

Quantum Computers

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This paper first considers sequential quantum machines (SQMs). The SQMs that possess an isometric transition operator and the SQMs that are factorizable or strongly factorizable are characterized. Quantum Turing machines (QTMs) are studied next and an alternative proof of the result that characterizes the unitary evolution of a QTM is given. It is shown that any QTM can be represented in terms of two quantum printers which are much simpler than a QTM. Unidirectional QTMs are studied and it is shown that their corresponding quantum printers are closely related to each other. A simple method for constructing unidirectional QTMs is given. Finally, a preliminary development of generalized QTMs and quantum pushdown automata is presented.

1. INTRODUCTION

This article is a continuation of ref. 2, where basic properties of quantum automata were discussed. Although the present article is essentially self-contained, we shall occasionally refer to ref. 2 for certain concepts and notation. We now continue our exploration of the hierarchy of quantum computers by moving from quantum automata to quantum machines that have a more complex structure.

We begin in Section 2 with a review of some properties of isometric and unitary operators that will be needed in the sequel. We point out that unitarity is not always necessary for the reversible action of a quantum computer and that an isometry is frequently sufficient. Section 3 considers sequential quantum machines (SQMs). We first characterize those SQMs that possess an isometric transition operator. We then characterize the SQMs that are factorizable and strongly factorizable. Roughly speaking, a factorizable SQM is one that can be decomposed into an internal part and an output part.

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Section 4 studies quantum Turing machines (QTMs). An alternative proof of the result [1] that characterizes the unitary evolution of a QTM is given. We review the concept of a quantum printer [2] and show that any QTM has a natural connection with two quantum printers. The advantage of this connection is that quantum printers are much simpler than QTMs. In particular, the transition operator of a quantum printer can be written as a finite product of quantum gates. We then characterize those pairs of quantum printers that generate a QTM.

Unidirectional QTMs are studied in Section 5. Their importance stems from the fact that any QTM can be simulated by a unidirectional QTM with slowdown by a factor of at most five [1]. We show that two quantum printers that generate a unidirectional QTM are closely related and this again gives a simplification. A simple method for constructing any unidirectional QTM is presented and examples are given.

Finally, Section 6 discusses generalized QTMs and quantum pushdown automata. Some of the results of Sections 4 and 5 are carried over to generalized QTMs. A preliminary development of quantum pushdown automata is given and isometric transition operators are characterized. For comprehensive bibliographies on quantum computers, see refs. 1, 2, and 4.

2. ISOMETRIC AND UNITARY OPERATORS

This section reviews some properties of isometric and unitary operators that will be needed in the sequel. In our work on quantum automata [2] all the Hilbert spaces were finite dimensional, in which case there was no difference between isometries and unitary operators. However, we must now deal with infinite-dimensional Hilbert spaces and we have to distinguish between these two types of operators.

If H_1 and H_2 are complex Hilbert spaces, a norm-preserving linear transformation $U: H_1 \rightarrow H_2$ is called an *isometric transformation*. Thus, $U: H_1 \rightarrow H_2$ satisfies $\|U\psi\| = \|\psi\|$ for all $\psi \in H_1$. If $H_1 = H_2 = H$, we call U an *isometry* on H . It is easy to show that U is an isometry if and only if $U^*U = 1$, where U^* is the adjoint of U and 1 is the identity operator on H . An isometry that also satisfies $UU^* = 1$ is called a *unitary* operator. If $\dim H < \infty$, then $U^*U = 1$ implies that $UU^* = 1$, so every isometry is unitary. However, if $\dim H = \infty$, then there exist isometries that are not unitary. For example, suppose H is a separable infinite-dimensional Hilbert space with orthonormal basis ψ_i , $i \in \mathbb{N}$. Define $U\psi_i = \psi_{i+1}$ and extend U to H by linearity and closure. Then U is an isometry, but U is not unitary because ψ_1 is not in the range of U . We denote the set of isometries on H by $\mathcal{I}(H)$ and the set of unitary operators on H by $\mathcal{U}(H)$. The following well-known result will be needed in the sequel [1, 2].

Theorem 2.1. Let S be an orthonormal basis for the Hilbert space H . (a) A bounded linear operator $U: H \rightarrow H$ is an isometry if and only if $\langle Us, Ut \rangle = \delta_{s,t}$ for every $s, t \in S$. (b) A linear operator $U: H \rightarrow H$ is unitary if and only if U is an isometry and $\|U^*s\| = 1$ for every $s \in S$.

Notice that $\mathcal{F}(H)$ is closed under multiplication because $U_1, U_2 \in \mathcal{F}(H)$ implies that

$$(U_1U_2)^*(U_1U_2) = U_2^*U_1^*U_1U_2 = U_2^*U_2 = 1$$

Moreover, if $U \in \mathcal{F}(H)$, then

$$\langle U\psi, U\phi \rangle = \langle U^*U\psi, \phi \rangle = \langle \psi, \phi \rangle$$

so U preserves transition amplitudes (and norms), which is all that is needed for quantum probability theory [3]. Thus, to describe quantum computers, isometric evolutions are sufficient. Also, if $U \in \mathcal{F}(H)$, then U is injective because $U\psi = U\phi$ implies that

$$\psi = U^*U\psi = U^*U\phi = \phi$$

Hence, U gives a reversible action, which is a requirement of quantum mechanics. We now show that any isometry can be extended to a unitary operator.

Theorem 2.2. If $U \in \mathcal{F}(H)$, then the following statements hold:

(a) $P = UU^*$ is a projection operator and UH is the closed subspace PH of H .

(b) $U: H \rightarrow UH$ is a bijection and $U^{-1} = U^*$.

(c) If H is separable, then there exists a Hilbert space H_1 containing H such that U has a unitary extension to H_1 .

Proof. (a) Since $P = P^*$ and

$$P^2 = UU^*UU^* = UU^* = P$$

P is a projection operator. To show that $UH = PH$, we have

$$U\psi = UU^*U\psi = PU\psi$$

Hence, $U\psi \in PH$ and $UH \subseteq PH$. Also,

$$P\psi = UU^*\psi = U(U^*\psi)$$

so that $P\psi \in UH$ and $PH \subseteq UH$.

(b) Since $U^*U = 1$ and it follows from (a) that $UU^* = 1_{UH}$ we have that $U^{-1} = U^*$.

(c) Let H_0 be a separable, infinite-dimensional Hilbert space and let $H_1 = H \oplus H_0$. Now H is a closed subspace of H_1 and U is a bijective

isometric transformation from H onto $PH \subseteq H_1$. Since H_0 and $P^\perp H \oplus H_0$ are separable, infinite-dimensional Hilbert spaces, there exists a bijective isometric transformation $U_0: H_0 \rightarrow P^\perp H \oplus H_0$. Then $U_1 = U \oplus U_0 \in \mathcal{U}(H_1)$ and U_1 extends U . ■

We denote the unit sphere of a Hilbert space H by \hat{H} . The restriction of an isometry to \hat{H} is an injection and the restriction of a unitary operator to \hat{H} is a bijection.

3. SEQUENTIAL QUANTUM MACHINES

Let O be a finite alphabet with n letters and let H_0 be a Hilbert space of dimension n . We identify the letters of O with an orthonormal basis for H_0 . Denoting the n -fold tensor product of H_0 with itself by $\otimes^n H_0$, let

$$K = \mathbb{C} \oplus H_0 \oplus \otimes^2 H_0 \oplus \cdots \oplus \otimes^n H_0 \oplus \cdots$$

be the tensor algebra over H_0 . (This corresponds to a full Fock space in quantum field theory.) We identify $1 \in \mathbb{C}$ with the empty word λ , and writing a basis element $y_1 \otimes \cdots \otimes y_m$ of $\otimes^m H_0$, $y_i \in O$, $i = 1, \dots, m$, as $y_1 y_2 \cdots y_m$, we can view this basis element as a word in O^* of length m . Thus, there is a one-to-one correspondence between an orthonormal basis of K and the words in O^* and we identify corresponding elements.

A *sequential quantum machine* (SQM) is a 5-tuple $\mathfrak{M} = (S, s_0, I, O, \delta)$, where S is a finite set of internal states, $s_0 \in S$ is the start state, I and O are finite input and output alphabets, and $\delta: I \times S \times O \times S \rightarrow \mathbb{C}$ is a transition amplitude function that satisfies

$$\sum_{y \in O, t \in S} \delta(x, s, y, t) \delta(x, s', y, t)^* = \delta_{s, s'} \tag{3.1}$$

for every $x \in I$, $s, s' \in S$. In (3.1), the symbol asterisk denotes the complex conjugation operation. We interpret $\delta(x, s, y, t)$ as the transition amplitude that \mathfrak{M} prints y and enters state t after scanning x in the current state s . Let H be a complex Hilbert space whose dimension is the cardinality of S . We identify S with a fixed orthonormal basis for H and call S a *computational basis* for H [2]. The *transition operator* $U: I \rightarrow \mathcal{F}(H \otimes K)$ is defined by letting

$$U(x)s \otimes y_m \cdots y_1 = \sum_{y, t} \delta(x, s, y, t) t \otimes y y_m \cdots y_1$$

and extending $U(x)$ to $H \otimes K$ by linearity and closure. More precisely, $U(x)$ is first extended to the subspace spanned by the basis elements $s \otimes y_m \cdots y_1$, $s \in S$, $y_i \in O$, $m = 0, 1, \dots$, where $y_0 = 1 \in \mathbb{C}$, by linearity. Since, as we shall show in Lemma 3.1, $\|U(x)\| = 1$, $U(x)$ has a unique bounded extension to $H \otimes K$. The next result shows that $U(x)$ is indeed an isometry.

