |\square^{(0)}\rangle, |\square^{(1)}\rangle, |\blacktriangleright^{(0)}\rangle, |\blacktriangleright^{(1)}\rangle\right\}$. The *state* of the system is a vector in the span of the basis vectors.

Let us now construct a sequence of configurations, corresponding to the progression of a computation with the circuit $\tilde{V}_x$. We view the qudit chain as R blocks of length $2n$ and mark their boundaries $\|$. To highlight the parity of the sites, we also draw $|$ after every even, non-boundary site.

In the initial configuration, the first block holds qubits at odd-numbered sites, interspersed with ◎s. The rest of the chain consists of ◯s:

$$\underbrace{\|\blacktriangleright\,◎\,|\square\,◎\,|\cdots|\square\,◎\,|\square\,◯}_{\text{the first block of length } 2n}\|◯\,◯\,|◯\,◯\,|\cdots \tag{4}$$

The qubit content of the $\blacktriangleright$ and $\square$ sites carries the initial n-qubit input to the circuit V'_x (the ancillae and the witness). Each step of the computation is a 2-local unitary operation applied to two adjacent particles, resulting in a change of configuration (building up an orthogonal sequence), and possibly a change in the state of the qubit content (doing the computation). Let us now write the rules for building up the circuit $\tilde{V}_x$.

We choose a list of transition rules (for configurations) and list them in Table 1. Each rule connects configurations that differ in two particular neighboring spots, and are connected by a 2-local unitary transformation. The sequence of these transformations (as applied sequentially to the initial configuration) defines the 2-local gates of the circuit $\tilde{V}_x$. This assignment of unitaries is unique by construction, as we choose the transition rules so that for any configuration arising from the initial one, there is always exactly one rule that possibly applies to it (see also Table 2 for a part of the sequence of configurations for $n = 3$). We ensure this uniqueness by rules involving up to 4 particles in the rules. However, in Section 4 we will write a Hamiltonian made from 2-local terms that checks[e] these transitions.

Let us explain the logic behind the rules. Rule 1 applies the unitary from the modified, nearest-neighbor circuit V'_x. The rest of the rules ensure the orthogonalization and locality properties. Initially, the qubits are placed at the odd sites, separated by ◎s. If we want them to interact, we have to move them together, which is what rules 2 and 3 do. The nearest-neighbor gates from V'_x are then performed at the $\blacktriangleright\square$ junctions using rule 1. The ◯ label marks sites that the computation hasn't reached yet, while the ⊗ sites will not be used again. The ⟵ (a pusher state) serves to move the qubits to the right.

The computation can be divided into R "rounds", each corresponding to the application of a "round" of gates from V'_x, and then moving the qubit block $2n$ positions to the right. Let us look at the two phases of a round of computation in detail, referring to Table 2 (a $n = 3$ qubit example).

The goal of the first phase of the computation is gate application. It involves rules 2 and 1, moving the $\blacktriangleright$ qubit from the left end of the chain while applying the gates from a given "round". When $\blacktriangleright$ reaches the front end of the chain, rule 4 creates a the "pusher" state ⟵. After $2n-1$ applications of rule 5, the pusher gets to the left end of the qubit sequence, where it disappears through rule 6. This first phase thus moves $\blacktriangleright$ n times, makes $n-1$ gate applications, adds 1 pusher creation, $2n-1$ pushes and 1 killing of ⟵, altogether making $4n$ steps.

[e] To "check" a transition means adding an energy penalty to terms that do not have the same amplitude for both of the states involved in the transition.

1. $\blacktriangleright|\square \longleftrightarrow U_m(\square|\blacktriangleright)$ performs a two-qubit gate U_m (location-dependent) on the qubit content of the two particles, while shifting the active site to the right.
2. (a) $|\blacktriangleright\circledcirc| \longleftrightarrow |\circledcirc\blacktriangleright|$ moves an "active" qubit $\blacktriangleright$ to the right (not near a block boundary),
   (b) $\|\blacktriangleright\circledcirc| \longleftrightarrow \|\otimes\blacktriangleright|$ is applicable when a block boundary is to the left of it,
   (c) $|\blacktriangleright\bigcirc\| \longleftrightarrow |\circledcirc\blacktriangleright\|$ is applicable when a block boundary is in front of it.
3. (a) $\otimes|\square\circledcirc\,\vdots\square \longleftrightarrow \otimes|\otimes\square\,\vdots\square$ moves the leftmost qubit (not after a boundary),
   (b) $\square\,\vdots\square\circledcirc\,\vdots\square \longleftrightarrow \square\,\vdots\circledcirc\,\square\,\vdots\square$ moves a qubit $\square$ to the right, only noting correct parity, regardless of the boundary location. We denote this using the symbol $\vdots$.
   (c) $\square\,\vdots\square\bigcirc|\bigcirc \longleftrightarrow \square\,\vdots\circledcirc\,\square|\bigcirc$ moves the rightmost qubit (not before a boundary).
   (d) $\otimes\,\vdots\square\bigcirc\,\vdots\bigcirc \longleftrightarrow \otimes\,\vdots\otimes\,\square\,\vdots\bigcirc$ a special rule ensuring that if there is a *single* qubit in the chain, it can still move. Rule 3(d) does not actually apply to any legal configuration.
4. (a) $\blacktriangleright\|\bigcirc\bigcirc \longleftrightarrow \square\|\ominus\bigcirc$ creates a left-moving pusher $\ominus$ at the front near a boundary $\|$.
   (b) $\square|\bigcirc\bigcirc \longleftrightarrow \square|\ominus\bigcirc$ introduces $\ominus$ when away from a block boundary.
5. (a) $\square\,\vdots\ominus \longleftrightarrow \ominus\,\vdots\square$ pushes $\ominus$ left and a qubit to the right (not caring for the boundary).
   (b) $\vdots\circledcirc\ominus\,\vdots \longleftrightarrow \vdots\ominus\circledcirc\,\vdots$ does the same with $\ominus$ and $\circledcirc$, at locations with this parity.
6. (a) $\otimes\ominus\|\square \longleftrightarrow \otimes\otimes\|\blacktriangleright$ kills the pusher $\ominus$ at the left end of the qubits at a boundary $\|$, changing the last qubit to $\blacktriangleright$, allowing the next round of gate applications to begin.
   (b) $\otimes\ominus|\square \longleftrightarrow \otimes\otimes|\square$ simply kills the pusher, when away from the boundary. $\ominus$.

Table 1. The transition rules, which together with a carefully chosen initial state (4) define the 2-local gates of the circuit $\tilde{V}_x$. Note that some of these rules are 2-local, some 3-local and some even 4-local, which helps them identify their intended locations uniquely. However, the transformations themselves are only 2-local. See also Table 2 for an example of a progression of configurations and the unique applicability of these rules. We will later write a Hamiltonian H_{prop} with only 2-local terms checking these transitions.

The second phase (which is repeated $n-1$ times) moves the qubits to the right until they are all within the next block. It takes n applications of rule 3 to move all the qubits one step to the right. Then we create the pusher $\ominus$, move it to the left ($2n-1$ steps) and kill it. Altogether, this takes $3n+1$ steps. If we now are not at the boundary, the second phase repeats. If we are at a block boundary $\|$, the second phase concludes, and the "round" of computation concludes as well, as all the qubits have now moved $2n$ positions to the right. A new "round" of computation (with the particle $\blacktriangleright$ starting to move) starts according to rule 2. Summing it up, a whole "round" of computation consists of $4n+(n-1)(3n+1) = 3n^2+2n-1$ steps. During each "round", $n-1$ gates from V'_x are applied and the qubits are moved over to the next block of qudits. This happens for each of the first $R-1$ blocks. In the last block, after the gates are applied, the computation comes to a halt in the state: $\|\otimes^{2n(R-1)}\|\otimes\square|\circledcirc\square|\cdots|\circledcirc\square|\circledcirc\blacktriangleright\|$. Also, without loss of generality, we take all the gates in the very first round to be identities. This allows us to verify that the ancilla qubits (laid out on the left of the qubit sequence) all start out in the correct state $|0\rangle$.

The entire computation with $(R-1)$ regular rounds and a last round with $2n$ steps (until $\blacktriangleright$ reaches the right end) together take $K=(R-1)(3n^2+2n-1)+2n$ steps, corresponding to $K+1$ configurations of the qudits. Also note that a configuration is never repeated in the course of the computation – all of the $K+1$ configurations are distinct, and therefore orthogonal.

3.1 Legal configurations

At the moment, we are interested only in the (legal) configurations that we want to appear during a computation. Of course, the whole Hilbert space is much larger, containing many other states. We will call those illegal, and want them to be "detectable". For now, we will not deal with these other states until Section 4.1.

Let the set of *legal* configurations $C_0,\ldots,C_K$ be the $K+1$ configurations that can be obtained by applying the rules in Table 1 starting with the initial configuration (4). The legal configurations correspond to the $K+1$ (including the initial state) intermediate computational states generated by the circuit $\tilde{V}_x$. We call all other configurations *illegal*.

We will now look at the properties shared by the legal configurations. It will be convenient to look at pairs of particles at locations $(2i-1,2i)$ and $(2i+1,2i+2)$. Table 3 lists the allowed pairs of symbols and which ones can be adjacent to each other. The pairs play the roles of "dead" (labeled x, particles not to be used anymore), "done" (labeled D, qubits to the left of the active site), "active" (labeled A, the active site), "ready" (labeled R, qubits to the right of the active site) and "unborn" (labeled u, "unborn" particles, not used yet) from the construction in [9]. There, the legal states were of the form (x$\cdots$x) (D$\cdots$D) A (R$\cdots$R) (u$\cdots$u), with a single active site. Here (z$\cdots$z) stands for a variable-length string made from the letter "z".

