Models of Quantum Turing Machines

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Abstract

Quantum Turing machines are discussed and reviewed in this paper. Most of the paper is concerned with processes defined by a step operator T that is used to construct a Hamiltonian H according to Feynman's prescription. Differences between these models and the models of Deutsch are discussed and reviewed. It is emphasized that the models with H constructed from T include fully quantum mechanical processes that take computation basis states into linear superpositions of these states.

The requirement that T be distinct path generating is reviewed. The advantage of this requirement is that Schrödinger evolution under H is one dimensional along distinct finite or infinite paths of nonoverlapping states in some basis B_T. It is emphasized that B_T can be arbitrarily complex with extreme entanglements between states of component systems.

The new aspect of quantum Turing machines introduced here is the emphasis on the structure of graphs obtained when the states in the B_T paths are expanded as linear superpositions of states in a reference basis such as the computation basis B_C. Examples are discussed that illustrate the main points of the paper. For one example the graph structures of the paths in B_T expanded as states in B_C include finite stage binary trees and concatenated finite stage binary trees with or without terminal infinite binary trees. Other examples are discussed in which the graph structures correspond to interferometers and iterations of interferometers.

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I. INTRODUCTION

Quantum computation is a field with much activity in recent years. Most work on models of quantum computers has been concerned with networks of quantum gates [1–3]. Models based on quantum Turing machines [4–8] have also been described. Networks of quantum gates are appealing because they are similar to integrated circuits in that they are built up from simple elementary quantum gates. Also working physical models of quantum computers are likely to have this network structure.

Networks of quantum gates are characterized by the fact that the complexity of the computation appears explicitly in the complexity of the layout and interconnections of the quantum gates and qubit lines making up the network. Because of this networks of more than a few gates are hard to conceptualize as physical models. For complex networks heirarchical descriptions in terms of simpler component networks are useful. Examples are the networks for the discrete Fourier transform [2] and Shor's Algorithm [9,10].

Quantum Turing machines (QTMs) are quite different in that the complexity of the computation is not reflected in the physical model. Instead the complexity is reflected in the dynamical description of the model either as a unitary operator describing the possible finite time interval steps or in the description of the Hamiltonian for the model. The physical model, consisting of a finite state head interacting with one (or if needed for convenience more than one) qubit lattice, remains fixed for the different models.

In this paper the discussion will be limited to quantum Turing machines. An interesting aspect of these systems is that they can be expanded in different directions to illustrate different properties. For example the description of the Hamiltonian can be easily expanded to include the presence of finite potential barriers on computation paths where the potential distribution is computable. These result in reflections of the computation back along the computation paths [11]. An example of this has been discussed in detail elsewhere [12,13]. Also the physical model of QTMs is a natural basis for expansion into a model of quantum robots interacting with an environment [14].

In this paper step operators T for each QTM are first defined by conditions on matrix elements in the computation basis. This follows the definition of Deutsch [5]. These operators can either be used to represent model steps occurring in a finite time interval, as was done by Deutsch, or they can be used to directly construct a Hamiltonian according to Feynman's prescription [15]. This was the method used by Benioff. Differences between these two types of models are discussed in Section III.

Another definition of T as a finite sum of elementary step operators is given in Section IV. This definition, much used by the author in earlier work [6,8], has the advantage that description of a step operator with a specified set of elementary steps is easier under this definition than with the matrix element definition. It is seen that, for the particular form of the unitary operators appearing in the elementary step sum, the matrix element definition is more general in that final state correlations between changes in the head state, head position, and scanned qubit state are included. Both definitions include initial state correlations and include steps that take computation basis states into linear superpositions of these states.

In most of this paper QTM step operators T will be used to construct model Hamiltonians according to Feynman's prescription [15]. In this case the requirement that T be distinct path generating much simplifies the dynamics of the system. The main consequence of this

requirement, which is reviewed and discussed in Section V, is that Schrödinger evolution of the computation corresponds to one dimensional motion along paths of states in some basis B_T. The paths are defined by iterations of T and $T^\dagger$ on states in B_T. The dependence on T is indicated by the subscript. Basis dependent (matrix) and basis independent (operator) descriptions of this property are reviewed. The form of the eigenfunctions and spectrum for Hamiltonians constructed from Ts that are distinct path generating is also summarized. A sum over paths representation of e^{-iHt} for H constructed from step operators that are distinct path generating is described. Section V concludes with a review of the fact that there is no effective way to determine in general if a step operator is distinct path generating.