Lemma 3.1. $U(x)$ is an isometry if and only if δ satisfies (3.1).

Proof. If $U(x) \in \mathcal{F}(H \otimes K)$, then

$$\begin{aligned} & \sum_{y,t} \delta(x, s, y, t) \delta(x, s', y, t)^* \\ &= \sum_{y,t} \sum_{y',t'} \delta(x, s, y, t) \delta(x, s', y', t')^* \langle t \otimes y, t' \otimes y' \rangle \\ &= \left\langle \sum_{y,t} \delta(x, s, y, t) t \otimes y, \sum_{y',t'} \delta(x, s', y', t') t' \otimes y' \right\rangle \\ &= \langle U(x)s \otimes \lambda, U(x)s' \otimes \lambda \rangle = \delta_{s,s'} \end{aligned}$$

Conversely, suppose that δ satisfies (3.1). As in the previous computation, we have

$$\langle U(x)s \otimes z, U(x)s' \otimes z' \rangle = \delta_{s,s'} \delta_{z,z'}$$

for all $s, s' \in S, z, z' \in O^*$. An arbitrary element ϕ in the subspace spanned by the basis elements can be represented by a finite sum of the form $\phi = \sum \alpha_{i,j} s_i \otimes z_j, s_i \in S, z_j \in O^*$. We then have

$$\begin{aligned} \|U(x)\phi\|^2 &= \left\langle U(x) \sum_{i,j} \alpha_{i,j} s_i \otimes z_j, U(x) \sum_{i',j'} \alpha_{i',j'} s_{i'} \otimes z_{j'} \right\rangle \\ &= \sum_{i,j} \sum_{i',j'} \alpha_{i,j} \alpha_{i',j'}^* \langle U(x)s_i \otimes z_j, U(x)s_{i'} \otimes z_{j'} \rangle \\ &= \sum_{i,j} |\alpha_{i,j}|^2 = \|\phi\|^2 \end{aligned}$$

It follows that the unique bounded linear extension of $U(x)$ to $H \otimes K$ is an isometry. ■

Notice that $U(x)$ is not unitary because λ is not in the range of $U(x)$. Also $U(x)$ is *local* in the sense that

$$U(x): H \otimes (\otimes^n H_0) \rightarrow H \otimes (\otimes^{n+1} H_0)$$

In this way, $U(x)$ is a kind of creation operator. We call the elements of $(H \otimes K)^{\otimes n}$ *configurations* on \mathfrak{M}^n and the vector $\phi_0 = s_0 \otimes \lambda$ is called the *initial configuration*. We extend the definition of U to $U: I^* \rightarrow \mathcal{F}(H \otimes K)$ by defining $U(\lambda) = 1$ and $U(w) = U(x_k) \cdots U(x_1)$ for any $w = x_k \cdots x_1 \in I^*$.

The SQM \mathfrak{M} operates as follows. Upon receiving a word $w = x_k \cdots x_1 \in I^*$, \mathfrak{M} scans the letter x_1 and enters the configuration $U(x_1)\phi_0 \in H \otimes H_0$. An output letter y_1 is printed with probability

$$p_{\mathfrak{M}}(y_1|x_1) = \sum_s |\langle U(x_1)\phi_0, s \otimes y_1 \rangle|^2$$

After scanning the letter x_2 , \mathfrak{M} enters the configuration

$$U(x_2x_1)\phi_0 = U(x_2)U(x_1)\phi_0 \in H \otimes (\otimes^2 H_0)$$

An output word y_2y_1 is printed with probability

$$p_{\mathfrak{M}}(y_2y_1|x_2x_1) = \sum_s |\langle U(x_2x_1)\phi_0, s \otimes y_2y_1 \rangle|^2$$

Finally, after the entire input word w is scanned, an output word of length k is printed and the probability that this word is $y_k \cdots y_1$ becomes

$$p_{\mathfrak{M}}(y_k \cdots y_1|x_k \cdots x_1) = \sum_s |\langle U(w)\phi_0, s \otimes y_k \cdots y_1 \rangle|^2$$

As with q-automata [2], the probability of an output can be computed in terms of a sum of amplitudes over computational paths. For example,

$$\begin{aligned} p_{\mathfrak{M}}(y_2y_1|x_2x_1) &= \sum_s |\langle U(x_1)\phi_0, U(x_2)*s \otimes y_2y_1 \rangle|^2 \\ &= \sum_s \left| \sum_{t,y} \langle U(x_1)\phi_0, t \otimes y \rangle \langle U(x_2)t \otimes y, s \otimes y_2y_1 \rangle \right|^2 \end{aligned}$$

An SQM $\mathfrak{M} = (S, s_0, I, O, \delta)$ is *factorizable* if

$$\delta(x, s, y, t) = \delta_1(x, s, y) \delta_2(x, s, t)$$

for some functions $\delta_1: I \times S \times O \rightarrow \mathbb{C}$ and $\delta_2: I \times S \times S \rightarrow \mathbb{C}$. It then follows that

$$\sum_y \delta_2(x, s, y) \delta_1(x, s', y)^* \sum_t \delta_2(x, s, t) \delta_2(x, s', t)^* = \delta_{s,s'}$$

for every $x \in I, s, s' \in S$. We say that \mathfrak{M} is *strongly factorizable* if there exist $U_T: I \rightarrow \mathcal{U}(H)$ and $U_O: I \times S \rightarrow \mathcal{F}(K)$ such that

$$U(x)s \otimes z = U_T(x)s \otimes U_O(x, s)z \tag{3.2}$$

for every $x \in I, s \in S, z \in O^*$. We call U_T the *state operator* and U_O the *output operator* for \mathfrak{M} .

Theorem 3.2. An SQM \mathfrak{M} is factorizable if and only if for every $x \in I, s \in S$, and $z \in O^*$ there exist $\psi \in H$ and $\phi \in K$ such that $U(x)s \otimes z = \psi \otimes \phi$.

Proof. If \mathfrak{M} is factorizable, then

$$\begin{aligned} U(x)s \otimes z &= \sum_{y,t} \delta_1(x, s, y) \delta_2(x, s, t)t \otimes yz \\ &= \sum_t \delta_2(x, s, t)t \otimes \sum_y \delta_1(x, s, y)yz \end{aligned}$$

Letting $\psi = \sum_t \delta(x, s, t)t$ and $\phi = \sum_y \delta_1(x, s, y)yz$ gives the result. Conversely, suppose that $U(x)s \otimes z = \psi \otimes \phi$ for some $\psi \in H$, $\phi \in K$. Then

$$U(x)s \otimes \lambda = \psi(x, s) \otimes \phi(x, s)$$

for some $\psi(x, s) \in H$, $\phi(x, s) \in K$. Since

$$U(x)s \otimes \lambda = \sum_{y,t} \delta(x, s, y, t)t \otimes y$$

we have

$$\begin{aligned} \delta(x, s, y, t) &= \langle U(x)s \otimes \lambda, t \otimes y \rangle = \langle \psi(x, s) \otimes \phi(x, s), t \otimes y \rangle \\ &= \langle \psi(x, s), t \rangle \langle \phi(x, s), y \rangle \end{aligned}$$

Letting $\delta_1(x, s, y) = \langle \phi(x, s), y \rangle$ and $\delta_2(x, s, t) = \langle \psi(x, s), t \rangle$ gives the result. ■

Theorem 3.3. An SQM \mathfrak{M} is strongly factorizable if and only if \mathfrak{M} is factorizable and

$$\sum_y |\delta_1(x, s, y)|^2 = 1, \quad \sum_t \delta_2(x, s, t) \delta_2(x, s', t)^* = \delta_{s,s'} \quad (3.3)$$

for every $x \in I$, $s, s' \in S$.