Connecting subsequent pairs according to the rules listed in Table 3 imposes a particular form for the legal states (brackets indicate variable-length, possibly empty substrings)

$$(\mathrm{x}\cdots\mathrm{x})[qubits](\mathrm{u}\cdots\mathrm{u}) \tag{5}$$

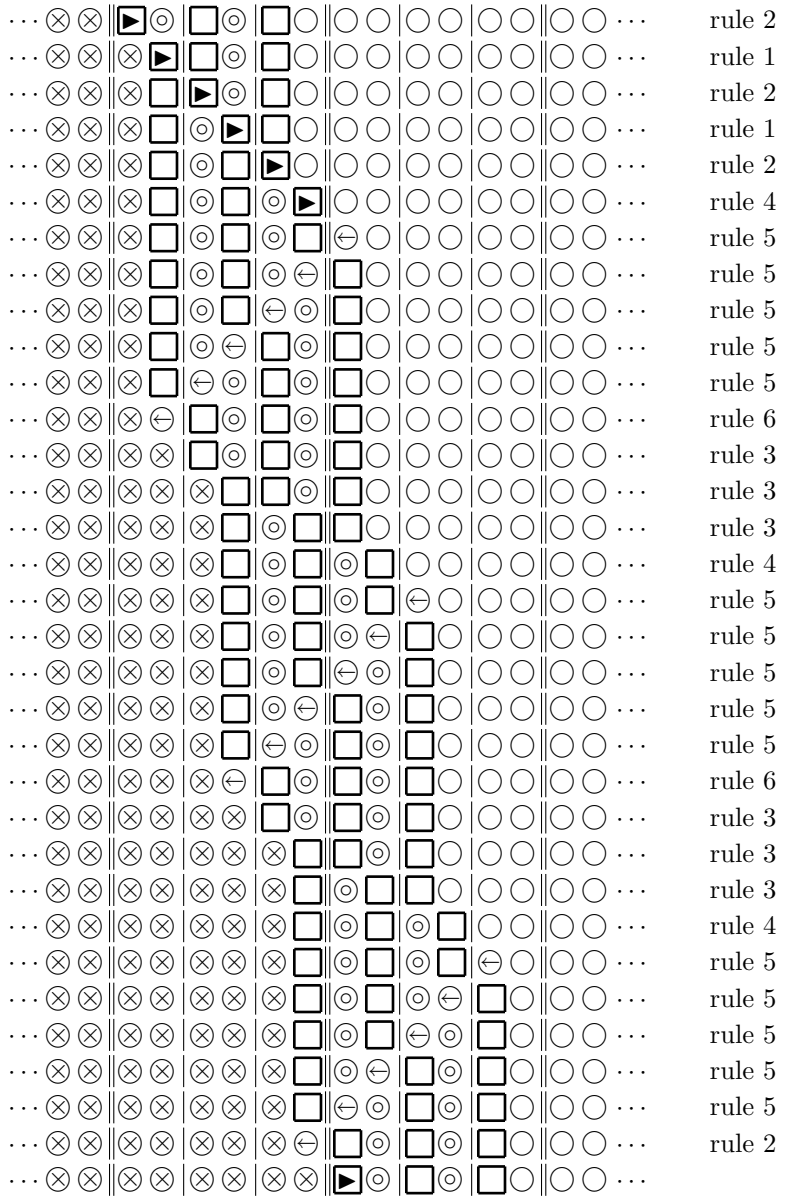


Table 2. The configurations occurring in one cycle of the computation with $n = 3$ qubits. The rules whose application brings the state to the next one are listed on the right.

where [*qubits*] is a *nonzero* string of the form

$$\mathrm{A}_x(\mathrm{R}\cdots\mathrm{R})\ \mathrm{R}_u \tag{6}$$
$$(\mathrm{D}_x\mathrm{D}\cdots\mathrm{D})\mathrm{A}_1(\mathrm{R}\cdots\mathrm{R})\ \mathrm{R}_u \tag{7}$$
$$\mathrm{D}_x\ (\mathrm{D}\cdots\mathrm{D})\mathrm{A}_p(\mathrm{R}\cdots\mathrm{R})\ \mathrm{R}_u \tag{8}$$
$$\mathrm{D}_x\ (\mathrm{D}\cdots\mathrm{D})\mathrm{A}_2(\mathrm{R}\cdots\mathrm{R}\mathrm{R}_u) \tag{9}$$
$$\mathrm{D}_x\ (\mathrm{D}\cdots\mathrm{D})\mathrm{A}_u \tag{10}$$
$$(\mathrm{R}\cdots\mathrm{R})\ \mathrm{R}_u \tag{11}$$
$$\mathrm{D}_x\ (\mathrm{D}\cdots\mathrm{D})\quad(\mathrm{R}\cdots\mathrm{R})\ \mathrm{R}_u \tag{12}$$
$$\mathrm{D}_x\ (\mathrm{D}\cdots\mathrm{D}). \tag{13}$$

The first five options involve an "active" pair, while the last three have no "active" pair in them. Furthermore, note that the whole [*qubits*] string cannot be empty, because the rightmost particle of the whole chain cannot be ⊗, the leftmost one cannot be ◯ and the combination ⊗◯ is illegal. Next, for legal configurations, the number of particles holding qubits needs to be exactly n.

Let us have a closer look at the legal [*qubits*] strings with an active site (▶ or ⟜), which translates to a single active pair (A_x, A_1, A_p, A_2 or A_u). One example is ‖⊗□|▶◎|□◯‖ (which is of the type $\mathrm{D}_x\mathrm{A}_1\mathrm{R}_u$). In the case there is no D_x pair, the active pair has to be $\mathrm{A}_x(6)$ or $\mathrm{A}_1(7)$ – an example is the sequence ‖⊗▶|□◎|□◯‖ (with pairs $\mathrm{A}_x\mathrm{RR}_u$). In the case there is no R_u pair, the active pair has to be of the A_2 or A_u, as in e.g. ‖⊗□|◎□|◎□‖⟜◯| (this is $\mathrm{D}_x\mathrm{DDA}_u$).

The other three types of legal substrings [*qubits*] do not have an active pair. First, we could have a done qubit pair on the right end as in |⊗□‖◎□|◎□| (simply $\mathrm{D}_x\mathrm{DD}$ without any R's). Second, observe that two neighboring □ particles can appear at positions $(2i, 2i+1)$, when coming from two consecutive pairs as in |⊗□|◎□‖□◯| (read as $\mathrm{D}_x\mathrm{DR}_u$). Finally, it is possible to have a ready qubit pair on the left end as in |□◎‖□◎|□◯| (simply RRR_u without any D's).

The location of the [*qubits*] substring matters. For a legal configuration with a ▶ symbol, the string [*qubits*] must fit exactly between two block boundaries as ‖[*qubits*]‖ (see Table 2). On the other hand, the string [*qubits*] without the symbol ▶ always has runs across a block boundary somewhere. These two properties later help us check that we do not have too few or too many qubits or whether the qubits are properly aligned between the boundaries, ruling out illegal but locally undetectable states.

4 The Hamiltonian

We aim to construct a Hamiltonian corresponding to a circuit $\tilde{V}_x$ such that the ground state energy of the Hamiltonian is $E \le a$ for 'yes' instances ($x \in L$) and $E \ge b$ for the 'no' instances, where a and b have a $1/poly(n)$ separation. We will show the history state of the computation on the witnesses for 'yes' instances has a low energy. Our Hamiltonian is a sum of four terms:

$$H := J_{\mathrm{in}}H_{\mathrm{in}} + J_{\mathrm{prop}}H_{\mathrm{prop}} + J_{\mathrm{pen}}H_{\mathrm{pen}} + H_{\mathrm{out}}.$$

The coefficients J_{in}, J_{prop}, and J_{pen} will later be chosen to be some polynomials in n. For the term H_{prop}, any valid history state (a uniform superposition of legal configurations whose

		allowed to be followed by										
property	*symbol pair*	x	D_x	D	A_x	A_1	A_p	A_2	A_u	R	R_u	u
dead: x	⊗⊗	✓	✓		✓	✓				✓	✓	
dead+done: D_x	⊗□			✓		✓	✓	✓	✓	✓	✓	✓
done: D	◎□			✓		✓	✓	✓	✓	✓	✓	✓
active leftmost: A_x	⊗▶, ⊗⟵									✓	✓	
active gate 1: A_1	▶◎									✓	✓	
active pusher: A_p	◎⟵, ⟵◎									✓	✓	
active gate 2: A_2	◎▶									✓	✓	✓
active rightmost: A_u	▶○, ⟵○											✓
ready: R	□◎									✓	✓	
ready+unborn: R_u	□○											✓
unborn: u	○○											✓

Table 3. Building up the legal configuration structure from pairs of symbols (unlisted symbol pairs do not appear in legal configurations). We list symbol pairs allowed at positions $(2i-1, 2i)$ and their designated followups at positions $(2i+1, 2i+2)$. Note the mirror symmetry of the table across the antidiagonal. The allowed configurations of the whole chain must then have form $(\mathrm{x}\cdots\mathrm{x})[qubits](\mathrm{u}\cdots\mathrm{u})$, with a substring $[qubits]$ given by (6)-(13), with at most one active pair. Further restrictions come into play from considering the block boundary locations (see Table 5) the number of "qubits" and their proper alignment with respect to the block boundaries.

qubit content comes corresponds to the computation with the gates from $\tilde{V}_x$) will be a zero-energy state. The term H_{in} raises the energy of states which do not have ancilla qubits initialized to 0, which is required in the circuit $\tilde{V}_x$. The role of H_{out} is to raise the energy of the states which encode computations that are not accepted. Finally, the terms in H_{pen} penalize (i.e. raise the energy of) locally detectable illegal configurations which do not have the proper form as described by equations (5)-(13) in Section 3.1.

We start with the ancilla-checking term H_{in}, defined as

$$H_{\mathrm{in}} := |▶^{(1)}\rangle\langle▶^{(1)}|_1 + \sum_{i=2}^{n-m} |□^{(1)}\rangle\langle□^{(1)}|_{2i-1}.$$

By raising the energy of states with qubit content $|1\rangle$, it ensures that in a low-energy state candidate the ancilla qubits (the first $n-m$) are all initially (in the initial configuration (4) they are located at odd positions in the first block) in the $|0\rangle$ state. Without loss of generality, we assume that the first round of V'_x consists of identity gates. This is necessary when we want the ancilla qubits to remain unpenalized by H_{in} until they are moved from the first block into the second block.

The term $H_{\mathrm{out}} := |▶^{(0)}\rangle\langle▶^{(0)}|_{2nR}$ checks that when the computation finishes (the ▶ state appears at the very right end of the qudit chain), the qubit content of the output qubit is $|1\rangle$. For computations that do not accept, the output qubit state is $|0\rangle$ and H_{out} penalizes this.