Fully quantum mechanical computations are included because B_T can be arbitrarily complex with extreme entanglements between the component system states. Examples will be given to show this and to show that T takes computation basis states into linear superpositions of computation basis states. Thus distinct path generation is not limited to descriptions of a "classical Turing machine made of quantum components" [2]. Demonstration of this point, which was also made in [8], is one of the goals of this paper.

The main novel feature introduced in this paper is an emphasis on the graph structure aspects of the paths in B_T when the states in B_T are expanded into superpositions of states in a fixed basis. Stated differently the main interest here is not in the outcome of a process such as a quantum computation. Instead the interest is in the graph properties of the computation paths relative to a fixed basis, such as the computation basis. Because of this aspect there is some overlap between this work and other work in the literature [16–18] describing motion of systems in graphs of interconnected quantum wires.

These properties are illustrated in Section VI by discussion of examples chosen to illustrate various points. All the examples are fully quantum mechanical in that they take computation basis states into linear superpositions of these states. The first example, the erasure? operator, is given to show that there are step operators, which at first glance appear to describe irreversible processes, in fact describe reversible processes. The second example, product qubit transformations followed by add 1, describes generation of a linear superpositions of states corresponding to all numbers up to 2^{n-1} and adding 1 to each. Depending on the initial states graph structures corresponding to one or more iterated binary trees with finite numbers of stages are generated. Also a terminal infinite binary tree may or may not be appended.

The third group of examples is introduced to show that closed graphs with loops are included. In particular the graph structure of the examples corresponds to that of interferometers in coordinate space. The examples show that depending on the initial state, iterated loops corresponding to successive opening and closing of interferometer type structures are included. It is seen that activities in each arm can be different although they must be such that differences in states in each arm must be removed coherently when the arms are closed.

II. THE PHYSICAL MODEL

The physical model used here corresponds to one-tape quantum Turing machines. Extension to machines with more than one tape, as in Bennett's description of reversible machines [19] is straightforward. The model consists of a two-way infinite one dimensional lattice of systems each of which can assume states in a finite dimensional Hilbert space. if the space

is two dimensional, the systems are referred to as qubits. This term will be used here even if the dimensionality is greater than two. It is often convenient but not necessary to consider the lattice as spin systems, e.g. spin 1/2 systems for binary qubits.

A head which can assume any one of a finite number of orthogonal states $|l\rangle$ with $l = 1, 2, \cdots, L$ moves along the lattice interacting with qubits at or next to its location on the lattice. Elementary QTM actions include one or more of (1) head motion one lattice site to the right or left, (2) change of the state of the qubit scanned or read by the head, (3) change of the head state. What happens depends on the states of the head and scanned qubit.

Here the system states are all assumed to lie in a separable Hilbert space $\mathcal{H}$. Based on the above description a particular basis, the computation basis, defined by the set of states $\{|l, j, \underline{s}\rangle\}$ and which spans $\mathcal{H}$, is used. Here l, j refer to the internal state and lattice position of the head. The qubit lattice computation basis state $|\underline{s}\rangle = \otimes_{m=-\infty}^{\infty} |\underline{s}_m\rangle$ where $\underline{s}_m = 0$ or 1 is the state of the qubit at lattice site m. From now on the computation basis will be denoted by B_C.

In order to keep $\mathcal{H}$ separable (a denumerable basis), it is necessary to impose some condition on $|\underline{s}\rangle$. Here it will be required that $\underline{s}_m \neq 0$ for at most a finite number of values of m. This condition, the 0 tail state condition, is one of many that can be imposed to keep the basis denumerable. Models of QTMs without tail conditions would have to be described by quantum field theory on a lattice to take account of the presence of an infinite number of degrees of freedom.

III. THE STEP OPERATOR

Models of QTMs in the literature [5,6,8,12] can be described by step operators T that correspond to single steps of a computation. In terms of matrix elements between states in B_C, T must satisfy a locality condition given by superpositions of states in B_C:

$$\langle l', j', \underline{s}'|T|l, j, \underline{s}\rangle = \langle \underline{s}'_{\neq j}|\underline{s}_{\neq j}\rangle \langle l', j', \underline{s}'_{j'}|\tilde{T}|l, j, \underline{s}_j\rangle \tag{1}$$

Here $|\underline{s}\rangle = |\underline{s}_{\neq j}\rangle|\underline{s}_j\rangle$ where $|\underline{s}_j\rangle$ is the state of the site j qubit.

This condition states that single step changes in the state of the lattice qubits are limited to the qubit at the position of the head.