Proof. Suppose \mathfrak{M} is factorizable and satisfies (3.3). For any $x \in I$, define $U_T(x): H \rightarrow H$ by

$$U_T(x)s = \sum_t \delta_2(x, s, t)t$$

and for any $x \in I$, $s \in S$, define $U_O(x, s): K \rightarrow K$ by letting

$$U_O(x, s)z = \sum_y \delta_1(x, s, y)yz$$

and extending $U_O(x, s)$ to K by linearity and closure. Then

$$\begin{aligned} \langle U_T(x)s, U_T(x)s' \rangle &= \left\langle \sum_t \delta_2(x, s, t)t, \sum_{t'} \delta_2(x, s', t')t' \right\rangle \\ &= \sum_{t,t'} \delta_2(x, s, t) \delta_2(x, s', t')^* \langle t, t' \rangle \\ &= \sum_t \delta_2(x, s, t) \delta_2(x, s', t)^* = \delta_{s,s'} \end{aligned}$$

It follows from Theorem 2.1 that $U_T: I \rightarrow \mathcal{U}(H)$. Moreover,

$$\begin{aligned}
\langle U_O(x, s)z, U_O(x, s)z' \rangle &= \left\langle \sum_y \delta_1(x, s, y)yz, \sum_{y'} \delta_1(x, s, y')y'z' \right\rangle \\
&= \sum_{y, y'} \delta_1(x, s, y) \delta_1(x, s, y')^* \langle yz, y'z' \rangle \\
&= \sum_y |\delta_1(x, s, y)|^2 \delta_{z, z'} = \delta_{z, z'}
\end{aligned}$$

Again, by Theorem 2.1, $U_O: I \times S \rightarrow \mathcal{F}(K)$. For $x \in I, s \in S, z \in Q^*$ we have

$$\begin{aligned}
U(x)s \otimes z &= \sum_{y, t} \delta(x, s, y, t)t \otimes yz \\
&= \sum_{y, t} \delta_1(x, s, y) \delta_2(x, s, t)t \otimes yz \\
&= \sum_t \delta_2(x, s, t)t \otimes \sum_y \delta_1(x, s, y)yz \\
&= U_T(x)s \otimes U_O(x, s)z
\end{aligned}$$

so \mathfrak{M} is strongly factorizable.

Conversely, suppose that \mathfrak{M} is strongly factorizable. Then there exist maps $U_T: I \rightarrow \mathcal{U}(H), U_O: I \times S \rightarrow \mathcal{F}(K)$ such that (3.2) holds. Define $\delta_1: I \times S \times O \rightarrow \mathbb{C}$ by

$$\delta_1(x, s, y) = \langle U_O(x, s)\lambda, y \rangle$$

and $\delta_2: I \times S \times S \rightarrow \mathbb{C}$ by

$$\delta_2(x, s, t) = \langle U_T(x)s, t \rangle$$

We then have

$$\begin{aligned}
\delta(x, s, y, t) &= \langle U(x)s \otimes \lambda, t \otimes y \rangle \\
&= \langle U_T(x)s \otimes U_O(x, s)\lambda, t \otimes y \rangle \\
&= \langle U_T(x)s, t \rangle \langle U_O(x, s)\lambda, y \rangle \\
&= \delta_1(x, s, y) \delta_2(x, s, t)
\end{aligned}$$

and we conclude that \mathfrak{M} is factorizable. Since

$$U_T(x)s \otimes U_O(x, s)\lambda = U(x)s \otimes \lambda = \sum_t \delta_2(x, s, t)t \otimes \sum_y \delta_1(x, s, y)y$$

we have $U_O(x, s)\lambda = \sum_y \delta_1(x, s, y)y$. Hence,

$$\sum_y |\delta_1(x, s, y)|^2 = \|U_O(x, s)\lambda\|^2 = 1$$

Moreover, $U_T(x)s = \sum_t \delta_2(x, s, t)t$, so we have

$$\sum_t \delta_2(x, s, t) \delta_2(x', t)^* = \langle U_T(x)s, U_T(x)s' \rangle = \delta_{s,s'}$$

Hence, (3.3) holds. ■

If \mathfrak{M} is strongly factorizable, then (S, s_0, I, δ_2) is a quantum automaton [2, 4]. We extend U_O to $U_O: (I \times S)^* \rightarrow \mathcal{F}(K)$ by defining $U_O(\lambda) = 1$ and

$$U_O((x_j, s_j) \cdots (x_1, s_1)) = U_O(x_j, s_j) \cdots U_O(x_1, s_1)$$

Theorem 3.4. If \mathfrak{M} is strongly factorizable, then

$$\begin{aligned} U(x_k \cdots x_1)\phi_0 &= \sum_{i_1, \dots, i_{k-1}} \langle U_T(x_1)s_0, s_{i_1} \rangle \langle U_T(x_2)s_{i_1}, s_{i_2} \rangle \\ &\quad \times \cdots \langle U_T(x_{k-1})s_{i_{k-2}}, s_{i_{k-1}} \rangle U_T(x_k)s_{i_{k-1}} \\ &\quad \otimes U_O((x_k, s_{i_{k-1}}) \cdots (x_1, s_0))\lambda \end{aligned}$$

Proof. We have that

$$\begin{aligned} U(x_k \cdots x_1)\phi_0 &= U(x_k) \cdots U(x_1)s_0 \otimes \lambda \\ &= U(x_k) \cdots U(x_2)[U_T(x_1)s_0 \otimes U_O(x_1, s_0)\lambda] \\ &= U(x_k) \cdots U(x_2) \sum_{i_1} \langle U_T(x_1)s_0, s_{i_1} \rangle s_{i_1} \otimes U_O(x_1, s_0)\lambda \\ &= U(x_k) \cdots U(x_3) \sum_{i_1} \langle U_T(x_1)s_0, s_{i_1} \rangle U(x_2)[s_{i_1} \otimes U_O(x_1, s_0)\lambda] \\ &= U(x_k) \cdots U(x_3) \sum_{i_1} \langle U_T(x_1)s_0, s_{i_1} \rangle U_T(x_2)s_{i_1} \\ &\quad \otimes U_O((x_2, s_{i_1})(x_1, s_0))\lambda \end{aligned}$$

Continuing this process, we obtain the result. ■

Two SQMs \mathfrak{M} and \mathfrak{M}' with the same input and output alphabets are *equivalent* if $p_{\mathfrak{M}}(u|v) = p_{\mathfrak{M}'}(u|v)$ for every $u \in O^*$, $v \in I^*$ of the same length. Simple examples show that not every SQM is equivalent to a factorizable one. We close this section with an open problem.

Problem 1. Let \mathfrak{M} and \mathfrak{M}' be SQMs with n and n' states, respectively and the same input and output alphabets. Is it true that \mathfrak{M} and \mathfrak{M}' are equivalent if and only if $p_{\mathfrak{M}}(u|v) = p_{\mathfrak{M}'}(u|v)$ for all words u, v of length $n + n' - 1$? (This holds for stochastic sequential machines [5].)

4. QUANTUM TURING MACHINES

A *quantum machine* (QM) is a triple $M = (I, S, \delta)$, where I is a finite alphabet with an identified blank symbol $\#$, S is a finite set of states with

identified start state s_0 and final state s_f , and $\delta: I \times S \times I \times S \times \{L, R\} \rightarrow \mathbb{C}$ is a transition amplitude function. The QM has a two-way infinite tape of cells indexed by the integers \mathbb{Z} and a single read–write head that moves one cell at a time along the tape. A *configuration* or *instantaneous description* of M is a complete description of the contents of the tape, the location of the tape head, and the state $s \in S$ of the finite control. At any time only a finite number of tape cells can contain nonblank letters. In the *initial configuration* of M the tape head is at cell 0, called the *start cell*, and M is in the state s_0 . An initial configuration has *input* $w \in (I \setminus \#)^*$, where w is written on the tape cells 0, 1, 2, . . . , m and all other tape cells are blank. The machine M *halts* for input w if M eventually enters the final state s_f . We interpret $\delta(x, s, y, t, d)$, $x, y \in I$, $s, t \in S$, $d \in \{L, R\}$, as the transition amplitude that M prints y , enters state t , and moves its tape head left or right when its current letter on the tape head is x and its current state is s .

Let H be the Hilbert space with computational basis B indexed by the configurations of M . An element $\psi \in B$ has the form $\psi = n \otimes s \otimes w$, where $n \in \mathbb{Z}$ is the address of the tape cell at the tape head, $s \in S$ is the current state, and w is the word printed on the tape. We assume that w has each of its letters indexed by the address of the cell that the letter occupies and $w_m \in I$ is the letter in the m th cell. The *evolution operator* for M is the linear operator $U: H \rightarrow H$ that satisfies

$$Un \otimes s \otimes w = \sum_{y,t,d} \delta(w_n, s, y, t, d)n(d) \otimes t \otimes w(y, n) \quad (4.1)$$

where $n(L) = n - 1$, $n(R) = n + 1$, and

$$w(y, n)_m = \begin{cases} y & \text{if } m = n \\ w_m & \text{if } m \neq n \end{cases}$$

A QM M is a *quantum Turing machine* (QTM) if $U \in \mathcal{U}(H)$. It is shown in ref. 1 that if $U \in \mathcal{F}(H)$, then $U \in \mathcal{U}(H)$. Their proof relies on a detailed analysis of the operation of M and a study of the “infinite matrix” U . We shall give an alternative proof that is straightforward and algebraic. For $d \in \{L, R\}$ we define

$$d' = \begin{cases} L & \text{if } d = R \\ R & \text{if } d = L \end{cases}$$

Lemma 4.1. The adjoint of U satisfies

$$U^*n \otimes t \otimes w = \sum_{x,s,d} \delta(x, s, w_{n(d)}, t, d')^*n(d) \otimes s \otimes w(x, n(d)) \quad (4.2)$$