In defining the remaining terms of the Hamiltonian, we will need to be able to distinguish between different kinds of configurations of the chain. We classify three types:

1. *legal* configurations are defined in Section 3.1 to be the configurations $C_0, \ldots, C_K$ occur-

1. $\otimes \| \blacktriangleright\!\!\square \circledcirc \,|\, (\square \circledcirc)^{n-2} \,|\, \square\bigcirc \,\|\, (\bigcirc\bigcirc)^{n} \,\|\, \bigcirc$ (2b)
2. $\otimes \| \otimes \blacktriangleright\!\!\square \,|\, (\square \circledcirc)^{n-2} \,|\, \square\bigcirc \,\|\, (\bigcirc\bigcirc)^{n} \,\|\, \bigcirc$ (1)
3. For i from 0 to $n-3$:
   (a) $\otimes \| \otimes \square \,|\, (\circledcirc \square)^{i} \,|\, \blacktriangleright\!\!\square \circledcirc \,|\, (\square \circledcirc)^{n-i-3} \,|\, \square\bigcirc \,\|\, (\bigcirc\bigcirc)^{n} \,\|\, \bigcirc$ (2a)
   (b) $\otimes \| \otimes \square \,|\, (\circledcirc \square)^{i} \,|\, \circledcirc \blacktriangleright\!\!\square \,|\, (\square \circledcirc)^{n-i-3} \,|\, \square\bigcirc \,\|\, (\bigcirc\bigcirc)^{n} \,\|\, \bigcirc$ (1)
4. $\otimes \| \otimes \square \,|\, (\circledcirc \square)^{n-2} \,|\, \blacktriangleright\!\!\square\bigcirc \,\|\, (\bigcirc\bigcirc)^{n} \,\|\, \bigcirc$ (2c)
5. $\otimes \| \otimes \square \,|\, (\circledcirc \square)^{n-2} \,|\, \circledcirc \blacktriangleright\!\!\square \,\|\, (\bigcirc\bigcirc)^{n} \,\|\, \bigcirc$ (4a)
6. $\otimes \| \otimes \square \,|\, (\circledcirc \square)^{n-1} \,\|\, \circlearrowleft\!\!\bigcirc \,|\, (\bigcirc\bigcirc)^{n-1} \,\|\, \bigcirc$ (5a)
7. For j from 0 to $n-2$:
   (a) For k from 0 to $n-2$:
      i. $\otimes \| (\otimes\otimes)^{j} \,|\, \otimes \square \,|\, (\circledcirc \square)^{n-k-2} \,|\, \circledcirc \circlearrowleft \,|\, (\square \circledcirc)^{k} \,|\, \square\bigcirc \,|\, (\bigcirc\bigcirc)^{n-j-1} \,\|\, \bigcirc$ (5b)
      ii. $\otimes \| (\otimes\otimes)^{j} \,|\, \otimes \square \,|\, (\circledcirc \square)^{n-k-2} \,|\, \circlearrowleft \circledcirc \,|\, (\square \circledcirc)^{k} \,|\, \square\bigcirc \,|\, (\bigcirc\bigcirc)^{n-j-1} \,\|\, \bigcirc$ (5a)
   (b) $\otimes \| (\otimes\otimes)^{j} \,|\, \otimes \circlearrowleft \,|\, (\square \circledcirc)^{n-1} \,|\, \square\bigcirc \,|\, (\bigcirc\bigcirc)^{n-j-1} \,\|\, \bigcirc$ (6b)
   (c) $\otimes \| (\otimes\otimes)^{j} \,|\, \otimes \otimes \,|\, (\square \circledcirc)^{n-1} \,|\, \square\bigcirc \,|\, (\bigcirc\bigcirc)^{n-j-1} \,\|\, \bigcirc$ (3a)
   (d) For l from 0 to $n-3$:
   $\otimes \| (\otimes\otimes)^{j+1} \,|\, \otimes \square \,|\, (\circledcirc \square)^{l} \,|\, (\square \circledcirc)^{n-l-2} \,|\, \square\bigcirc \,|\, (\bigcirc\bigcirc)^{n-j-1} \,\|\, \bigcirc$ (3b)
   (e) $\otimes \| (\otimes\otimes)^{j+1} \,|\, \otimes \square \,|\, (\circledcirc \square)^{n-2} \,|\, \square\bigcirc \,|\, (\bigcirc\bigcirc)^{n-j-1} \,\|\, \bigcirc$ (3c)
   (f) $\otimes \| (\otimes\otimes)^{j+1} \,|\, \otimes \square \,|\, (\circledcirc \square)^{n-2} \,|\, \circledcirc \square \,|\, (\bigcirc\bigcirc)^{n-j-1} \,\|\, \bigcirc$ (4b)
   (g) $\otimes \| (\otimes\otimes)^{j+1} \,|\, \otimes \square \,|\, (\circledcirc \square)^{n-2} \,|\, \circledcirc \square \,|\, \circlearrowleft\!\!\bigcirc \,|\, (\bigcirc\bigcirc)^{n-j-2} \,\|\, \bigcirc$ (5a)
8. For i from 0 to $n-2$:
   (a) $\otimes \| (\otimes\otimes)^{n-1} \,|\, \otimes \square \,|\, (\circledcirc \square)^{n-i-2} \,|\, \circledcirc \circlearrowleft \,|\, (\square \circledcirc)^{i} \,|\, \square\bigcirc \,\|\, \bigcirc$ (5b)
   (b) $\otimes \| (\otimes\otimes)^{n-1} \,|\, \otimes \square \,|\, (\circledcirc \square)^{n-i-2} \,|\, \circlearrowleft \circledcirc \,|\, (\square \circledcirc)^{i} \,|\, \square\bigcirc \,\|\, \bigcirc$ (5a)
9. $\otimes \| (\otimes\otimes)^{n-1} \,|\, \otimes \circlearrowleft \,\|\, (\square \circledcirc)^{n-1} \,|\, \square\bigcirc \,\|\, \bigcirc$ (6a)
10. $\otimes \| (\otimes\otimes)^{n} \,\|\, \blacktriangleright\!\!\square \circledcirc \,|\, (\square \circledcirc)^{n-2} \,|\, \square\bigcirc \,\|\, \bigcirc$

Table 4. The general form of the sequence of legal configurations in one round of computation. The middle block boundary is not shown in steps 7 and 8. The full computation ends at Step 5 without the trailing circles. A particular example for $n = 3$ is shown in Table 2.

ring during the computation with a circuit $\tilde{V}_x$ when starting with the initial configuration (4) with n qubits. All other configurations are *illegal*.

2. *locally detectable illegal* configurations are those that contain a pair of neighboring qudits labeled by a pair of symbols that does not occur in the legal configurations. These can be identified and penalized locally by means of a projector onto such a pair.

3. *locally undetectable illegal* configurations are those that are not detectable by local projections, but are still not legal, as they do not appear in the legal progression of a computation. As shown in Lemma 4.2.4, these states have too many or too few qubits, or an improperly aligned [*qubits*] block.

4.1 The penalty Hamiltonian

The role of H_{pen} is to ensure that there are no locally detectable illegal configurations in the computation. That is, we wish to leave the legal states unpenalized while raising the energy of the locally detectable illegal ones by projecting on neighboring pairs of symbols that do not occur in a proper course of computation described in Section 3. We call such pairs *forbidden*. Since we have 6 different symbols in the construction, there are 36 possible neighboring pairs. Furthermore, we can distinguish 5 types of location pairs depending on the parity of the positions and their position with respect to the block boundaries $\|$ as listed on the right in Table 5. We list the 56 allowed pairs of symbols in Table 5, which gives us $36 \times 5 - 56 = 124$ types of projector terms

$$|XY\rangle\langle XY|_{i,i+1}, \tag{14}$$

where $XY \in \{\otimes, \bigcirc, \circledcirc, \ominus, \square, \blacktriangleright\}^{\otimes 2}$ is a forbidden pair at a location $(i, i{+}1)$. For example, the forbidden pair $\otimes\bigcirc$ (disallowed in all 5 types of locations) is energetically penalized by

$$\sum_{f=1}^{5} H_{\mathrm{pen},f} = \sum_{i=1}^{2nR-1} \mathbb{I}_{1,\ldots,i-1} \otimes |\otimes\bigcirc\rangle\langle\otimes\bigcirc|_{i,i+1} \otimes \mathbb{I}_{i+2,\ldots,2nR}, \tag{15}$$

while the pair $\square\square$ is forbidden on even-parity sites (type A,C,E), and is penalized by

$$\sum_{f=93}^{95} H_{\mathrm{pen},f} = \sum_{i=1}^{nR} \mathbb{I}_{1,\ldots,2i-2} \otimes |\square\square\rangle\langle\square\square|_{2i-1,2i} \otimes \mathbb{I}_{2i+1,\ldots,2nR}. \tag{16}$$

To take the qubit content of the $\square$ particles into account, as in [9] we use the notation $|A\rangle\langle B| := \sum_s |a_s\rangle\langle b_s|$, meaning that subspace B is mapped to subspace A in some prescribed way specified by the pairing of the basis vectors. Thus, $|\square\square\rangle\langle\square\square|$ preserves the qubit contents as $|\square\square\rangle\langle\square\square| := \sum_{s,t=0}^{1} |\square^{(s)}\square^{(t)}\rangle\langle\square^{(s)}\square^{(t)}|$.

Furthermore, to rule out configurations without any qubit-holding particles, we need to penalize the symbols $\{\bigcirc, \square, \ominus, \circledcirc\}$ at the leftmost qudit (only $\otimes$ or $\blacktriangleright$ can appear there) and project onto $\{\otimes, \square, \ominus, \circledcirc\}$ on the rightmost qudit (only $\blacktriangleright$ or $\bigcirc$ are allowed at the right end). Together, the Hamiltonian imposing an energy penalty on configurations containing any of the forbidden pairs is

$$H_{\mathrm{pen}} = \sum_{f=1}^{124} H_{\mathrm{pen},f} + H_{\mathrm{left}} + H_{\mathrm{right}}. \tag{17}$$

X \ Y	⊗	◯	◎	⟵	□	▶
⊗	✓	—	—	ACE	ABCE	CD
◯	—	✓	—	—	—	—
◎	—	—	—	ACE	✓	AE
⟵	—	ACE	ACE	—	BD	—
□	—	ABCE	✓	BD	BD	B
▶	—	DE	AC	—	B	—

A:	$\vert\cdot\ \cdot\vert$	$i = 2(k-1)n + 2j' + 1$
B:	$\cdot\vert\cdot$	$i = 2(k-1)n + 2j$
C:	$\Vert\cdot\ \cdot\vert$	$i = 2(k-1)n + 1$
D:	$\cdot\Vert\cdot$	$i = 2k'n$
E:	$\vert\cdot\ \cdot\Vert$	$i = 2kn - 1$
		$1 \le k \le R$
		$1 \le k' \le R-1$
		$1 \le j \le n-1$
		$1 \le j' \le n-2$

Table 5. The 56 allowed pairs XY of symbols at positions $(i, i+1)$ in the $d = 8$ construction according to H_{pen}. There are 5 types of locations (A, B, C, D, E) for the pair, according to location parity and block-boundary position. For each of the 36 symbol combinations, we list its allowed location types. The forbidden pairs implied by this table are penalized by H_{pen} (17).

Observe that H_{pen} only catches illegal configurations with *locally detectable* errors, and there exist illegal configurations that are not locally detectable, i.e., that have zero energy under H_{pen}, such as this one with too many qubits

$$\Vert\otimes\otimes\vert\square\circledcirc\vert\square\circledcirc\Vert\square\circledcirc\vert\square\bigcirc\vert\bigcirc\bigcirc\Vert. \tag{18}$$

To identify these states as illegal, we will have to show they propagate into states with forbidden pairs. First, though, we want to ensure this propagation, which is the topic of the next section.

4.2 The propagation Hamiltonian

We want to check whether the computation on the line of qudits proceeds correctly, in a linear sequence of configurations $C_0 \leftrightarrow \cdots \leftrightarrow C_t \leftrightarrow C_{t+1} \leftrightarrow C_{t+2} \leftrightarrow \cdots \leftrightarrow C_K$ (see Section 3 and the example in Table 2), ensuring the intended unitary operations are applied in the correct order. The propagation-checking Hamiltonian H_{prop} should have a low energy only for a state which is a superposition of all the legal configurations, with the gates applied to their qubit content as planned.

