

Revisiting the simulation of quantum Turing machines by quantum circuits

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Abstract

Yao (1993) proved that quantum Turing machines and uniformly generated quantum circuits are polynomially equivalent computational models: $t \geq n$ steps of a quantum Turing machine running on an input of length n can be simulated by a uniformly generated family of quantum circuits with size quadratic in t , and a polynomial-time uniformly generated family of quantum circuits can be simulated by a quantum Turing machine running in polynomial time. We revisit the simulation of quantum Turing machines with uniformly generated quantum circuits, which is the more challenging of the two simulation tasks, and present a variation on the simulation method employed by Yao together with an analysis of it. This analysis reveals that the simulation of quantum Turing machines can be performed by quantum circuits having depth linear in t , rather than quadratic depth, and can be extended to variants of quantum Turing machines, such as ones having multi-dimensional tapes. Our analysis is based on an extension of a method of Arrighi, Nesme, and Werner (2011) that allows for the localization of causal unitary evolutions.

1 Introduction

The Turing machine model of computation, proposed by Turing in his landmark 1937 paper [Tur37], is a cornerstone of computability and complexity theory: it provides a simple and clean mathematical abstraction of what it means to compute, upon which a rigorous theory of computation may be constructed. It is therefore natural that in the early days of quantum computing, researchers investigated quantum variants of the Turing machine model, and used these variants as a foundation from which to study the power of quantum computing [Deu85, DJ92, BV93, BV97, Sim94, Sim97, Sho94, ADH97].

In retrospect, however, it is reasonable to consider the quantum Turing machine model to be a rather cumbersome model, and not a particularly effective tool with which to reason that quantum algorithms can be efficiently implemented on a quantum computer.

The quantum circuit model offers a more usable alternative. Quantum circuits were first described by Deutsch in 1989 [Deu89], although the now standard acyclic variant of the quantum circuit model was proposed and investigated a few years later by Yao [Yao93]. Yao considered the complexity theoretic aspects of quantum circuits, which were ignored by Deutsch for the most part, proving that (up to a polynomial overhead) quantum Turing machines and uniformly generated quantum circuits (i.e., families of quantum circuits that can be efficiently described by classical Turing machine computations) are equivalent in computational power. Specifically, Yao proved that $t \geq n$ steps of a quantum Turing machine running on an input of length n can be simulated by a uniformly generated family of quantum circuits with size quadratic in t , and that a polynomial-time uniformly generated family of quantum circuits can be simulated by a quantum Turing machine running in polynomial time. By the mid- to late-1990s, quantum circuits effectively supplanted quantum Turing machines as the computational model of choice in the study of quantum algorithms and complexity theory—a shift made possible by Yao’s proof that the models are equivalent. The simulation of quantum circuit families by quantum Turing machines is quite straightforward, and for this reason we will not discuss it further and will instead focus on the simulation of quantum Turing machines by quantum circuits.

In this paper we present a variation on Yao’s simulation method; the essential idea behind the simulation we present is the same as Yao’s, but the technical details are somewhat different. We do not claim that our simulation achieves a quantitative improvement over Yao’s simulation, but we believe nevertheless that there is value in an alternative simulation and analysis, and also in a discussion that fills in some of the details absent from Yao’s original paper (which appeared only as an extended abstract in a conference proceedings). One small advantage of our simulation is that it allows one to essentially read off an explicit description of the quantum circuits that perform the simulation from a simple formula, whereas Yao’s simulation requires that one uses linear algebra to solve for a suitable circuit description. We observe that the simulation of quantum Turing machines by quantum circuits can be parallelized, resulting in quantum circuits having depth linear in t rather than depth quadratic in t , while still having size quadratic in t . (This is true of our simulation, and although it is not the case for the precise simulation presented by Yao, it is not difficult to achieve a similar parallelization by slightly modifying his simulation.) We also observe that both simulations can be extended to variants of quantum Turing machines such as ones having multi-dimensional tapes.

Our analysis is based on an extension of a result of Arrighi, Nesme, and Werner [ANW11] that allows for the localization of causal unitary evolutions. This extension concerns unitary evolutions that are only causal when restricted to certain subspaces, and may potentially find other uses, as might also our introduction of a model of quantum Turing machines with a finite tape loop.

Paper organization

The remainder of this paper is organized as follows. First, in Section 2, we discuss the classic simulation of deterministic Turing machines by Boolean circuits. While this simulation cannot be applied directly to quantum Turing machines, it is useful to refer to it and to view the method as a foundation of the quantum simulation. In Section 3 we

discuss the quantum Turing machine model at a formal level, and also introduce the notion of a quantum Turing machine with a finite tape loop, which simplifies somewhat the study of bounded computations of quantum Turing machines. In Section 4 we discuss the localization of causal unitary evolutions, as described by Arrighi, Nesme, and Werner [ANW11], and prove an extension of their result to unitary evolutions that are only causal when restricted to certain subspaces. While it is key to the simulation we consider, this section is completely independent of the notion of quantum Turing machines, and might potentially be useful in other contexts. In Section 5 we present and analyze a simulation of quantum Turing machines by quantum circuits, compare the simulation with Yao’s original simulation, and briefly discuss how the simulation can be applied to variants of quantum Turing machines.

2 The classic Boolean circuit simulation of deterministic Turing machines

To explain our variation on Yao’s method for simulating quantum Turing machine computations with quantum circuits, and the challenges that both simulations overcome, it is helpful to recall the classic simulation of deterministic Turing machines by Boolean circuits. This discussion also serves as an opportunity to introduce some notation that will be useful when discussing quantum circuit simulations of quantum Turing machines. This classical simulation method, variants of which appear in [Sav72, PF79] and as standard material in textbooks on computational complexity, can informally be described as a “solid state” implementation of a Turing machine.

For the sake of simplicity, we will assume that the deterministic Turing machine to be simulated has state set $Q = \{1, \dots, m\}$ and tape alphabet $\Gamma = \{0, \dots, k - 1\}$, where the tape symbol 0 represents the blank symbol. The tape is assumed to be two-way infinite, with squares indexed by the set of integers \mathbb{Z} . The computation begins with the tape head scanning the tape square indexed by 0, with the input string written in the squares indexed by $1, \dots, n$ and all other tape squares containing the blank symbol, and with the starting state 1. The evolution of the Turing machine is specified by a transition function

$$\delta : Q \times \Gamma \rightarrow Q \times \Gamma \times \{-1, +1\}; \tag{1}$$

if the machine is in the state $p \in Q$, the tape head is scanning a square that holds the symbol $a \in \Gamma$, and it is the case that

$$\delta(p, a) = (q, b, D), \tag{2}$$

then in one step the machine will change state to q , overwrite the currently scanned tape square with the symbol b , and move the tape head in the direction D (where $D = -1$ indicates a movement to the left and $D = +1$ indicates a movement to the right).

Suppose that t steps of the Turing machine’s computation are to be simulated, and assume that the length of the input string satisfies $n \leq t$. Note that it is not possible for the tape head to leave the region of the tape indexed by the set $\{-t, \dots, t\}$, and no tape square outside of this region will ever store a non-blank symbol within these t steps.

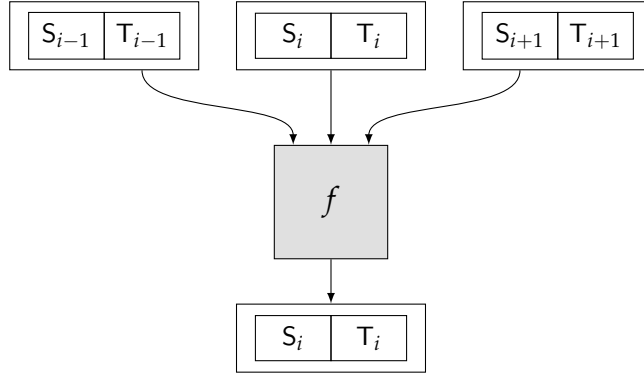


Figure 1: The information corresponding to cell i in the Turing machine is a function of the information in the previous time step for cells $\{i - 1, i, i + 1\}$. The shaded box labeled f represents the function that determines the updated contents of (S_i, T_i) given the contents of (S_{i-1}, T_{i-1}) , (S_i, T_i) , and (S_{i+1}, T_{i+1}) prior to being updated.

For each of the $2t + 1$ tape squares indexed by $\{-t, \dots, t\}$, one imagines two registers: one register stores information that indicates whether or not the tape head is currently scanning this tape square, and if it is, the current state of the Turing machine, while the other register stores the symbol that is currently written in the corresponding tape square. More precisely, we define registers

$$S_{-t}, \dots, S_t \quad \text{and} \quad T_{-t}, \dots, T_t, \quad (3)$$

where each register S_i holds an element of the set $\{0, \dots, m\}$ and each register T_i holds an element of the set $\{0, \dots, k - 1\}$. If S_i holds 0, then the tape head is not positioned over the square indexed by i , while if S_i holds $p \in \{1, \dots, m\}$, then the tape square is positioned over the tape square indexed by i and the current state of the Turing machine is p . In either case, the symbol written in the tape square indexed by i is stored in T_i . The simulation begins with a pre-processing step that initializes these registers appropriately for a given input string.

To simulate one step of the Turing machine's computation, each of the registers (3) is simultaneously updated. The contents of the pair (S_i, T_i) after being updated depend only on the contents of the registers (S_{i-1}, T_{i-1}) , (S_i, T_i) , and (S_{i+1}, T_{i+1}) prior to the update, as is suggested by Figure 1. This local dependence is enabled by the fact that the Turing machine's state is stored locally in the register S_j that corresponds to the tape head location j , along with the fact that the tape head cannot move more than one square on each computation step. For example, if (S_i, T_i) stores $(0, c)$ for some $c \in \{0, \dots, k - 1\}$, then after being updated, T_i will continue to store c , as the absence of the tape head at square i prevents the tape contents of square i from changing. However, after being updated, S_i might potentially contain any element of $\{0, \dots, m\}$; for example, if (S_{i+1}, T_{i+1}) stores (p, a) and $\delta(p, a) = (q, b, -1)$, then the updated contents of S_i will become q , indicating that the tape head has moved over square i and that the current state has become q . In the same situation the updated contents of (S_{i+1}, T_{i+1}) will become $(0, b)$.

