Space-Time Circuit-to-Hamiltonian Construction and Its Applications

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Abstract. The circuit-to-Hamiltonian construction translates dynamics (a quantum circuit and its output) into statics (the groundstate of a circuit Hamiltonian) by explicitly defining a quantum register for a clock. The standard Feynman-Kitaev construction uses one global clock for all qubits while we consider a different construction in which a clock is assigned to each interacting qubit. This makes it possible to capture the spatio-temporal structure of the original quantum circuit into features of the circuit Hamiltonian. The construction is inspired by the original two-dimensional interacting fermionic model in [1]. We prove that for one-dimensional quantum circuits the gap of the circuit Hamiltonian is appropriately lower-bounded, partially using results on mixing times of Markov chains, so that the applications of this construction for QMA (and partially for quantum adiabatic computation) go through. For one-dimensional quantum circuits, the dynamics generated by the circuit Hamiltonian corresponds to diffusion of a string around the torus.

1. Introduction

In [2] Feynman considered how to simulate a quantum circuit by unitary dynamics generated by a time-independent Hamiltonian H. Imagine that the quantum circuit consists of L unitary gates $U_1, \ldots, U_L$ on n qubits. Feynman's idea was to introduce a clock-register $|t\rangle$ with time t running from $t = 0$ to L such that for each unitary gate U_t in the circuit, we have a term H_t in the Hamiltonian H, i.e.

$$H_t = U_t \otimes |t\rangle \langle t-1| + U_t^\dagger \otimes |t-1\rangle \langle t| \,, \quad H = \sum_{t=1}^{L} H_t.$$

Alternatively, one can construct a Hamiltonian $H_{circuit}$ such that the groundstate of $H_{circuit} = \sum_{t=1}^{L} H_t$ is the *history state* of the quantum circuit [3]. We then take ‡

$$H_t = -U_t \otimes |t\rangle \langle t-1| - U_t^\dagger \otimes |t-1\rangle \langle t| + |t\rangle \langle t| + |t-1\rangle \langle t-1| \geq 0.$$

The zero energy groundstate of the *circuit Hamiltonian* $H_{circuit}$ is

$$|\psi_{history}\rangle = \frac{1}{\sqrt{L+1}} \sum_{t=0}^{L} U_t \ldots U_1 \, |\xi\rangle \otimes |t\rangle \,,$$

‡ Sometimes a prefactor of $\frac{1}{2}$ is included to make H_t a projector.

for any input state $|\xi\rangle$ to the circuit. It is not hard to analyze the spectrum of $H_{circuit}$ as one can transform the dependence on the specific gates $U_1, \ldots, U_L$ away by a unitary transformation $W = \sum_{t=0}^{L} U_t \ldots U_1 \otimes |t\rangle\langle t|$ such that $W^\dagger H_{circuit}(U_1, \ldots, U_L)W = H_{circuit}(U_1 = I, \ldots, U_L = I)$. This unitarily-transformed circuit Hamiltonian corresponds to that of a particle (whose location is t) moving on a 1D line: the eigenvalues of $H_{circuit}$ are $\lambda_k = 2(1 - \cos q_k)$ with $q_k = \frac{\pi k}{L+1}$ for $k = 0, \ldots, L$. The gap above the ground-space of $H_{circuit}$ is thus easily lowerbounded as $\Omega(L^{-2})$, corresponding to the lowest $k \neq 0$ eigenstate. If one is given the history state, one can measure the clock register t and, with probability $1/(L+1)$, obtain the output of the quantum circuit. In order to increase the probability of getting the output to some constant, one can pad the quantum circuit with, say, L identity gates at the end, so that the probability of measuring any time $t \in [L, 2L]$ is approximately $1/2$. For all times in this interval, the qubits are in the output state of the quantum circuit.

The circuit-to-Hamiltonian construction can be directly used as a model for universal quantum adiabatic computation [4]. We assume that the quantum circuit which we wish to simulate by an adiabatic computation is efficient, i.e. $L = \text{poly}(n)$ where $\text{poly}(n)$ is some polynomial in n. A simple way to go from the circuit Hamiltonian to an adiabatic algorithm is to construct a continuous family of circuit Hamiltonians $H_{circuit}(U_1(\epsilon), \ldots, U_L(\epsilon)) = H_{circuit}[\epsilon]$ depending on a parameter $\epsilon \in [0, 1]$. For $\epsilon = 0$, we have $\forall i\ U_i(\epsilon = 0) = I$ while for $\epsilon = 1$, we have $U_i(\epsilon = 1) = U_i$ such that we smoothly interpolate between I and U_i for intermediate values of ϵ [5] (Such smooth deformations always exists as one can continuously deform any element to I in a Lie-group $U(n)$).

The adiabatic computation starts in the groundstate of $H_{circuit}[\epsilon = 0]$ and ϵ is gradually increased to evolve to the groundstates of $H_{circuit}[\epsilon \neq 0]$. The smoothness in the interpolation is required such that first and second-derivatives of $H_{circuit}[\epsilon]$ with respect to ϵ are polynomially bounded in n, so that the explicit formulation of the quantum adiabatic theorem in e.g. [6] applies. As each $H_{circuit}[\epsilon]$ on the path has the same gap $\Omega(L^{-2}) = \frac{1}{\text{poly}(n)}$, the simulation arrives at the history state of the quantum circuit in polynomial time [6]. Note that this adiabatic path requires that the ground-state of the initial circuit Hamiltonian can be 'trivially' prepared, see the discussion in Sec. 3.4.

Nagaj [7] has suggested that for any quantum circuit one can define a circuit Hamiltonian whose dynamics correspond to a particle moving on a *circle* instead of a line. We will use this idea in this paper as it is easier to analyze, so let us give some details, see Fig. (1). We define a *circular* clock register $t = 0, \ldots 2L-1$ where we identify $t = 2L$ with $t = 0$ ($t \in Z_{2L}$). The idea is to use the sequence of unitary gates $U_1, \ldots, U_L$ of the quantum circuit for the two different ways one can go from $t = 0$ to the opposite point on the circle, $t = L$, see Fig. (1). More generally, we define some new, yet to be specified, gates $U_{L+1}, \ldots U_{2L}$ and take as before

$$t \in [1, 2L]\text{: } H_t = -\left(U_t \otimes |t\rangle\langle t-1| + h.c.\right) + |t\rangle\langle t| + |t-1\rangle\langle t-1|\,.$$

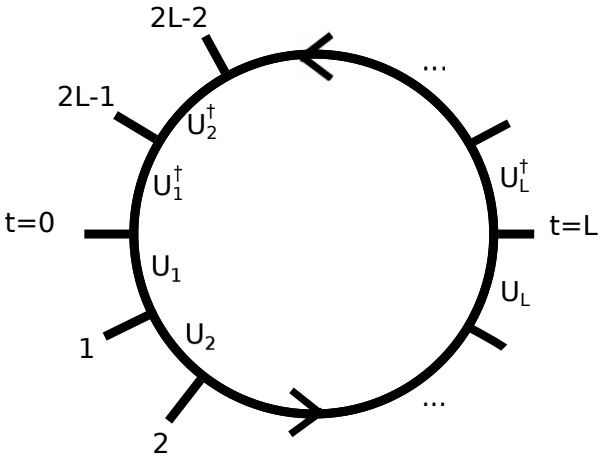


Figure 1: Representation of the Feynman-Kitaev circuit-to-Hamiltonian construction with circular time [7]. At $t = L$, the qubits are in the output state of the quantum circuit while evolving further along the circle will undo the evolution. The evolution from any point, say $t = 0$, to another point t on the circle is well-defined, even though the evolution can happen via two different paths.

Let $H_{circuit} = \sum_{t=1}^{2L} H_t$. As $H_{circuit}$ is a sum of positive-semidefinite operators, it only has a zero energy if all terms H_t have zero energy. W.l.o.g. we can take the groundstate to be of the form $\sum_{t=0}^{2L-1} |\psi_t\rangle |t\rangle$ which is a zero energy state if and only if

$$t \in [1, 2L]\colon\ |\psi_t\rangle = U_t |\psi_{t-1}\rangle .$$

This implies that the unitary evolution from a state $|\psi_t\rangle$ around the entire circle must act as I on the state $|\psi_t\rangle$. Equivalently, we have $U_{2L} \ldots U_{L+1} U_L \ldots U_1 |\xi\rangle = |\xi\rangle$ where $|\xi\rangle = |\psi_{t=0}\rangle$. Depending on the choice for $U_{L+1}, \ldots, U_{2L}$, this defines a *subspace* of states $|\xi\rangle$. When we choose $U_t = U_{2L-t+1}^\dagger$ for $t = L+1, \ldots, 2L$, the subspace $|\xi\rangle$ is the whole space and the history state of the circuit is

$$|\psi_{history}\rangle = \frac{1}{\sqrt{2L}} \sum_{t=0}^{2L-1} U_t \ldots U_2 U_1 |\xi\rangle \otimes |t\rangle , \forall\, \xi \tag{1}$$

where the latter part (for $t > L$) of the evolution unravels the earlier part. An additional observation is that if the original quantum circuit contains some I gates here and there, then the gates need not explicitly be included in the unraveling evolution, in order for there to be a zero energy history state for any ξ.

Note that the history state of this circular time construction, Eq. (1), contains the output of the original circuit when we measure time and find $t = L$. As before, we can pad the original circuit with I gates at the end such that we have a window of time around $t = L$ when the qubits are in the output state of the original quantum circuit. Hence, one can realize quantum adiabatic computation with such circular-time model similar as in the linear-time model.

Before we introduce the novel circuit-to-Hamiltonian construction, we remark that the circuit-to-Hamiltonian construction has an intimate connection with the cosmology

ideas of Page and Wootters [8, 9] which, in our language, posit that there is no observable difference between a universe which evolves according to the circuit dynamics versus a universe which simply finds itself in the groundstate of the circuit Hamiltonian $H_{circuit}$.

1.1. Space-Time Circuit-to-Hamiltonian Construction

We consider a quantum circuit on n qubits with single and two-qubit gates $U_i, i = 1, \ldots, S$ where S is the *size* of the circuit. As some gates can be executed in parallel on different qubits, the circuit also has a certain *depth* $D \leq S$. The circuit may have a geometric structure, i.e. only nearest-neighbor qubits on some d-dimensional lattice or space interact. The space-time circuit-to-Hamiltonian defines a circuit Hamiltonian $H_{circuit}$ whose properties relate to the geometric structure and the depth D of this quantum circuit.

Each gate U_i in this circuit will correspond to a term in $H_{circuit}$. The gates can be labeled as $U_h^1[q]$ for a single-qubit gate acting at time-step (depth) $t = 1, \ldots, D$ on qubit q, or a two-qubit gate $U_t^2[q, p]$ acting at time-step t on qubits q and p.

The construction that we will analyze later has circular time, see Sec. 1.4, but for simplicity we first define the model with linear time. For *each* qubit q in the original circuit, we define a clock register $|t\rangle_q$ with $t = 0, \ldots, D$. Thus the global clock in the Feynman-Kitaev construction gets replaced by a *time-configuration* $|t_1, \ldots, t_n\rangle_{1,\ldots n}$. Consider a single qubit gate $U_t^1[q]$ acting on qubit q at time-step t in the quantum circuit. For each such gate, there is a term $H_t^1[q]$ in $H_{circuit}$ of the standard form, i.e.

$$H_t^1[q] = -\left(U_t^1[q] \otimes |t\rangle \langle t-1|_q + h.c.\right) + |t\rangle \langle t|_q + |t-1\rangle \langle t-1|_q .$$

Clearly, if the quantum circuit were to consist of single qubit gates only, the history state would be a tensor product of history states, one for each qubit independently. In such a scenario, the clocks of the qubits can be completely unsychronized and measure different times.