For now, let us look only at the states from the span of the legal configurations, where we want H_{prop} to give an energy penalty to all states except the history states corresponding to the circuit $\tilde{V}_x$. We would like to construct it as $H_{\text{prop}} = \sum_{t=0}^{K-1} H_t$, where H_t checks the transition from the state $|\psi_t\rangle$ to $|\psi_{t+1}\rangle$. For a candidate low-energy state that has a nonzero overlap with $|\psi_t\rangle$, it should insist that it has to have the *same* amplitude as the state $|\psi_{t+1}\rangle$. Any two legal configurations are orthogonal, so if locality did not matter, it would suffice to use projections onto the states $|\psi_t\rangle$ as in (2) in Section 2. However, we want our Hamiltonian to be 2-local.

The computation of the circuit $\tilde{V}_x$ on an initial state runs according to the rules in Table 1, which are (up to) 4-local. A rule $LNOR \leftrightarrow LPQR$ applied at some location corresponds to a transition between states $|\psi_t\rangle = |\cdots LNOR \cdots\rangle$ and $|\psi_{t+1}\rangle = |\cdots LPQR \cdots\rangle$. In the language of Hamiltonians, this transition is facilitated by

$$\left(\mathbb{I} \otimes \left(|LPQR\rangle\langle LNOR| + |LNOR\rangle\langle LPQR| \right) \otimes \mathbb{I}\right) |\psi_t\rangle = |\psi_{t+1}\rangle$$

To penalize states whose overlap with the states $|\psi_t\rangle$ and $|\psi_{t+1}\rangle$ is not the same, we would use

$$\mathbb{I}\otimes\left(|LNOR\rangle\langle LNOR|+|LPQR\rangle\langle LPQR|\right)\otimes\mathbb{I}$$
$$-\mathbb{I}\otimes\left(|LPQR\rangle\langle LNOR|+|LNOR\rangle\langle LPQR|\right)\otimes\mathbb{I},$$

which within the subspace spanned by $|\psi_t\rangle$ and $|\psi_{t+1}\rangle$ projects[f] onto a state proportional to $|\psi_t\rangle-|\psi_{t+1}\rangle$. The equal superposition of the two states is thus an eigenvector with eigenvalue 0. However, we want to use 2-local, not 4-local operators. If we simply involved only the two particles that actually change ($NO \leftrightarrow PQ$), it would be possible that the resulting terms like $|PQ\rangle\langle NO|$ would apply to several places in a given configuration, leading to a branching of the legal configuration sequence, instead of producing a simple connected line $C_0 \leftrightarrow \cdots \leftrightarrow C_t \leftrightarrow C_{t+1} \leftrightarrow \cdots \leftrightarrow C_K$. This could doom the construction by giving some energy to history states. However, we will now show how to construct H_t from several 2-qudit terms that can "pick out" and "check" the intended transitions between the configurations C_t and C_{t+1}. The trick involves 2-local terms on surrounding qudits as well.

Let us look at a forward application of a rule that changes the qudits $(i, i+1)$, taking them from a sub-configuration $NO_{(i,i+1)}$ to a sub-configuration $PQ_{(i,i+1)}$. We constructed the legal configurations (see Table 4) so that this rule is applicable only to a configuration that is uniquely identifiable by a sub-configuration $XY_{(j,j+1)}$ on some nearby qudits $(j, j+1)$. Similarly, the backwards applicability of this rule is uniquely identifiable by a sub-configuration $ZW_{(k,k+1)}$ on some nearby qudits $(k, k+1)$. We now write a Hamiltonian checking the application of this rule as

$$H^{(\mathrm{rule})}_{\mathrm{prop},i} = |XY\rangle\langle XY|_{j,j+1} + |ZW\rangle\langle ZW|_{k,k+1} - |PQ\rangle\langle NO|_{i,i+1} - |NO\rangle\langle PQ|_{i,i+1}\,. \quad (19)$$

In the simplest case, $XY = NO$, $ZW = PQ$ and $i = j = k$, so that XY, ZW, NO, PQ all involve the same pair of particles $(i, i+1)$. For a more complicated case, let us look at rule 4(b) $\square|\bigcirc\bigcirc \longleftrightarrow \square|\ominus\bigcirc$ from Table 1. The forward applicability of the rule is uniquely identified by the substring $\square|\bigcirc$ on the first two particles, while the backwards applicability of this rule is uniquely identified by the substring $\ominus\bigcirc$ on the second and third particles. The Hamiltonian term checking this rule will be given in (27).

Let us now look at an example from a unary clock construction, to see that history states retain a zero-energy for a Hamiltonian of the type (19).

4.2.1 Analogy with [7]

As an example, we recall [7], where the propagation Hamiltonian was reduced from 3-local to 2-local. There, checking the progress of a unary clock register $|s\rangle = |1\cdots 1_s 0\cdots 0\rangle$ can be done with a 3-local Hamiltonian

$$H_t = \big(|100\rangle\langle 100| + |110\rangle\langle 110| - |110\rangle\langle 100| - |100\rangle\langle 110|\big)_{t,t+1,t+2}, \quad (20)$$

uniquely picking the states $|t\rangle$ and $|t+1\rangle$ for which the transition rule $100 \leftrightarrow 110$ applies. Instead, we can make it out of 2-local (and 1-local) terms

$$H'_t = |10\rangle\langle 10|_{t,t+1} + |10\rangle\langle 10|_{t+1,t+2} - |1\rangle\langle 0|_{t+1} - |0\rangle\langle 1|_{t+1}. \quad (21)$$

[f] Up to a constant, as it equals $2\,|\alpha\rangle\langle\alpha|$ with $|\alpha\rangle = \frac{1}{\sqrt{2}}(|\psi_t\rangle + |\psi_{t+1}\rangle)$.

with the first two terms uniquely identifying the places where the rule should apply, while the last two (transition) terms are ambiguous in their applicability. The price for the decrease in locality are "mistimed" transitions such as $|11\mathbf{1}100\rangle \to |11\mathbf{0}100\rangle$ in the unary clock register. However, observe that the expectation value of this Hamiltonian in the uniform superposition of unary clock states is zero, i.e.

$$\frac{1}{T+1}\sum_{r,s=0}^{T}\langle r|\, H'_t|s\rangle = 0,$$

because the mistimed transitions in H'_t take the state out of the legal subspace, to states orthogonal to any of the proper unary clock states. On the other hand, the transitions taking place at proper places are easily shown to result in 0 energy. Thus, the restriction of H'_i to the legal clock subspace spanned by $\{|0\rangle, |1\rangle, \ldots, |T\rangle\}$ works exactly as the Hamiltonian $H^{\text{unary}}_{\text{prop},i} = |t\rangle\langle t| + |t+1\rangle\langle t+1| - |t+1\rangle\langle t| - |t+1\rangle\langle t|$ from (2). We conclude that a correct history state (a superposition of all legal states) has expectation energy zero under the decreased-locality propagation-checking Hamiltonian (21) from [7].

The projector terms in H'_t thus picked the applicability place uniquely, while the mistimed transitions coming from the last two terms took the state out of the legal subspace (to non-unary clock states). We will now use this insight to construct our H_{prop} from 2-local terms. However, our task is more complicated, because the unary-clock propagation rule $100 \to 110$ for a certain location applied just once in a sequence of proper clock states. In our case, a rule for moving a qubit (or a gate particle) at a given location in the chain could connect configurations $C_t \leftrightarrow C_{t+1}$ as well as some other configurations $C_{t'} \leftrightarrow C_{t'+1}$ with the data in the chain shifted by a few positions.

4.2.2 Explicit form of the propagation-checking terms

Instead of writing the propagation Hamiltonian as a sum of terms H_t, we choose to write it out as a sum of terms $H^{(\text{rule }\rho)}_{\text{prop},i}$ corresponding to different rules ρ applied at location pairs $(i, i+1)_\rho$ wherever rule ρ is applicable. This generalization is required because one rule ρ for a pair of particles can facilitate legal transitions between several configuration pairs. The propagation Hamiltonian is then

$$H_{\text{prop}} = \sum_{\rho=1}^{6}\sum_{(i,i+1)_\rho} H^{(\text{rule }\rho)}_{\text{prop},i}. \tag{22}$$

and we want its application to a state $|\psi_t\rangle$ (corresponding to a legal configuration C_t with $2 \le t \le K$) to result in

$$H_{\text{prop}}\,|\psi_t\rangle = 2\,|\psi_t\rangle - |\psi_{t-1}\rangle - |\psi_{t+1}\rangle + \text{illegal but locally detectable states.} \tag{23}$$

The propagation term corresponding to rule 1 ($\blacktriangleright|\square \longleftrightarrow U_m(\square|\blacktriangleright)$) in Table 1 is simple, as it involves only the sites i and $i+1$ and does not create bad transitions. We want to check the transfer of $\blacktriangleright$ to the right and the application of the gate U_{t_i} (corresponding to the location i) to the qubit content of the two neighboring sites. This is done by

$$H^{(\text{rule }1)}_{\text{prop},i} = \quad |\blacktriangleright\square\rangle\langle\blacktriangleright\square|_{i,i+1} + \quad |\square\blacktriangleright\rangle\langle\square\blacktriangleright|_{i,i+1} \tag{24}$$

$$- U_{t_i}|\square\blacktriangleright\rangle\langle\blacktriangleright\square|_{i,i+1} - U^\dagger_{t_i}|\blacktriangleright\square\rangle\langle\square\blacktriangleright|_{i,i+1}, \tag{25}$$

and this term appears only for locations $(i, i+1)$ of the type B in Table 5.

We continue with rule 2 ($|\blacktriangleright\!\circledcirc| \longleftrightarrow |\circledcirc\!\blacktriangleright|$, $\|\blacktriangleright\!\circledcirc| \longleftrightarrow \|\otimes\!\blacktriangleright|$, $|\blacktriangleright\!\bigcirc\| \longleftrightarrow |\circledcirc\!\blacktriangleright\|$) for moving the $\blacktriangleright$ from position i to $i+1$. Depending on the location in the chain, the Hamiltonian term reads

$$\begin{aligned} H_{\mathrm{prop},i}^{(\text{rule 2})} &= |\blacktriangleright O\rangle\langle\blacktriangleright O|_{i,i+1} + |P\blacktriangleright\rangle\langle P\blacktriangleright|_{i,i+1} \\ &\quad - |P\blacktriangleright\rangle\langle\blacktriangleright O|_{i,i+1} - |\blacktriangleright O\rangle\langle P\blacktriangleright|_{i,i+1}, \end{aligned} \tag{26}$$

with $PO = \circledcirc\circledcirc$ for locations $(i, i+1)$ of type A, $PO = \otimes\circledcirc$ for locations of type C, and $PO = \circledcirc\bigcirc$ for locations of type E.