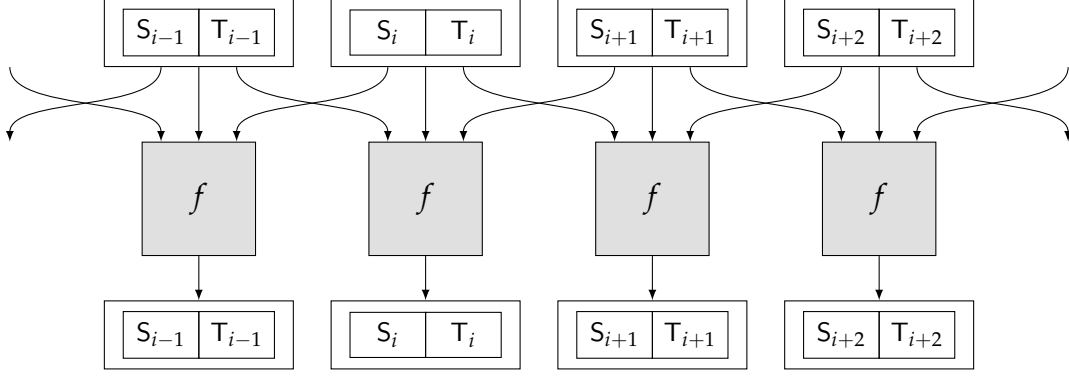


Figure 2: To simulate one step of a Turing machine computation, each pair of registers is simultaneously updated. The same function f describes the update for each pair of registers.

One could of course give an explicit description of this update rule, for a given transition function δ , but doing so for the sake of this discussion is not particularly helpful. Instead, it suffices to observe that there exists a function

$$f : (\{0, \dots, m\} \times \{0, \dots, k-1\})^3 \rightarrow \{0, \dots, m\} \times \{0, \dots, k-1\}, \quad (4)$$

also depicted in Figure 1, that describes the update rule. Figure 2 illustrates the update being applied simultaneously to every pair of registers.

It should be noted that for inputs of the form

$$((q_1, a_1), (q_2, a_2), (q_3, a_3)) \quad (5)$$

where two or more of the elements q_1, q_2, q_3 are contained in the set $\{1, \dots, m\}$, the output of f may be defined arbitrarily; such an input could only arise from a Turing machine configuration having two or more tape heads, which never happens in a valid Turing machine computation. Also note that a special case must be made for the register pairs in the leftmost column (i.e., (S_{-t}, T_{-t})) and the rightmost column (i.e., (S_t, T_t)) as there are no register pairs to the left or right, respectively, to feed into the function f that determines how these registers update. However, the missing inputs will always be $(0, 0)$, representing the absence of the tape head and a blank symbol stored on the tape, and so they can be “hard-coded” into the corresponding copies of the function f .

To simulate t steps of the Turing machine computation, one envisions a network consisting of $t + 1$ rows, each having the $2t + 1$ register pairs $(S_{-t}, T_{-t}), \dots, (S_t, T_t)$, as suggested by Figure 3. The registers in the top row (which corresponds to time 0) are initialized by the pre-processing step suggested previously, so that collectively they describe the initial configuration of the Turing machine on the input string of interest, and their updates are performed in the indicated pattern. Subsequent rows of register pairs will then collectively describe the configuration of the Turing machine on subsequent computation steps, and in particular the bottom row will describe the configuration after t steps. A final post-processing step may be appended so that a description of the final Turing

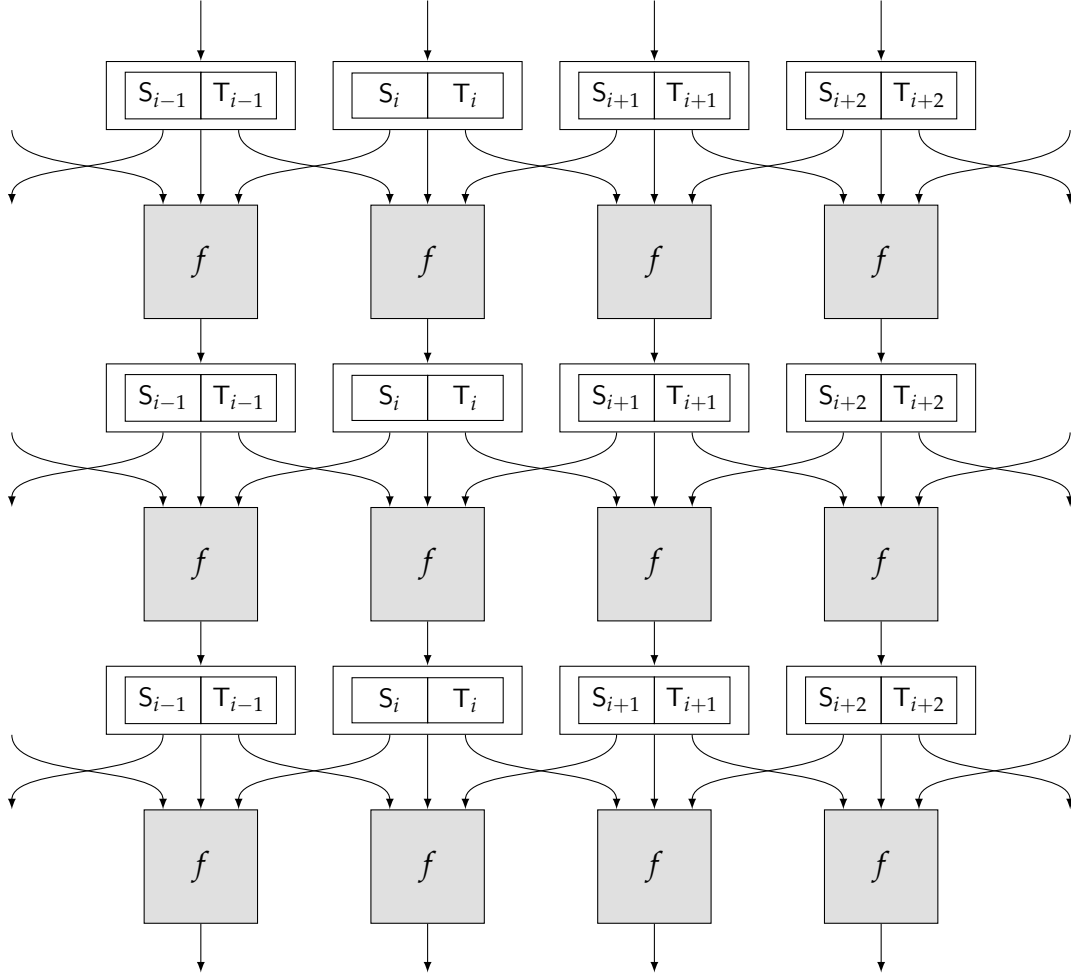


Figure 3: The pattern of connections among the registers corresponding to individual tape squares, along with copies of the function f that performs the local updates on these registers.

machine configuration is produced that conforms to some alternative encoding scheme, if that is desired.

Assuming that the states of the $2t + 1$ register pairs $(S_{-t}, T_{-t}), \dots, (S_t, T_t)$ are encoded as binary strings, that the computation represented by the function f is implemented as a (constant-size) Boolean circuit, and that the pre-processing and post-processing steps suggested above have size at most $O(t^2)$ and depth at most $O(t)$, which is ample size and depth to handle a wide range of input and output encoding schemes, one obtains a Boolean circuit simulation of the original Turing machine having linear depth and quadratic size. The circuits also conform to a simple and regular pattern, and can therefore be uniformly generated in logarithmic-space (and hence polynomial-time) by a deterministic Turing machine.

Now, it is not at all clear how this classic deterministic Turing machine simulation can be extended to a quantum circuit simulation of quantum Turing machines. A first

guess for how this might be done is to somehow replace the function f by a unitary operation that describes the evolution of local parts of the quantum Turing machine—but the function f does not even have input and output sets of the same cardinality. One might therefore hope to replace the function f with a unitary operation that transforms each triple of register pairs $(S_{i-1}, T_{i-1}), (S_i, T_i), (S_{i+1}, T_{i+1})$ in a way that is consistent with one step in the quantum Turing machine’s evolution. Two complications arise: one is that it is unclear how “overlapping” unitary transformations are to be performed in a consistent way, given that these operations will generally not commute, and another is that some quantum Turing machine evolutions fail to be unitary when restricted to a finite portion of the machine’s tape. (For example, even the trivial Turing machine evolution in which the tape head moves right on each step without changing state or modifying the tape contents induces a non-invertible transformation when restricted to any finite region of the tape.) Yao’s simulation method does indeed overcome these obstacles, but requires additional ideas in order to do this.

3 Quantum Turing machines

In this section we describe the quantum Turing machine model, which was first introduced by Deutsch [Deu85] and later studied in depth by Bernstein and Vazirani [BV93, BV97]. Quantum Turing machines generalize Turing machines to the quantum realm by allowing them to transition in superposition, subject to constraints that ensure that the overall evolution of the Turing machine is unitary.

Similar conventions will be followed for quantum Turing machines as for deterministic Turing machines, as discussed in the previous section. In particular, we assume for simplicity that quantum Turing machines have a state set of the form $Q = \{1, \dots, m\}$ and a tape alphabet of the form $\Gamma = \{0, \dots, k - 1\}$, for some choice of positive integers m and k , and where the tape symbol 0 represents the blank symbol. Again the tape is assumed to be two-way infinite, with squares indexed by the set of integers \mathbb{Z} , and computations begin with the state 1, with the tape head scanning the tape square indexed by 0, and with the input string written in the squares indexed $1, \dots, n$ and all other tape squares containing the blank symbol.