For every two qubit gate $U_t^2[q, p]$ acting on qubits p and q at time $t_q = t_p = t$ in the quantum circuit, we have in $H_{circuit}$ the term

$$\begin{aligned} H_t^2[q, p] = &-\left(U_t^2[q, p] \otimes |t, t\rangle \langle t-1, t-1|_{q,p} + h.c.\right) \\ &+ |t, t\rangle \langle t, t|_{q,p} + |t-1, t-1\rangle \langle t-1, t-1|_{q,p} . \end{aligned} \tag{2}$$

Note that $H_t^2[q, p] \geq 0$ always has zero energy when the clocks of qubits q and p measure unequal times. We take $H_{circuit} = \sum_{t=1}^{D} H_t$ where H_t is a sum over all $H_t^2[q, p]$ and $H_t^1[q]$ for various q, p, corresponding to gates $U_t^2[q, p]$ and $U_t^1[q]$ which act in parallel at time t.

1.2. Proper Time-Configurations

We consider the zero energy states of this circuit Hamiltonian. First we define what we call *improper* time-configurations $|t_1, \ldots, t_n\rangle$. Improper configurations are the time-configurations in which, of at least one pair of qubits, say, the pair (q, p) which

interacts in some two-qubit gate $U_t^2[q,p]$ in the quantum circuit, it holds that either $(t_q < t) \wedge (t_p \geq t)$ or $(t_p < t) \wedge (t_q \geq t)$. Informally, this means that one qubit has gone through the gate while its partner qubit has not yet gone through the gate. If one would evolve with $H_{circuit}$ starting from the all-synchronized state $|t_1 = 0, \ldots, t_n = 0\rangle \otimes |\xi\rangle$, then clearly the resulting state would not have any support on improper time-configurations as qubits always go together through two-qubit gates by Eq. (2). Stated differently, $H_{circuit}$ preserves the space of proper time-configurations and its eigenstates split into a sectors of proper and improper eigenstates.

On the space of improper time-configurations, one can easily find zero energy eigenstates for $H_{circuit}$, but we will not be interested in these states. If we apply this construction for quantum adiabatic computation, we can start in the space of proper time-configurations and remain there. If we apply the construction to QMA, we need to do some additional work, see Section 3.1.

We consider zero energy states in the space of proper time-configurations. We restrict ourselves to quantum circuits which only employ two-qubit gates §. For such quantum circuits, a proper time-configuration $|t_1, \ldots, t_n\rangle$ has zero energy when, for *every* two-qubit gate $U_t^2[q,p]$ in the circuit, the clock-times t_q and t_p are either $(t_q \neq t_p)$, or $(t_p = t_q \neq t) \wedge (t_p = t_q \neq t-1)$ as then each term $H_t^2[q,p]$ has zero energy with respect to $|t_1, \ldots, t_n\rangle$. Such configurations do not evolve and we could call these configurations *light-like*. If one would give each qubit q a spatial location r_q, then one can informally say that for these configurations, the space-time intervals of any pair of space-time points (r_q, t_q) and (r_p, t_p) is light-like. We could call the remaining proper configurations space-like, as in these time-configurations there is no causal relation between any pair of points (r_q, t_q) and (r_p, t_p).

Let us illustrate these notions with quantum circuits that will mostly concern us, namely one-dimensional quantum circuits with nearest-neighbor qubits interacting in two-qubit gates, depicted in Fig.(2). The quantum circuit in Fig.(2)(a) has a beginning and an end and periodic boundary condition in space, but some two-qubit gates are missing in the circuit so that the (red) line represents a light-like configuration. The quantum circuit in Fig. (2)(b) has no light-like configurations. Note that n and D are both even.

Fig. (3) is an example of a quantum circuit with periodic boundary conditions in both space and time which does have unavoidable light-like configurations, see Section 1.4.

For quantum adiabatic computation, the light-like configurations are harmless as we can avoid starting the computation in such non-evolving configurations. For the application to QMA, the existence of light-like configurations must be avoided as the goal is to construct a Hamiltonian where the existence of a zero energy groundstate depends on the computation done by the quantum circuit. If there are light-like configurations,

§ Single-qubit gates can always be absorbed into two-qubit gates. The presence of single-qubit gates would lead to some differences, for example the presence of gapped excitations in $H_{circuit}$ which are localized in space-time.

it is not clear how to modify $H_{circuit}$ to make such configurations have non-zero energy. As we see, it is simple to avoid light-like configurations by ensuring that the quantum circuit has two-qubit and single-qubit (possibly I) gates throughout which propagate the clocks.

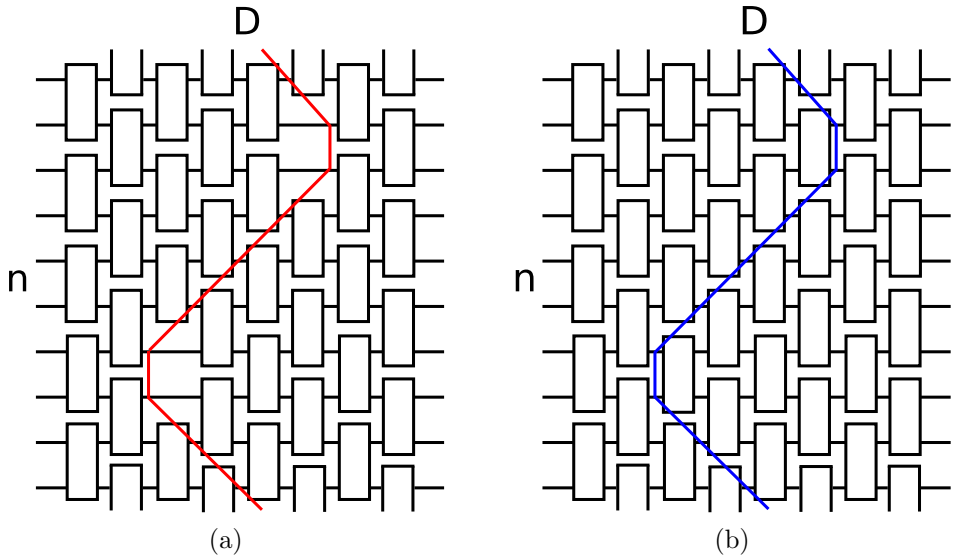


Figure 2: (a) One-dimensional quantum circuit on n qubits and depth D where the (red) line indicates a zero energy light-like time configuration. (b) One-dimensional quantum circuit on n qubits with nearest-neighbor interactions on a circle and depth D (n and D both even) which is analyzed in this paper. The (blue) line is not a light-like configuration but evolves under $H_{circuit}$.

1.3. Relation with the fermionic ground-state model of [1, 10, 11]

In [1] the authors formulated a (fermionic) model which allows for universal quantum computation by adiabatically modifying a circuit Hamiltonian [11]. Imagine we have a quantum circuit on n qubits, e.g. the one in Fig. (2)(b), of depth D. With every qubit q, we associate $2(D+1)$ fermionic modes with creation operators $a_t^\dagger[q], b_t^\dagger[q], t = 0, \ldots, D$. One can view these $2n(D+1)$ modes as the state-space of n spin-1/2 fermions, where each fermion can be localized at sites on a one-dimensional (time)-line of length $D+1$. The spin-state of the n fermions represents the state of the computation while the clock of each qubit is represented by where the fermion is on the one-dimensional line. Let $C_t[q] = \begin{bmatrix} a_t[q] \\ b_t[q] \end{bmatrix}$. Then for each single qubit gate $U_t^1[q]$, there is a term in the circuit Hamiltonian $H_{circuit}$ equal to

$$H_t^1[q] = [C_t^\dagger - \lambda C_{t-1}^\dagger \, {U_t^1}^\dagger][C_t - \lambda U_t^1 \, C_{t-1}],$$

where we have dropped the label $[q]$ for readibility. This is a fermion hopping term for the qth fermion from site $t-1$ to t and vice-versa, while U_t^1 acts on the internal spin

degree of freedom. By including the onsite terms $C_t^\dagger C_t$ and $C_{t-1}^\dagger C_{t-1}$ one ensures that $H_t^1[q] \geq 0$. The parameter $\lambda \in [0,1]$ can tune the relative strength of the hopping, but we will take $\lambda = 1$ for the rest of the paper. In order for the circuit Hamiltonian to represent the action of a quantum circuit with some single qubit gates, we must require that the fermionic occupation number $N[q] = \sum_{t=0}^{D} n_t[q] = 1$ with $n_t[q] \equiv a_t^\dagger[q]a_t[q] + b_t^\dagger[q]b_t[q]$, or that one qubit is represented by a single hopping fermion. If the original quantum circuit is universal, it will also involve CNOT gates (or controlled-U gates). The authors in [1] represent a CNOT gate between qubit c (control) and g (target) at time t by the following two terms $H_t^{CNOT}[c,g] = H_t^I[c,g] + H_t^{NOT}[c,g]$ in the circuit Hamiltonian, i.e.

$$\begin{aligned} H_t^I[c,g] = \quad & a_t^\dagger[c]a_t[c]\; n_t[g] + a_{t-1}^\dagger[c]a_{t-1}[c]\; n_{t-1}[g] \\ & - \left(a_t^\dagger[c]a_{t-1}[c]\left(a_t^\dagger[g]a_{t-1}[g] + b_t^\dagger[g]b_{t-1}[g]\right) + h.c.\right), \\ H_t^{NOT}[c,g] = {} & b_t^\dagger[c]b_t[c]n_t[g] + b_{t-1}^\dagger[c]b_{t-1}[c]n_{t-1}[g] \\ & - \left(b_t^\dagger[c]b_{t-1}[c]\left(a_t^\dagger[g]b_{t-1}[g] + b_t^\dagger[g]a_{t-1}[g]\right) + h.c.\right) \end{aligned} \tag{3}$$

Note that for a general controlled-U gate, we could take $H_t^{CU}[c,g] = H_t^I[c,g] + H_t^U[c,g]$ with the formal definition

$$\begin{aligned} H_t^U[c,g] = {} & b_t^\dagger[c]b_t[c]\; n_t[g] + b_{t-1}^\dagger[c]b_{t-1}[c]\; n_{t-1}[g] \\ & - \left(b_t^\dagger[c]b_{t-1}[c]\; C_t^\dagger[g]UC_{t-1}[g] + h.c.\right) \end{aligned}$$

For such two-qubit gates, the fermions corresponding to qubits c and g both hop forward or backward and the internal spin-state of fermion g is changed depending on the internal state of fermion c. If the original quantum circuit is 1-dimensional, then the circuit Hamiltonian describes a fairly natural interacting fermion system in 2D and thus may thus be a physically attractive system for realizing quantum adiabatic computation [11] or quantum walks [12]. Note that these interactions preserve the condition that $\forall q,\ N[q] = 1$. The authors in [11] propose to use the parameter λ to adiabatically turn the dynamics of the terms $H_t^1[q]$ (and similarly $H_2^t[q]$) on.

First, we would like to note that this model of interacting fermions can be unitarily mapped onto the space-time circuit model introduced in Section 1.1 by the following steps (see [13] for details). Instead of fermions, one can represent each qubit q by a double line of $2(D+1)$ qubits as the interactions remain local under a Jordan-Wigner transformation. Then we unitarily switch the representation of the internal state of the fermion at site t from a 'dual rail' representation $\alpha|01\rangle + \beta|10\rangle$ to $|1\rangle \otimes (\alpha|0\rangle + \beta|1\rangle)$ (while the state with no fermion in either mode at site t is mapped onto $|0\rangle \otimes |0\rangle$ and the state with two fermions at site t, which does not occur as $N[q] = 1$, gets mapped onto $|1\rangle \otimes |1\rangle$). Note that of the $2(D+1)$ qubits representing one qubit in the original circuit, after the transformation, D qubits are in the $|0\rangle$ state and can be mentally discarded. One can see that under this transformation each qubit obtains its own clock which is realized as a $D+1$ qubit register $|t\rangle = |0\rangle_1|0\rangle_2 \ldots |0\rangle_t|1\rangle_{t+1}|0\rangle_{t+2} \ldots |0\rangle_{D+1}$. This clock representation is usually called a pulse clock, as opposed to a domain wall clock which was originally introduced in [3]. In our formulation of the circuit Hamiltonian we have

not yet specified a particular clock realization; we discuss this in Section 3.2.

As the fermionic circuit Hamiltonian in the sector $N[q] = 1$ for all qubits q, is unitarily related to the circuit Hamiltonian in Section 1.1, the spectrum of the Hamiltonians is the same. In [11, 10] the authors provide bounds on the gap above the ground-space. In [11] a penalty term H_{causal} is added to $H_{circuit}$ which ensures that improper configuration have at least some constant energy, see Eq. (26) in Section 3.