The operator $\tilde{T}$ describes the interactions of the head with qubits on the lattice. Since the interaction is localized to the qubit at the head position, $\tilde{T}$ can be described as an operator on the Hilbert space spanned by states of the form $|l, j, s\rangle$. This corresponds to the head in state $|l\rangle$ at position j and the site j qubit in state $|s\rangle$.[1]

Another condition on T is that head motion on the lattice is limited to at most one site in either direction. Also all lattice sites are equivalent (space is homogenous). These conditions are given respectively by

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[1]In general the states have the form $|l, j, s, k\rangle$ that describe the head at site j and the qubit at site k. However since T (and $\tilde{T}$) have nonzero matrix elements only for states of the form $|l, j, s, j\rangle$ where $k = j$, the two j positions are combined.

$$\tilde{T} = \sum_{j=-\infty}^{\infty} \sum_{\Delta=-1}^{1} P_{j+\Delta} \tilde{T} P_j$$

$$\langle l', j' + \Delta, s' | \tilde{T} | l, j', s' \rangle = \langle l', j + \Delta, s' | \tilde{T} | l, j, s \rangle \tag{2}$$

for all j, j' and all $\Delta = -1, 0, 1$. P_j is the projection operator for the head at site j.

This definition differs in some inessential details from that given by Deutsch [5] for QTMs. One difference is that the possibility that $\Delta = 0$ is included. This addition is not essential in that it has been shown [7] that for every QTM that includes steps with no change in the head position there is an equivalent (slower) QTM which excludes these steps (i.e. $\Delta = -1, 1$ only). Also systems with $\Delta = 0$ excluded are simpler to analyze.

In the QTM models of Deutsch, T describes the transformation associated with a finite time interval t. Thus T is also required to be unitary. Iterations of T give the successive transformations at times that are integer multiples of t. The implicit existence of Hamiltonians that generate these transformations was assumed.

Models of QTMs described by Benioff [6,8,12] differ from those of Deutsch in that T is used directly to construct a Hamiltonian according to Feynman's prescription: [15]

$$H = K(2 - T - T^{\dagger}) \tag{3}$$

where K is a constant. This definition has the property that if $T = Y$ where Y describes free head motion with no interaction along the lattice ($Y|l, j, \underline{s}\rangle = |l, j+1, \underline{s}\rangle$), then H is the kinetic energy of free head motion on the lattice. As such it is equivalent to the symmetrized discrete version of the second derivative, $-(\hbar^2/2m)d^2/dx^2$. As defined H is local as the head interacts only with qubits at or next to its location. Also the requirement that T be unitary is dropped.

As noted above the main difference between the two types of models is that in those of Deutsch T is unitary and it describes changes occurring in a finite time interval. In the models of Benioff T is used to directly construct a Hamiltonian H with the changes in a finite time interval t given by e^{-iHt}. In this case T need not be unitary.

One consequence of these differences is that in the models of Benioff e^{-iHt} is not local even though H is local. In the models of Deutsch [5] T represents the model evolution in a finite time interval and is supposed to be local. This requirement is not realistic in the sense that there is no local Hamiltonian H that satisfies $T = e^{-iHt}$ for finite t. This is easily seen by examination of the terms in a power series expansion of e^{-iHt} where H has a finite but nonzero spatial range.

Of course from a practical standpoint, even though e^{-iHt} is not exactly local, it is approximately local in that matrix elements between sufficiently separated space positions are extremely small. Otherwise it would not be possible to isolate systems for carrying out experiments.

IV. T AS A SUM OF ELEMENTARY STEP OPERATORS

The conditions given on T by Eqs. 1 and 2 for T used in the Hamiltonian of Eq. 3 were done in a way to emphasize the similarities between the two types of QTM models. However it is often quite useful to define T as a finite sum

$$T = \sum_{l,s} T_{l,s} \tag{4}$$

over elementary step operators $T_{l,s}$. This method has been used by the author to model QTMs [4,6,8,12] as this description makes it relatively clear what elementary steps are needed to accomplish a specific computation. It also is easier to see how the different elementary step operators interconnect in a QTM.

The elementary step operator $T_{l,s}$ describes the single step that occurs in case the head is in state $|l\rangle$ and the qubit at the head location is in state $|s\rangle$. $T_{l,s}$ is defined by,

$$T_{l,s} = \gamma_{l,s} \sum_{j=-\infty}^{\infty} w_{l,s} Q_l v_{l,s} P_{s,j} u_{l,s} P_j \tag{5}$$

where $Q_l, P_j, P_{s,j}$ are respective projection operators for the head in internal state $|l\rangle$, at site j, and the site j qubit in state $|s\rangle$. $\gamma_{l,s}$ is a numerical constant.