The transition function of a quantum Turing machine takes the form

$$\delta : Q \times \Gamma \rightarrow \mathbb{C}^{Q \times \Gamma \times \{-1, +1\}}, \quad (6)$$

meaning that $\delta(p, a)$ is a complex vector indexed by the set $Q \times \Gamma \times \{-1, +1\}$ for every $p \in Q$ and $a \in \Gamma$. The interpretation of a transition function δ of the form (6) is as follows: for each choice of states $p, q \in Q$, tape symbols $a, b \in \Gamma$, and a direction $D \in \{-1, +1\}$, the complex number $\delta(p, a)[q, b, D]$ represents the *amplitude* with which a quantum Turing machine whose current state is p and whose tape head is scanning the symbol a will change state to q , write b to the tape, and move its tape head in direction D . Not all transition functions of this form describe valid quantum Turing machines; only those transition functions that induce global unitary evolutions, to be discussed shortly, are valid. We note that this definition can easily be relaxed so that the tape head of a quantum

Turing machine is not required to move left or right on each step, but instead can remain stationary, by allowing the transition function to take the form

$$\delta : Q \times \Gamma \rightarrow \mathbb{C}^{Q \times \Gamma \times \{-1,0,+1\}}, \quad (7)$$

but in the interest of simplicity we will focus on transition functions of the form (6) in the discussion that follows.

In order to obtain a computational model that does not permit difficult or impossible to compute information to be somehow hidden inside of a given transition function, it is important that the complex numbers $\delta(p, a)[q, b, D]$ are drawn from a reasonable set, such as a finite set like

$$\left\{ 0, \pm 1, \pm i, \pm \frac{1}{\sqrt{2}}, \pm \frac{i}{\sqrt{2}} \right\} \quad (8)$$

or a set for which rational approximations can be efficiently computed. Adleman, DeMarras, and Huang [ADH97] discuss the importance of such assumptions. For the sake of this paper, however, we will mostly ignore this issue: the simulation to be analyzed places no restrictions on the complex numbers appearing in δ , but any computationally offensive properties possessed by δ will be inherited by the quantum circuits that result from the simulation.

In order to specify the global evolution of a quantum Turing machine that a given transition function δ induces, we must clarify the notion of a *configuration* of a Turing machine, which is a classical description of the machine's state, tape head location, and tape contents. The state and tape head location of a Turing machine correspond to elements of the sets Q and \mathbb{Z} , respectively, while the contents of a Turing machine tape can be described by a function $T : \mathbb{Z} \rightarrow \Gamma$, which specifies that the tape symbol $T(j)$ is stored in the tape square indexed by j , for each integer j . The *support* of such a function is defined as

$$\text{supp}(T) = \{j \in \mathbb{Z} : T(j) \neq 0\}, \quad (9)$$

which is the set of tape square indices that do not contain the blank symbol 0. We are only concerned with those functions T that have finite support, given that we only consider computations that begin with a finite-length input string written on an otherwise blank tape, and therefore the set of all configurations of a Turing machine forms a countably infinite set.

For a given function $T : \mathbb{Z} \rightarrow \Gamma$, an index $i \in \mathbb{Z}$, and a tape symbol $a \in \Gamma$, let us write $T_{i,a}$ to denote the function defined as

$$T_{i,a}(j) = \begin{cases} a & \text{if } j = i \\ T(j) & \text{if } j \neq i. \end{cases} \quad (10)$$

Thus, if the contents of a Turing machine tape are described by T , and then the symbol a overwrites the contents of the square indexed by i , then the resulting tape contents are described by $T_{i,a}$.

For a fixed choice of Q and Γ , let \mathcal{H} denote the Hilbert space of complex vectors indexed by the set of configurations of a Turing machine with state set Q and tape alphabet Γ . That is, \mathcal{H} is the Hilbert space whose standard basis includes the vectors $|p, i, T\rangle$,

where $p \in Q, i \in \mathbb{Z}$, and $T : \mathbb{Z} \rightarrow \Gamma$ has finite support. The global evolution of a quantum Turing machine whose transition function is δ can now be specified by the operator U_δ on \mathcal{H} defined by the action

$$U_\delta |p, i, T\rangle = \sum_{q,a,D} \delta(p, T(i)) [q, a, D] |q, i + D, T_{i,a}\rangle \quad (11)$$

on standard basis states, and extended to all of \mathcal{H} by linearity.

Bernstein and Vazirani [BV93] identified conditions on the transition function δ that cause the operator U_δ to be unitary. To be more precise, they identified conditions under which U_δ is an isometry, and proved that U_δ is necessarily unitary whenever it is an isometry. Although the specific conditions they identify are not relevant to this paper, it is a simple matter to recall them:

1. The set of vectors $\{\delta(p, a) : p \in Q, a \in \Gamma\}$ is orthonormal.
2. For all triples $(p_0, a_0, b_0), (p_1, a_1, b_1) \in Q \times \Gamma \times \Gamma$, one has

$$\sum_{q \in Q} \delta(p_0, a_0) [q, b_0, +1] \overline{\delta(p_1, a_1) [q, b_1, -1]} = 0. \quad (12)$$

One may note, in particular, that these conditions are easily checked for a given transition function δ , as they express a finite number of orthonormality relations.

Classical Turing machine definitions usually specify that some states are to be considered as *halting states*, with the understanding being that a Turing machine continues to compute so long as it has not entered a halting state, and then stops once a halting state is reached. Stopping conditions for quantum Turing machines are more subtle. Deutsch [Deu85] suggested that periodic measurements could determine when a quantum Turing machine computation is to be terminated, whereas Bernstein and Vazirani [BV93, BV97] considered quantum Turing machine computations that run for a predetermined number of steps. We will adopt the second convention, which is particularly well-suited to the simulation of quantum Turing machines by quantum circuits: we simply consider that the number of steps t of a quantum Turing machine to be simulated by a quantum circuit is fixed and hard-coded into the circuit.

Variants of quantum Turing machines

As is the case for classical Turing machines, one may consider variants of quantum Turing machines, such as quantum Turing machines with multiple tapes, with tapes having a fixed dimension larger than one, with tape heads that have greater freedom in their movements, and so on. The quantum Turing machine definition suggested above can be extended to handle such variants in a natural way. For example, a quantum Turing machine with 3 tapes could be described by a transition function of the form

$$\delta : Q \times \Gamma^3 \rightarrow \mathbb{C}^{Q \times (\Gamma \times \{-1, +1\})^3}, \quad (13)$$

with $\delta(p, a_1, a_2, a_3)[q, b_1, D_1, b_2, D_2, b_3, D_3]$ indicating the amplitude with which a quantum Turing machine in state p and reading the symbols a_1 , a_2 , and a_3 on its tapes will transition to state q , write the symbols b_1 , b_2 , and b_3 on its tapes, and move the tape heads in directions D_1 , D_2 , and D_3 .

Unfortunately, it becomes increasingly difficult to check that a given transition function induces a unitary global evolution when the Turing machine variant becomes more complex. For example, Ozawa and Nishamura [ON00] identified relatively simple conditions guaranteeing unitary evolutions for quantum Turing machine transition functions allowing for stationary tape head movements, and rather complex conditions for two-tape quantum Turing machines. We do not investigate the difficulty of checking whether a transition function of a given quantum Turing machine variant induces a unitary evolution, but simply assume that a transition function must induce a unitary global evolution in order for it to be considered valid. If one attempts to apply the simulation method we describe to a quantum Turing machine whose global evolution is not unitary, it will result in a non-unitary circuit.

For the most part, we will not focus too much on the technical aspects of any of the possible variants of quantum Turing machines. It is the case, however, that the simulation method we describe extends easily to some interesting variants of the quantum Turing machine model. This point will be revisited later in the paper after the simulation and its analysis have been presented.

Quantum Turing machines with looped tapes

For a given quantum Turing machine M having state set Q and tape alphabet Γ , one has that the Hilbert space \mathcal{H} with respect to which the global quantum states of M are defined is infinite-dimensional. On the other hand, any finite-length computation of M will only involve a finite-dimensional subspace of this Hilbert space. More concretely, if M runs for $t \geq n$ steps on an input of length n , then its tape head will never leave the portion of the tape indexed by elements of the set $\{-t, \dots, t\}$, and all tape squares outside of this region will contain blank symbols for the duration of the computation.

For this reason, it is tempting to imagine the tape has been truncated in such a case, so that every relevant classical configuration of M takes the form (p, i, T) for $i \in \{-t, \dots, t\}$ and $\text{supp}(T) \subseteq \{-t, \dots, t\}$. One may imagine that any quantum state of M reached at any point during such a computation is represented by a unit vector in the finite-dimensional Hilbert space whose standard basis includes precisely those elements $|p, i, T\rangle$ for which $i \in \{-t, \dots, t\}$ and $\text{supp}(T) \subseteq \{-t, \dots, t\}$. A problem arises, however, which is that this space is generally not invariant under the action of the evolution operator U_δ ; and defining a matrix from this operator by discarding rows and columns corresponding to tape heads or non-blank tape symbols outside of the region indexed by $\{-t, \dots, t\}$ may result in a non-unitary (and possibly non-normal) matrix.

A simple way to address this issue is to imagine that the tape has been formed into a loop rather than truncated. Specifically, for every positive integer N , one may consider a Turing machine tape loop whose squares are indexed by the set $\mathbb{Z}_N = \{0, 1, \dots, N-1\}$, and where tape head movements are calculated modulo N . Specifically, we will define a finite-dimensional Hilbert space \mathcal{H}_N whose standard basis contains all elements of the

form $|p, i, T\rangle$ where $p \in Q$, $i \in \mathbb{Z}_N$, and T takes the form

$$T : \mathbb{Z}_N \rightarrow \Gamma. \quad (14)$$

(No assumption on the finiteness of the support of T is required in this case, of course, as \mathbb{Z}_N is finite.) The transition function δ now defines an operator

$$U_{\delta, N} \in L(\mathcal{H}_N) \quad (15)$$

for every choice of a positive integer N by precisely the same formula (11) as before, except that the expression $i + D$ is understood to refer to addition modulo N . We observe that if U_δ is unitary, then $U_{\delta, N}$ is necessarily unitary for every choice of $N \geq 5$.