The authors claim that the lowest nonzero eigenvalue of $H_{circuit}$ in the space of proper time configurations is $\Omega(S^{-4})$ where S is the size of the quantum circuit. The proof of this claim is however not contained in [11], but the authors refer back to section C in [10] where this result seems to be claimed for any quantum circuit consisting of single qubit and two-qubit gates. However, the arguments in Section C in [10] make no reference to having to exclude improper time-configurations which can easily be constructed to have zero energy. We believe that the gap analysis in these papers misses several essential and interesting aspects of the space-time circuit-to-Hamiltonian construction and warrants a more thorough mathematical investigation. This is what we set out to do in this paper.

1.4. Space-Time Circuit-to-Hamiltonian Construction with Circular Time

The construction in Sec. 1.1 gets modified when the clock registers represent a circular time. For *each* qubit q in the original circuit, we define an individual clock register $|t\rangle_q$ with $t \in Z_{2D}$. For simplicity, we again assume that the quantum circuit only contains two-qubit gates. One possible construction is to take $H_{circuit} = \sum_{t=1}^{2D} H_t$ where H_t is a sum over terms $H_t^2[q,p]$ corresponding to all the gates which occur in parallel at time-step t in the original circuit, i.e. Eq. (2) for $t \in [1, D]$. For $t \in [D+1, 2D]$ we take terms corresponding to the inverses of all the gates which occur at time-step $2D-t+1$. However, if we apply this to the circuit in Fig. (2)(b), we loose the alternating structure of the quantum circuit at times $t = 0$ and $t = D$. We can simply avoid this by assuming that in the last time-step of the circuit only I gates are performed on all qubits. Instead of undoing this gate in the next time-step at $t = D+1$, we 'undo' it in the last time-step $t = 2D$. Thus the terms H_t for $t \in [1, D]$ correspond again to the original two-qubit gates. The terms H_t with $t \in [D+1, 2D-1]$ correspond to the inverses of gates happening at time-steps $2D - t$ and the last term H_{2D} corresponds to the (trivial I) gates happening at time $t = D$ in the original quantum circuit. In this way, we can wrap the alternating gate structure around a cyclinder, Fig. (3).

What are the zero energy states for such ciruit Hamiltonian? First consider the possibility for improper time-configurations. A two-qubit gate $U^2[q,p]$ occurring at time t in the quantum circuit gets mapped onto two terms in $H_{circuit}$ in general. The gate specifies two complementary time intervals between the two gate-terms, I_t and I_t^c with $I_t \cup I_t^c = Z_{2D}$. For example, for the unraveling choice above, all gates at timesteps $t \in [1, D)$, the intervals are $I_t = [t, 2D-t-1]$ and $I_t^c = [2D-t, t-1]$ and for the I-gates at $t = D$, the intervals are $[D, 2D-1]$ and $[0, D-1]$.

A time-configuration $t_1, \ldots, t_n$ is called improper if there exists at least one pair of such qubits (q, p) interacting at time t in the original circuit, for which either $(t_q \in I_t) \wedge (t_p \in I_t^c)$ or $(t_p \in I_t) \wedge (t_q \in I_t^c)$.

Next, we consider zero energy light-like configurations. If we impose periodic boundaries conditions in space and take circular time with $n = 2kD$ with integer $k = 1, 2, \ldots$, one can construct light-like configurations, see Fig. (3). The configuration with (even) $n = 2kD$ makes a homologically nontrivial loop around the torus in both directions (one always makes a nontrivial loop around the space-direction). For $n < 2D$ and two-qubit gates throughout the quantum circuit, we note that it is not possible to have light-like configurations.

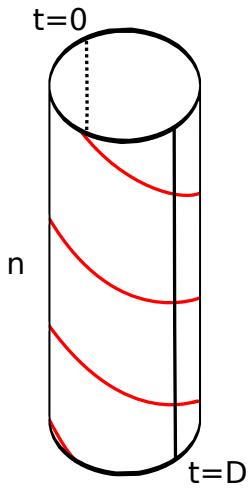


Figure 3: Space-Time Cylinder with circumference $2D$ and length n with $n = 6D$, based on quantum circuit in Fig. (2b). We identify the top and bottom of cylinder (periodic boundaries in space) to make a torus. The red line represents a zero energy light-like time configuration, a closed time-loop. Such zero energy loops can be constructed whenever $n = 2kD$ with integer k.

2. Gap of the Circuit Hamiltonian

In this section we will do the technical work of lowerbounding the gap of the circuit Hamiltonian for one-dimensional quantum circuits with closed boundary conditions in space, Fig. (2)(b), in which the circuit Hamiltonian is constructed using circular time as in Sec. 1.4. We start with some observations which hold for more general quantum circuits. We consider the gap of the circuit Hamiltonian in the space of proper time-configurations. Such proper time configurations will be denoted as $|\mathbf{t}\rangle$. We can associate a graph and its Laplacian with the circuit Hamiltonian on this proper subspace spanned by $|\mathbf{t}\rangle$. Let $G = (V, E)$ be a graph with vertices $\mathbf{t} \in V$ representing proper time-configurations and let E be the set of undirected edges of the graph. There exists an

edge $e = (\mathbf{t}, \mathbf{t}') \in E$ between proper time-configurations $\mathbf{t} \neq \mathbf{t}'$ iff

$$\langle \mathbf{t} | \, H_{circuit} \, | \mathbf{t}' \rangle = -V(\mathbf{t} \leftarrow \mathbf{t}') \neq 0,$$

for some unitary $V(\mathbf{t} \leftarrow \mathbf{t}')$, i.e. $V(\mathbf{t} \leftarrow \mathbf{t}')$ is the particular single-qubit or two-qubit gate of the quantum circuit which connects $\mathbf{t}'$ to $\mathbf{t}$. The Laplacian of the graph underlying the circuit Hamiltonian is defined as

$$L(G)_{\mathbf{t},\mathbf{t}'} = \begin{cases} \deg(\mathbf{t}), & \mathbf{t} = \mathbf{t}' \\ -1, & (\mathbf{t}, \mathbf{t}') \in E \\ 0 & else. \end{cases}$$

If G is a *connected* graph then by some number of applications of $H_{circuit}$ one can get from any proper time-configuration to any other one. We will be only interested in *connected graphs*: this precludes the existence of light-like configurations, or more generally disconnected clusters of proper time-configurations. It may be clear that for the one-dimensional quantum circuit with two-qubit gates throughout with a circular time and $2D > n$, Fig. (2b), $H_{circuit}$ corresponds to a connected graph. For a connected graph, one can always construct a path from the 'origin' time-configuration $\mathbf{t} = (0, 0, \ldots 0) = \mathbf{0}$ to any other $\mathbf{t}$. It may also be clear that there is a *unique* unitary transformation $V(\mathbf{t} \leftarrow \mathbf{0}) = V(\mathbf{t} \leftarrow \mathbf{t}_m) \ldots V(\mathbf{t}_2 \leftarrow \mathbf{t}_1) V(\mathbf{t}_1 \leftarrow \mathbf{0})$ which one can associate with such a path (of length $m + 1$) ‖. Using this composite unitary transformation $V(\mathbf{t} \leftarrow \mathbf{0})$ we can transform away the dependence of $H_{circuit}$ on the particular unitary gates. That is, let

$$W = \sum_{proper\, \mathbf{t}} V(\mathbf{t} \leftarrow \mathbf{0}) \, |\mathbf{t}\rangle \, \langle \mathbf{t}| \,, \tag{4}$$

then

$$W^\dagger H_{circuit}(\{U\}, G) W = H_{circuit}(\{U = I\}, G) = \sum_{\mathbf{t},\mathbf{t}'} L(G)_{\mathbf{t},\mathbf{t}'} \, |\mathbf{t}\rangle \, \langle \mathbf{t}'| \,. \tag{5}$$

The standard Feynman-Kitaev construction is a simple example of this in which the underlying graph is a one-dimensional line or circle and is thus connected. The space-time circuit-to-Hamiltonian construction generalizes this to high-dimensional graphs whose vertices are no longer points but strings (for one-dimensional circuits) or membranes (for two-dimensional quantum circuits) etc.

From the spectral theory of Laplacians on graphs [14], one can get some standard results, e.g.

Proposition 2.1. *The lowest eigenvalue of the Laplacian of a connected graph $G = (V, E)$ is zero and corresponds to a unique vector which is the uniform superposition over all vertices.*

‖ Note that the path may not be unique as the order in which the gates are executed is not unique, but the induced unitary transformation will nonetheless be unique.

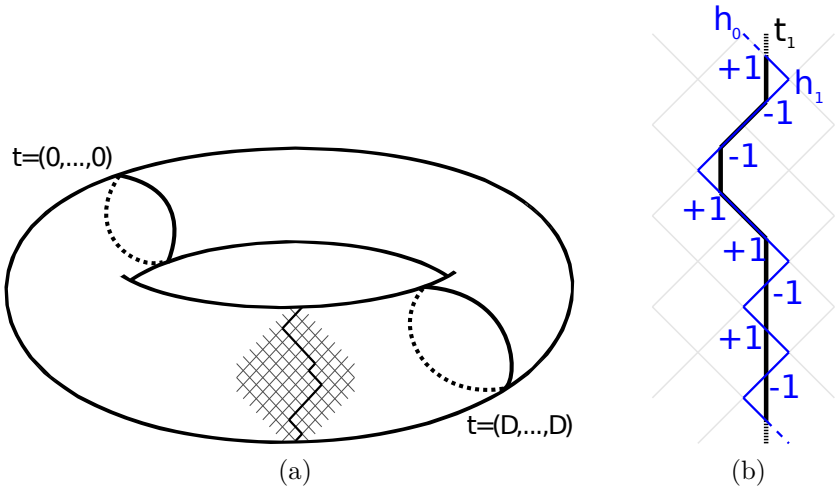
This directly implies that for circuit Hamiltonians with underlying connected graph $G = (V, E)$, the unique ground-state in the space of proper time-configurations is the history state

$$|\psi_{history}\rangle = \frac{1}{\sqrt{|V|}} \sum_{proper\ \mathbf{t}} V(\mathbf{t} \leftarrow \mathbf{0}) \, |\xi\rangle \otimes |\mathbf{t}\rangle \, , \forall \xi.$$

The second smallest eigenvalue of the Laplacian of a graph (and thus the gap of the circuit Hamiltonian) is called the algebraic connectivity. Various techniques have been developed to bound this eigenvalue [14], in particular using the theory of random walks on graphs and their mixing times.

For the one-dimensional quantum circuit in Fig. (2)(b), with the circular-time $H_{circuit}$, the graph is translationally-invariant in the 'time direction'. Due to the periodic boundaries conditions in space, the proper time-configurations corresponds to strings which wind around the torus, see Fig. 3. This model is identical to the model considered in [15]. Our question, namely bounding the mixing time of the process of diffusion of a closed string, is slightly different from the problem solved in that paper. The problem of diffusion of a domain wall (of an ferromagnetic Ising model at $T = 0$ where the Ising spin $+1$ or -1 represents whether a gate has been done or not) has also been considered in the condensed-matter literature, see e.g. [16, 17].

2.1. One-dimensional Quantum Circuits: FM Heisenberg Model Coupled to a Counter



(a) (b)

Figure 4: (a) The proper time configurations of the quantum circuit in Fig. (2)(b), using the circular-time construction, can be represented as a single string which winds around the torus. The dynamics of the circuit Hamiltonians corresponds to diffusion of this string. The square plaquettes represent the gates and the string forms the boundary of the gates that have already been executed. (b) Relabeling of the string variables using the boundary point h_0 which is next to the time t_1 of qubit 1 and the variables x_i with $(-1)^{x_i} = \pm 1$ which indicate whether the string continues left or right.