Proof. For any $n' \otimes s' \otimes w' \in B$ we have

$$\begin{aligned}
& \langle Un \otimes s \otimes w, n' \otimes s' \otimes w' \rangle \\
&= \left\langle \sum_{y,t,d} \delta(w_n, s, y, t, d) n(d) \otimes t \otimes w(y, n), n' \otimes s' \otimes w' \right\rangle \\
&= \sum_{y,t,d} \delta(w_n, s, y, t, d) \langle n(d), n' \rangle \langle t, s' \rangle \langle w(y, n), w' \rangle \\
&= \delta(w_n, s, y, s', d) \delta_{n',n(d)} \delta_{w',w(y,n)} \quad (4.3)
\end{aligned}$$

On the other hand, the operator in (4.2) acting on $n' \otimes s' \otimes w'$ gives

$$\begin{aligned}
& \left\langle n \otimes s \otimes w, \sum_{x,t,d} \delta(x, t, w'_{n'(d)}, s', d') n'(d) \otimes t \otimes w'(x, n'(d)) \right\rangle \\
&= \sum_{x,t,d} \delta(x, t, w'_{n'(d)}, s', d') \langle n, n'(d) \rangle \langle s, t \rangle \langle w, w'(x, n'(d)) \rangle \\
&= \delta(x, s, w'_{n'(d)}, s', d') \delta_{n,n'(d)} \delta_{w,w'(x,n'(d))} \quad (4.4)
\end{aligned}$$

If the right side of (4.3) is nonzero, then it equals $\delta(w_n, s, y, s', d)$, where $n' = n(d)$, $w' = w(y, n)$. If the right side of (4.4) is nonzero, then it equals $\delta(x, s, w'_{n'(e)}, s', e')$, where $n = n'(e)$ and

$$w = w'(x, n'(e)) = w'(x, n)$$

Now $n' = n(d) = n'(e)(d)$ implies that $e = d'$. Also,

$$w'_{n'(e)} = w'_n = y$$

and $x = w_n$. Hence, the right side of (4.4) is also $\delta(w_n, s, y, s', d)$. Similar reasoning show that if (4.3) or (4.4) vanishes, then so does the other. ■

Theorem 4.2. For a QM $M = (I, S, \delta)$ the following statements are equivalent. (a) M is a QTM. (b) $U \in \mathcal{F}(H)$. (c) δ satisfies

$$\sum_{y,t,d} \delta(x, s, y, t, d) \delta(x', s', y, t, d)^* = \delta_{x,x'} \delta_{s,s'} \quad (4.5)$$

$$\sum_t \delta(x, s, y, t, R) \delta(x', s', y', t, L)^* = 0 \quad (4.6)$$

Proof. That (a) implies (b) is trivial. To show that (b) implies (c), suppose that $U \in \mathcal{F}(H)$. Assume that $w'_m = w_m$ for $m \neq n$, $w_n = x$, and $w'_n = x'$. We then have

$$\begin{aligned}
\delta_{x,x'} \delta_{s,s'} &= \langle Un \otimes s \otimes w, Un \otimes s' \otimes w' \rangle \\
&= \left\langle \sum_{y,t,d} \delta(x, s, y, t, d) n(d) \otimes t \otimes w(y, n), \right.
\end{aligned}$$

$$\begin{aligned}
 & \left\langle \sum_{y',t',e} \delta(x', s', y', t', e)n(e) \otimes t' \otimes w'(y', n) \right\rangle \\
 &= \sum_{y,t,d} \sum_{y',t',e} \delta(x, s, y, t, d) \delta(x', s', y', t', e)^* \\
 &\quad \times \langle n(d), n(e) \rangle \langle t, t' \rangle \langle w(y, n), w'(y', n) \rangle \\
 &= \sum_{y,t,d} \sum_{y',t',e} \delta(x, s, y, t, d) \delta(x', s', y', t', e)^* \delta_{d,e} \delta_{t,t'} \delta_{y,y'} \\
 &= \sum_{y,t,d} \delta(x, s, y, t, d) \delta(x', s', y, t, d)^*
 \end{aligned}$$

so (4.5) holds. Assume that $w'_m = w_m$ for $m \neq n, m \neq n + 2, w_n = x, w_{n+2} = y', w'_n = y,$ and $w'_{n+2} = x'$. We then have

$$\begin{aligned}
 0 &= \langle Un \otimes s \otimes w, U(n + 2) \otimes s' \otimes w' \rangle \\
 &= \left\langle \sum_{z,t,d} \delta(x, s, z, t, d)n(d) \otimes t \otimes w(z, n)' \right. \\
 &\quad \left. \sum_{z',t',e} \delta(x', s', z', t', e)(n + 2)(e) \otimes t' \otimes w'(z', n + 2) \right\rangle \\
 &= \sum_{z,t,d} \sum_{z',t',e} \delta(x, s, z, t, d) \delta(x', s', z', t', e)^* \\
 &\quad \times \langle n(d), (n + 2)(e) \rangle \langle t, t' \rangle \langle w(z, n), w'(z', n + 2) \rangle \\
 &= \sum_{z,z',t} \delta(x, s, z, t, R) \delta(x', s', z', t, L)^* \langle w(z, n), w'(z', n + 2) \rangle
 \end{aligned}$$

But $\langle w(z, n), w'(z', n + 2) \rangle = 0$ unless $z = w'_n = y$ and $z' = w_{n+2} = y'$, in which case $\langle w(z, n), w'(z', n + 2) \rangle = 1$. Hence, (4.6) holds.

To show that (c) implies (a), suppose that (4.5) and (4.6) hold. It follows from our calculations in the previous paragraph that $\|U\psi\| = \|\psi\|$ for every $\psi \in B$ and that $\langle U\psi, U\phi \rangle = 0$ for every $\psi, \phi \in B$ with $\psi \neq \phi$. As in the proof of Lemma 3.1, $\|U\psi\| = \|\psi\|$ for every ψ in the subspace spanned by the basis elements. Hence, the operator U satisfying (4.1) has a unique extension to a bounded linear operator on H . We conclude that $U \in \mathcal{F}(H)$. By Theorem 2.1(b), if $\|U^*\psi\| = 1$ for every $\psi \in B$, then $U \in \mathcal{U}(H)$. Applying Lemma 4.1, we have

$$\begin{aligned}
 \|U^*n \otimes t \otimes w\|^2 &= \sum_{x,s,d} |\delta(x, s, w_{n(d)}, t, d)|^2 \\
 &= \sum_{x,s} |\delta(x, s, w_{n(L)}, t, R)|^2 + \sum_{x,s} |\delta(x, s, w_{n(R)}, t, L)|^2 \quad (4.7)
 \end{aligned}$$

We now show that for any $y, y' \in I$ we have

$$J_{y,y'} = \sum_{x,s} |\delta(x, s, y, t, R)|^2 + \sum_{x,s} |\delta(x, s, y', t, L)|^2 = 1 \quad (4.8)$$

Letting $w_{n(L)} = y, w_{n(R)} = y'$, it follows from (4.7) that

$$J_{y,y'} = \|U^*n \otimes t \otimes w\| \leq \|U^*\|^2 = \|U\| = 1$$

Denoting the cardinality of S by $|S|$, by (4.5) we have

$$\begin{aligned} |S| \sum_{y,y'} J_{y,y'} &= \sum_{t \in S} \sum_{y,y'} J_{y,y'} \\ &= \sum_{x,s} \left[\sum_{y,y',t} |\delta(x, s, y, t, R)|^2 + \sum_{y,y',t} |\delta(x, s, y', t, L)|^2 \right] \\ &= |I| \sum_{x,s} \left[\sum_{y,t} |\delta(x, s, y, t, R)|^2 + \sum_{y',t} |\delta(x, s, y', t, L)|^2 \right] \\ &= |I| \sum_{x,s} \sum_{y,t,d} |\delta(x, s, y, t, d)|^2 = |I| \sum_{x,s} 1 = |I|^2 |S| \end{aligned}$$

Hence,

$$\sum_{y,y'} J_{y,y'} = |I|^2$$

and since $J_{y,y'} \leq 1$ we have $J_{y,y'} = 1$. It follows from (4.7) and (4.8) that $\|U^*\psi\| = 1$ for every $\psi \in B$, so $U \in \mathcal{O}l(H)$. Thus, M is a QTM. ■

A QTM M operates as follows. The initial configuration has the form $\psi_0 = 0 \otimes s_0 \otimes w_0 \in B$, where s_0 is the start state and w_0 is the input word. After the i th time step, M is in the superposition configuration $U^i\psi_0 \in \hat{H}$. The probability that M halts at time i becomes

$$\sum_{n,w} |\langle U^i\psi_0, n \otimes s_f \otimes w \rangle|^2$$

Of course, there are only a finite number of nonzero terms in this summation. The probability that the word w is printed on the tape at time i becomes

$$\sum_{n,s} |\langle U^i\psi_0, n \otimes s \otimes w \rangle|^2$$

Again, there are only a finite number of nonzero terms in this summation. As with a SQM, the action of U is local on H .