A simulation of a quantum Turing machine on an input string of length n for $t \geq n$ steps can immediately be obtained from a simulation of the same machine on a tape loop of size $N = 2t + 1$ (or any choice of N larger than $2t + 1$). For this reason we will focus on quantum Turing machines with tapes formed into loops, whose size will be a function of the input length and number of steps for which the machine is to be simulated. Viewing quantum Turing machine computations as taking place on a tape loop is just a minor convenience that allows us to work entirely with finite-dimensional Hilbert spaces and removes the need for special cases at the edges of the tape region indexed by $-t, \dots, t$.

4 Localizing causal unitary evolutions

This section of the paper is concerned with a relationship between causality and localizability of unitary operators, first described by Arrighi, Nesme, and Werner [ANW11]. Our presentation of this relationship will differ somewhat from theirs, however, and we will require a generalization of their findings that is concerned with operators whose causality holds only on certain subspaces of a tensor product space. Although the relationship between causality and localizability to be discussed is a key to our analysis of the simulation of quantum Turing machines by quantum circuits, the section itself is independent of quantum Turing machines.

We will begin with a definition of causality, which includes both the cases in which causality holds on an entire space (as considered by Arrighi, Nesme, and Werner) or just on a subspace.

Definition 1. Let X , Y , and Z be registers having associated Hilbert spaces \mathcal{X} , \mathcal{Y} , and \mathcal{Z} , respectively, and let $U \in U(\mathcal{X} \otimes \mathcal{Y} \otimes \mathcal{Z})$ be a unitary operator.

1. The operator U is $Y \rightarrow X$ causal if, for every pair of states $\rho, \sigma \in D(\mathcal{X} \otimes \mathcal{Y} \otimes \mathcal{Z})$ satisfying $\text{Tr}_{\mathcal{Z}}(\rho) = \text{Tr}_{\mathcal{Z}}(\sigma)$, one has

$$\text{Tr}_{\mathcal{Y} \otimes \mathcal{Z}}(U\rho U^*) = \text{Tr}_{\mathcal{Y} \otimes \mathcal{Z}}(U\sigma U^*). \quad (16)$$

2. The operator U is $Y \rightarrow X$ causal on a subspace $\mathcal{V} \subseteq \mathcal{X} \otimes \mathcal{Y} \otimes \mathcal{Z}$ if, for every pair of states $\rho, \sigma \in D(\mathcal{X} \otimes \mathcal{Y} \otimes \mathcal{Z})$ satisfying $\text{im}(\rho) \subseteq \mathcal{V}$, $\text{im}(\sigma) \subseteq \mathcal{V}$, and $\text{Tr}_{\mathcal{Z}}(\rho) = \text{Tr}_{\mathcal{Z}}(\sigma)$, one has

$$\text{Tr}_{\mathcal{Y} \otimes \mathcal{Z}}(U\rho U^*) = \text{Tr}_{\mathcal{Y} \otimes \mathcal{Z}}(U\sigma U^*). \quad (17)$$

The intuition behind this definition is that a unitary operator U is $Y \rightarrow X$ causal if the state of X after the application of the operator U is completely determined by the state of (X, Y) before the application of U . A natural way to view this situation is that X represents some local region of interest, Y represents a neighborhood of X (excluding X itself), and Z represents everything outside of this neighborhood. If U is $Y \rightarrow X$ causal, then changes to X induced by U are effectively caused by the state of (X, Y) and are not influenced by the state of Z . The restriction of this property to a subspace \mathcal{V} of $\mathcal{X} \otimes \mathcal{Y} \otimes \mathcal{Z}$ requires only that this property holds for states fully supported on \mathcal{V} .

Next we will prove two lemmas that lead naturally to the main result of the section. The first lemma establishes a simple but useful technical condition on causal unitary operators.

Lemma 2. *Let $X, Y,$ and Z be registers having associated Hilbert spaces $\mathcal{X}, \mathcal{Y},$ and $\mathcal{Z},$ respectively, let $\mathcal{V} \subseteq \mathcal{X} \otimes \mathcal{Y} \otimes \mathcal{Z}$ be a subspace, and let $U \in \mathbf{U}(\mathcal{X} \otimes \mathcal{Y} \otimes \mathcal{Z})$ be a $Y \rightarrow X$ causal unitary operator on the subspace \mathcal{V} . For every Hermitian operator $H \in \mathbf{Herm}(\mathcal{X} \otimes \mathcal{Y} \otimes \mathcal{Z})$ satisfying $\text{im}(H) \subseteq \mathcal{V}$ and $\text{Tr}_{\mathcal{Z}}(H) = 0,$ and every operator $X \in \mathbf{L}(\mathcal{X}),$ one has*

$$\langle H, U^*(X \otimes \mathbb{1}_{\mathcal{Y}} \otimes \mathbb{1}_{\mathcal{Z}})U \rangle = 0. \quad (18)$$

Proof. The statement is trivial when $H = 0,$ so assume H is nonzero, and let

$$H = P - Q \quad (19)$$

be the Jordan-Hahn decomposition of $H,$ meaning that $P, Q \in \mathbf{Pos}(\mathcal{X} \otimes \mathcal{Y} \otimes \mathcal{Z})$ are the unique positive semidefinite operators satisfying (19) and $PQ = 0.$ The assumption $\text{Tr}_{\mathcal{Z}}(H) = 0$ implies that $\text{Tr}_{\mathcal{Z}}(P) = \text{Tr}_{\mathcal{Z}}(Q),$ and in particular

$$\text{Tr}(P) = \lambda = \text{Tr}(Q) \quad (20)$$

for some positive real number $\lambda > 0.$ Moreover, by the assumption $\text{im}(H) \subseteq \mathcal{V},$ one has that $\text{im}(P) \subseteq \mathcal{V}$ and $\text{im}(Q) \subseteq \mathcal{V}.$ Thus, the density operators $\rho = P/\text{Tr}(P)$ and $\sigma = Q/\text{Tr}(Q)$ satisfy

$$H = \lambda(\rho - \sigma) \quad \text{and} \quad \text{Tr}_{\mathcal{Z}}(\rho) = \text{Tr}_{\mathcal{Z}}(\sigma), \quad (21)$$

as well as $\text{im}(\rho) \subseteq \mathcal{V}$ and $\text{im}(\sigma) \subseteq \mathcal{V}.$ By the assumption that U is causal on $\mathcal{V},$ it follows that

$$\langle H, U^*(X \otimes \mathbb{1}_{\mathcal{Y}} \otimes \mathbb{1}_{\mathcal{Z}})U \rangle = \lambda \langle \text{Tr}_{\mathcal{Y} \otimes \mathcal{Z}}(U\rho U^*) - \text{Tr}_{\mathcal{Y} \otimes \mathcal{Z}}(U\sigma U^*), X \rangle = 0, \quad (22)$$

as required. \square

The second lemma draws an implication from the structure suggested in the previous lemma that will lead naturally to the notion of localizability, provided that the subspace in question is suitably aligned with the underlying tensor product structure of the global space. (Note that the Hilbert space \mathcal{W} in this lemma plays the role of $\mathcal{X} \otimes \mathcal{Y}$ in the definition of causality.)

Lemma 3. Let \mathcal{W} and \mathcal{Z} be finite-dimensional Hilbert spaces, let $\{\Delta_1, \dots, \Delta_n\} \subseteq \text{Proj}(\mathcal{W})$ and $\{\Lambda_1, \dots, \Lambda_n\} \subseteq \text{Proj}(\mathcal{Z})$ be orthogonal sets of nonzero projection operators, and let

$$\Pi = \sum_{k=1}^n \Delta_k \otimes \Lambda_k. \quad (23)$$

For every operator $A \in \text{L}(\mathcal{W} \otimes \mathcal{Z})$ such that $\langle H, A \rangle = 0$ for all Hermitian operators H with $\text{im}(H) \subseteq \text{im}(\Pi)$ and $\text{Tr}_{\mathcal{Z}}(H) = 0$, there exists an operator $W \in \text{L}(\mathcal{W})$ such that

$$\Pi A \Pi = \Pi(W \otimes \mathbb{1}_{\mathcal{Z}})\Pi. \quad (24)$$

If, in addition, A is a unitary operator and $[A, \Pi] = 0$, then there exists a unitary operator W that satisfies (24).

Proof. Suppose $Z \in \text{U}(\mathcal{Z})$ is any unitary operator satisfying

$$[\mathbb{1}_{\mathcal{X}} \otimes Z, \Pi] = 0. \quad (25)$$

For an arbitrarily chosen Hermitian operator $H \in \text{Herm}(\mathcal{X} \otimes \mathcal{Z})$, one has

$$\langle H, \Pi A \Pi - (\mathbb{1}_{\mathcal{X}} \otimes Z) \Pi A \Pi (\mathbb{1}_{\mathcal{X}} \otimes Z^*) \rangle = \langle K, A \rangle \quad (26)$$

for

$$K = \Pi H \Pi - (\mathbb{1}_{\mathcal{X}} \otimes Z^*) \Pi H \Pi (\mathbb{1}_{\mathcal{X}} \otimes Z). \quad (27)$$

The operator K is Hermitian and satisfies $\text{im}(K) \subseteq \text{im}(\Pi)$ and $\text{Tr}_{\mathcal{Z}}(K) = 0$, and therefore by the assumptions of the lemma the quantity represented by (26) is zero. Because this is so for every choice of $H \in \text{Herm}(\mathcal{X} \otimes \mathcal{Z})$, it follows that

$$\Pi A \Pi = (\mathbb{1}_{\mathcal{X}} \otimes Z) \Pi A \Pi (\mathbb{1}_{\mathcal{X}} \otimes Z^*), \quad (28)$$

which is equivalent to

$$[\mathbb{1}_{\mathcal{X}} \otimes Z, \Pi A \Pi] = 0. \quad (29)$$

Now, the set of all unitary operators $Z \in \text{U}(\mathcal{Z})$ for which (25) is satisfied includes those operators for which $[Z, \Lambda_k] = 0$ for all $k \in \{1, \dots, n\}$, from which it follows that

$$\Pi A \Pi = \sum_{k=1}^n W_k \otimes \Lambda_k \quad (30)$$

for some choice of $W_1, \dots, W_n \in \text{L}(\mathcal{X})$ satisfying $W_k = \Delta_k W_k \Delta_k$ for each $k \in \{1, \dots, n\}$. By setting

$$W = W_1 + \dots + W_n + (\mathbb{1}_{\mathcal{X}} - \Delta_1 - \dots - \Delta_n), \quad (31)$$

one obtains an operator satisfying

$$\Pi A \Pi = \sum_{k=1}^n \Delta_k W \Delta_k \otimes \Lambda_k = \Pi(W \otimes \mathbb{1}_{\mathcal{Z}})\Pi. \quad (32)$$

Finally, if A is unitary and $[A, \Pi] = 0$, then A is a unitary operator when restricted to $\text{im}(\Pi)$, which implies that each W_k in (30) is unitary when restricted to $\text{im}(\Delta_k)$. The operator W defined in (31) is therefore unitary, which completes the proof. \square

Remark 4. Note that if one allows $\{\Delta_1, \dots, \Delta_n\}$ not to be mutually orthogonal, the decomposition for $\Pi A \Pi$ given by (30) can still be obtained. However, now the operator defined in (31) does not satisfy the relation in (32) because the images of the operators W_1, \dots, W_n may overlap.