We start with a convenient relabeling of the proper time-configurations $\mathbf{t}$ as (τ, x) where $\tau \in Z_D$ and bitstring $x = x_1, x_2, \ldots, x_n$. Let t_1 be the time of one designated qubit, say, qubit 1. We assume as in Fig. (2)(b) that the first gate on qubit 1 is between qubits 1 and 2. Let $h_0 = t_1 + \frac{1}{2}$ if t_1 is even and $h_0 = t_1 - \frac{1}{2}$ if t_1 is odd so that h_0 takes on values $\frac{1}{2} + 2\tau$ with $\tau \in Z_D$, see Fig. (4)(b). Each proper time-configuration can be associated with the half integers $h \equiv h_0, h_1, \ldots, h_{n-1}$ ($h_n = h_0$) at the vertices in Fig. (4)(b) such that $(-1)^{x_i} = h_i - h_{i-1}$. Hence $\mathbf{t} \equiv (h_0, \ldots, h_{n-1}) \equiv (\tau, x_1, \ldots, x_n)$ with $x_i = 0, 1$. It is important to note that the periodic boundary conditions in space imply that $\sum_{i=1}^{n}(-1)^{x_i} = 0$ or $\sum_{i=1}^{n} Z_i = 0$, i.e. an equal number of 'spins' are up or down.

This relabeling also immediately gives us the number of vertices in the graph $G = (V, E)$ as $|V| = D\binom{n}{n/2}$. We consider the action of the circuit Hamiltonian (omitting the unitary gates due to Eq. (5) with this relabeling. Terms in $H_{circuit}$ which correspond to gates between qubits 1 and n act on h_0 and the 'spin' states x_1 and x_n. By such term h_0 can be mapped onto $h_0 \pm 2$ or the counter variable τ to $\tau \pm 1$.

Terms which correspond to gates between the other qubits do not act on the counter τ but *only* on the spin states. For adjacent variables $|x_i = 0, x_{i+1} = 1\rangle \leftrightarrow |x_i = 1, x_{i+1} = 0\rangle$ while $|x_i = 1, x_{i+1} = 1\rangle$ or $|x_i = 0, x_{i+1} = 0\rangle$ are left unchanged. The dynamics of the internal variables x corresponds to that of the isotropic ferromagnetic spin-1/2 Heisenberg model with the condition $\sum_{i=1}^{n} Z_i = 0$. More precisely, the circuit Hamiltonian (in the proper time-config. subspace) is unitarily equivalent to

$$\begin{aligned}\tilde{H}_{circuit} = & \sum_{i=1}^{n-1}(\sigma_i^+\sigma_i^-\sigma_{i+1}^-\sigma_{i+1}^+ + h.c) - \sum_{i=1}^{n-1}(\sigma_i^+\sigma_{i+1}^- + h.c.) \\ & + \left(\sigma_n^+\sigma_n^-\sigma_1^-\sigma_1^+ + h.c\right) - \left(\sigma_1^-\sigma_n^+ \sum_{\tau=0}^{D-1} |\tau - 1\rangle\langle\tau| + h.c.\right). \end{aligned} \tag{6}$$

The eigenstates of $\tilde{H}_{circuit}$ with respect to the counter variable τ are simple plane-waves, i.e.

$$\begin{aligned} |\psi_k\rangle &= \frac{1}{\sqrt{D}} \sum_{\tau=0}^{D-1} e^{2\pi i k\tau/D} |\tau\rangle, \quad k = 0, \ldots D-1, \\ \tilde{H}_{circuit} |\psi_k\rangle &= H(k) |\psi_k\rangle, \end{aligned} \tag{7}$$

where

$$H(k) = \frac{n-1}{2} - \frac{1}{2}\sum_{i=1}^{n-1}(X_iX_{i+1} + Y_iY_{i+1} + Z_iZ_{i+1}) + \Delta(k), \tag{8}$$

with

$$\Delta(k) = \frac{1}{2}(1 - Z_1Z_n) - \sigma_1^-\sigma_n^+ e^{2\pi ik/D} - \sigma_1^+\sigma_n^- e^{-2\pi ik/D} \geq 0. \tag{9}$$

The eigenstates (and eigenvalues) of $\tilde{H}_{circuit}$ are thus the eigenstates of $H(k)$ in tensorproduct with the plane-wave states $|\psi_k\rangle$. $H(k = 0)$ is the ferromagnetic (spin-$\frac{1}{2}$)

Heisenberg chain with periodic boundary conditions (in the sector with $\sum_i Z_i = 0$), i.e.

$$H(k=0) = \frac{n}{2} - \frac{1}{2}\sum_{i=1}^{n}(X_iX_{i+1} + Y_iY_{i+1} + Z_iZ_{i+1}) \geq 0. \tag{10}$$

This model can be analyzed using the Bethe ansatz, see e.g. [18]. Note that the condition $\sum_i Z_i = 0$ is not the usual one studied in physics: one can interpret it as there being $n/2$ particles (out of n) which by the dynamics of $H(k)$ can interchange positions on a circle. The model $H(k \neq 0)$ corresponds to a ferromagnetic Heisenberg chain with a *partially twisted boundary*. It may be possible to determine the full spectrum of the partially-twisted Heisenberg chain $H(k)$ with a Bethe ansatz, but here we focus on determining the lowest eigenvalues.

The unique groundstate of $\tilde{H}_{circuit}$ is the zero energy groundstate of $H(k=0)$, the state $\frac{1}{\sqrt{D\binom{n}{n/2}}}\sum_{\tau=0}^{D-1}\sum_{x:\sum(-1)^{x_i}=0}|\tau, x\rangle$.

The gap of the ferromagnetic Heisenberg chain $H(k=0)$ for n spins with $\sum_i Z_i = 0$ has been lowerbounded, e.g. by using the connection to the theory of Markov chains, see Theorem 2.5 in Section 2.1.1. In order to lowerbound the gap of $\tilde{H}_{circuit}$, we also need to lowerbound the groundstate energies for any $H(k \neq 0)$. Let us outline the remainder of our proof. We have $H(k) = A + B$ where A is the ferromagnetic Heisenberg chain with *open boundaries*, i.e. let

$$A \equiv \frac{n-1}{2} - \frac{1}{2}\sum_{i=1}^{n-1}(X_iX_{i+1} + Y_iY_{i+1} + Z_iZ_{i+1}) \geq 0 \tag{11}$$

and $B \equiv \Delta(k \neq 0)$. We will invoke the following lemma

Lemma 2.2 (Kitaev[3])**.** *Let $A \geq 0$ and $B \geq 0$ and let $\ker(A)/\ker(B)$ be their respective nullspaces, where $\ker(A) \cap \ker(B) = \{0\}$. Let $\lambda_1(A)$ ($\lambda_1(B)$) be the smallest nonzero eigenvalue of A (B). Then*

$$A + B \geq \min(\lambda_1(A), \lambda_1(B)) \cdot (1 - \cos(\theta)).$$

with $\cos(\theta) = \max_{\psi_B \in \ker(B), \psi_A \in \ker(A)} |\langle\psi_A|\psi_B\rangle|$.

Thus if we can bound the gap of A (see Lemma 2.6 in Section 2.1.1) and bound the gap of the boundary term $\Delta(k \neq 0)$ (this is simple as it involves two qubits) and bound the angle between the two null-spaces $\ker(A)$ and $\ker(B)$ (see Lemma 2.4), we can obtain a lowerbound on the smallest eigenvalue of $H(k \neq 0)$. Together with the lowerbound on the gap of $H(k=0)$, Theorem 2.5, this will prove the following result:

Theorem 2.3. *The smallest non-zero eigenvalue λ_1 of the space-(circular) time Hamiltonian $H_{circuit}$ of a one-dimensional, depth D (with $2D > n$), quantum circuit on n qubits as in Fig. (2)(b) in the space of proper time-configurations, is bounded as*

$$\lambda_1(H_{circuit}) = \lambda_1(\tilde{H}_{circuit}) \geq \frac{3\pi^2 n}{D^2(n-1)^2(n+1)(n/2+1)} + O\left(\frac{1}{n^3D^4}\right). \tag{12}$$

Proof: As we argued before, the spectrum of $H_{circuit}$ is that of $\tilde{H}_{circuit}$ is that of $H(k)$ for all k. Theorem 2.5 shows that $\lambda_1(H(k=0)) = \Omega(\frac{1}{n^2})$, but $H(k \neq 0)$ may have lower nonzero eigenvalues. We invoke Lemma 2.2. We have $\lambda_1(B) \geq 2$ by direct calculation and we use Lemma 2.6 to lowerbound $\lambda_1(A)$. The angle between the null-spaces $\ker(A)$ and $\ker(B)$ is given in Lemma 2.4. This results in Eq. (12). □

Lemma 2.4 (Angle between Subspaces)**.** *Let A be the open-boundary Heisenberg chain defined in Eq.(11) and let B be the boundary term $B = \Delta(k \neq 0)$ defined in Eq. (9) and* $\cos(\theta) = \max_{\psi_B \in \ker(B), \psi_A \in \ker(A)} |\langle \psi_A | \psi_B \rangle|$. *Then*

$$1 - \cos(\theta) \geq \frac{\pi^2 n}{4D^2(n-1)} + O\left(\frac{1}{D^4}\right).$$

Proof: The groundstate $|\psi_A^0\rangle = \binom{n}{n/2}^{-1/2} \sum_{x:\sum_i (-1)^{x_i}=0} |x\rangle$ of A is unique, see also Section 2.1.1. Thus we consider

$$1 - \cos(\theta) = \min_{\psi_B \in \mathrm{Ker}(B)} \left(1 - \sqrt{F(\psi_A^0, \psi_B)}\right),$$

with the fidelity $F(\sigma, \rho) = \left(\mathrm{Tr}\sqrt{\rho^{1/2}\sigma\rho^{1/2}}\right)^2$ for two arbitrary density matrices σ and ρ. We can use the monotonicity of fidelity under taking partial traces, i.e. $F(\rho_A^0, \rho_B) \geq F(\psi_A^0, \psi_B)$ [19] for the reduced density matrices ρ_A^0 and $\rho_B(k)$ for qubits 1 and n. The reduced density matrix of ψ_A^0 equals

$$\rho_A^0 = \frac{n-2}{4(n-1)} \left(|00\rangle\langle 00| + |11\rangle\langle 11|\right) + \frac{n}{2(n-1)} |\eta_0\rangle\langle\eta_0|,$$

with $|\eta_0\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$. The space $\ker B$ is spanned by vectors of the form $|00\rangle \otimes |\psi_{00}\rangle$,$|11\rangle \otimes |\psi_{11}\rangle$ and $|\eta_k\rangle \otimes |\psi_{\eta_k}\rangle$ with $|\eta_k\rangle = \frac{1}{\sqrt{2}}(|01\rangle + e^{-2\pi i k/D}|10\rangle)$. Here $|\psi_{00}\rangle, |\psi_{11}\rangle, |\psi_{\eta_k}\rangle$ are orthogonal as they contain a different number of particles (remember $\sum_i Z_i = 0$). As the states in the nullspace of B are not fully symmetric under all permutations of particles, the null-spaces of A and B have zero intersection. A reduced density matrix $\rho_B(k)$ can thus be parametrized as

$$\rho_B(k) = |\alpha|^2 |00\rangle\langle 00| + |\beta|^2 |11\rangle\langle 11| + |\gamma|^2 |\eta_k\rangle\langle\eta_k|,$$

with $|\alpha|^2 + |\beta|^2 + |\gamma|^2 = 1$, so that

$$\mathrm{Tr}\left(\rho_B^{1/2}(k)\, \rho_A^0\, \rho_B^{1/2}(k)\right)^{1/2} = (|\alpha| + |\beta|)\sqrt{\frac{n-2}{4(n-1)}} + |\gamma|\sqrt{\frac{n}{2(n-1)}}|\langle\eta_0|\eta_k\rangle|.$$

Using the Cauchy-Schwartz inequality and $|\langle\eta_0|\eta_k\rangle|^2 = \frac{1+\cos(2\pi k/D)}{2}$ we can upperbound

$$\sqrt{F(\rho_A^0, \rho_B(k))} \leq \sqrt{\frac{2(n-2)}{4(n-1)} + \frac{n(1+\cos(2\pi k/D))}{4(n-1)}}.$$

This fidelity is clearly maximized for the lowest non-zero momentum $k = 1$ (or $k = D-1$) so that, using the Taylor expansion for the cosine and square-root, we can bound

$$\sqrt{F(\psi_A^0, \psi_B)} \leq 1 - \frac{\pi^2 n}{4D^2(n-1)} + O\left(\frac{1}{D^4}\right).$$