The propagation terms for rule 4 ($\blacktriangleright\|\bigcirc\bigcirc \longleftrightarrow \square\|\ominus\bigcirc$, $\square|\bigcirc\bigcirc \longleftrightarrow \square|\ominus\bigcirc$) govern the creation of the symbol $\ominus$. We now involve three particles, but again, only two at a time, leaving the Hamiltonian 2-local:

$$\begin{aligned} H_{\mathrm{prop},i}^{(\text{rule 4})} &= |X\bigcirc\rangle\langle X\bigcirc|_{i,i+1} + |\ominus\bigcirc\rangle\langle\ominus\bigcirc|_{i+1,i+2} \\ &\quad - |\square\ominus\rangle\langle X\bigcirc|_{i,i+1} - |X\bigcirc\rangle\langle\square\ominus|_{i,i+1} \end{aligned} \tag{27}$$

with $X = \blacktriangleright$ at locations of the type D and $X = \square$ at locations of the type B. Only the projector term identifying the backwards applicability of rule 4 involves a particle pair different from $(i, i+1)$.

Rule 5 ($\square\|\ominus \longleftrightarrow \ominus\|\square$, $\|\circledcirc\ominus\| \longleftrightarrow \|\ominus\circledcirc\|$) pushes $\ominus$ to the left, and its checking Hamiltonian is again simple:

$$\begin{aligned} H_{\mathrm{prop},i}^{(\text{rule 5})} &= |X\ominus\rangle\langle X\ominus|_{i,i+1} + |\ominus X\rangle\langle\ominus X|_{i,i+1} \\ &\quad - |\ominus X\rangle\langle X\ominus|_{i,i+1} - |X\ominus\rangle\langle\ominus X|_{i,i+1} \end{aligned} \tag{28}$$

with $X = \circledcirc$ at locations of the type ACE and with $X = \square$ at locations of the type BD.

The Hamiltonian for rule 6 ($\otimes\ominus\|\square \longleftrightarrow \otimes\otimes\|\blacktriangleright$, $\otimes\ominus|\square \longleftrightarrow \otimes\otimes|\square$) kills the symbol $\ominus$ and mirrors the ones for rule 4:

$$\begin{aligned} H_{\mathrm{prop},i}^{(\text{rule 6})} &= |\otimes\ominus\rangle\langle\otimes\ominus|_{i-1,i} + |\otimes W\rangle\langle\otimes W|_{i,i+1} \\ &\quad - |\otimes W\rangle\langle\ominus\square|_{i,i+1} - |\ominus\square\rangle\langle\otimes W|_{i,i+1} \end{aligned} \tag{29}$$

with $W = \blacktriangleright$ at locations of the type D and $W = \square$ at locations of the type B.

Rule 3 is the most complicated one since its definition is 4-local. We reduce the locality by looking only at qudit pairs $(i-1, i)$ and $(i+1, i+2)$ to identify the applicability of this rule to states $|\psi_t\rangle$ and $|\psi_{t+1}\rangle$ which can be connected by an application of rule 3. Note that the pair $(i, i+1)$ has to be of the type ACE.

We begin by writing out the propagation terms corresponding to each of the possible transitions in rule 3. Rule 3b ($\square\|\square\circledcirc\|\square \longleftrightarrow \square\|\circledcirc\square\|\square$) applies to pairs $(i, i+1)$ of type A, C, and E:

$$\begin{aligned} H_{\mathrm{prop},i}^{(\text{rule } 3b)} &= |\square\square\rangle\langle\square\square|_{i-1,i} + |\square\square\rangle\langle\square\square|_{i+1,i+2} \\ &\quad - |\circledcirc\square\rangle\langle\square\circledcirc|_{i,i+1} - |\square\circledcirc\rangle\langle\circledcirc\square|_{i,i+1}. \end{aligned} \tag{30}$$

Rule 3a ($\otimes|\square\circledcirc\!\!\!\!\square\square \longleftrightarrow \otimes|\otimes\square\!\!\!\!\square\square$) applies to pairs $(i, i+1)$ of type A and E:

$$H_{\mathrm{prop},i}^{(\text{rule } 3a)} = |\otimes\square\rangle\langle\otimes\square|_{i-1,i} + |\square\square\rangle\langle\square\square|_{i+1,i+2} - |\otimes\square\rangle\langle\square\circledcirc|_{i,i+1} - |\square\circledcirc\rangle\langle\otimes\square|_{i,i+1}. \tag{31}$$

Rule 3c ($\square\!\!\!\!\square\square\bigcirc|\bigcirc \longleftrightarrow \square\!\!\!\!\square\circledcirc\square|\bigcirc$) acts on pairs of type A and C:

$$H_{\mathrm{prop},i}^{(\text{rule } 3c)} = |\square\square\rangle\langle\square\square|_{i-1,i} + |\square\bigcirc\rangle\langle\square\bigcirc|_{i+1,i+2} - |\circledcirc\square\rangle\langle\square\bigcirc|_{i,i+1} - |\square\bigcirc\rangle\langle\circledcirc\square|_{i,i+1}. \tag{32}$$

Finally, rule 3d ($\otimes\!\!\!\!\square\bigcirc\!\!\!\!\bigcirc \longleftrightarrow \otimes\!\!\!\!\otimes\square\!\!\!\!\bigcirc$) handles a special type of illegal configuration that contains only a single qubit-holding particle. In combination with rules 4-6, it helps to move this qubit until it reaches a locally-detectable illegal configuration. For locations $(i, i+1)$ of type A, C and E, we write

$$H_{\mathrm{prop},i}^{(\text{rule } 3d)} = |\otimes\square\rangle\langle\otimes\square|_{i-1,i} + |\square\bigcirc\rangle\langle\square\bigcirc|_{i+1,i+2} - |\otimes\square\rangle\langle\square\bigcirc|_{i,i+1} - |\square\bigcirc\rangle\langle\otimes\square|_{i,i+1}. \tag{33}$$

To obtain the overall Hamiltonian for rule 3, we do not simply sum these four terms, as we would include the terms $|\otimes\square\rangle\langle\otimes\square|_{i-1,i}$, $|\square\bigcirc\rangle\langle\square\bigcirc|_{i+1,i+2}$, $|\square\square\rangle\langle\square\square|_{i-1,i}$, $|\square\square\rangle\langle\square\square|_{i+1,i+2}$ twice. The function of these projectors is to pick out the 'before' and 'after' configurations of the corresponding transition rule. Since we want each legal configuration to picked out exactly once, we include them only in a single copy, i.e.

$$\begin{aligned}
H_{\mathrm{prop},i}^{(\text{rule } 3)} &= |\square\square\rangle\langle\square\square|_{i-1,i} + |\square\square\rangle\langle\square\square|_{i+1,i+2} && (34)\\
&+ |\otimes\square\rangle\langle\otimes\square|_{i-1,i} + |\square\bigcirc\rangle\langle\square\bigcirc|_{i+1,i+2} && (35)\\
&- |\circledcirc\square\rangle\langle\square\circledcirc|_{i,i+1} - |\square\circledcirc\rangle\langle\circledcirc\square|_{i,i+1} && (36)\\
&- |\otimes\square\rangle\langle\square\bigcirc|_{i,i+1} - |\square\bigcirc\rangle\langle\otimes\square|_{i,i+1} && (37)\\
&- |\otimes\square\rangle\langle\square\circledcirc|_{i,i+1} - |\square\circledcirc\rangle\langle\otimes\square|_{i,i+1} \quad \text{only at location types AE} && (38)\\
&- |\circledcirc\square\rangle\langle\square\bigcirc|_{i,i+1} - |\square\bigcirc\rangle\langle\circledcirc\square|_{i,i+1} \quad \text{only at location types AC} && (39)
\end{aligned}$$

where the first four lines apply at locations $(i, i+1)$ of the types ACE, and the last two lines apply only at the location types listed (AE and AC). The projector terms in this Hamiltonian term applied to a legal configuration now gives something nonzero only when rule 3 could be applied to this legal configuration – and induces exactly *one* forward and *one* backward legal transition. Possibly, it could also induce illegal transitions, which lead to illegal states detectable by H_{pen}). On the other hand, when rule 3 (in its 4-local form) is not applicable to a given configuration, we get no projection terms, only transitions to illegal states.

Note that we need to fix the prescriptions at the ends of the chain. We do this by omitting the particles with positions with $i-1<1$, $i+1>2nR$ or $i+2>2nR$, e.g., using only a single-particle projector $|\square\rangle\langle\square|_1$ as the first term in (34) at the location pair (1,2). Together, all these terms make up H_{prop}.

4.2.3 Applying the propagation Hamiltonian: examples

Let us see the Hamiltonian for rule 3 in action. We list a few examples, applying it in a location of the type E (with a block boundary on the right), first to legal configurations:

a legal configuration	applying $H_{\mathrm{prop},i}^{(\text{rule 3})}$ for $(i, i+1) = (5, 6)$ gives
$C_1 = \otimes\otimes\vert\otimes\square\vert\square\circledcirc\Vert\square\bigcirc\vert\bigcirc\bigcirc\cdots$	$+\otimes\otimes\vert\otimes\square\vert\square\circledcirc\Vert\square\bigcirc\vert\bigcirc\bigcirc\cdots$ (projection) $-\otimes\otimes\vert\otimes\square\vert\circledcirc\square\Vert\square\bigcirc\vert\bigcirc\bigcirc\cdots$ (legal transition) $-\otimes\otimes\vert\otimes\square\vert\otimes\square\Vert\square\bigcirc\vert\bigcirc\bigcirc\cdots$ (locally detectable)
$C_2 = \otimes\otimes\vert\otimes\otimes\vert\square\circledcirc\Vert\square\circledcirc\vert\square\bigcirc\cdots$	$+\otimes\otimes\vert\otimes\otimes\vert\square\circledcirc\Vert\square\circledcirc\vert\square\bigcirc\cdots$ (projection) $-\otimes\otimes\vert\otimes\otimes\vert\otimes\square\Vert\square\circledcirc\vert\square\bigcirc\cdots$ (legal transition) $-\otimes\otimes\vert\otimes\otimes\vert\circledcirc\square\Vert\square\circledcirc\vert\square\bigcirc\cdots$ (locally detectable)
$C_3 = \otimes\square\vert\circleddash\circledcirc\vert\square\circledcirc\Vert\square\bigcirc\vert\bigcirc\bigcirc\cdots$	$-\otimes\square\vert\circleddash\circledcirc\vert\circledcirc\square\Vert\square\bigcirc\vert\bigcirc\bigcirc\cdots$ (locally detectable) $-\otimes\square\vert\circleddash\circledcirc\vert\otimes\square\Vert\square\bigcirc\vert\bigcirc\bigcirc\cdots$ (locally detectable)

For the first configuration C_1, the pair (5,6) is indeed where rule 3 should apply. Thus we get a projection from (34), and a legal transition from (36). There is an additional illegal transition from (38), locally detectable by the illegal pair $\square\otimes$. The second configuration C_2 should transform forward by applying rule 3. The configuration is projected by (35), has a legal transition from (38) and an extra illegal one from (36) with the bad substring $\otimes\circledcirc$. For the third configuration C_3, rule 3 should not apply (the proper-transition producing rule is now rule 5, involving $\circleddash$) – thus we get nothing from the projection terms (34)-(35). Instead, we get two transitions to illegal states – (36) creates a state with a bad substring $\circledcirc\circledcirc$ and (38) makes a state detectable by the pair $\circledcirc\otimes$.