In our previous study of quantum automata, we considered a quantum computer called a quantum printer [2]. Let I and S be as for a QTM. A

quantum printer is a triple $P = (I, S, \delta)$ where $\delta: I \times S \times I \times S \rightarrow \mathbb{C}$ is a transition amplitude function that satisfies

$$\sum_{y,t} \delta(x, s, y, t) \delta(x', s', y, t)^* = \delta_{x,x'} \delta_{s,s'}$$

The quantum printer P operates as follows. Suppose we have an infinite one-way tape divided into cells numbered $-1, 0, 1, 2, \dots$. The printer P has a tape head that begins at cell 0 and moves one cell to the right at each time step. The original tape is blank in every cell so P begins in state s_0 with # in every cell. At time 0, P scans its current state s_0 and the # in cell -1 . Then P prints letter y in cell 0 and enters state s with amplitude $\delta(\#, s_0, y, s)$ and moves its tape head to cell 1. Then P scans the printed letter, say y , in cell 0 and its current state, say s , prints letter z and enters state t with amplitude $\delta(y, s, z, t)$ and moves its tape head to cell 2. This process continues until P enters its final state s_f and halts. Of course, P can also be interpreted as moving to the left on a one-way left infinite tape.

As with a QTM, the action of P is most easily given in terms of its associated evolution operator. We form a finite-dimensional complex Hilbert space H_0 with an orthonormal basis identified with the elements of $I \times S$. Thus, $I \times S$ is the computational basis for H_0 and we denote its elements by $x \otimes s$, $x \in I$, $s \in S$. We define the evolution operator $U_P: H_0 \rightarrow H_0$, by

$$U_P x \otimes s = \sum_{y,t} \delta(x, s, y, t) y \otimes t$$

and it follows that $U_P \in \mathcal{U}(H_0)$. Since a quantum printer P is much more limited than a QTM, the Hilbert space H_0 for P is finite dimensional and its evolution operator U_P is much simpler. In particular, U_P can be represented by a finite unitary matrix. Nevertheless, we shall show that there is a natural connection between a QTM and quantum printers.

Lemma 4.3. If $M = (I, S, \delta)$ is a QTM and $a, b \in \mathbb{C}$ with $|a| = |b| = 1$, then $P = (I, S, \gamma)$ is a quantum printer for

$$\gamma(x, s, y, t) = a\delta(x, s, y, t, L) + b\delta(x, s, y, t, R)$$

Proof. Applying (4.5) and (4.6), we have

$$\begin{aligned} & \sum_{y,t} \gamma(x, s, y, t) \gamma(x', s', y, t)^* \\ &= \sum_{y,t} [a\delta(x, s, y, t, L) + b\delta(x, s, y, t, R)] \\ & \quad \times [a^*\delta(x', s', y, t, L)^* + b^*\delta(x', s', y, t, R)^*] \\ &= \sum_{y,t,d} \delta(x, s, y, t, d) \delta(x', s', y, t, d)^* \end{aligned}$$

$$\begin{aligned}
& + ab^* \sum_{y,t} \delta(x, s, y, t, L) \delta(x', s', y, t, R)^* \\
& + ba^* \sum_{y,t} \delta(x, s, y, t, R) \delta(x', s', y, t, L)^* \\
& = \delta_{x,x'} \delta_{s,s'}
\end{aligned}$$

The result now follows. ■

The next result can be proved using the fact that $UU^* = 1$, but it is easier to prove using Lemma 4.3.

Corollary 4.4. If $M = (I, S, \delta)$ is a QTM, then

$$\sum_{x,s,d} \delta(x, s, y, t, d) \delta(x, s, y', t', d)^* = \delta_{y,y'} \delta_{t,t'} \quad (4.9)$$

$$\sum_{x,s} \delta(x, s, y, t, L) \delta(x, s, y', t', R)^* = 0 \quad (4.10)$$

for every $y' \in I, t' \in S$.

Proof. Define $\alpha, \beta: I \times S \times I \times S \rightarrow \mathbb{C}$ by

$$\alpha(x, s, y, t) = \delta(x, s, y, t, L) + \delta(x, s, y, t, R) \quad (4.11)$$

$$\beta(x, s, y, t) = \delta(x, s, y, t, L) - \delta(x, s, y, t, R) \quad (4.12)$$

By Lemma 4.3, $\alpha(x, s, y, t)$ are the entries of a unitary matrix A , so $AA^* = 1$. It follows that

$$\begin{aligned}
\delta_{y,y'} \delta_{t,t'} & = \sum_{x,s} \alpha(x, s, y, t) \alpha(x, s, y', t')^* \\
& = \sum_{x,s,d} \delta(x, s, y, t, d) \delta(x, s, y', t', d)^* \\
& \quad + \sum_{x,s,d} \delta(x, s, y, t, d) \delta(x, s, y', t', d')^* \quad (4.13)
\end{aligned}$$

A similar observation for β leads to

$$\begin{aligned}
\delta_{y,y'} \delta_{t,t'} & = \sum_{x,s,d} \delta(x, s, y, t, d) \delta(x, s, y', t', d)^* \\
& \quad - \sum_{x,s,d} \delta(x, s, y, t, d) \delta(x, s, y', t', d')^* \quad (4.14)
\end{aligned}$$

Adding (4.13) and (4.14) gives (4.9). Hence,

$$\sum_{x,s,d} \delta(x, s, y, t, d) \delta(x, s, y', t', d')^* = 0$$

so that

$$\operatorname{Re} \sum_{x,s} \delta(x, s, y, t, L) \delta(x, s, y', t', R)^* = 0$$

Now let

$$\alpha'(x, s, y, t) = \delta(x, s, y, t, L) + i\delta(x, s, y, t, R)$$

By reasoning as before, we have

$$\begin{aligned} \delta_{y,y'} \delta_{t,t'} &= \sum_{x,s,d} \delta(x, s, y, t, d) \delta(x, s, y', t', d)^* \\ &\quad - i \left[\sum_{x,s} \delta(x, s, y, t, L) \delta(x, s, y', t', R)^* \right. \\ &\quad \left. - \sum_{x,s} \delta(x, s, y, t, R) \delta(x, s, y', t', L)^* \right] \end{aligned}$$

Hence,

$$\operatorname{Im} \sum_{x,s} \delta(x, s, y, t, L) \delta(x, s, y', t', R)^* = 0$$

so (4.10) holds. ■

Corresponding to a QTM $M = (I, S, \delta)$ we have two quantum printers $P = (I, S, \alpha)$, $Q = (I, S, \beta)$, where α and β are defined as in (4.11), (4.12). Since α, β give finite-dimensional unitary matrices A and B , applying results in refs. 1 and 2, we can write A and B as finite products of quantum gates. Since

$$\begin{aligned} \delta(x, s, y, t, L) &= \frac{1}{2}\alpha(x, s, y, t) + \frac{1}{2}\beta(x, s, y, t) \\ \delta(x, s, y, t, R) &= \frac{1}{2}\alpha(x, s, y, t) - \frac{1}{2}\beta(x, s, y, t) \end{aligned} \tag{4.15}$$

it follows that $\delta(x, s, y, t, L)$ and $\delta(x, s, y, t, R)$ can be written in terms of a finite number of quantum gates. In this sense, quantum gates can be employed in constructing a QTM. If α, β satisfy (4.15), we say that the quantum printers $P = (I, S, \alpha)$, $Q = (I, S, \beta)$ generate the QTM $M = (I, S, \delta)$. Of course, we have just shown that any QTM is generated by a pair of quantum printers. The converse does not hold in the sense that an arbitrary pair of quantum printers need not generate a QTM. The next result characterizes generating pairs of quantum printers.

Lemma 4.5. A pair of quantum printers $P = (I, S, \alpha)$, $Q = (I, S, \beta)$ generate a QTM $M = (I, S, \delta)$ if and only if

$$\sum_t [\alpha(x, s, y, t) - \beta(x, s, y, t)][\alpha(x', s', y', t) + \beta(x', s', y', t)]^* = 0 \quad (4.16)$$

for every $x, x', y, y' \in I, s, s' \in S$.

Proof. If P and Q generate M , then (4.16) follows from (4.6). Conversely, suppose that (4.16) holds and δ is given by (4.15). Then (4.6) follows immediately. To show that (4.5) holds we have

$$\begin{aligned} & \sum_{y,t,d} \delta(x, s, y, t, d) \delta(x', s', y, t, d)^* \\ &= \frac{1}{4} \sum_{y,t} [\alpha(x, s, y, t) + \beta(x, s, y, t)][\alpha(x', s', y, t) + \beta(x', s', y, t)]^* \\ & \quad + \frac{1}{4} \sum_{y,t} [\alpha(x, s, y, t) - \beta(x, s, y, t)][\alpha(x', s', y, t) - \beta(x', s', y, t)]^* \\ &= \frac{1}{2} \sum_{y,t} \alpha(x, s, y, t) \alpha(x', s', y, t)^* + \frac{1}{2} \sum_{y,t} \beta(x, s, y, t) \beta(x', s', y, t)^* \\ &= \delta_{x,x'} \delta_{s,s'} \quad \blacksquare \end{aligned}$$

Let $M = (I, S, \delta)$ be a QTM with evolution operator U . Even though U^* gives the reverse operation of M , we cannot consider U^* as the evolution operator of a QTM. Indeed, by (4.2), $U^*n \otimes t \otimes w$ depends on the letters $w_{n(d)}$ to the left and right of the tape head instead of the letter w_n at the tape head. Thus, U^* does not act like the evolution operator of a QTM. We may then ask whether $M' = (I, S, \delta')$ is a QTM, where

$$\delta'(x, s, y, t, d) = \delta(y, t, x, s, d)$$

The answer in general is no. Although (4.9) shows that (4.5) holds for δ' , (4.10) gives a weaker condition than (4.6), and (4.6) need not hold for δ' . We shall give an example to show this in the next section.