□

2.1.1. Heisenberg Chain With (Open) Boundaries: connection with Markov chains We use the known connection between the Heisenberg model and a particle interchange model, see e.g. [18]. Let $P_{i,i+1}$ be a transposition (permutation) of particles at i and $i+1$, i.e. $P_{i,i+1}\left|01\right\rangle_{i,i+1} = \left|10\right\rangle_{i,i+1}$, $P_{i,i+1}\left|10\right\rangle_{i,i+1} = \left|01\right\rangle_{i,i+1}$ and $P_{i,i+1}\left|11\right\rangle_{i,i+1} = \left|11\right\rangle_{i,i+1}$ and $P_{i,i+1}\left|00\right\rangle_{i,i+1} = \left|00\right\rangle_{i.i+1}$. We can define the symmetric, stochastic Markov matrices $P(x,y) = \frac{1}{n-1}\sum_{i=1}^{n-1}\left\langle y\right| P_{i,i+1}\left|x\right\rangle$ and $\tilde{P}(x,y) = \frac{1}{n}\sum_{i=1}^{n}\left\langle y\right| P_{i,i+1}\left|x\right\rangle$ on the space of bitstrings $\left|x\right\rangle$ with $\sum_i (-1)^{x_i} = 1$, or the space with $n/2$ particles (out of n). The Hamiltonians in Eqs. (11), (10) can then be written as $A = (n-1) - \sum_{i=1}^{n-1} P_{i,i+1}$ or $\left\langle y\right| A\left|x\right\rangle = (n-1)(\delta_{xy} - P(x,y))$ and $H(k=0) = n - \sum_{i=1}^{n} P_{i,i+1}$ or $\left\langle y\right| H(k=0)\left|x\right\rangle = n(\delta_{xy} - \tilde{P}(x,y))$.

The Markov processes given by $P(x,y)$ and $\tilde{P}(x,y)$ are both reversible, irreducible and aperiodic. Thus P and $\tilde{P}$ has a unique fixed point $\pi(x) = \binom{n}{n/2}^{-1}$ (see e.g. [20]). The second largest eigenvalue of P ($\tilde{P}$) determines the smallest non-zero eigenvalue of the Heisenberg chain with open (closed) boundary. The second largest eigenvalue of $\tilde{P}$ has previously been bounded, i.e.

Theorem 2.5 (Theorem 3.1 in [21], see also [18])**.** *Let $\tilde{P}$ be the reversible, irreducible Markov chain defined above with eigenvalues $\tilde{\beta}_0 = 1 > \tilde{\beta}_1 > \tilde{\beta}_2 \geq \ldots$. Then the second largest eigenvalue of $\tilde{P}$ is*

$$\tilde{\beta}_1 \leq 1 - \frac{12}{(n+1)(n/2+1)n},$$

which directly implies that

$$\lambda_1(H(k=0)) \geq \frac{12}{(n+1)(n/2+1)}.$$

To bound the second largest eigenvalue of the Markov chain P, we relate this Markov process to that of $\tilde{P}$ and use the method of Markov chain comparison introduced in [21]. Essentially, we are applying the ideas which prove Theorem 2.5 to our particular case without any change. The idea is to show how to simulate (the flow through) the Markov process $\tilde{P}$, which can use the boundary permutation $P_{1,n}$, using the possible transitions of P, but without overloading the edges of the graph underlying P too much. Diaconis and Saloff-Coste [21] prove that for two Markov chains P and $\tilde{P}$ with the same state space and the same unique fixed point, we have

$$\beta_1 \leq 1 - \frac{1}{\Omega}(1 - \tilde{\beta}_1), \tag{13}$$

with the quantity Ω defined as follows. Let $E = \{(x,y); P(x,y) > 0\}$ be the edges of the Markov chain P and let $\tilde{E} = \{(x,y); \tilde{P}(x,y) > 0\}$, the edges of the Markov chain $\tilde{P}$. Note that $E \subseteq \tilde{E}$ in our case as in the process given by P we have $\binom{n-2}{n/2-1}$ fewer edges, corresponding to all pairs (x,y) which are related by a particle hopping between positions 1 and n. Let this difference set be $\mathrm{Dif} = \tilde{E} - E$. For each edge $(x,y) \in \tilde{E}$ one constructs a path $x_0 = x, x_1, x_2, ..., x_k = y$ with $P(x_i, x_{i+1}) > 0$ from x to y. In our case, for elements in $E \cap \tilde{E}$, we take the path to be of length 1 as $P(x,y) > 0$. For elements

$(x, y) \in \text{Dif}$ we construct an explicit path γ_{xy} of length at most $n-1$ below. Note that one constructs paths for $x \to y$ and $y \to x$.

One defines $\tilde{E}(e)$ as the number of paths which go through the edge $e \in E$, i.e. $\tilde{E}(e) = \{(x, y) \in \tilde{E} | e \in \gamma_{xy}\}$. For a given edge e, there is at least one path that goes through it, namely the path of length 1, but as we need to reroute all the flow for $(x, y) \in \text{Dif}$, there will be other paths corresponding to elements in Dif which pass through this edge as well. The quantity Ω for a given set of paths γ_{xy} is defined as

$$\Omega = \max_{(z,w)\in E} \left(\frac{1}{\pi(z)P(z,w)} \sum_{\tilde{E}(z,w)} |\gamma_{xy}| \tilde{\pi}(x) \tilde{P}(x,y) \right).$$

The goal is thus to choose a set of paths γ_{xy} such that Ω is small. In our case, the expression for Ω can be simplified since

$$\max_{x,y,z,w:P(z,w)>0} \frac{\tilde{P}(x,y)}{P(z,w)} = \frac{n-1}{n}.$$

Furthermore, the length of the paths γ_{xy} below is at most $n-1$, so that

$$\Omega = \frac{(n-1)^2}{n} \max_{e\in E} \sum_{\tilde{E}(e)} 1.$$

There are $\binom{n-2}{n/2-1}$ pairs (x, y) of the form $(x = 1\, z\, 0, y = 0\, z\, 1)$ where z is a $n-2$ bit string for which we have to construct a path using transpositions $01 \leftrightarrow 10$ between neighboring positions $1, 2 \ldots, n$. A good path is constructed in [21] and consists of swapping the particle on, say, the left boundary to the first group of 11s, then taking the rightmost 1 in that group and swapping it forward to the next group of 11s etc. until the particle is at the right end of the chain. Then we go back and 'clean up' to revert the $n-2$ bits in the middle back to the initial z. The length of this path, –the number of transpositions–, is at most $n-1$, as shown in [21]. Furthermore, as argued in Ref. [21], given a (directed) edge $e = (x_i, x_{i+1})$ on the graph, one can reconstruct from which x one came and to what y one is going. This implies that the number of such paths swapping particles at the left and right boundary which go through a particular edge is just 1 and $\Omega = 4(n-1)$. These arguments prove the lemma:

Lemma 2.6. *Let $P(x, y)$ be the Markov chain associated with the open-boundary Heisenberg model defined in Eq. (11), with eigenvalues $\beta_0 = 1 > \beta_1 \geq \beta_2 \geq \ldots$. By Eq. (13) [21] and the arguments above we have*

$$\beta_1 \leq 1 - \frac{12}{(n-1)^2(n+1)(n/2+1)}$$

This implies that

$$\lambda_1(A) \geq \frac{12}{(n+1)(n/2+1)(n-1)} = \Theta(n^{-3}).$$

3. Application to QMA and Quantum Adiabatic Computation

3.1. Quantum Merlin Arthur

The complexity class QMA (Quantum Merlin Arthur) [3] is the quantum equivalent of the class NP (or its probabilistic variant MA). Informally, in QMA the classical proof or witness and the classical verifier of NP are replaced by a quantum proof $|\xi\rangle$ and a quantum verifier. The formal definition is

Definition 3.1 (QMA [3, 22])**.** A promise problem $L = L_{yes} \cup L_{no} \subseteq \{0,1\}^*$ belongs to QMA iff there exist a polynomial $p(n)$ and a uniformly generated family of quantum circuits $\{C_n\}$ such that for all n and all $x \in \{0,1\}^n$,

$$x \in L_{yes} \Rightarrow \exists\, \xi, \quad \mathbf{Pr}[C_n(x,\xi) = 1] \geq 2/3, \quad \text{(Completeness)}$$
$$x \in L_{no} \Rightarrow \forall\, \xi, \quad \mathbf{Pr}[C_n(x,\xi) = 1] \leq 1/3. \quad \text{(Soundness)}$$

The completeness and soundness errors $(\frac{2}{3}, \frac{1}{3})$ can be amplified to $(1-\epsilon, \epsilon)$ where $\epsilon = 2^{-\mathrm{poly}(n)}$ [3, 23], thus making these errors exponentially small, without increasing the number of qubits of the witness ξ.

To prove that a computational (promise) problem is QMA-complete, one needs to prove that (1) the problem is contained in the complexity class QMA and (2) that the problem is QMA-hard. The general 'local Hamiltonian' problem has been shown to be in QMA, e.g.

Proposition 3.2 ([3])**.** *Let $H = \sum_i H_i$ be a Hamiltonian on n qubits with $||H_i|| = O(1)$ and each H_i acts on $O(1)$ qubits non-trivially. We have the following promise: either there exists a state ψ, $\langle\psi| H |\psi\rangle \leq a$ (*YES*) or $\forall\psi, \langle\psi| H |\psi\rangle \geq b$ (*NO*) for some given a, b (described by some* poly(n) *bits) with $|a-b| \geq \frac{1}{\mathrm{poly}(n)}$. The problem of deciding between YES and NO is in the class* QMA*.*

The idea behind the containment in QMA is simple: if YES, Merlin (the prover) can give Arthur (the verifier) a ground-state and Arthur can estimate the energy of this state with $1/\mathrm{poly}(n)$ precision using an efficient quantum circruit. If this answer is NO, then Merlin cannot give any state which has low enough energy to fool Arthur.

Using the circuit-to-Hamiltonian construction, Kitaev proved that 5-local Hamiltonian problem (where each H_i acts on at most 5 qubits) is QMA-complete [3]. Since then, many variants of the local Hamiltonian problem have been shown to be QMA-complete or QMA_1-complete, such as 1D local Hamiltonians [24]. See [25, 26] and references therein for the most recent results. Various new results for QMA-complete problems have so far come about by modifications of the circuit-to-Hamiltonian construction, different realizations of clocks and the use of perturbation gadgets [27]. We now show how the space-time circuit-to-Hamiltonian construction can also be used to give QMA-completeness results.

As the general local Hamiltonian problems is contained in QMA, it is the second part of the QMA-completeness which concerns us here. We construct a map from any class of problems $L = L_{yes} \cup L_{no}$ in QMA to a Hamiltonian such that:

- if $x \in L_{yes}$, then the Hamiltonian $H(x)$ has eigenvalue lower than or equal to some a, see Sec. 3.1.1.
- if $x \in L_{no}$, then all eigenvalues of the Hamiltonian are larger than or equal to b where $|a-b| \geq \frac{1}{\text{poly(n)}}$, see Sec. 3.1.2.

A property that any promise problem L in QMA possesses is the existence of the verification circuits C_n with the properties in Definition 3.1. The quantum circuit C_n takes as input the unspecified quantum proof $|\xi\rangle$ provided by Merlin and some initial input qubits in a set S_{in} set to $|0\rangle$ or $|1\rangle$ with $|S_{in}| = m < n$. The instance x is also part of this input set of qubits. Whether qubits in S_{in} are set to 0 or 1 plays no role in the proof, so for notational simplicity we require the qubits in S_{in} to be $|0\rangle$.

W.l.o.g. we can take the verification circuit to be of the form, Fig. (2), as such one-dimensional quantum circuits with only two-qubit gates are universal. The circuit acts on n qubits and has depth D which is a some polynomial in n. Let q_{out} be the output qubit of the circuit C_n, so that $\mathbf{Pr}[C_n(x,\xi) = 1] = \mathbf{Pr}[q_{out} = 1]$.