Remark 5. Note that our proof for Lemma 3 will still go through if the space \mathcal{Z} is allowed to be an infinite-dimensional separable Hilbert space, as can be checked for example through [Con00, Tak13, Jon15].

Finally, we state the main theorem of the section, which connects the property of a unitary operator being causal with the notion of *localizability*, which simply means that an operator can be represented as a tensor product of one operator with the identity operator. The original result of Arrighi, Nesme, and Werner that this theorem generalizes states that if U is a $Y \rightarrow X$ causal unitary operator and $X \in \mathcal{U}(\mathcal{X})$ is a unitary operator on \mathcal{X} , then

$$U^*(X \otimes \mathbb{1}_{\mathcal{Y} \otimes \mathcal{Z}})U = W \otimes \mathbb{1}_{\mathcal{Z}} \quad (33)$$

for some unitary operator $W \in \mathcal{U}(\mathcal{X} \otimes \mathcal{Y})$. As has already been suggested, the generalization represented by the theorem that follows concerns unitary operators that are only causal on some subspace that is suitably aligned with the tensor product structure of $\mathcal{X} \otimes \mathcal{Y} \otimes \mathcal{Z}$.

Theorem 6. Let \mathcal{X} , \mathcal{Y} , and \mathcal{Z} be complex Euclidean spaces, let $\{\Delta_1, \dots, \Delta_n\} \subseteq \text{Proj}(\mathcal{X} \otimes \mathcal{Y})$ and $\{\Lambda_1, \dots, \Lambda_n\} \subseteq \text{Proj}(\mathcal{Z})$ be orthogonal sets of nonzero projection operators, let

$$\Pi = \sum_{k=1}^n \Delta_k \otimes \Lambda_k, \quad (34)$$

and let $U \in \mathcal{U}(\mathcal{X} \otimes \mathcal{Y} \otimes \mathcal{Z})$ be a unitary operator that is $Y \rightarrow X$ causal on $\text{im}(\Pi)$. For every operator $X \in \mathcal{L}(\mathcal{X})$, there exists an operator $W \in \mathcal{L}(\mathcal{X} \otimes \mathcal{Y})$ such that

$$\Pi U^*(X \otimes \mathbb{1}_{\mathcal{Y} \otimes \mathcal{Z}})U \Pi = \Pi(W \otimes \mathbb{1}_{\mathcal{Z}})\Pi. \quad (35)$$

If, in addition, X is unitary and $[U^*(X \otimes \mathbb{1}_{\mathcal{Y} \otimes \mathcal{Z}})U, \Pi] = 0$, then W may also be taken to be unitary.

Proof. Let $\mathcal{W} = \mathcal{X} \otimes \mathcal{Y}$ and $A = U^*(X \otimes \mathbb{1}_{\mathcal{Y} \otimes \mathcal{Z}})U$. By Lemma 2 the operator A satisfies the requirements of Lemma 3, which in turn implies the theorem. \square

5 Circuit simulation of quantum Turing machines

In this section we present a simulation of quantum Turing machines by quantum circuits based on the simulation method of Yao, together with its analysis. As has already been mentioned, there are technical differences between the simulation we present and the one originally proposed by Yao, and these differences are described briefly later in the section.

Simulation structure

Following the same conventions that were described in Section 3, we will assume that the quantum Turing machine M to be simulated has state set $Q = \{1, \dots, m\}$ and tape alphabet $\Gamma = \{0, \dots, k-1\}$, and has a transition function

$$\delta : Q \times \Gamma \rightarrow \mathbb{C}^{Q \times \Gamma \times \{-1, +1\}} \quad (36)$$

that induces a unitary global evolution. It will also be assumed that some input alphabet $\Sigma \subseteq \{1, \dots, k-1\}$ has been specified, and that the computation of the quantum Turing machine M on an input string $x \in \Sigma^n$ is to be simulated for $t \geq n$ steps. The simulation can be performed for fewer than n steps, but the assumption that $t \geq n$ allows us to write t rather than $\max\{n, t\}$ in various places throughout the proof, and little generality is lost in disregarding Turing machine computations that are not even long enough to read their entire input string.

Quantum circuits operate on qubits, of course, but it is convenient to first describe a circuit simulation of quantum Turing machines that operates on collections of registers whose classical state sets relate to the sets Γ and Q , rather than on qubits. (The classical Turing machine simulation in Section 2 was described in a similar style.) More precisely, the simulation described below makes use of registers whose classical state sets are either $\{0, \dots, k-1\}$ or $\{-m, \dots, m\}$. The gates in these circuits will operate on at most six registers, three of each of the two sizes just mentioned. In both cases, these are constant-size registers, each such register can be replaced by a constant number of qubits, and the operations on these registers that appear in the simulation can be replaced by constant-size quantum circuits acting on these qubits. In such a replacement, elements of the sets $\{0, \dots, k-1\}$ or $\{-m, \dots, m\}$ would be encoded as binary strings of the appropriate length, and an arbitrary choice for such encodings may be selected.

The simulation includes pre-processing and post-processing steps that will be discussed shortly. The main part of the simulation functions in an iterative manner that resembles the classical simulation described in Section 2. That is, it consists of a concatenation of t identical circuit *layers*, each of which simulates a single step of the Turing machine. Also similar to the classical case, the simulation will make use of a collection of registers

$$(S_{-t}, T_{-t}), \dots, (S_t, T_t) \quad (37)$$

to represent those tape squares indexed by integers in the range $\{-t, \dots, t\}$; each register S_i indicates the presence or absence of the tape head at the square indexed by i , as well as the Turing machine's state if the head is present at this location, while T_i represents the contents of the tape square indexed by i .

We will set $N = 2t + 1$, which is assumed to be at least 5, and imagine that the Turing machine M runs on a tape loop of length N rather than a two-way infinite tape. (One may choose N to be larger than $2t + 1$ without compromising the simulation. It turns out that it is both natural and convenient to choose N to be the smallest multiple of 3 that is at least $2t + 1$, as will become clear later in the section.) As was mentioned in Section 3, there is essentially no difference between the two cases, as the tape head never has time to cross the division between the tape squares indexed by t and $-t$ (or, equivalently, t and $t + 1$,

as tape square indices are equated modulo N). The transition function δ induces a unitary operator $U_{\delta,N}$ on the Hilbert space \mathcal{H}_N whose standard basis corresponds to the set of possible configurations of M running on a tape loop of length N , as defined in Section 3. Hereafter we will write U rather than $U_{\delta,N}$ for brevity, as δ and N may safely be viewed as being fixed for the purposes of this description.

Next, let us be more precise about the registers (37). As suggested above, we will view the indices of these registers as representing elements of \mathbb{Z}_N , so that they may alternatively be written (without changing their order) as $(S_{N-t}, T_{N-t}), \dots, (S_{N-1}, T_{N-1}), (S_0, T_0), \dots, (S_t, T_t)$. The classical state set of each register S_i is $\{-m, \dots, m\}$ and the classical state set of each T_i is $\{0, \dots, k-1\}$. Note, in particular, that this choice differs from the classical case, in which each S_i stores an element of $\{0, \dots, m\}$. In essence, the states $-1, \dots, -m$ will function as “inactive copies” of the states $1, \dots, m$; this is a simple but key trick that allows Yao’s simulation method to work. For each $i \in \mathbb{Z}_N$ we will let \mathcal{S}_i and \mathcal{T}_i denote the Hilbert spaces associated with S_i and T_i , respectively, and we will let

$$\mathcal{K}_N = (\mathcal{S}_0 \otimes \mathcal{T}_0) \otimes \dots \otimes (\mathcal{S}_{N-1} \otimes \mathcal{T}_{N-1}) \quad (38)$$

be the combined Hilbert space of the entire sequence $(S_0, T_0), \dots, (S_{N-1}, T_{N-1})$. The spaces $\mathcal{S}_0, \dots, \mathcal{S}_{N-1}$ are of course equivalent to one another, as are the spaces $\mathcal{T}_0, \dots, \mathcal{T}_{N-1}$, and when we wish to refer generally to any one of these spaces without specifying which one it is, we will simply write \mathcal{S} or \mathcal{T} without a subscript.