5. UNIDIRECTIONAL QUANTUM TURING MACHINES

For a QTM $M = (I, S, \delta)$ define the operators Δ_L, Δ_R on the finite-dimensional Hilbert space H_0 with computational basis $I \times S$ by

$$\begin{aligned} \Delta_L x \otimes s &= \sum_{y,t} \delta(x, s, y, t, L) y \otimes t \\ \Delta_R x \otimes s &= \sum_{y,t} \delta(x, s, y, t, R) y \otimes t \end{aligned}$$

It follows from (4.5) and (4.6) that $\Delta_L\Delta_L^* + \Delta_R\Delta_R^* = 1$ and $\Delta_R\Delta_L^* = 0$. Moreover, (4.9) and (4.10) give that $\Delta_L^*\Delta_L + \Delta_R^*\Delta_R = 1$ and $\Delta_R^*\Delta_L = 0$. For $a, b \in \mathbb{C}$ with $|a| = |b| = 1$, define the operator A on H_0 by $A = a\Delta_L + b\Delta_R$. Then A is unitary because

$$\begin{aligned} AA^* &= (a\Delta_L + b\Delta_R)(a^*\Delta_L^* + b^*\Delta_R^*) \\ &= \Delta_L\Delta_L^* + \Delta_R\Delta_R^* + ba^*\Delta_R\Delta_L^* + ab^*\Delta_L\Delta_R^* = 1 \end{aligned}$$

This gives an alternative proof of Lemma 4.3. We say that M is *commutative* if $\Delta_R\Delta_L = \Delta_L\Delta_R$.

Lemma 5.1. Suppose a QTM $M = (I, S, \delta)$ is generated by the quantum printers P and Q with evolution operators U_P, U_Q , respectively. Then M is commutative if and only if $U_P U_Q = U_Q U_P$.

Proof. Since $U_P = \Delta_L + \Delta_R, U_Q = \Delta_L - \Delta_R$, we have the following equivalent equations:

$$\begin{aligned} U_P U_Q &= U_Q U_P \\ (\Delta_L + \Delta_R)(\Delta_L - \Delta_R) &= (\Delta_L - \Delta_R)(\Delta_L + \Delta_R) \\ \Delta_L^2 - \Delta_L\Delta_R + \Delta_R\Delta_L - \Delta_R^2 &= \Delta_L^2 + \Delta_L\Delta_R - \Delta_R\Delta_L - \Delta_R^2 \\ \Delta_R\Delta_L &= \Delta_L\Delta_R \quad \blacksquare \end{aligned}$$

A QTM $M = (I, S, \delta)$ is *unidirectional* [1] if

$$\delta(x, s, y, t, R) \delta(x', s', y', t, L)^* = 0 \tag{5.1}$$

for all values of the arguments. Notice that (5.1) is a strengthening of (4.6). Equation (5.1) says that any state of M can be entered from only one direction. It is shown in ref. 1 that any QTM can be simulated by a unidirectional QTM with slowdown by a factor of at most five. For this reason one can frequently assume without loss of generality that a QTM is unidirectional.

Lemma 5.2. Two quantum printers $P = (I, S, \alpha), Q = (I, S, \beta)$ generate a unidirectional QTM if and only if for every $t \in S$ either $\alpha(x, s, y, t) = \beta(x, s, y, t)$ for every $x, y \in I, s \in S$ or $\alpha(x, s, y, t) = -\beta(x, s, y, t)$ for every $x, y \in I, s \in S$.

Proof. If P and Q generate a unidirectional QTM $M = (I, S, \delta)$, then (5.1) implies that

$$[\alpha(x, s, y, t) - \beta(x, s, y, t)][\alpha(x', s', y', t) + \beta(x', s', y', t)]^* = 0 \tag{5.2}$$

for every value of the arguments. Fix $t \in S$. If there exist $x', y' \in I, s' \in S$ such that the second factor in (5.2) is nonzero, then $\alpha(x, s, y, t) = \beta(x, s,$

y, t for every $x, y \in I, s \in S$. If there exist $x, y \in I, s \in S$ such that the first factor in (5.2) is nonzero, then $\alpha(x', s', y', t) = -\beta(x', s', y', t)$ for every $x', y' \in I, s' \in S$. Conversely, suppose the second statement of the lemma holds. Then (4.16) holds, so by Lemma 4.5, P and Q generate a QTM $M = (I, S, \delta)$. Moreover, (5.1) clearly holds, so M is unidirectional. ■

Let $P = (I, S, \alpha), Q = (I, S, \beta)$ be quantum printers with evolution operators A, B , respectively, considered as unitary matrices on the Hilbert space H_0 with computational basis $I \times S$. Suppose that P and Q generate a unidirectional QTM $M = (I, S, \delta)$. Applying Lemma 5.2, we have $S = S_L \cup S_R$ and $S_L \cap S_R = \emptyset$, where

$$\begin{aligned} S_L &= \{t \in S: \alpha(x, s, y, t) = \beta(x, s, y, t) \text{ for all } x, y \in I, s \in S\} \\ &= \{t \in S: \delta(x, s, y, t, R) = 0 \text{ for all } x, y \in I, s \in S\} \\ S_R &= \{t \in S: \alpha(x, s, y, t) = -\beta(x, s, y, t) \text{ for all } x, y \in I, s \in S\} \\ &= \{t \in S: \delta(x, s, y, t, L) = 0 \text{ for all } x, y \in I, s \in S\} \end{aligned}$$

Letting $r(t)$ be the characteristic function of S_R , we have

$$A^*B(x, s, y, t) = (-1)^{r(t)} \delta_{x,y} \delta_{s,t} \tag{5.3}$$

Indeed,

$$\begin{aligned} A^*B(x, s, y, t) &= \sum_{y',t'} A^*(x, s, y', t')B(y', t', y, t) \\ &= \sum_{y',t'} \alpha(y', t', x, s) \beta(y', t', y, t) \end{aligned} \tag{5.4}$$

Since B is unitary, it follows from Lemma 5.2 that the right side of (5.4) vanishes if $x \neq y$ or $s \neq t$. If $x = y$ and $s = t$, then the right of (5.4) is 1 or -1 depending on whether $t \in S_L$ or $t \in S_R$, respectively. We conclude that A^*B is a diagonal matrix with diagonal elements ± 1 , where -1 appears in precisely those entries for which $t \in S_R$. A simple example is a *one-way* QTM in which $\Delta_R = 0$ or $\Delta_L = 0$. In the first case, $A = B$ and $A^*B = 1$, and in the second case $B = -A$ and $A^*B = -1$.

In the general situation, letting $D = A^*B$, we have that $B = AD$. Hence,

$$\begin{aligned} \Delta_L &= \frac{1}{2}A + \frac{1}{2}B = \frac{1}{2}A + \frac{1}{2}AD = A(\frac{1}{2}1 + \frac{1}{2}D) \\ \Delta_R &= \frac{1}{2}A - \frac{1}{2}B = \frac{1}{2}A - \frac{1}{2}AD = A(\frac{1}{2}1 - \frac{1}{2}D) \end{aligned} \tag{5.5}$$

Now $P_L = \frac{1}{2}I + \frac{1}{2}D$ and $P_R = \frac{1}{2}I - \frac{1}{2}D$ are diagonal matrices with 0 or 1 entries. It is clear that P_L and P_R are the projections of H_0 onto the subspaces generated by $I \times S_L$ and $I \times S_R$, respectively. We conclude that Δ_L can be written as a product of quantum gates and P_L , and Δ_R is the same product of quantum gates and P_R .

Lemma 5.2 gives a simple method for constructing any unidirectional QTM. Just take any unitary matrix A on the Hilbert space H_0 with computational basis $I \times S$. Let $S = S_L \cup S_R$ be a partition of S and define $\Delta_L = AP_L$ and $\Delta_R = AP_R$, where P_L and P_R are the projections of H_0 onto the subspaces generated by $I \times S_L$ and $I \times S_R$, respectively. Then

$$\delta(x, s, y, t, L) = \langle \Delta_L x \otimes s, y \otimes t \rangle$$

$$\delta(x, s, y, t, R) = \langle \Delta_R x \otimes s, y \otimes t \rangle$$

and $M = (I, S, \delta)$ is a unidirectional QTM.