For every qubit in the quantum circuit, one can define a past causal cone of qubits, namely those qubits which could have influenced the state of that qubit at the end of the computation. It is important to note that we may assume w.l.o.g. that the qubits in the set S_{in} are in the past causal cone of the output qubit q_{out}. If they are not, then these qubits are not needed to produce this output so we could omit them. The Hamiltonian which corresponds to a verification circuit is

$$H = H_{circuit} + H_{in} + H_{out} + H_{causal} \tag{14}$$

where $H_{circuit}$ is the space-time circuit Hamiltonian of the verification circuit in Fig. (2)(b) with circular time. Recall that we have shown that the unique zero energy ground-state (space) of this $H_{circuit}$ is of the form

$$\begin{aligned} |\psi_{history}\rangle &= \frac{1}{\sqrt{D\binom{n}{n/2}}} \sum_{proper\ \mathbf{t}} V(\mathbf{t} \leftarrow \mathbf{0}) \, |\phi_{in}\rangle \otimes |\mathbf{t}\rangle \,, \\ |\phi_{in}\rangle &= \sum_{y \in \{0,1\}^m} \alpha_y \, |\xi_y\rangle \, |y\rangle_{S_{in}} \,. \end{aligned} \tag{15}$$

Here y are the input-qubits in S_{in} and $|\xi_y\rangle$ is a general input state of the other qubits. One makes the following choice for H_{in} and H_{out}:

$$\begin{aligned} H_{in} &= \sum_{p \in S_{in}} |1\rangle \langle 1|_p \otimes |t=0\rangle \langle t=0|_p \,, \\ H_{out} &= |0\rangle \langle 0|_{q_{out}} \otimes |t=D\rangle \langle t=D|_{q_{out}} \,. \end{aligned} \tag{16}$$

The term H_{causal} is a penalty term for improper time-configurations. It is a sum of terms, one for each two-qubit gate in the original quantum circuit. Let there be a gate acting at time t on qubits $[q,p]$ in the original quantum circuit. Let $\Pi(t_q \in I_t) = \sum_{s \in I_t} |s\rangle \langle s|_q$

where the interval I_t (and I_t^c) were defined in Section 1.4. Such projector acts on the time register of qubit q and has eigenvalue 1 if $t_q \in I_t$ (and 0 otherwise). The penalty term corresponding to this gate equals

$$H_{causal}([q,p],t) = \Pi(t_q \in I_t)\Pi(t_p \in I_t^c) + \Pi(t_p \in I_t)\Pi(t_q \in I_t^c). \tag{17}$$

H_{causal} commutes with H_{in} and H_{out} as all terms are diagonal in the same basis. Each term $H_{causal}([q,p],t)$ commutes with $H_{circuit}$ as follows. First of all, $H_{causal}([q,p],t)$ commutes with the two terms which represent the gate $U_t^2[q,p]$ in the circuit Hamiltonian, as $H_{causal}([q,p],t)H_t^2[q,p] = 0$ etc. It obviously commutes with any $H_t^2[q',p']$ with $q' \neq q$ and $p' \neq p$. Lastly, it commutes with any $H_{t'}^2[q,p']$ or $H_{t'}^2[q',p]$ or $H_{t'}^2[q,p]$ as these terms can propagate the clock of one qubit or both qubits, but they cannot propagate the times of these clocks out of the complementary intervals I_t and I_t^c. In other words, these last terms commute with the individual projectors $\Pi(t_q \in I_t)$,$\Pi(t_p \in I_t), \Pi(t_p \in I_t^c), \Pi(t_q \in I_t^c)$. The commutativity implies that the eigenstates of H either reside in the subspace where $H_{causal} = 0$, i.e. the proper time-configuration subspace, or the subspace where H_{causal} has its lowest nonzero eigenvalue which is 1. In this way we impose an energy penalty on improper time-configurations and we can ignore them in the remainder of the analysis.

In the next two sections, we do the technical work of establishing both aspects of the map where the final results are expressed in Eq. (18) and Eq. (19). Note that the difference between a and b scales as $1/S^2$ where S is the size of the verification circuit, if ϵ is sufficiently small. This proof is very analogous to the standard proof, first given in [3], with similar results, but the notation and some of details are a bit more cumbersome.

3.1.1. Yes-instance ⇒ (almost) zero energy groundstate We assume that there exists an input witness state $|\xi\rangle$ such that the verification circuit C_n has $q_{out} = 1$ with probability $1-\epsilon$. We construct a low-energy state for the Hamiltonian H in Eq. (14) as the history state, Eq. (15), with $|\phi_{in}\rangle = |\xi\rangle\,|y = 00\ldots0\rangle$. The terms H_{in}, H_{prop} and H_{causal} have zero energy with respect to this state, thus

$$\begin{aligned}&\langle\psi_{history}|\, H\, |\psi_{history}\rangle = \langle\psi_{history}|\, H_{out}\, |\psi_{history}\rangle \\ &= \frac{1}{D\binom{n}{n/2}} \sum_{\mathbf{t}:t_{q_{out}}=D} \langle\xi, 00\ldots0|\, V^\dagger(\mathbf{t} \leftarrow \mathbf{0})\, |0\rangle\, \langle 0|_{q_{out}}\, V(\mathbf{t} \leftarrow \mathbf{0})\, |\xi, 00\ldots0\rangle\,.\end{aligned}$$

Note that the proper times $\mathbf{t}$ with $t_{q_{out}} = D$ are times such that $V(\mathbf{t} \leftarrow \mathbf{0})$ is the product of a set of elementary gates which *includes all gates which are in the past causal cone of* q_{out}. Said differently, it includes all gates which are needed to produce the correct circuit outcome for the output qubit q_{out}. Hence $\langle\xi, 00\ldots0|\, V^\dagger(\mathbf{t} \leftarrow \mathbf{0})\, |0\rangle\, \langle 0|_{q_{out}}\, V(\mathbf{t} \leftarrow \mathbf{0})\, |\xi, 00\ldots0\rangle \leq \epsilon$. The number of $\mathbf{t}$ for which $t_{q_{out}} = D$ is simply $\binom{n-1}{\frac{n}{2}-1}$ as fixing the time for one qubit fixes the counter τ and the first bit of the bit string x. Thus

$$\langle\psi_{history}|\, H\, |\psi_{history}\rangle \leq \frac{\epsilon}{2D} \equiv a. \tag{18}$$

3.1.2. No-instance ⇒ ground-state energy of Hamiltonian bounded away from zero We start from the assumption that for all inputs $|\xi\rangle |00\dots0\rangle_{S_{in}}$ to the verification circuit C_n, $\mathbf{Pr}[q_{out}=1] \leq \epsilon$. Due to the presence of H_{causal} and the fact that $H_{circuit}$ preserves the subspace of proper time-configurations, the eigenstates of H in the space of improper time configurations have energy penalty at least 1. We thus consider the spectrum of $H_{circuit} + H_{in} + H_{out}$ in the space of proper time configurations.

We apply Lemma 2.2 with $A = H_{circuit}(\{U\})$ and $B = H_{in} + H_{out}$ which have no common null-space as the quantum circuit never outputs $q_{out} = 1$ for some correctly initialized input state by assumption. The final result is the following lowerbound

Lemma 3.3. *For a no-instance the smallest eigenvalue of the Hamiltonian H can be lowerbounded as*

$$\lambda_1(H) \geq \Omega\left(\frac{1}{D^2n^2}\right)\left(\frac{1}{4D} - O\left(\frac{\epsilon}{D}\right)\right) \equiv b \tag{19}$$

Proof: Theorem 2.3 provides the lower-bound on $\lambda_1(H_{circuit})$. Consider B and note that the set $\{\mathbf{t}: t_{q_{out}} = D\}$ is disjoint from the sets $\{\mathbf{t}: t_{p\in S_{in}} = 0\}$ as we have assumed that the qubits in S_{in} are in the past causal cone of q_{out} thus their clocks cannot read $t = 0$ while the clock of the output qubit reads D! This means that $\lambda_1(B) \geq 1$. To apply Lemma 2.2, we need to bound the angle between the null-spaces of A and B. The nullspace of A only contains the history states $\psi_{history}$ in Eq. (15). The goal is to upperbound $\cos^2(\theta) = \max_{\psi_{history}} \langle\psi_{history}| \Pi_B |\psi_{history}\rangle$ where Π_B is the projector onto the nullspace of B. We can write $|\psi_{history}\rangle = \alpha_I |\psi_I\rangle + \alpha_{NI} |\psi_{NI}\rangle$ where ψ_I is a state which is properly initialized, i.e. $|\phi^I_{in}\rangle = |\xi, 00\dots0\rangle$ and ψ_{NI} is some state which is not properly initialized. We have

$$\begin{aligned}\langle\psi_{history}| \Pi_B |\psi_{history}\rangle = |\alpha_I|^2 \langle\psi_I| \Pi_B |\psi_I\rangle + |\alpha_{NI}|^2 \langle\psi_{NI}| \Pi_B |\psi_{NI}\rangle \\ + 2Re(\alpha_I\alpha^*_{NI} \langle\psi_{NI}| \Pi_B |\psi_I\rangle).\end{aligned} \tag{20}$$

We will separately determine the maximum values of $\langle\psi_I| \Pi_B |\psi_I\rangle$ and $\langle\psi_{NI}| \Pi_B |\psi_{NI}\rangle$ and the crossterm $|\langle\psi_{NI}| \Pi_B |\psi_I\rangle|$. We start with some basic observations. The nullspace of B is a direct sum of spaces $\ker(B) = \ker(B)_{out} \oplus \ker(B)_{in} \oplus \ker(B)_{int}$ with the three orthogonal null-spaces:

$$\begin{aligned}\ker(B)_{out} &= \text{span}\left(|1\rangle_{q_{out}} |v\rangle \otimes |\mathbf{t}: t_{q_{out}} = D\rangle, \forall |v\rangle \in (\mathcal{C}^2)^{\otimes n-1}\right)\\ \ker(B)_{in} &= \text{span}\Big(|w\rangle |00\dots0\rangle_{S(x)} \otimes |\mathbf{t}: \forall p \in S(x),\ (t_p = 0)\rangle,\\ &\qquad \forall S(x) \neq \emptyset \subseteq S_{in}, \forall |w\rangle \in (\mathcal{C}^2)^{\otimes n-1}\Big)\\ \ker(B)_{int} &= \text{span}\left(|\xi\rangle \otimes |\mathbf{t}: (\forall p, t_p \neq 0) \wedge (t_{q_{out}} \neq D)\rangle, \forall |\xi\rangle \in (\mathcal{C}^2)^{\otimes n}\right).\end{aligned}$$

We have $\Pi_B = \Pi_{in} + \Pi_{out} + \Pi_{int}$ where Π_{in}, Π_{out} and Π_{int} are the projectors onto these three null-spaces. As Π_{int} is diagonal in the $\mathbf{t}$-basis, we have

$$\langle\psi_{history}| \Pi_{int} |\psi_{history}\rangle = \frac{|\{\mathbf{t}: (t_{q_{out}} \neq D) \wedge (\forall p \in S_{in}, t_p \neq 0)\}|}{D\binom{n}{n/2}},$$

independent of initialization or the witness state.