For each configuration (p, i, T) of M running on a tape loop of length N , one may associate a classical state

$$f(p, i, T) \in (\{0, \dots, m\} \times \{0, \dots, k-1\})^N \quad (39)$$

of the register pairs $(S_0, T_0), \dots, (S_{N-1}, T_{N-1})$ in a similar way to what is done in the classical simulation described in Section 2. That is, each register T_j stores $T(j)$ for $j \in \mathbb{Z}_N$, the register S_i stores p , which is an element of the set $\{1, \dots, m\}$, and every other register S_j , for $j \neq i$, stores 0. None of the registers S_0, \dots, S_{N-1} stores a negative value. One can also define an isometry $A \in U(\mathcal{H}_N, \mathcal{K}_N)$ based on this correspondence between configurations and classical register states as

$$A = \sum_{(p,i,T)} |f(p, i, T)\rangle \langle p, i, T|, \quad (40)$$

where the sum is over all configurations of M on a tape loop of length N . It may be observed that the projection AA^* is alternatively described as the projection onto the space spanned by classical states of the registers $(S_0, T_0), \dots, (S_{N-1}, T_{N-1})$ that correspond to valid Turing machine configurations, meaning that none of the registers S_0, \dots, S_{N-1} contain negative values and exactly one of these registers contains a positive value.

Simulation procedure

The pre-processing step of the simulation initializes $(S_0, T_0), \dots, (S_{N-1}, T_{N-1})$ to the standard basis state corresponding to the initial configuration of M on input x . Each circuit

layer in the main part of the simulation will induce a unitary transformation that agrees with AUA^* on the subspace $\text{im}(A)$. The final post-processing step transforms the state of the registers $(S_0, T_0), \dots, (S_{N-1}, T_{N-1})$ into whatever output form is desired for the simulation. The state of these registers will be fully supported on $\text{im}(A)$, so a standard basis measurement of these registers after the completion of the main part of the simulation would necessarily yield a state corresponding to a valid configuration of M .

The main challenge of the simulation is to efficiently implement the layers in the main part of the simulation, each of which performs a transformation that agrees with AUA^* on $\text{im}(A)$. To this end, define a reversible (and therefore unitary) transformation

$$F|p\rangle = |-p\rangle \quad (41)$$

for every $p \in \{-m, \dots, m\}$, which may be regarded as an operator acting on \mathcal{S} , or equivalently on \mathcal{S}_i for any choice of $i \in \mathbb{Z}_N$. Note that F is not a phase flip, it is a permutation of the standard basis states $|-m\rangle, \dots, |m\rangle$. For each index $i \in \mathbb{Z}_N$, define F_i to be the unitary operator acting on \mathcal{K}_N that is obtained by tensoring F on the register \mathcal{S}_i with the identity operator on all of the remaining registers. Notice that the operators F_0, \dots, F_{N-1} mutually commute, and that their product $F_0 \cdots F_{N-1}$ is equivalent to F being performed independently on every one of the registers $\mathcal{S}_0, \dots, \mathcal{S}_{N-1}$.

Next, define two unitary operators:

$$V = AUA^* + (\mathbb{1} - AA^*) \quad \text{and} \quad W = (F_0 \cdots F_{N-1})V^*(F_0 \cdots F_{N-1})V. \quad (42)$$

The subspace $\text{im}(A)$ is evidently an invariant subspace of V , as is its orthogonal complement $\text{im}(A)^\perp$, upon which V acts trivially. The operator $F_0 \cdots F_{N-1}$ maps $\text{im}(A)$ into $\text{im}(A)^\perp$, as each standard basis state corresponding to a configuration is transformed into a standard basis state for which one of the registers $\mathcal{S}_0, \dots, \mathcal{S}_{N-1}$ contains a negative value. Specifically, $|f(p, i, T)\rangle$ is transformed into a standard basis state in which the register \mathcal{S}_i contains the value $-p$. The operator

$$(F_0 \cdots F_{N-1})V^*(F_0 \cdots F_{N-1}) \quad (43)$$

therefore acts trivially on $\text{im}(A)$, implying that V and W act identically on $\text{im}(A)$.

Now consider the operator $V^*(F_0 \cdots F_{N-1})V$, which may alternatively be written

$$V^*(F_0 \cdots F_{N-1})V = (V^*F_0V) \cdots (V^*F_{N-1}V). \quad (44)$$

As F_0, \dots, F_{N-1} mutually commute, so do the operators $V^*F_0V, \dots, V^*F_{N-1}V$. It therefore suffices that each circuit layer in the main part of the simulation applies these operators, in an arbitrary order, followed by the operator $F_0 \cdots F_{N-1}$ (or, equivalently, F applied independently to each of the registers $\mathcal{S}_0, \dots, \mathcal{S}_{N-1}$).

Locality

It remains to prove that each of the operators V^*F_iV can be localized, specifically to the registers $(\mathcal{S}_{i-1}, T_{i-1}), (\mathcal{S}_i, T_i), (\mathcal{S}_{i+1}, T_{i+1})$, when restricted to a suitable subspace that contains $\text{im}(A)$. Fix $i \in \mathbb{Z}_N$, define $X = (\mathcal{S}_i, T_i)$ and $Y = (\mathcal{S}_{i-1}, T_{i-1}, \mathcal{S}_{i+1}, T_{i+1})$, and let Z

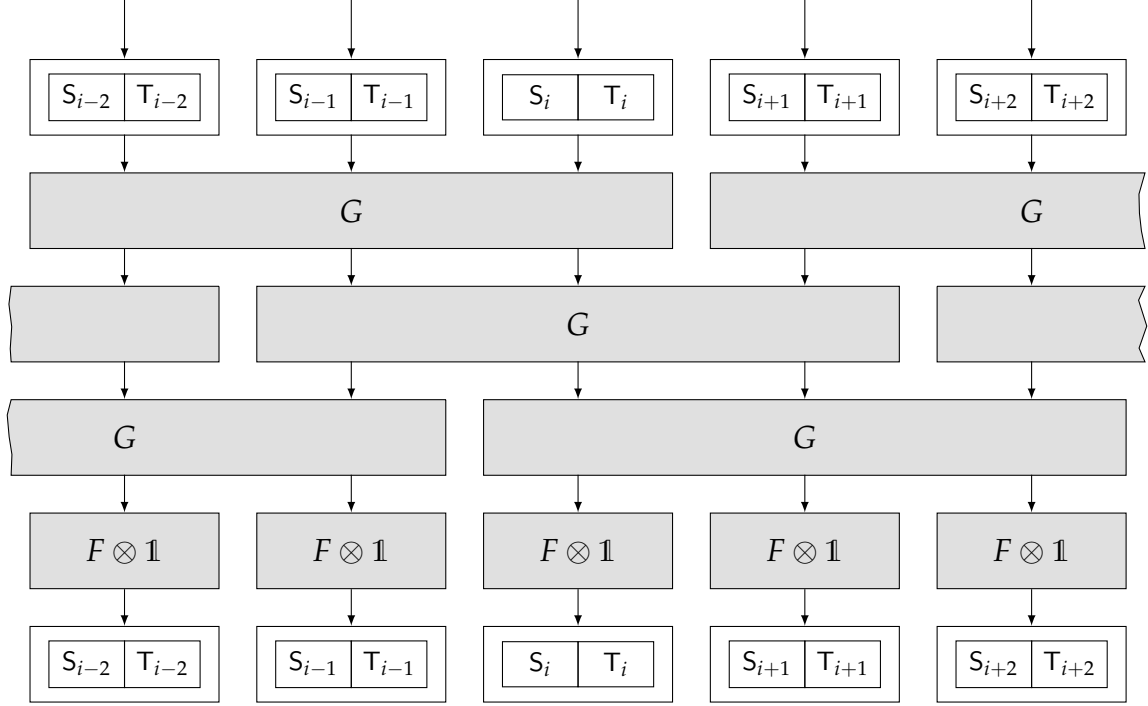


Figure 4: Each Turing machine step is simulated by one circuit layer in the main part of the simulation, which consists of a pattern of unitary operations as illustrated. (Note that if the number of register pairs is not divisible by 3, then one or two additional G transformations may need to be performed on separate levels so that G is applied once to each triple $(S_{i-1}, T_{i-1}), (S_i, T_i), (S_{i+1}, T_{i+1})$. Alternatively, N can be increased to the nearest multiple of 3 without affecting the validity of the simulation.)

denote all of the remaining registers among $(S_0, T_0), \dots, (S_{N-1}, T_{N-1})$ that do not appear in X or Y . For each $a \in \{0, 1\}$, define $\Delta_a \in \text{Proj}(\mathcal{X} \otimes \mathcal{Y})$ to be the projection onto the space spanned by standard basis states of (X, Y) in which precisely a of the registers S_{i-1}, S_i, S_{i+1} contain a nonzero (either positive or negative) value, and define $\Lambda_a \in \text{Proj}(\mathcal{Z})$ similarly, but replacing S_{i-1}, S_i, S_{i+1} with those registers among S_0, \dots, S_{N-1} that appear in Z rather than (X, Y) . Finally, define a projection

$$\Pi = \Delta_0 \otimes \Lambda_1 + \Delta_1 \otimes \Lambda_0. \quad (45)$$

In words, Π is the projection onto the space spanned by standard basis states of the registers $(S_0, T_0), \dots, (S_{N-1}, T_{N-1})$ in which exactly one of the registers S_0, \dots, S_{N-1} contains a nonzero value (representing exactly one tape head, either active or inactive). The expression (45) reveals that this projection is aligned with the tensor product structure of $\mathcal{X} \otimes \mathcal{Y} \otimes \mathcal{Z}$ in a suitable way to allow for Theorem 6 to be applied to the situation under consideration.

It is evident that the operator V is $Y \rightarrow X$ causal on the subspace $\text{im}(\Pi)$: for an arbitrary state $\rho \in D(\mathcal{K}_N)$ satisfying $\rho = \Pi\rho\Pi$, the state $(V\rho V^*)[S_i, T_i]$ (i.e., the state of (S_i, T_i) obtained by tracing out all other registers from $V\rho V^*$) is uniquely determined by

the state $\rho[S_{i-1}, T_{i-1}, S_i, T_i, S_{i+1}, T_{i+1}]$. By Theorem 6 there must therefore exist a unitary operator $G \in U(\mathcal{X} \otimes \mathcal{Y})$, or equivalently $G \in U((\mathcal{S} \otimes \mathcal{T})^{\otimes 3})$, such that

$$\Pi(G \otimes \mathbb{1}_{\mathcal{Z}})\Pi = \Pi V^*((F \otimes \mathbb{1}) \otimes \mathbb{1}_{\mathcal{Y} \otimes \mathcal{Z}})V\Pi. \quad (46)$$

Note that G has no dependence on i because the behavior of M is the same for every tape square. The circuit suggested by Figure 4, in which G is applied to each consecutive triple $(S_{i-1}, T_{i-1}), (S_i, T_i), (S_{i+1}, T_{i+1})$, followed by F on each of the registers S_0, \dots, S_{N-1} , therefore agrees with W on $\text{im}(\Pi)$. Given that $\text{im}(A) \subseteq \text{im}(\Pi)$, this operator also agrees with W on $\text{im}(A)$.