Let us look at one more example, checking what $H_{\mathrm{prop},i}^{(\text{rule 3})}$ does to an illegal, allowed but not locally detectable configuration. This special case is crucial for detecting configurations with badly aligned blocks or with too few/too many qubits.

an allowed but illegal configuration	applying $H_{\mathrm{prop},i}^{(\text{rule 3})}$ for the middle pair
$C_4 = \cdots\otimes\otimes\vert\square\bigcirc\Vert\bigcirc\bigcirc\cdots$	$+\otimes\otimes\vert\otimes\otimes\vert\square\bigcirc\Vert\bigcirc\bigcirc\vert\bigcirc\bigcirc\cdots$ (projection) $-\otimes\otimes\vert\otimes\otimes\vert\otimes\square\Vert\bigcirc\bigcirc\vert\bigcirc\bigcirc\cdots$ (loc. detectable)

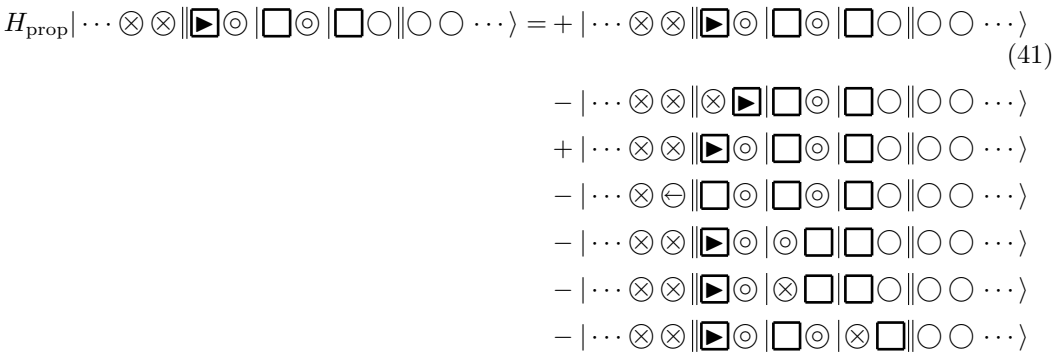
(40)

The configuration C_4 is projected once by (35) and an illegal transition from (37) makes a configuration with a forbidden pair $\square\Vert\bigcirc$. Note that we did not obtain a legal transition, even though rule 3 was applicable and gave us a projection term. In Section 6.2 we will translate this into a lower bound on the ground state energy for such states.

4.2.4 Classifying the legal and illegal transitions

When H_{prop} (22) acts on a state of the system, it induces changes in the configuration (besides sometimes performing a two-qubit unitary operation). This construction differs from the one in [9] in that the changes can occur at more than one location along the chain. This is readily apparent when one considers the action of the whole propagation Hamiltonian on the state with a configuration such as $\cdots\otimes\otimes\Vert\blacksquare\circledcirc\vert\square\circledcirc\vert\square\bigcirc\Vert\bigcirc\bigcirc\cdots$ (the first line in Table 2).

We obtain



(41)

with the first 2 terms coming from (26), connected with rule 2 for moving the ▶ particle, the second 2 terms coming from (29), connected with backward application of rule 6 for making ⊖ disappear. These 4 terms are exactly what we would like. However, we also obtain the three transitions to locally detectable states on the 5-7th lines, due to (36)-(38), connected with rule 3 for moving a qubit □. The way the legal and locally detectable terms are produced by H_{prop} in our construction obeys certain rules.

We can check that H_{prop} acting on a state $|\psi_t\rangle$ with a *legal* configuration (i.e. one appearing in a computation as in Table 2, with a correct number of qubits, properly aligned between boundaries) produces a superposition $H_{\text{prop}}|\psi_t\rangle$ that contains

1. The original legal state with amplitude 2 (for two rules that apply to it), except for $t = 0$ and $t = K$, where the amplitude is 1 (only a single rule applies to those two states).

2. Two new legal configurations: one due to a 'forward' transition to $|\psi_{t+1}\rangle$ and one due to a 'backward' transition to $|\psi_{t-1}\rangle$. Note that for $t = 0$ and $t = K$ we only get one legal transition.

3. Some illegal terms, which are all locally detectable with H_{pen} (such as the 5th line in (41), with the illegal combination ◎◎).

Points 1 and 2 are a property of our construction with projector terms uniquely picking out only the "active" spots in a given configuration. We discuss the verification of point 3 (verifying that transition terms applied at inappropriate times are always locally detectable) in the next section.

Note that there exist allowed (not containing one of the forbidden pairs) configurations that are not locally detectable (such as the configuration C_4 in (40) with a single qubit). These are either improperly aligned or have an incorrect number of qubits. For some of these states, H_{prop} gives only one transition to another allowed state, while it still projects onto the state twice – this will be used to show the energy of such locally undetectable states is still high. For example the configuration from (40) is projected twice by the terms in H_{prop} corresponding to rules 3 and (the backwards application of) 6.

Lemma A configuration that does not contain any of the forbidden pairs (i.e. those penalized by H_{pen}) is either one of the legal configurations (configurations that occur in the course of

a computation), or (i) has a [qubits] string of incorrect length, or (ii) has a [qubits] string of the right length, but improperly aligned with the block boundaries.

Proof: Careful checking of the allowed pairs at positions $(i, i+1)$ for odd i and even i from Table 5 implies the allowed joining of symbol pairs given in Table 3). This in turn restricts the legal/allowed configurations to form $(\mathrm{x}\cdots\mathrm{x})[qubits](\mathrm{u}\cdots\mathrm{u})$ where $[qubits]$ is a nonzero string with the structure (5)-(13).

The only configurations that are not ruled out by these considerations are: (i) the legal configurations, (ii) configurations with a $[qubits]$ string of the wrong length (not containing exactly n qubits), (iii) configurations with a $[qubits]$ string with the right number of qubits, but improperly aligned with the blocks (e.g. $\cdots\otimes|\otimes\square\|\circledcirc\square|\blacktriangleright\circledcirc|\square\bigcirc|\bigcirc\cdots$ which eventually evolves to $\cdots\otimes|\otimes\square\|\circledcirc\square|\circledcirc\square|\blacktriangleright\bigcirc|\bigcirc\cdots$ with a bad pair $|\blacktriangleright\bigcirc|$ indicative of a misaligned block). □

5 Completeness

Suppose there exists a witness, $|\xi\rangle$, that is accepted by V_x with probability $\geq 1-\epsilon$. Beginning with the initial state $|\psi_0\rangle$ (4) that has n qubits with qubit content $|0^{n-m}\rangle\otimes|\xi\rangle$, we get the history state $|\eta\rangle = \frac{1}{\sqrt{K+1}}\sum_{t=0}^{K}|\psi_t\rangle$ associated with circuit $\tilde{V}_x$. The configurations occurring in this superposition are exactly the legal configurations. Given that all the ancilla qubits were initially in the $|0\rangle$ state, H_{in} evaluates to zero on $|\eta\rangle$. Since all the configurations in the superposition are legal, H_{pen} also evaluates to zero.

We next note the following facts about the legal configurations to be used in the claim.

Fact 2 *Any legal configuration can contain at most one substring on the lefthand side of the transition rules 1–6. This means that to any legal configuration, at most one of the transition rules can apply in the forward direction. Furthermore, a legal configuration can contain at most one substring $XY_{(j,j+1)}$ (and thus be connected to a single projector term of the type $|XY\rangle\langle XY|_{j,j+1}$ in all of $H^{rule\ \rho}_{prop,i}$ (19)).*

The first part of this fact can be verified by inspection of the list of legal configurations in Table 2 and the transitions that can be applied to them in Table 1. To check the second part (about the projector terms), in Table 5 we list the substrings XY identifying active spots in legal configurations from the projector terms of the type $|XY\rangle\langle XY|_{j,j+1}$ in all of the $H^{\mathrm{rule}\ \rho}_{\mathrm{prop},i}$. An inspection of the legal sequence again shows that each state in it has only one spot where one of the substrings XY appears (at a proper location with respect to the boundaries).

Fact 3 *Any legal configuration can contain at most one substring from the righthand side of the transition rules 1–6 (i.e. at most one transition rule applies to it in the backward direction). Furthermore, a legal configuration can contain at most one substring $ZW_{(k,k+1)}$ (and thus be connected to a single projector term of the type $|ZW\rangle\langle ZW|_{k,k+1}$ in all of $H^{rule\ \rho}_{prop,i}$ (19)).*

location type	XY (for a forward transition)	ZW (for a backward transition)
(A) $\vert\ \cdot\ \cdot\ \vert$	$\vert\circledcirc\ominus\vert, \vert\otimes\ominus\vert$	$\vert\ominus\circledcirc\vert, \vert\ominus\bigcirc\vert$
(B) $\cdot\vert\cdot$	$\blacksquare\vert\square, \square\vert\square, \otimes\vert\square, \square\vert\bigcirc, \square\vert\ominus$	$\square\vert\blacksquare, \square\vert\square, \otimes\vert\square, \square\vert\bigcirc, \ominus\Vert\square$
(C) $\Vert\ \cdot\ \cdot\ \vert$	$\Vert\circledcirc\ominus, \Vert\otimes\ominus$	$\Vert\ominus\circledcirc, \Vert\ominus\bigcirc, \Vert\otimes\blacksquare$
(D) $\cdot\Vert\cdot$	$\blacksquare\Vert\bigcirc, \square\Vert\ominus$	$\otimes\Vert\blacksquare, \ominus\Vert\square$
(E) $\vert\ \cdot\ \cdot\Vert$	$\circledcirc\ominus\Vert, \otimes\ominus\Vert, \blacksquare\bigcirc\Vert$	$\ominus\circledcirc\Vert, \ominus\bigcirc\Vert$

Table 6. Substrings identifying active spots in legal configurations. We list all of the substrings appearing in the projector terms of the type $|XY\rangle\langle XY|_{j,j+1}$ and $|ZW\rangle\langle ZW|_{k,k+1}$ from all of the $H^{\text{rule }\rho}_{\text{prop},i}$ terms (24), (26), (34), (27), (28) and (29). Finding a substring XY of a legal configuration C_t uniquely indicates that the configuration is connected to some configuration C_{t+1} ahead of it. Similarly, finding a substring ZW uniquely locates a backward transition to some C_{t-1}.