By assumption on the verification circuit we have for all proofs $|\phi_{in}^I\rangle = |\xi, 00\ldots0\rangle$

$$\begin{aligned}\langle\psi_I|\,\Pi_{out}\,|\psi_I\rangle &= \frac{1}{D\binom{n}{n/2}}\sum_{\mathbf{t}:t_{q_{out}}=D}\langle\phi_{in}^I|\,V^\dagger(\mathbf{t}\leftarrow\mathbf{0})\,|1\rangle\,\langle 1|_{q_{out}}\,V(\mathbf{t}\leftarrow\mathbf{0}\,|\phi_{in}^I\rangle\\ &\leq \frac{\epsilon}{2D},\end{aligned}$$

where we used that *all* $V(\mathbf{t}\leftarrow\mathbf{0})$ with $t_{q_{out}}=D$ are evolutions which lead to the correct output of the verification circuit. This implies that for all proofs ψ_I, we have

$$\langle\psi_I|\,\Pi_B\,|\psi_I\rangle = 1-\frac{1-\epsilon}{2D}. \tag{21}$$

Consider next $\langle\psi_{NI}|\,\Pi_B\,|\psi_{NI}\rangle$. We have $\langle\psi_{NI}|\,\Pi_B\,|\psi_{NI}\rangle \leq \max_{\psi_{NI}}\langle\psi_{NI}|\,\Pi_{out}\,|\psi_{NI}\rangle + \max_{\psi_{NI}}\langle\psi_{NI}|\,\Pi_{int}+\Pi_{in}\,|\psi_{NI}\rangle$. The first term is maximized when we assume that all improperly initialized states lead to $q_{out}=1$. We focus on upperbounding the last term $\langle\psi_{NI}|\,\Pi_{in}\,|\psi_{NI}\rangle$. We write

$$\Pi_{in} = \sum_{S\neq\emptyset\in S_{in}}|00\ldots\rangle\langle00\ldots|_S\otimes P_S, \tag{22}$$

with P_S the projector onto all $|\mathbf{t}\rangle$ for which $(\forall p\in S, t_p=0)\wedge(\forall p\in S_{in}\backslash S, t_p\neq 0)$. Let the state ψ_{NI} be initialized to some $|\phi_{in}^{NI}\rangle = \sum_{y\neq00\ldots0\in\{0,1\}^m}|\xi_y\rangle\otimes|y\rangle_{S_{in}}$. We note that the projector Π_{in} in Eq. (22) acts diagonally on the basis $|y\rangle_{S_{in}}$ which implies that the input state ϕ_{in}^{NI} initialized with a $|y\rangle_{S_{in}}$ which 'incurs a minimal penalty' is the one which for which $\langle\psi_{NI}|\,\Pi_{in}\,|\psi_{NI}\rangle$ is maximized. For this particular y, all qubits in S_{in} are set to 0, except for one qubit, call it qubit q_1, whose state is set to 1. Let this particular subset of qubits which is initialized to 0 be $T\subseteq S_{in}$ ¶. Taking $|\psi_{NI}\rangle$ initialized with $|\phi_{in}^{NI}\rangle = |\xi\rangle\,|100\ldots0\rangle_{S_{in}}$, one has:

$$\begin{aligned}\langle\psi_{NI}|\,\Pi_{in}\,|\psi_{NI}\rangle &= \sum_{\emptyset\neq S\subseteq S_{in}}\frac{\mathrm{Rank}(P_S)}{D\binom{n}{n/2}}\mathrm{Tr}(|10\ldots0\rangle\langle10\ldots0|_{S_{in}}\,|0\ldots0\rangle\langle00\ldots0|_S)\\ &= \sum_{\emptyset\neq S\subseteq T}\frac{\mathrm{Rank}(P_S)}{D\binom{n}{n/2}} = \sum_{\emptyset\neq S\subseteq S_{in}}\frac{\mathrm{Rank}(P_S)}{D\binom{n}{n/2}} - \sum_{\emptyset\neq S\in S_{in}:q_1\in S}\frac{\mathrm{Rank}(P_S)}{D\binom{n}{n/2}}.\end{aligned}$$

Note that for a properly initialized state we have

$$\langle\psi_I|\,\Pi_{in}\,|\psi_I\rangle = \sum_{\emptyset\neq S\subseteq S_{in}}\frac{\mathrm{Rank}(P_S)}{D\binom{n}{n/2}}$$

Furthermore

$$\begin{aligned}\sum_{\emptyset\neq S\subseteq S_{in}:q_1\in S}\mathrm{Rank}(P_S) &= \sum_{q_1\in S\in S_{in}}|\{\mathbf{t}\colon(\forall p\in S,t_p=0)\wedge(\forall p\in S_{in}\backslash S,t_p\neq0)\}|\\ &= |\{\mathbf{t}\colon t_{q_1}=0\}| = \binom{n-1}{\frac{n}{2}-1}.\end{aligned}$$

¶ In order to not have any dependence on the particular choice for qubit 1, we assume for simplicity that the number of qubits in S_{in} is even, that the qubits are adjacent to each other and that they all interact among each other at the first time-step.

This gives

$$\max_{\psi_{NI}} \langle\psi_{NI}|\,\Pi_B\,|\psi_{NI}\rangle = 1 - \frac{1}{2D}. \tag{23}$$

Lastly, we bound the 'crossterm' $|\,\langle\psi_{NI}|\,\Pi_B\,|\psi_I\rangle\,|$. Following the slightly different proof technique in [24], we can write $\Pi_B = \Pi_{final}\Pi_{init}$ where Π_{init} is the projector onto the entire nullspace of H_{in} and Π_{final} is the projector onto the null-space of H_{out}. The projectors Π_{init} and Π_{final} commute as the set $\{\mathbf{t}\colon t_{q_{out}} = D\}$ is disjoint from the sets $\{\mathbf{t}\colon t_{p\in S_{in}} = 0\}$. We have

$$|\,\langle\psi_{NI}|\,\Pi_{final}\Pi_{init}\,|\psi_I\rangle\,| \leq |\,\langle\psi_{NI}|\,\Pi_{final}\,|\psi_I\rangle\,|.$$

As Π_{final} is diagonal in the basis $\mathbf{t}$ and a properly initialized state $V(\mathbf{t}\leftarrow\mathbf{0})\,|\psi_{in}^I\rangle\otimes|\mathbf{t}\rangle$ is orthogonal to $V(\mathbf{t}\leftarrow\mathbf{0})\,|\psi_{in}^{NI}\rangle\otimes|\mathbf{t}\rangle$, we can bound

$$\begin{aligned}&|\,\langle\psi_{NI}|\,\Pi_{final}\,|\psi_I\rangle\,| \leq \\ &\frac{1}{D\binom{n}{n/2}}\sum_{\mathbf{t}:t_{q_{out}=D}} |\,\langle\psi_{in}^{NI}|\,V^\dagger(\mathbf{t}\leftarrow\mathbf{0})\,|1\rangle\,\langle 1|_{q_{out}}\,V(\mathbf{t}\leftarrow\mathbf{0})\,|\psi_{in}^I\rangle\,| \leq \frac{\sqrt{\epsilon}}{2D}\end{aligned} \tag{24}$$

All contributions, Eqs. (21),(23),(24) together with Eq. (20) give

$$\langle\psi_{history}|\,\Pi_B\,|\psi_{history}\rangle \leq 1 - \frac{1}{2D} + \frac{\epsilon}{2D} + \frac{\sqrt{\epsilon}}{D}, \tag{25}$$

which is bounded away from 1 by approximately $\frac{1}{2D}$ for exponentially small (in n or D) ϵ. Using Lemma 2.2 then gives Eq. 19. □.

3.2. Clock Realizations

The space-time circuit Hamiltonians $H_{circuit}$ used so far are not $O(1)$-local Hamiltonians, –they are not sums of terms each of which acts on O(1) qubits non-trivially,– as the clock of each qubit is realized by a $O(\log D)$-qubit register. In order to prove that the lowest eigenvalue problem for $O(1)$-local Hamiltonians is QMA-complete, one can realize such clock as a pulse or domain wall clock (see e.g. [7]). In particular for the domain-wall clock introduced by Kitaev [3], terms such as $|t\rangle\langle t-1|$ are 3-local. For the QMA-application, one then considers a Hamiltonian $H = H_{circuit}+H_{in}+H_{out}+H_{causal}+H_{clock}$ where H_{clock} gives a $O(1)$ penalty to any state of the time-registers which does not represent time. This implies that the lowest-energy states are in the space where the time-registers do represent time and one applies the arguments in the previous sections to this subspace. Using the domain wall clock in the space-time circuit-to-Hamiltonian construction gives rise to 8-local terms as $|t,t\rangle\langle t-1,t-1|$ is 6-local. Similarly, the term H_{causal} translates into a 4-local term as a term of the form $|t\rangle\langle t|$ is 2-local for a domain wall clock, e.g. [7]. This implies that this use of the space-time circuit-to-Hamiltonian construction is less efficient in terms of locality than the Feynman-Kitaev construction which is 5-local.

3.3. QMA-completeness of two-dimensional interacting fermions

We can also prove QMA-completeness for the fermionic model of [11] ([13]) which indirectly realizes a pulse clock for each qubit q. The terms of the circuit Hamiltonian are in Eq. (4) in Section 1.3. Note that we can only represent two-qubit gates which are controlled-U operations. However, given a supply of qubits initialized to the state $|1\rangle$, a one-dimensional quantum circuit with only such controlled-U gates is universal. The circuit Hamiltonian will correspond to that of an interacting fermion model in two spatial dimensions with periodic boundary conditions in both directions (a torus), as we work with the circular time circuit-to-Hamiltonian construction. Aside from the circuit Hamiltonian one needs the fermionic equivalent of the terms H_{in}, H_{out} and H_{causal}. To represent the input state $|00\ldots0\rangle_{S_{in}}$, one takes

$$H_{in} = \sum_{q\in S_{in}} b_0^\dagger[q] b_0[q],$$

such that the modes $b_0[q]$ (corresponding to those qubits being in the state $|1\rangle$ at time 0) are never occupied. If we translate this back to qubits, this corresponds to the term H_{in} in Eq. (16). Similarly, for H_{out}, Eq. (16), one takes

$$H_{out} = a_D^\dagger[q_{out}] a_D[q_{out}].$$

Lastly, H_{causal} (given in [11]) is the fermionic equivalent of Eq. (17). For a gate in the original quantum circuit at time t between qubits q and p, one can take

$$H_{causal}([q,p],t) = n(t_q \in I_t) n(t_p \in I_t^c) + n(t_p \in I_t) n(t_q \in I_t^c), \tag{26}$$

where $n(t_q \in I_t) = \sum_{t_q\in I_t} n_{t_q}[q]$ with number operator n_{t_q} (previously defined in Sec. 1.3). Again H_{causal} commutes with all other terms H_{in}, H_{out} and $H_{circuit}$. This form of H_{causal} is not local on the two-dimensional lattice however. If we wish to prove QMA-completeness of the ground-state energy problem of a two-dimensional interacting fermion model, then one can replace H_{causal} by a local version H_{causal}^{loc}. The idea is that the proper time-configurations of the quantum circuit in Fig. (2)(b) are very constrained, or the space-time is tightly knit. Consider Fig. (5). In between all two-qubit gates, –which themselves form a checkerboard pattern–, one places two triangle operator constraints. The triangle operator between three fermionic sites a, b and c with control site at the top labeled a, see Fig. (5) reads $H_{triangle} = n_a(1 - n_b - n_c)$. It is important to note that we work in the Fock space where $N[q] = 1$ which means that $\langle n_b + n_c\rangle \leq 1$ and $H_{triangle} \geq 0$ for the triangle operators in the picture. The zero energy subspace of $H_{triangle}$ is the direct sum of the Fock-space with $n_a = 0$, the space with $n_a = 1$ and $n_b = 1$, and the space with $n_a = 1$ and $n_c = 1$. Thus the triangle operator expresses the constraint that *if there is a particle at 1, there should also be a particle at 2 or 3*. In the spaces between the gates, one puts two triangle operators. Note that the triangle operators all commute as all number operators $n_t[q]$ mutually commute.

It is not hard to see that all triangle operators have energy zero if and only if the fermionic Fock states represent a proper time-configuration. In addition, we want to establish that the sum over all triangle operators commutes with $H_{circuit}$, H_{in} and

H_{out}. When this is the case, the lowest improper Fock state has at least energy 1 and thus in order to determine the lowest nonzero eigenvalue of H, one only needs to look at the space of proper Fock states. Consider a gate term $H_t^{CU}[q,p]$ with qubits q,p as control and target qubits in Eqs. (3),(4), as in Fig. (5) with the number operators n_1, n_2 and n_3 and n_4 at the corners of the gate. We wish to show that all triangle operators commute with $H_t^{CU}[q,p]$. We consider the gate interaction $H_t^{CU}[q,p]$ on the states partially labeled by $n_1,n_2,n_3,n_4,\{n_{else}\}$ where $\{n_{else}\}$ are the number operators for all the other fermionic sites on the lattice (the full state specification includes the spin-degree but is not relevant for the next arguments).