As an aside, one may observe that the operator V is not $Y \rightarrow X$ causal on the entire space \mathcal{K}_N , for any selection of $i \in \mathbb{Z}_N$. For example, if S_j contains nonzero values for two or more distinct choices of $j \in \mathbb{Z}_N$ (which would represent an invalid “multi-headed” configuration), then V will act trivially on all local regions, regardless of their states. This explains why we have stated and proved Theorem 6, as opposed to directly making use of the results of Arrighi, Nesme, and Werner [ANW11].

Behavior of the local gate G

The action of the operation G on standard basis states, which can be recovered directly from the equation (46), is as follows:

1. For $p_1, p_2, p_3 \in \{1, \dots, m\}$ and $a_1, a_2, a_3 \in \Gamma$, G acts trivially on the following standard basis states:

$$\begin{aligned} &|0, a_1\rangle|p_2, a_2\rangle|0, a_3\rangle, \\ &|-p_1, a_1\rangle|0, a_2\rangle|0, a_3\rangle, \\ &|0, a_1\rangle|0, a_2\rangle|-p_3, a_3\rangle. \end{aligned} \quad (47)$$

In the first of these cases F_i acts as the identity and V cancels V^* , while in the other two cases all three of those operators act as the identity.

Similarly, G may be taken to act trivially on all choices of standard basis states of the form

$$|q_1, a_1\rangle|q_2, a_2\rangle|q_3, a_3\rangle \quad (48)$$

for which two or more of the values q_1, q_2 , and q_3 are nonzero. (The action of G can, in fact, be chosen arbitrarily on the space spanned by such states, so long as this space is invariant under the action of G .)

2. For $p_2 \in \{1, \dots, m\}$ and $a_1, a_2, a_3 \in \Gamma$, the action of G on standard basis states of the form $|0, a_1\rangle|-p_2, a_2\rangle|0, a_3\rangle$ is as follows:

$$\begin{aligned} G : |0, a_1\rangle|-p_2, a_2\rangle|0, a_3\rangle &\mapsto \\ &\sum_{\substack{p_1 \in \{1, \dots, m\} \\ b_1 \in \Gamma}} \overline{\delta(p_1, b_1)[p_2, a_1, +1]} |p_1, b_1\rangle|0, a_2\rangle|0, a_3\rangle \\ &+ \sum_{\substack{p_3 \in \{1, \dots, m\} \\ b_3 \in \Gamma}} \overline{\delta(p_3, b_3)[p_2, a_3, -1]} |0, a_1\rangle|0, a_2\rangle|p_3, b_3\rangle. \end{aligned} \quad (49)$$

3. For $p_1, p_3 \in \{1, \dots, m\}$ and $a_1, a_2, a_3 \in \Gamma$, the action of G on standard basis states of the forms $|p_1, a_1\rangle|0, a_2\rangle|0, a_3\rangle$ and $|0, a_1\rangle|0, a_2\rangle|p_3, a_3\rangle$ is as follows:

$$\begin{aligned}
G : |p_1, a_1\rangle|0, a_2\rangle|0, a_3\rangle \mapsto & \\
& \sum_{\substack{q_2 \in \{1, \dots, m\} \\ b_1 \in \Gamma}} \delta(p_1, a_1)[q_2, b_1, +1]|0, b_1\rangle|-q_2, a_2\rangle|0, a_3\rangle \\
& + \sum_{\substack{q_1 \in \{1, \dots, m\} \\ r_0 \in \{1, \dots, m\} \\ b_1 \in \Gamma, c_1 \in \Gamma}} \delta(p_1, a_1)[r_0, c_1, -1]\overline{\delta(q_1, b_1)[r_0, c_1, -1]}|q_1, b_1\rangle|0, a_2\rangle|0, a_3\rangle.
\end{aligned} \tag{50}$$

and

$$\begin{aligned}
G : |0, a_1\rangle|0, a_2\rangle|p_3, a_3\rangle \mapsto & \\
& \sum_{\substack{q_2 \in \{1, \dots, m\} \\ b_3 \in \Gamma}} \delta(p_3, a_3)[q_2, b_3, -1]|0, a_1\rangle|-q_2, a_2\rangle|0, b_3\rangle \\
& + \sum_{\substack{q_3 \in \{1, \dots, m\} \\ r_4 \in \{1, \dots, m\} \\ b_3 \in \Gamma, c_3 \in \Gamma}} \delta(p_3, a_3)[r_4, c_3, +1]\overline{\delta(q_3, b_3)[r_4, c_3, +1]}|0, a_1\rangle|0, a_2\rangle|q_3, b_3\rangle.
\end{aligned} \tag{51}$$

For a given quantum Turing machine M , the actions expressed in the second and third items above can be simplified by making use of the conditions of Bernstein and Vazirani required for δ to induce a global unitary evolution. We have described the transitions without making such simplifications to illustrate how the transitions can simply be read off from the equation (46). Note that in the third case, one might expect from (46) that there would be terms where the head ends up outside the considered range of cells. For example, in (50) we might expect to have a term where the head first goes left with the application of V and then goes left again with the application of V^* . However, we know from our application of Theorem 6 that such terms cannot exist, which means that the corresponding coefficients that would be derived from δ must be zero for any choice of quantum Turing machine.

Recapitulation

In summary, the simulation of M for t steps on a given input string x of length $n \leq t$ is as follows:

1. (Pre-processing step) For $N = 2t + 1$, initialize registers $(S_0, T_0), \dots, (S_{N-1}, T_{N-1})$ so that their state represents the initial configuration of M on input x , running on a tape loop of length N .
2. (Main part) Let G be the unitary operator determined by the transition function δ of M as described above. Concatenate t identical copies of a circuit that first applies G to every triple of register pairs $(S_{i-1}, T_{i-1}), (S_i, T_i), (S_{i+1}, T_{i+1})$, for i ranging over

the set \mathbb{Z}_N , and then applies F to each of the registers S_0, \dots, S_{N-1} . The copies of G can be applied in an arbitrary order, such as the one suggested in Figure 4 that allows for these operations to be parallelized.

3. (Post-processing step) Transform the standard basis states of the registers $(S_0, T_0), \dots, (S_{N-1}, T_{N-1})$ that represent a configuration of M on a tape loop of length N into whatever configuration encoding is desired for the output.

Complexity of the simulation

As was already suggested, each of the registers S_0, \dots, S_{N-1} and T_0, \dots, T_{N-1} may be viewed as a constant-size collection of qubits, and the standard basis states of these registers may be encoded as a binary string of an appropriate length, and therefore the entire simulation described above may be implemented as a quantum circuit. Each of the registers has constant size, and can therefore be represented by a constant number of qubits.

Let us first make the simplifying assumption that the operation G , which acts on a constant number of qubits for any fixed choice of a quantum Turing machine, is available as a single quantum gate. The total number of gates required by the main part of the simulation is therefore $O(t^2)$, and the depth required is $O(t)$. The pre-processing step can be performed by circuits having constant depth and size linear in t , and therefore the pre-processing step and the main part of the simulation can together be performed by quantum circuits of size $O(t^2)$ and depth $O(t)$.

The cost of the post-processing step depends on the desired form for the output of the simulation. For a natural choice of an encoding scheme in which each configuration (p, i, T) is described as a sequence of integers $p \in \{1, \dots, m\}$, $i \in \{-t, \dots, t\}$, and $T(-t), \dots, T(t) \in \{0, \dots, k-1\}$, all expressed in binary notation, the post-processing step can be performed by a circuit with size $O(t \log(t))$ and depth $O(\log(t))$. For a wide range of alternative encoding schemes for Turing machine configurations, the post-processing step can be performed by circuits whose size and depth are within the bounds $O(t^2)$ and $O(t)$ obtained for the main part of the simulation. For any such output form, the total number of gates required by the simulation is therefore $O(t^2)$ and the depth is $O(t)$.

The circuits that result from the simulation described above are evidently logarithmic-space uniformly generated (and therefore polynomial-time uniformly generated). To be more precise, for every quantum Turing machine M , there exists a deterministic Turing machine running in logarithmic space that, on input $1^n 0 1^t$, outputs a description of the quantum circuit that simulates M on inputs of length n for t steps. This follows from the observation that these circuits all conform to the same simple and regular pattern—the dependence on M is captured entirely by the specific choice for G and the size (always considered a constant) of the state set and alphabet of M .

If one is not satisfied with the assumption that G is made available as a single quantum gate from which the quantum circuits that simulate a given quantum Turing machine can be constructed, then the cost of implementing or approximating G must be considered. This issue is, of course, not specific to the simulation of quantum Turing machines, but rather is a more fundamental issue—and for this reason we will not discuss it in depth.