Fact 4 *For a legal configuration C_t, there can be multiple places containing one of the substrings $NO_{(i,i+1)}$ or $PQ_{(i,i+1)}$ from all of the terms in $H^{rule\ \rho}_{prop,i}$ (19). However, exchanging any $NO \to PQ$ in C_t leads to locally detectable illegal configurations for all cases except one, which gives the legal (following) configuration C_{t+1}. Similarly, exchanging any $PQ \to NO$ in C_t leads to locally detectable illegal configurations for all cases except one, which gives the legal (preceding) configuration C_{t-1}.*

We have chosen the PQ's and NO's so that they work properly where they should, and always produce locally detectable illegal configurations when used at "wrong times" (i.e. improper locations). This can be checked by careful inspection of the transition rules and terms in $H^{\text{rule }\rho}_{\text{prop},i}$.

Claim 5 *For any history state $|\eta\rangle$ with an initial configuration C_0 from (4), $\langle\eta|H_{\text{prop}}|\eta\rangle = 0$.*

Proof: Let us see what happens when we apply H_{prop} to a state $|\psi_t\rangle$ with a legal configuration C_t. The propagation Hamiltonian is made from terms of the type (19), with projection terms built from substrings XY and ZW, and transition terms exchanging substrings NO for PQ and vice versa.

First, due to Fact 2, a legal configuration C_t contains only one substring $XY_{(j,j+1)}$, and this projection term will apply, producing $|\psi_t\rangle$. Second, due to Fact 4, the corresponding transition term $NO_{(i,i+1)} \to PQ_{(i,i+1)}$ will apply, producing the state $-|\psi_{t+1}\rangle$. Possibly, other transition terms for other substrings $NO \to PQ$ will apply at a different (or the same) location, but these all produce locally detectable configurations, which are orthogonal to legal ones. Third, due to Fact 3 we get a single projection term because of the unique substring $ZW_{(k,k+1)}$, producing $|\psi_t\rangle$ again. Fourth, again due to Fact 4, we get a single legal transition to $-|\psi_{t-1}\rangle$, and possible other, illegal, detectable states.

In sum, the action of H_{prop} on $|\psi_t\rangle$ (for $1 \le t \le K-1$) produces, $-|\psi_{t-1}\rangle + 2|\psi_t\rangle -$

$|\psi_{t+1}\rangle$ in the legal subspace, and a vector that lies in the space of locally detectable illegal configurations. For the endpoint states, we only get $H_{\text{prop}}|\psi_0\rangle = |\psi_0\rangle - |\psi_1\rangle +$ illegal states, and $H_{\text{prop}}|\psi_K\rangle = |\psi_K\rangle - |\psi_{K-1}\rangle +$ illegal states. Observe that within the legal subspace, both the rows and columns of the matrix form of H_{prop} sum to zero. Looking now at a history state $|\eta\rangle$, a uniform superposition of legal states (for a given initial state), we obtain $\langle\eta| H_t |\eta\rangle = 0$, since $H_{\text{prop}}|\eta\rangle = 0$ when restricted to the legal subspace, and the illegal terms produced by H_{prop} are orthogonal to $|\eta\rangle$. □

With the propagation Hamiltonian evaluating to zero on a proper history state, we have

$$\langle\eta|J_{\text{in}}H_{\text{in}} + J_{\text{prop}}H_{\text{prop}} + J_{\text{pen}}H_{\text{pen}}|\eta\rangle = 0.$$

Consider now the last remaining term in the Hamiltonian, $\langle\eta|H_{\text{out}}|\eta\rangle$. Since H_{out} acts only on the state with ▶ on the last qubit, this term equals $\frac{1}{K+1}\langle\psi_K|H_{\text{out}}|\psi_K\rangle = \frac{p_0}{K+1}$, where p_0 is the probability that the output qubit is zero in the final step. Since the computation accepts with probability $1 - p_0 \geq 1 - \epsilon$, we have $\langle\eta| H_{\text{out}} |\eta\rangle \leq \frac{\epsilon}{K+1}$. Finally,

$$\langle\eta| H |\eta\rangle = \langle\eta| J_{\text{in}}H_{\text{in}} + J_{\text{prop}}H_{\text{prop}} + J_{\text{pen}}H_{\text{pen}} + H_{\text{out}} |\eta\rangle \leq \frac{\epsilon}{K+1}. \tag{42}$$

This concludes our completeness proof, showing that the energy for a proper history state corresponding to the verifying computation on a well-accepted witness $|\xi\rangle$ is close to zero. Therefore, the ground state energy of H is also small, in fact it is upper-bounded by $a = \frac{\epsilon}{K+1}$, where $K = (R-1)(3n^2 + 2n - 1) + 2n$, with R a polynomial in n.

6 Soundness

We now need to show that in the case that there exists no witness that is accepted by V_x with probability greater than ϵ, the ground state energy of H is bounded away from zero.

We partition the set of configurations into minimal sets S that are invariant under the action of H_{prop}. The invariant sets are of three types:

1. Sets that contain legal configurations and locally detectable illegal configurations.
2. Sets that contain only locally detectable illegal configurations.
3. Sets that contain only illegal configurations, some of which are not locally detectable

As we have seen previously, the action of H_{prop} on a legal configuration produces legal 'forward' and 'backward' transitions, besides transitions to illegal configurations.

Illegal configurations that are not locally detectable either have the wrong number of qubits or have the right number of qubits but are incorrectly aligned[g] with the blocks. Since the transition rules do not change the number of two-state sites in a configuration nor change the alignment of the [*qubits*] string, legal configurations cannot transition to illegal configurations that are not locally detectable. Similarly, illegal configurations that are not locally detectable can only turn into other non-locally detectable illegal configurations, or into locally detectable illegal configurations.

[g] An example of a locally undetectable, misaligned sequence: $\cdots \otimes$ ☐‖◎ ☐|◎ ▶|☐○ |○ ○ ‖○ ○ $\cdots$ The block length is 4, and when the ▶ particle eventually reaches the front of the [*qubits*], it will happen away from a sequence boundary – there we'll be able to detect it.

A vector belonging to a subspace of type 2 has energy $\geq J_{\text{pen}}$, due to the presence of at least one locally detectable illegal pair that is penalized by H_{pen}. We now need to show that vectors from spaces of type 1 and 3 have high energy. We do this by repeated use of the Projection Lemma, a technique introduced in [7]. The lemma allows us to bound the ground state energy of our Hamiltonian by restricting it to progressively smaller subspaces of the Hilbert space.

Lemma 1 (Projection Lemma, [7] Lemma 1) *Let $H = H_1 + H_2$ be the sum of two Hamiltonians operating on some Hilbert space $\mathcal{H} = S + S^{\perp}$. Suppose the Hamiltonian H_2 is such that S is a zero eigenspace and the eigenvectors in $S^{\perp}$ have eigenvalue at least $J > 2||H_1||$. Then,*

$$\lambda(H_1|_S) - \frac{\|H_1\|^2}{J - 2\|H_1\|} \leq \lambda(H) \leq \lambda(H_1|_S) \tag{43}$$

where $\lambda(A)$ denotes the lowest eigenvalue of an operator A.

6.1 Type 1 subspace

We consider the action of H on $\mathcal{H}_1$, the space spanned by configurations of type 1. We apply the projection lemma with

$$H_1 = J_{\text{in}} H_{\text{in}} + J_{\text{prop}} H_{\text{prop}} + H_{\text{out}},\ H_2 = J_{\text{pen}} H_{\text{pen}}.$$

Let S_{pen} be the subspace of $\mathcal{H}_1$ that is spanned by legal configurations. Then $S_{\text{pen}} \subseteq \mathcal{H}_1$ is the zero eigenspace of H_2. On $S_{\text{pen}}^{\perp}$, H_2 has energy $\geq J_{\text{pen}}$. Since $\|H_1\| \leq poly(n)$, we can pick J_{pen} to be some polynomial such that $J_{\text{pen}} > 2\|H_1\|$, allowing us to apply the projection lemma:

$$\lambda(H) \geq \lambda(H_1|_{S_{\text{pen}}}) - 1/8. \tag{44}$$

Now we bound the lowest eigenvalue of $H_1|_{S_{\text{pen}}}$,

$$H_1|_{S_{\text{pen}}} = H_{\text{out}}|_{S_{\text{pen}}} + J_{\text{in}} H_{\text{in}}|_{S_{\text{pen}}} + J_{\text{prop}} H_{\text{prop}}|_{S_{\text{pen}}}.$$

We apply the projection lemma again, with

$$H_1' = H_{\text{out}}|_{S_{\text{pen}}} + J_{\text{in}} H_{\text{in}}|_{S_{\text{pen}}},\ H_2' = J_{\text{prop}} H_{\text{prop}}|_{S_{\text{pen}}}.$$

To simplify the analysis of the eigenvalues of H_{prop}, we rotate to a different basis – one in which all the gates from V_x are just the identity operator. We define the unitary matrix W:

$$W = \sum_{t=0}^{K} U_t \cdots U_1 \otimes |t\rangle\langle t|$$

where $|t\rangle$ represents the configuration in the t-th step of the computation, and $U_t, \ldots, U_1$ are

the first t unitary operations performed on the qubit content of the particles. Then we have,

$$W^\dagger H_{\text{prop}}|_{S_{\text{pen}}} W = I \otimes \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} & 0 & 0 & \cdots & 0 & 0 \\ -\frac{1}{2} & 1 & -\frac{1}{2} & 0 & \cdots & \cdots & 0 \\ 0 & -\frac{1}{2} & 1 & -\frac{1}{2} & \ddots & & \\ 0 & 0 & -\frac{1}{2} & \ddots & \ddots & & \vdots \\ \vdots & & & \ddots & & & 0 \\ 0 & & & & & 1 & -\frac{1}{2} \\ 0 & 0 & & \cdots & 0 & -\frac{1}{2} & \frac{1}{2} \end{bmatrix}_{(K+1)\times(K+1)} . \tag{45}$$

This matrix has only one zero-eigenvector, namely the valid history state. Therefore $S_{\text{prop}} \subset S_{\text{pen}} \subset \mathcal{H}_1$ the set of correct history states (disregarding initial state of ancilla qubits). This matrix has second largest eigenvalue $\geq \frac{1}{2(K+1)^2}$ (see Appendix 1). Therefore, in $S_{\text{prop}}^{\perp}$, H_2' has minimum energy $\geq J_{\text{prop}} \cdot \frac{1}{2(K+1)^2}$. Choosing J_{prop} so that $\frac{J_{\text{prop}}}{2(K+1)^2} > 2\|H_1'\|$, the projection lemma gives us:

$$\lambda(H_1|_{S_{\text{pen}}}) \geq \lambda(H_1'|_{S_{\text{prop}}}) - \frac{1}{8}. \tag{46}$$

We now apply the projection lemma a third time, to $H_1'|_{S_{\text{prop}}}$, with

$$H_1'' = H_{\text{out}}|_{S_{\text{prop}}},\ H_2'' = J_{\text{in}} H_{\text{in}}|_{S_{\text{prop}}}.$$

H_2'' has zero eigenspace $S_{in} \subset S_{\text{prop}} \subset S_{\text{pen}} \subset \mathcal{H}_1$, the set of history states with correctly initialized ancilla qubits. Since H_2'' is in the standard basis and applies to vectors that are history states with 0 on the ancilla input (i.e., in $S_{in}^{\perp}$), H_2'' has minimum energy $O\left(\frac{1}{K+1}\right)$. Therefore, J_{in} can be chosen so that $\frac{J_{\text{in}}}{K+1} > 2\|H_1''\|$. Then

$$\lambda(H_1'|_{S_{\text{prop}}}) \geq \lambda(H_1''|_{S_{in}}) - \frac{1}{8}, \tag{47}$$

and $H_1''|_{S_{in}} = H_{\text{out}}|_{S_{in}}$. For any input state $|\xi, 0\rangle$, the circuit V_x accepts with probability $< \epsilon$. Therefore, for any $|\eta\rangle \in S_{in}$, we have $\langle\eta|H_{\text{out}}|\eta\rangle > (1-\epsilon)/(K+1)$. In particular, this is true for the eigenvector $|\eta\rangle$ of H_{out} with the lowest eigenvalue. Therefore $\lambda(H_{\text{out}}|_{S_in}) \geq (1-\epsilon)/(K+1)$.