For a simple example, let $|I| = |S| = 2$ and let

$$A = \frac{1}{2} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 \\ -\sqrt{2} & 0 & 0 & \sqrt{2} \\ 0 & \sqrt{2} & -\sqrt{2} & 0 \end{bmatrix}$$

For $S = \{t_1, t_2\}$, let $S_L = \{t_1\}$, $S_R = \{t_2\}$. Then $P_L = \text{diag}(1, 0, 1, 0)$, $P_R = \text{diag}(0, 1, 0, 1)$, and

$$\Delta_L = AP_L = \frac{1}{2} \begin{bmatrix} 1 & 0 & 1 & 0 \\ 1 & 0 & -1 & 0 \\ -\sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & -\sqrt{2} & 0 \end{bmatrix}$$

$$\Delta_R = AP_R = \frac{1}{2} \begin{bmatrix} 0 & 1 & 0 & 1 \\ 0 & -1 & 0 & 1 \\ 0 & 0 & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 & 0 \end{bmatrix}$$

We mentioned earlier that in contrast to (4.6), the equation

$$\sum_S \delta(x, s, y, t, R) \delta(x', s, y', t', L)^* = 0$$

need not hold for a QTM. The present example illustrates this fact. Indeed, we have

$$\begin{aligned} & \delta(x_2, t_2, x_1, t_2, R) \delta(x_1, t_2, x_1, t_1, L)^* \\ & + \delta(x_2, t_1, x_1, t_2, R) \delta(x_1, t_1, x_1, t_1, L)^* \\ & = \frac{1}{\sqrt{2}} \cdot \frac{1}{2} + 0 \cdot \frac{1}{2} \neq 0 \end{aligned}$$

We now apply Lemma 4.5 to obtain a simple example of a nonunidirectional QTM. Let I , S , and A be as in the previous example and let

$$B = \frac{1}{2} \begin{bmatrix} 1 & 1 & 1 & 1 \\ -1 & 1 & 1 & -1 \\ 0 & -\sqrt{2} & \sqrt{2} & 0 \\ \sqrt{2} & 0 & 0 & -\sqrt{2} \end{bmatrix}$$

To show that A and B are evolution operators for quantum printers that generate a QTM, we must verify (4.16). Notice that $\beta(x, s, y, t_1) = \alpha(x, s, y, t_2)$ and $\beta(x, s, y, t_2) = \alpha(x, s, y, t_1)$. Hence,

$$\begin{aligned} & [\alpha(x, s, y, t_1) - \beta(x, s, y, t_1)] [\alpha(x', s', y', t_1) + \beta(x', s', y', t_1)]^* \\ & + [\alpha(x, s, y, t_2) - \beta(x, s, y, t_2)] \\ & [\alpha(x', s', y', t_2) + \beta(x', s', y', t_2)]^* \\ & = [\alpha(x, s, y, t_1) - \alpha(x, s, y, t_2)] \\ & [\alpha(x', s', y', t_1) + \alpha(x', s', y', t_2)]^* \\ & + [\alpha(x, s, y, t_2) - \alpha(x, s, y, t_1)] \\ & [\alpha(x', s', y', t_2) + \alpha(x', s', y', t_1)]^* = 0 \end{aligned}$$

In this case

$$A^*B = \frac{1}{2} \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

so by the discussion following Lemma 5.2, the generated QTM is not unidirectional. To compute δ , we have

$$\begin{aligned} \Delta_L &= \frac{1}{2}A + \frac{1}{2}B = \frac{1}{2} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 \\ -1/\sqrt{2} & -1/\sqrt{2} & 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} & -1/\sqrt{2} & -1/\sqrt{2} \end{bmatrix} \\ \Delta_R &= \frac{1}{2}A - \frac{1}{2}B = \frac{1}{2} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & -1 & -1 & 1 \\ -1/\sqrt{2} & 1/\sqrt{2} & -1/\sqrt{2} & 1/\sqrt{2} \\ -1/\sqrt{2} & 1/\sqrt{2} & -1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix} \end{aligned}$$

6. GENERALIZED QTMs AND QUANTUM PUSHDOWN AUTOMATA

This section briefly discusses two generalizations of quantum computers considered previously. Our investigations of these are preliminary and a complete analysis will require further development.

A *generalized* QTM is the same as a QTM except that the tape can stay in the same position as well as move to the left or right. In this case

$$\delta: I \times S \times I \times S \times \{L, N, R\} \rightarrow \mathbb{C}$$

where N indicates no movement of the tape head. It is shown in ref. 1 that unlike ordinary Turing machines, a generalized QTM is more powerful than a QTM. The Hilbert space H and the computational basis B for a generalized QTM $M = (I, S, \delta)$ are the same as they were for a QTM. The evolution operator $U: H \rightarrow H$ for M satisfies

$$Un \otimes s \otimes w = \sum_{y,t,d} \delta(x, s, y, t, d)n(d) \otimes t \otimes w(y, n)$$

where $d \in \{L, N, R\}$, $n(L) = n - 1$, $n(N) = n$, $n(R) = n + 1$. It is easy to check that the adjoint U^* of U satisfies (4.2) except now $d \in \{L, N, R\}$ and

$$d' = \begin{cases} L & \text{if } d = R \\ N & \text{if } d = N \\ R & \text{if } d = L \end{cases}$$

The generalized counterpart of Theorem 4.2 holds except that in addition to Condition 4.5 with $d \in \{L, N, R\}$ and Condition 4.6, we need

$$\sum^t [\delta(x, s, y, t, N) \delta(x', s', y', t, L)^* + \delta(x, s, y, t, R) \delta(x', s', y', t, N)^*] = 0 \tag{6.1}$$

for every $x, y, x', y' \in I, s, s' \in S$.

To show that (6.1) is necessary, suppose $U \in \mathcal{F}(H)$, $w'_m = w_m$ for $m \neq n, m \neq n + 1$, $w_n = x, w_{n+1} = y', w'_n = y, w'_{n+1} = x'$. We then have

$$\begin{aligned} 0 &= \langle Un \otimes s \otimes w, U(n + 1) \otimes s' \otimes w' \rangle \\ &= \langle \sum_{z,t,d} \delta(x, s, z, t, d)n(d) \otimes t \otimes w(z, n), \\ &\quad \sum_{z',t',e} \delta(x', s', z', t', e)(n + 1)(e) \otimes t' \otimes w'(z', n + 1) \rangle \\ &= \sum_{z,t,d} \sum_{z',t',e} \delta(x, s, z, t, d) \delta(x', s', z', t, e)^* \end{aligned}$$

$$\begin{aligned} & \times \langle n(d), (n+1)(e) \rangle \langle t, t' \rangle \langle w(z, n), w'(z', n+1) \rangle \\ &= \sum_{z, z', t} \delta(x, s, z, t, N) \delta(x', s', z', t, L)^* \langle w(z, n), w'(z', n+1) \rangle \\ & \quad + \sum_{z, z', t} \delta(x, s, z, t, R) \delta(x', s', z', t, N)^* \langle w(z, n), w'(z', n+1) \rangle \end{aligned}$$

But $\langle w(z, n), w'(z', n+1) \rangle = 0$ unless $z = w'_n = y$ and $z' = w_{n+1} = y'$, in which case $\langle w(z, n), w'(z', n+1) \rangle = 1$. Hence, (6.1) holds. The rest of the proof of the generalized counterpart of Theorem 4.2 proceeds as in the proof of Theorem 4.2.

For a generalized QTM $M = (I, S, \delta)$, define the operators Δ_L, Δ_R on H_0 as in Section 5 and define the operator Δ_N by

$$\Delta_N x \otimes s = \sum_{y, t} \delta(x, s, y, t, N) y \otimes t$$

As before we have $\Delta_R \Delta_L^* = 0$ and

$$\Delta_L \Delta_L^* + \Delta_N \Delta_N^* + \Delta_R \Delta_R^* = 1$$

In addition, by (6.1) we have

$$\Delta_N \Delta_L^* + \Delta_R \Delta_N^* = 0$$

Lemma 6.1. Let $M = (I, S, \delta)$ be a generalized QTM and let $a, b, c \in \mathbb{C}$ with $|a| = |b| = |c| = 1, ca^* = bc^*$. Then the operator A on H_0 defined by

$$A = a\Delta_L + b\Delta_R + c\Delta_N$$

is unitary.