However, we do mention a couple of points regarding this issue that some readers may find to be helpful:

1. The operation G can be implemented exactly using a constant number of two-qubit gates, provided that one assumes that controlled-NOT gates and arbitrary single-qubit gates are available, through the method of [BBC⁺95]. The single-qubit gates required for an exact implementation naturally depend on the values $\delta(p, a)[q, b, D]$ taken by the transition function of M . As G is constant in size, the same complexity bounds described above remain valid in this case: the simulation requires size $O(t^2)$, depth $O(t)$, and is performed by logarithmic-space uniformly generated families of quantum circuits composed of controlled-NOT gates and a finite number of single-qubit gates (the selection of which depends on M).
2. If one is instead interested in a simulation with overall error ε using a fixed universal set of gates, then each G must be implemented with accuracy on the order of $O(\varepsilon/t^2)$. This is possible with circuits of size polylogarithmic in t and $1/\varepsilon$ by means of the Solovay–Kitaev theorem. The size and depth of the simulation in this case is as above, but multiplied by this polylogarithmic factor. This is true for arbitrary choices of the complex numbers $\delta(p, a)[q, b, D]$ that define the transition function of M ; the additional cost that may be incurred by difficult-to-compute numbers is paid only in circuit uniformity. That is, if computing highly accurate approximations of these numbers is computationally difficult, then the same will be true of computing accurate approximations of G by a fixed gate set. On the other hand, the Solovay–Kitaev theorem is known to have a computationally efficient constructive proof [KSV02, DN06], and if accurate approximations of the complex numbers defining the transition function can be efficiently computed, then the same will be true of the circuits approximating G .

Differences with Yao’s original simulation

Disregarding extremely minor, inconsequential differences in the way that the simulations encode information, the key difference between the simulation described above and Yao’s original simulation is that the operation G is different in the two simulations. Yao’s simulation is similar to the one presented above in that G is applied to the three register pair neighborhood associated with each tape square, and this operation must be applied once for each tape square in order to simulate one step of the quantum Turing machine’s computation. Yao takes G so that it directly implements the action of the Turing machine when the tape head presence is indicated by the middle register pair:

$$\begin{aligned}
 G : |0, a_1\rangle |p_2, a_2\rangle |0, a_3\rangle &\mapsto \\
 &\sum_{\substack{q_2 \in \{1, \dots, m\} \\ b_2 \in \Gamma}} \delta(p_2, a_2)[q_2, b_2, -1] |-q_2, a_1\rangle |0, b_2\rangle |0, a_3\rangle \\
 + \sum_{\substack{q_2 \in \{1, \dots, m\} \\ b_2 \in \Gamma}} \delta(p_2, a_2)[q_2, b_2, +1] |0, a_1\rangle |0, b_2\rangle |-q_2, a_3\rangle
 \end{aligned} \tag{52}$$

for each $p_2 \in Q$ and $a_1, a_2, a_3 \in \Gamma$. (Yao actually does this for quantum Turing machines allowing for stationary tape heads, but this is the form for quantum Turing machines that disallow for stationary tape heads.)

The operation G is then further constrained so that it acts trivially on a certain subspace. This requires that one considers the orthogonality relations induced by the unitary global evolution of M , specifically among the states obtained when M is run on configurations in which the tape head has distance one or two from the cell represented by the middle triple upon which G acts. Yao does not explicitly describe G , but observes that it may be obtained through basic linear algebra.

As analyzed by Yao, this leads to the correctness of a cascading construction, where the instances of G are executed from left to right. However, it is not difficult to see that if one wishes to parallelize this construction, it can be done so through a minor symmetry-inducing change in the definition of the subspace that G acts trivially on. After that, a given instance of G will commute with those instances applied to the two overlapping neighborhoods consisting of three register pairs.

Simulating variants of quantum Turing machines

The simulation method described above can be applied to variants of quantum Turing machines that exhibit a local causal behavior similar to ordinary (one-dimensional tape) quantum Turing machines. A very simple example, which we have already noted was considered in Yao's original paper, is that of a quantum Turing machine whose tape head may remain stationary, so that its transition function takes the form

$$\delta : Q \times \Gamma \rightarrow \mathbb{C}^{Q \times \Gamma \times \{-1,0,+1\}}. \quad (53)$$

There is essentially no difference in the analysis of this case from the one presented above, except that an explicit specification of the operation G , which is easily obtained from the equation (46), may be slightly more complicated than the one described above. This lack of substantial differences is a consequence of the fact that quantum Turing machines allowing for stationary heads have precisely the same causal structure that was required to invoke Theorem 6.

A different example that better illustrates the flexibility of the simulation method we have described is that of quantum Turing machines having multi-dimensional tapes.¹ It is not necessarily our intention to advocate further study of this arguably contrived quantum Turing machine variant—the discussion that follows is meant only to support the claim that our simulation and its analysis extend without complications to models other than the standard quantum Turing machine model with a single one-dimensional tape. We will consider just two-dimensional tapes in the interest of simplicity, but it will be apparent that the discussion may be extended to tapes of any constant dimension.

A natural way to define a quantum Turing machine with a two-dimensional tape is by a transition function of the form

$$\delta : Q \times \Gamma \rightarrow \mathbb{C}^{Q \times \Gamma \times \{-1,0,+1\} \times \{-1,0,+1\}}. \quad (54)$$

¹The word *tape* is perhaps a poor choice of a word to describe a multi-dimensional storage medium, but little would be gained in introducing a different term for such an object.

The interpretation of such a function is that the complex number

$$\delta(p, a)[q, b, D_1, D_2] \quad (55)$$

indicates the amplitude with which the machine will, when in state p and scanning a tape square containing the symbol a , change state to q , overwrite the symbol in the square being scanned with b , and move its tape head in the direction (D_1, D_2) on the tape. (For example, $(-1, +1)$ indicates a diagonal tape head movement, up and to the left.) A configuration of a two-dimensional tape Turing machine having state set Q and tape alphabet Γ is represented by a triple $(p, (i, j), T)$, where $p \in Q$ is a state, $(i, j) \in \mathbb{Z} \times \mathbb{Z}$ is a pair of integers representing the tape head location, and $T : \mathbb{Z} \times \mathbb{Z} \rightarrow \Gamma$ is a function with finite support that describes the contents of the two-dimensional tape. To simulate such a quantum Turing M for t steps on an input of length $n \leq t$, it may be imagined that the machine runs on a tape in the form of a torus indexed by $\mathbb{Z}_N \times \mathbb{Z}_N$, for $N = 2t + 1$, which is the natural two-dimensional analogue of a loop in one dimension.

The quantum circuit simulation described earlier naturally extends to this situation, with one register pair $(S_{i,j}, T_{i,j})$ being defined for each tape square. The roles played by these registers are similar to before: $S_{i,j}$ indicates whether or not the tape head is present at square (i, j) , and the state (active or inactive) if it is, and $T_{i,j}$ represents the tape symbol stored in tape square (i, j) . The transition function of M is assumed to define a unitary evolution, which in turn defines a unitary operator V acting on the state space \mathcal{K}_N (corresponding to the N^2 register pairs just described) in a similar manner to the one-dimensional case. This unitary operator acts trivially on the subspace of \mathcal{K}_N orthogonal to the standard basis states in which precisely one register $S_{i,j}$ contains a positive value and none contain negative values. The operator F , which may be applied to any register $S_{i,j}$, and the projection Π onto the subspace of \mathcal{K}_N spanned by standard basis states in which exactly one register $S_{i,j}$ contains a nonzero value, are defined in the same way as in the one-dimensional case.

In the one-dimensional case, the operation G acts on three register pairs, but in the two-dimensional case G acts on nine register pairs. Specifically, for each index (i, j) , the corresponding G operation acts on the register pairs having indices in the set

$$\{(i', j') : |i - i'| \leq 1, |j - j'| \leq 1\}, \quad (56)$$

which is equivalent to the set containing (i, j) and its 8 nearest neighbors on the torus $\mathbb{Z}_N \times \mathbb{Z}_N$. The register pairs indexed by elements in this set may be collected into compound registers as $X = (S_{i,j}, T_{i,j})$ and

$$Y = \begin{pmatrix} (S_{i-1,j-1}, T_{i-1,j-1}) & (S_{i,j-1}, T_{i,j-1}) & (S_{i+1,j-1}, T_{i+1,j-1}) \\ (S_{i-1,j}, T_{i-1,j}) & & (S_{i+1,j}, T_{i+1,j}) \\ (S_{i-1,j+1}, T_{i-1,j+1}) & (S_{i,j+1}, T_{i,j+1}) & (S_{i+1,j+1}, T_{i+1,j+1}) \end{pmatrix} \quad (57)$$

Taking Z to include all of the remaining register pairs aside from the ones included in X and Y , one may apply Theorem 6 to conclude that there exists a unitary operator G acting on (X, Y) such that

$$\Pi(G \otimes \mathbb{1}_Z)\Pi = \Pi V^*((F \otimes \mathbb{1}) \otimes \mathbb{1}_{Y \otimes Z})V \Pi. \quad (58)$$

For each possible standard basis state of the register pairs comprising X and Y , the action of G may effectively be read off from this equation. One observes the following:

1. For standard basis states of these registers for which none of the registers $S_{i,j}$ included in X and Y is nonzero, the action of G will necessarily be trivial.
2. For standard basis states of these registers for which two or more of the registers $S_{i,j}$ included in X and Y are nonzero, the action of G may be taken to be trivial. (The above equation implies that the subspace spanned by such states must be invariant under the action of G , but taking G to be the identity on this space is the simplest choice.)
3. For all remaining standard basis states, one may assume that every register of Z is in the standard basis state $(0, 0)$ for simplicity, although this choice will have no influence on the action that is recovered for G . By Theorem 6, the action of the operator on the right-hand side of the above equation will uniquely specify the action of G on the chosen standard basis state; and moreover the same theorem implies that G will be unitary.

As in the one-dimensional case, the action of G is independent of the choice of (i, j) , and the operators obtained by applying G to two neighborhoods corresponding to distinct choices of (i, j) will necessarily commute, even when the neighborhoods overlap. A simulation of M is obtained as before, by alternating between the application of G to the nine register pairs corresponding to the neighborhoods of $(S_{i,j}, T_{i,j})$ for every pair (i, j) with the application of F to every register $S_{i,j}$. This time the size of the resulting circuits is $O(t^3)$ rather than $O(t^2)$, while the depth remains linear in t .

Yao's original simulation can also be extended to quantum Turing machines with multi-dimensional tapes, although once again one is required to perform computations based on simple linear algebra—which become increasingly tedious as the dimension of the tape grows—to obtain a description of G .

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