Due to the $\forall q$, $N[q] = 1$ constraint, some of these n_{else} are constrained depending on $n_1,\ldots,n_4$, i.e. we only have $(n_1,n_2,n_3,n_4) = (1,0,1,0),(1,0,0,1),(0,1,0,1),(0,1,1,0),(0,0,1,0),(0,0,0,1),(1,0,0,0),(0,1,0,0)$ and $(0,0,0,0)$. $H_t^{CU}[q,p]$ has nontrivial action only in the subspace where $(n_1,n_2,n_3,n_4) = (1,0,1,0)$ and $(n_1,n_2,n_3,n_4) = (0,1,0,1)$, for all other (n_1,n_2,n_3,n_4) states it has zero energy. This means that the operators n_1+n_2, n_3+n_4 and $n_1n_3+n_1n_4$ commute with the gate interaction. The four triangle operators above and below the gate, see Fig. (5) involves only symmetric combination such as n_1+n_2 and n_3+n_4 and thus commute. The sum of the two triangle operators left and right to the gate can be written as $(n_1+n_2)-(n_1n_3+n_2n_4)-n_1n_5-n_2n_6$ where the first two terms in () are conserved quantities and thus commute. The last two terms commute separately as they only have support on the null-space of the gate interaction. Similarly the triangle operator, either on the left or the right of the gate, commutes with the gate interaction as the only term which involves, say n_3, is supported on the null-space of the gate interaction. Note that the triangle operators also commute with H_{in} and H_{out}. This means that the fermionic Hamiltonian $H = H_{circuit} + H_{in} + H_{out} + H_{causal}^{loc}$ is a quartic fermion Hamiltonian involving spin-1/2 fermionic sites. The quartic interaction involves at most 4 fermionic sites on a square lattice, see Fig. (5).

Another issue is H_{clock}. For adiabatic computation one can assume that there is at most one fermion per qubit q, i.e $N[q] = 1$, see Section 1.3. The arguments above and in the last sections show that the problem of deciding whether there is a state with energy less than or equal to a or larger than or equal to b ($|a-b| \geq \frac{1}{\mathrm{poly}(n)}$) for a two-dimensional interacting fermion Hamiltonians H on a torus, *in the sector where* $\forall q, N[q] = 1, N[q] = \sum_{t\in Z_{2D}} n_t[q]$ is QMA-complete. This result goes beyond the perturbative approach used in [28] as all terms in the Hamiltonians here are of strength $O(1)$. Considering eigenvalues of fermionic problems restricted to sectors with fixed number of fermions is not unnatural as fermion number is a conserved quantity in physical systems and one can tune a physical system such as a quantum dot so that one excess electron (above the Fermi energy) is available for interactions. Alternatively, we add a nonlocal penalty term H_{clock} to the Hamiltonian which enforces $N[q] = 1$, e.g. $H_{clock} = \sum_q (N[q]-1)^2$. However, as has been observed before [7], it is not clear how to enforce this constraint in a local one-dimensional manner (without making the vacuum state without fermions always have the lowest energy).

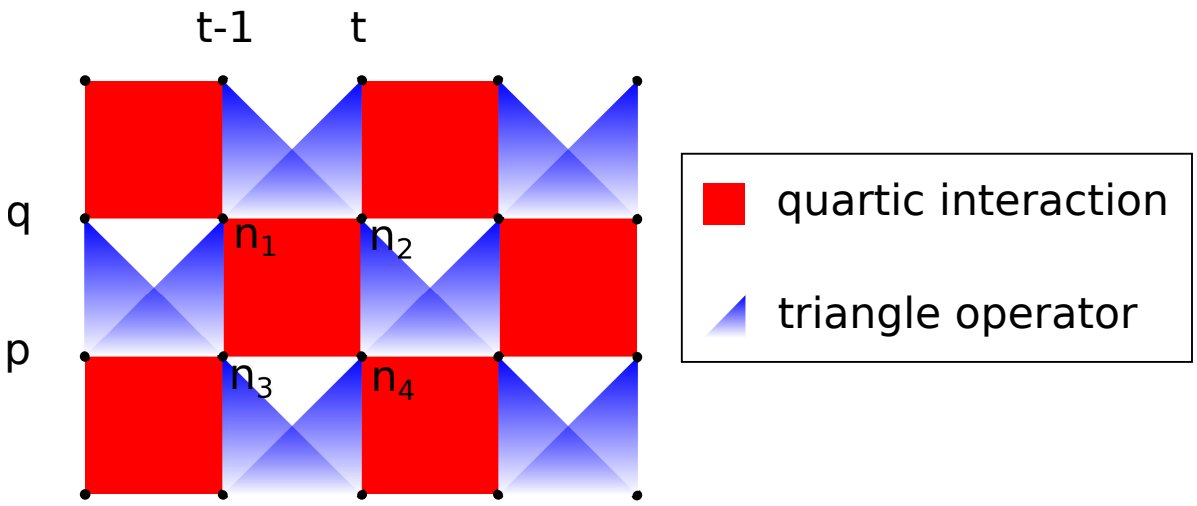


Figure 5: The black dots are fermionic sites, each with two modes (an $\uparrow$ or $\downarrow$ state, say). The (red) squares represent the quartic gate interactions and the (blue) triangle operators penalize improper fermionic configurations (improper time-configurations). A (blue) triangle operator with top corner a and bottom corners b and c equals $n_a(1-n_b-n_c)$. The lattice has periodic boundary conditions in both directions.

We note that these results also can be stated in terms of only qubits instead of fermions (using the Jordan-Wigner transformation). The terms $H_{in}, H_{out}, H^{loc}_{caus}$ remain local terms under this transformation. However the pulse clock condition $\forall q, N[q] = 1$ is somewhat less natural.

3.4. Quantum adiabatic computation

In order to use the space-time Hamiltonian construction for quantum adiabatic computation one has to (i) bound the gap above the ground-state for the quantum adiabatic path $H_{circuit}[\epsilon]$, $\epsilon \in [0,1]$, see Sec. (1), (ii) show that one can prepare the ground-state of the initial Hamiltonian $H_{circuit}[0]$ efficiently and (iii) show that one can read out the output state of the quantum circuit from the ground-state of the final Hamiltonian $H_{circuit}[1]$ on the adiabatic path.

(i) Theorem 2.3 shows that the gap of the circuit Hamiltonian for efficient one-dimensional quantum circuits is lowerbounded appropriately, by some $\frac{1}{\mathrm{poly}(n)}$. Together with the unitary relation between the fermionic model and the qubit circuit Hamiltonian, this shows that the two-dimensional interacting fermionic (or qubit) model could be used for quantum adiabatic computation, as proposed in [11].

(ii) For the Feynman-Kitaev construction, preparing the initial ground-state, as a uniform superposition over all times is not hard. For the space-time construction, it requires preparing the uniform sum over all proper time-configurations. One may expect that by simple cooling the system one can reach the ground-state. If we wish

to do all computation by quantum adiabatic techniques, one would have to show how to obtain this initial state as output state from another adiabatic path, as in [4], and prove that this adiabatic path has a $1/\mathrm{poly}(n)$ gap everywhere. In [11] the authors propose to execute the quantum adiabatic computation by gradually increasing the strength of the propagating part of each H_t (by the parameter λ). However, the gap of this adiabatic path is not fully analyzed in [11, 10] and goes beyond the results in this paper. We believe that it should be possible however to design an effcient quantum adiabatic path which starts from a simple (say, fermionic) state and ends up in the uniform superposition over all proper time-configurations. The intuition is that the Markov chain (related to the Laplacian of the graph underlying the circuit Hamiltonian) which starts in the proper time configuration $|\mathbf{t} = \mathbf{0}\rangle$, –equivalent to each fermion q being localized in the $a_0[q]$ or $b_0[q]$ mode–, efficiently mixes to the uniform mixture over all proper time configurations, as we have shown that the gap of the Laplacian is bounded away from zero by $1/\mathrm{poly}(n)$.

(iii) If one measures the time-configuration in the history state, the total probability to measure a configuration $\mathbf{t}$ in which a qubit q has $t_q = D$ is $\frac{1}{2D}$. This can be amplified to a constant by padding the quantum circuit with I gates as in the Feynman-Kitaev construction. One cannot avoid that the probability for *all* qubits to be at time D is exponentially small in n when the final state of the computation is the history state. Thus in order to read out the full final state of the quantum circuit, one would have to apply the adiabatic preparation of the history state in reverse to convert the history state to the state for which all the clocks read the time $t = D$.

4. Discussion

It would be interesting to do a similar analysis for two-dimensional quantum circuits with periodic boundary conditions in both space directions, using the circular-time construction. For two-dimensional quantum circuits, the vertices of the underlying graph G can be labeled by a 1-dimensional object (the spatial boundary of the two-dimensional quantum circuit) together with a set of internal degrees of freedom which represent a membrane with a fixed boundary.

The reason to use the circular-time construction is that the gap analysis for the space-time circuit Hamiltonian with open boundaries in time is much more involved. The internal state-space which is now represented by n qubits with $\sum_i Z_i = 0$ is then different at the two time-boundaries of the circuit as strings cannot cross the boundary. Using a combination of the Markov chains techniques in [29] and results on random walks on the space of Dyck paths [30], it may be possible to bound the gap of the circuit Hamiltonian.

We note that the circuit Hamiltonian in the altered representation, Eq. (6), could be used as a realization of a one-dimensional translationally-invariant cellular automaton

circuit. For such a cellular automaton circuit, we assume that the same set of two-qubit gates is applied at every depth: this implies that dynamics of the internal variable $|x\rangle$ do not need to depend on the counter τ [+].

It is not immediately clear what additional interest the space-time circuit-to-Hamiltonian construction has for further questions in quantum complexity and quantum adiabatic computation. It may be interesting to study the model for low depth $D \ll n$. We note that the angle between the null-spaces in the QMA-proof, see the proof of Lemma 3.3, is determined by the depth and not the size of the quantum circuit. One can observe that the number of qubits in the circuit enters the promise-gap of the QMA problem via the gap of the Heisenberg model only (and indirectly via the assumption that $2D > n$ which is invoked in Sec. 1.4 to avoid closed-time configurations). In addition, it is not clear that in order to access the state of qubit q_{out}, one needs to be in the ground-state of the circuit Hamiltonian. In particular, it is an open question whether there exists, in this construction, a $1/poly(n)$ wide- energy band of 'single-qubit informative states' for which any single qubit observable has the correct expectation, above the groundspace. The point is that deviations of the relative amplitudes of terms $V(\mathbf{t} \leftarrow \mathbf{0})\,|\phi_{in}\rangle \otimes |\mathbf{t}\rangle$ for various $\mathbf{t}$ with $t_{q_{out}} = D$ do not matter as all these paths lead to the correct output.

We should mention that one can get this dependence on the depth D in the Feynman-Kitaev construction by only applying the construction to those $O(D^2)$ gates in the causal cone of the output qubit, thus suitably reducing the size of the quantum circuit. However, using this size-reduction, the quantum adiabatic algorithm with runtime poly(D) can only accurately give the output of qubit $q_{\rm out}$. This would be in contrast with a *possible* quantum adiabatic algorithm, based on the space-time circuit to Hamiltonian construction, where one could read out the answer of *any* single qubit in time poly(D) (by being in the single-qubit informative subspace but not necessarily in the ground states itself).

Another applicaton of our analysis can be a different proposal for a universal quantum walk using a two-dimensional interacting fermion system (see such proposal in [12]). In [7] the standard Feynman-Kitaev construction and its spectral analysis were directly used to show how to do a universal random walk. One may expect that by initializing the fermions around the $t = 0$ modes and letting them evolve for a random time within a certain window, one could be guaranteed to find them in an interval where their internal state corresponds to the output state of the simulated quantum circuit.

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[+] However, one cannot work with circular time *and* keep the circuit completely translationally invariant as the circular time construction then requires one to add a single I-layer of gates which is not feasible under the cellular automaton assumption.

out the connection to the ideas of Page and Wootters and Guillaume Aubrun for pointing out Ref. [15]. BMT thanks the Isaac Newton Institute for Mathematical Sciences in Cambridge, UK for hosting the program on Mathematical Problems in Quantum Information Theory where some of this work was completed. BMT is happy to acknowledge no external funding as it would have distracted her from actually doing the research.

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