Proof. Applying our previous observations, we have

$$\begin{aligned} AA^* &= (a\Delta_L + b\Delta_R + c\Delta_N) (a^* \Delta_L^* + b^* \Delta_R^* + c^* \Delta_N^*) \\ &= \Delta_L \Delta_L^* + \Delta_R \Delta_R^* + \Delta_N \Delta_N^* + ab^* \Delta_L \Delta_R^* + ba^* \Delta_R \Delta_L^* \\ & \quad + ca^* \Delta_N \Delta_L^* + bc^* \Delta_R \Delta_N^* + ac^* \Delta_L \Delta_N^* + cb^* \Delta_N \Delta_R^* = 1 \quad \blacksquare \end{aligned}$$

For $a, b, c \in \mathbb{C}$ satisfying the conditions of Lemma 6.1, it follows that $P = (I, S, \gamma)$ is a quantum printer for

$$\gamma(x, s, y, t) = a \delta(x, s, y, tL) + b \delta(x, s, y, tR) + c \delta(x, s, y, tN)$$

Lemma 6.2. If $M = (I, S, \delta)$ is a generalized QTM, then there exist three quantum printers $P = (I, S, \alpha), Q = (I, S, \beta), T = (I, S, \gamma)$ such that

$$\begin{aligned} \delta(x, s, y, t, L) &= \frac{1}{4}(1-i)\alpha(x, s, y, t) + \frac{1}{4}(1+i)\beta(x, s, y, t) + \frac{1}{2}\gamma(x, s, y, t) \\ \delta(x, s, y, t, R) &= \frac{1}{4}(1+i)\alpha(x, s, y, t) + \frac{1}{4}(1-i)\beta(x, s, y, t) - \frac{1}{2}\gamma(x, s, y, t) \end{aligned}$$

$$\delta(x, s, y, t, N) = \frac{1}{2}\alpha(x, s, y, t) - \frac{1}{2}\beta(x, s, y, t)$$

Proof. Define the operators A, B, C on H_0 by

$$A = \Delta_L + \Delta_R + \Delta_N$$

$$B = \Delta_L + \Delta_R - \Delta_N$$

$$C = \Delta_L - \Delta_R + i\Delta_N$$

It follows from Lemma 6.1 that $A, B, C \in \mathcal{U}(H_0)$. Solving these three equations simultaneously, we obtain

$$\Delta_L = \frac{1}{4}(1 - i)A + \frac{1}{4}(1 + i)B + \frac{1}{2}C$$

$$\Delta_R = \frac{1}{4}(1 + i)A + \frac{1}{4}(1 - i)B + \frac{1}{2}C$$

$$\Delta_N = \frac{1}{2}A - \frac{1}{2}B$$

Letting $P = (I, S, \alpha)$, $Q = (I, S, \beta)$, $T = (I, S, \gamma)$ be the quantum printers with evolution operators A, B, C , respectively, we obtain the result. ■

If P, Q, T satisfy the conditions of Lemma 6.2, we say that P, Q, T generate M . Then Lemma 6.2 says that any generalized QTM is generated by three quantum printers. One can now continue the analysis of a generalized QTM as in Section 5, but we shall not pursue this here.

To better understand the concept of a quantum pushdown automaton, we first review its classical version. A *deterministic pushdown automaton* (DPDA) is a 4-tuple $\mathcal{A} = (S, I, T, \delta)$, where S is a finite set of internal control states with an identified start state $s_0 \in S$ and an identified set $S_f \subseteq S$ of final states, I is a finite input alphabet, T is a finite stack alphabet, and

$$\delta: I \times \{\lambda\} \cup T \times S \rightarrow S \times T^*$$

is a transition function. The DPDA \mathcal{A} has access to a stack which is an infinite memory that stores words in the alphabet T . The transition function δ allows \mathcal{A} to scan the input letter, the top stack letter, and its current control state. It then updates the control state, pops the top letter off the stack, and pushes a (possibly empty) word onto the top of the stack. If the word in the stack is empty so there is no top letter, we use λ in δ . An element $s \times w' \in S \times T^*$ is a *configuration* of \mathcal{A} . The start configuration for \mathcal{A} has the form $s_0 \times w'_0$. After reading a word $w \in I^*$, \mathcal{A} *accepts* w if \mathcal{A} is in a configuration $s \times \{\lambda\}$, where $s \in S_f$. The *language accepted* by \mathcal{A} is the set of all words that \mathcal{A} accepts. For example, the Dyck language of properly nested words of brackets.

$$\{\lambda, (, ((), () (), (() (), \dots\}$$

is accepted by a DPDA \mathcal{A} . In this case, $I = \{(,)\}$, $T = \{x\}$, and \mathcal{A} pushes

x onto the stack when it scans a (and pops an x off the stack when it scans a). If \mathcal{A} ever attempts to pop an x off an empty stack, then \mathcal{A} enters a reject configuration and stays there. A DPDQ does not lose any power if it is only allowed to push a single letter or the empty word at a time. In this case, it either pushes down a single new letter or pops off an old letter.

A *quantum pushdown automaton* (QPDA) is a 4-tuple $\mathcal{A} = (S, I, T, \delta)$, where S, I, T are as in a DPDA, but now δ is a transition amplitude function

$$\delta: I \times S \times \{\lambda\} \cup T \times S \times T \cup \{p\} \rightarrow \mathbb{C}$$

Then δ has the natural interpretation and we require that δ satisfies the following conditions:

$$\sum_{r,t} \delta(x, s, v, r, t) \delta(x, s', v, r, t)^* = \delta_{s,s'} \quad (6.2)$$

for every $v \in \{\lambda\} \cup T$, where $r \in S, t \in T \cup \{p\}$;

$$\sum_r \delta(x, s, v, r, p) \delta(x, s', v', r, p)^* = 0 \quad (6.3)$$

for every $v, v' \in \{\lambda\} \cup T$, with $v \neq v'$; and

$$\sum_r \delta(x, s, v, r, t) \delta(x, s', v', r, p)^* = 0 \quad (6.4)$$

for every $t \in T, v \in \{\lambda\} \cup T, v' \in T$.

Let H be the configuration Hilbert space with computational basis $S \times T^*$. For $x \in I$, define the *transition operator* $U(x): H \rightarrow H$ as follows. If $s \in S, u = u_k \cdots u_1 \in T^* \setminus \{\lambda\}$, then

$$U(x)s \otimes u = \sum_{r,t} \delta(x, s, u, r, t)r \otimes u(t) \quad (6.5)$$

where

$$u(t) = \begin{cases} ut & \text{if } t \in T \\ u_k \cdots u_2 & \text{if } t = p \end{cases}$$

and when $u = \lambda$, then $U(x)$ is also defined by (6.5) with

$$u(t) = \begin{cases} t & \text{if } t \in T \\ \lambda & \text{if } t = p \end{cases}$$

Theorem 6.3. The operator $U(x) \in \mathcal{F}(H)$ if and only if (6.2)–(6.4) hold.

Proof. Assume that $U(x) \in \mathcal{F}(H)$. Letting $u = u_k \cdots u_1, v \neq \lambda$, we have

$$\begin{aligned}
\delta_{s,s'} &= \langle U(x)s \otimes u, U(x)s' \otimes u \rangle \\
&= \left\langle \sum_{r,t} \delta(x, s, v, r, t)r \otimes u(t), \sum_{r',t'} \delta(x, s', v, r', t')r' \otimes u(t') \right\rangle \\
&= \sum_{r,t \in T} \sum_{r',t' \in T} \delta(x, s, v, r, t) \delta(x, s', v, r', t')^* \langle r, r' \rangle \langle u(t), u(t') \rangle \\
&\quad + \sum_{r,r'} \delta(x, s, v, r, p) \delta(x, s', v, r', p)^* \langle r, r' \rangle \langle u_k \cdots u_1, u_k \cdots u_1 \rangle \\
&= \sum_{r,t} \delta(x, s, v, r, t) \delta(x, s', v, r, t)^*
\end{aligned}$$

If $u = \lambda$ and hence $v = \lambda$, we get the same result. Hence, (6.2) holds. Letting $u = u_k \cdots u_1 v$, $u' = u_k \cdots u_1 v'$, $v, v' \in T$ with $v \neq v'$, we have

$$\begin{aligned}
0 &= \langle U(x)s \otimes u, U(x)s' \otimes u' \rangle \\
&= \sum_r \delta(x, s, v, r, p) \delta(x, s', v', r, p)^*
\end{aligned}$$

If $u = \lambda$, $u' = v' \in T$, we get the same result, so (6.3) holds. Letting $u = u_k \cdots u_1 v$, $u' = u_k \cdots u_1 v t_1 v'$, we have

$$\begin{aligned}
0 &= \langle U(x)s \otimes u, U(x)s' \otimes u' \rangle \\
&= \sum_r \delta(x, s, v, r, t_1) \delta(x, s', v', r, p)^*
\end{aligned}$$

If $u = v = \lambda$, we get the same result, so (6.4) holds.

Conversely, assume that (6.2)–(6.4) hold. To prove that $U(x) \in \mathcal{F}(H)$, it is sufficient to show that

$$\langle U(x)s \otimes u, U(x)s' \otimes u' \rangle = \delta_{s,s'} \delta_{u,u'}$$

That $\|U(x)s \otimes u\| = 1$ follows from (6.2). If $s \neq s'$, we have

$$\begin{aligned}
&\langle U(x)s \otimes u, U(x)s' \otimes u' \rangle \\
&= \sum_{r,t,t'} \delta(s, x, u_1, r, t) \delta(x, s', u'_1, r, t')^* \langle u(t), u'(t') \rangle
\end{aligned}$$

The right side vanishes unless $u(t) = u'(t')$ for some $t, t' \in T \cup \{p\}$. If $u = u'$, then the right side vanishes by (6.2). The other cases are given by (6.3) and (6.4). If $s = s'$ and $u \neq u'$, then we proceed in a similar way. ■

It can be shown that $U(x) \notin \mathcal{U}(H)$ in general. We leave a further study of QPDAs, including the languages they accept, to a later paper.

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