Combining (47) with (44) and (46), we have $\lambda(H) \geq \frac{5}{8} - \epsilon$.

Now we look at vectors from subspaces of type 3.

6.2 Type 3 subspace

A locally undetectable illegal configuration either (i) has the wrong number of qubits, or (ii) has the [*qubits*] string incorrectly aligned with the blocks.

Consider a (locally undetectable illegal) configuration with a ▶ site. The [*qubits*] string either crosses a block boundary, or is too short (or both). The ▶ moves right until it either hits the end of the [*qubits*] string or it hits a block boundary. If the end of the [*qubits*] string does not coincide with a block boundary, the configuration eventually evolves to contain either |▶◎‖ or |▶◯|, both of which are locally detectable. If the end of the [*qubits*] string does

coincide with the block boundary (this can only happen when the [*qubits*] string is too short), the qubits get moved over into the next block, where a ▶ is generated again, and, moving right, eventually produces a pair $|\blacktriangleright\bigcirc|$, which is locally penalized.

A locally undetectable illegal configuration with a ⊖ also eventually evolves into a locally detectable one: the ⊖ moves the [*qubits*] string to the right until the beginning of the [*qubits*] string coincides with the beginning of a block, and generates a ▶, at which point the above argument applies.

If our locally undetectable illegal configuration has neither ▶ or ⊖, i.e. its [*qubits*] substring consists only of □s (separated by ◎s), the qubits begin to move themselves to the right, eventually generating a ⊖ or ▶ flag, at which point, the previous arguments apply: the evolution does indeed result in a locally detectable configuration.

In all the above cases, a locally detectable illegal configuration is reached within polynomially many steps/transitions. To see this, consider a configuration with n' qubits. It takes $poly(n')$ steps to move the [*qubits*] string over one block, and by the preceding arguments, a locally checkable configuration must be reached at some point in this 'round' of computation. Since n' can be at most $2nR$, this number of steps (which we label K') must be polynomial in n. In other words, the transition rules eventually take the state outside $\mathcal{H}_3 =$ Span(configurations of type 3). We can treat the restriction of H_{prop} to $\mathcal{H}_3$ in much the same way as we did its restriction to $\mathcal{H}_1$.

We attempt to bound the lowest eigenvalue of $J_{\text{pen}}H_{\text{pen}} + J_{\text{prop}}H_{\text{prop}}$ on $\mathcal{H}_3$ using the projection lemma, with $H_1 = J_{\text{prop}}H_{\text{prop}}$ and $H_2 = J_{\text{pen}}H_{\text{pen}}$. The zero eigenspace of H_2 is the space of illegal states that are *not* locally detectable, $S_{\text{pen}} \subset \mathcal{H}_3$. H_2 has energy $\geq J_{\text{pen}}$ on $S_{\text{pen}}^{\perp}$. Choosing J_{pen} to be $poly(J_{\text{prop}}\|H_{\text{prop}}\|)$,

$$\lambda(H) \geq \lambda(H_1|_{S_{\text{pen}}}) - \frac{1}{8}. \tag{48}$$

We now need the lowest eigenvalue of $J_{\text{prop}}H_{\text{prop}}|_{S_{\text{pen}}}$. We rotate bases once again, using the unitary matrix W defined earlier, with the difference that $|t\rangle$ now represents the t-th configuration in the sequence of (locally undetectable) illegal configurations that arises from the transition rules and forms the steps of the 'computation'. This sequence of configurations terminates in a locally detectable illegal configuration on at least one end. (The other end of the sequence could be a locally undetectable illegal configuration from which there are no further transitions.) When we have a transition to a locally illegal configuration, the action of H_{prop} on the last nonlocally detectable illegal configuration ($|K'\rangle$) in the sequence is to pick this configuration out twice, i.e., there are two projectors onto this configuration in $H_{\text{prop}}|_{S_{\text{pen}}}$, with the result that, in the space of configurations, the last (or first, or both) diagonal element of $W^{\dagger}H_{\text{prop}}|_{S_{\text{pen}}}W$ is 1 instead of $\frac{1}{2}$.

In other words, $W^\dagger H_{\text{prop}}|_{S_{\text{pen}}} W$ looks like

$$I \otimes \begin{bmatrix} f & -\frac{1}{2} & 0 & 0 & \cdots & 0 & 0 \\ -\frac{1}{2} & 1 & -\frac{1}{2} & 0 & \cdots & \cdots & 0 \\ 0 & -\frac{1}{2} & 1 & -\frac{1}{2} & \ddots & & \\ 0 & 0 & -\frac{1}{2} & \ddots & \ddots & & \vdots \\ \vdots & & & \ddots & & & 0 \\ 0 & & & & & 1 & -\frac{1}{2} \\ 0 & 0 & & \cdots & 0 & -\frac{1}{2} & g \end{bmatrix}_{(K'+1)\times(K'+1)} \tag{49}$$

with $f = 1, g = \frac{1}{2}$ or $f = g = 1$. This is a matrix for a quantum walk on a line with particular boundary conditions.

The least eigenvalue of either of these matrices is $O\left(\frac{1}{(K'+1)^2}\right)$ (see Appendix 1). Since K' is a polynomial in n, choosing J_{prop} to be an appropriately large polynomial in n, we can lower-bound the energy of H on type-3 subspaces by some constant.

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Appendix A Eigenvalues

Here we analyze the eigenvalues of the three matrices in Section 6. Our matrices are of

the form:

$$\begin{bmatrix} f & -\frac{1}{2} & 0 & 0 & \cdots & 0 & 0 \\ -\frac{1}{2} & 1 & -\frac{1}{2} & 0 & \cdots & \cdots & 0 \\ 0 & -\frac{1}{2} & 1 & -\frac{1}{2} & \ddots & & \\ 0 & 0 & -\frac{1}{2} & \ddots & \ddots & & \vdots \\ \vdots & & & \ddots & & & 0 \\ 0 & & & & & 1 & -\frac{1}{2} \\ 0 & 0 & & \cdots & 0 & -\frac{1}{2} & g \end{bmatrix}_{(L+1)\times(L+1)} \tag{A.1}$$

where, in subspaces of type 1, $f = g = \frac{1}{2}$, and in subspaces of type 3, either (i) $f = g = 1$ or (ii) $f = 1$ and $g = \frac{1}{2}$ (we could also have $f = \frac{1}{2}$ and $g = 1$, but this doesn't change the eigenvalues).

We wish to solve the eigenvalue equation $Mx = \lambda x$, where M is our matrix, and $x = (x_0, x_1, x_2, \ldots, x_L)^T$. It is easy to see that x must satisfy the equations

$$-\frac{1}{2}x_{j-1} + x_j - \frac{1}{2}x_{j+1} = \lambda x_j \qquad \text{for } 1 \le j \le L-1. \tag{A.2}$$

We use the ansatz

$$x_j = A\cos k(j+c) + B\sin k(j+c). \tag{A.3}$$

where A, B, k and c are reals. Plugging this into (A.2):

$$-(\cos k)\,(A\cos k(j+c) + B\sin k(j+c)) = (\lambda - 1)\,(A\cos k(j+c) + B\sin k(j+c))$$
$$\lambda = 1 - \cos k$$

Any vector x with $x_j = A\cos k(j+c) + B\sin k(j+c)$ satisfies (A.2) with $\lambda = 1 - \cos k$. Now we apply the 'boundary conditions' in the first case ($f = g = \frac{1}{2}$). The eigenvectors and eigenvalues are

$$\lambda_m = 1 - \cos\left(\frac{m\pi}{L+1}\right),$$
$$|\psi_m\rangle = \sum_{j=0}^{L} \cos\left(\frac{m\pi}{L+1}(j+\frac{1}{2})\right)|j\rangle \qquad \text{for } m = 0, 1, \ldots, L.$$

We can check this by plugging into the boundary condition equations

$$\frac{1}{2}x_0 - \frac{1}{2}x_1 = (1-\cos k)x_0,$$
$$-\frac{1}{2}x_{L-1} + \frac{1}{2}x_L = (1-\cos k)x_L.$$

The lowest eigenvalue in this case is 0 (when $m = 0$). The second-lowest eigenvalue is

$$1 - \cos\left(\frac{\pi}{L+1}\right) > \left(\frac{1}{L+1}\right)^2 \left(\frac{\pi^2}{2!} - \frac{\pi^4}{4!(L+1)^2}\right)$$
$$= \Omega\left(\frac{1}{(L+1)^2}\right)$$

i.e., $1/poly(L)$, where L is the number of steps, as promised.

Now we consider the next set of boundary conditions $f = g = 1$ (subspace of type 3). We get eigenvalues and eigenvectors:

$$\lambda_m = 1 - \cos\left(\frac{(m+1)\pi}{L+1}\right),$$
$$|\psi_m\rangle = \sum_{j=0}^{L} \cos\left(\frac{(m+1)\pi}{L+2}(j+1)\right)|j\rangle \qquad \text{for } m = 0, 1, \ldots, L.$$

This is again easily checked by plugging into the equations

$$x_0 - \frac{1}{2}x_1 = (1 - \cos k)x_0,$$
$$-\frac{1}{2}x_{L-1} + x_L = (1 - \cos k)x_L.$$

The lowest eigenvalue here is $\lambda_0 = 1 - \cos\left(\frac{\pi}{L+2}\right)$, which is $\Omega(\frac{1}{(L+2)^2})$.

The final set of boundary conditions to consider is $f = 1, g = \frac{1}{2}$. The eigenvalues and eigenvectors in this case are:

$$\lambda_m = 1 - \cos\left(\frac{(2m+1)\pi}{2L+3}\right),$$
$$|\psi_m\rangle = \sum_{j=0}^{L} \sin\left(\frac{(2m+1)\pi}{2L+3}(j+1)\right)|j\rangle \qquad \text{for } m = 0, 1, \ldots, L.$$

The lowest eigenvalue here is $\lambda_0 = 1 - \cos\left(\frac{\pi}{2L+3}\right) = \Omega(\frac{1}{(2L+3)^2})$.