The operators $w_{l,s}, v_{l,s}, u_{l,s}$ act in the finite dimensional Hilbert space of head states, the two dimensional qubit Hilbert space, and in the space of head lattice position states respectively where they describe head and qubit state changes, and head motion. The operators $w_{l,s}, v_{l,s}, u_{l,s}$ are unitary in their respective spaces, and $u_{l,s}$ satisfies the condition that $\langle j'|u_{l,s}|j\rangle \neq 0$ only if $|j'-j| = 0, 1$. The possibility that these operators can be different for different values of l, s is indicated by the subscripts.

The form of the equation for $T_{l,s}$ shows projection operators on computation basis states followed by unitary operators. Depending on the process to be modelled it is sometimes useful to invert the order of the projection and unitary operators for one or more of the system components. An example would be to replace $w_{l,s}Q_l$ by $Q_l w_{l,s}$ in Eq. 5. This is the case if some component computation basis state is the desired final state. This will be seen in the first and third examples studied.

In most work using this form of T, $\gamma_{l,s} = 1$ for all l, s in the sum. The case $0 \leq \gamma_{l,s} \leq 1$ was considered elsewhere [12]. A detailed analysis of a simple case was done for which $\gamma_{l,s} < 1$ corresponded to the introduction of potential barriers in the computation paths [13,20]. For this example the distribution and widths of the potential barriers in the paths was quasiperiodic [21] and corresponded to a generalized substitution sequence [22–24].

This definition includes $T_{l,s}$ that take computation basis states into linear superpositions of the basis states. In particular $T|l, j, \underline{s}\rangle = |\underline{s}_{\neq j}\rangle \delta_{s,\underline{s}_j} T_{l,s}|l, j, s\rangle$ where

$$T_{l,s}|l, j, s\rangle = \gamma_{l,s} \sum_{l',j',s'} |l', j', s'\rangle \langle l'|w_{l,s}|l\rangle \langle s'|v_{l,s}|s\rangle \langle j'|u_{l,s}|j\rangle \tag{6}$$

Here $w_{l,s}$ and $v_{l,s}$ can be any L dimensional and 2 dimensional unitary operators respectively and $u_{l,s}$ can be such that the matrix elements $\langle j + \Delta|u_{l,s}|j\rangle$ are non zero for all three values of Δ.

The definition of T as a step operator that satisfies Eqs. 1 and 2 is somewhat more general than T defined as an l, s sum by Eq. 4 with $T_{l,s}$ defined by Eq. 5. To see this one notes that any T defined by Eqs. 4 and 5 satisfies Eqs. 1 and 2.

To examine the converse let T be a step operator that satisfies Eqs. 1 and 2. From these equations it follows that the corresponding operator $\tilde{T}$ and, as a result T, can always be expressed as an l, s sum in the form

$$T = \sum_{l,s} T P_{l,s} \tag{7}$$

where

$$P_{l,s} = \sum_{j=-\infty}^{\infty} Q_l P_{s,j} P_j \tag{8}$$

where the projection operators are as defined in Eq. 5. From this one sees that $TP_{l,s} = T_{l,s}$ if and only if

$$TP_{l,s} = \gamma_{l,s} w_{l,s} \otimes v_{l,s} \otimes u_{l,s} P_{l,s}. \tag{9}$$

This shows that the definition of $T_{l,s}$ given by Eq. 5 is restricted to uncorrelated unitary transformations of the head state and position and qubit state. That is the action of T defined by Eqs. 4 and 5 converts a computation basis state $|l, j, \underline{s}\rangle$ into $w_{l,s}|l\rangle u_{l,s}|j\rangle|\underline{s}_{\neq j}\rangle v_{l,s}|\underline{s}_j\rangle$ where $s = \underline{s}_j$. Correlation with the initial state is included through the l, s dependence of the different unitary operators in Eq. 5.

V. DISTINCT PATH GENERATION

Here the property of distinct path generation for step operators will be reviewed and discussed. This property is quite useful because the dynamics of any such process with a Hamiltonian given by Eq. 3 corresponds to one dimensional motion along distinct paths of states in some basis B. In this case the complexity of the process is contained in the complexity of the states in B and their ordering in paths. In particular the states in B can describe arbitrary entanglements among states of component systems in the model.

In general a path of states is an ordered set of states in a Hilbert space $\mathcal{H}$. Here the interest is in paths generated by operators T on $\mathcal{H}$ that represent the single steps of a process. If ψ_1 is a state in $\mathcal{H}$, then the set of states $\{T^n\psi_1,\ (T^\dagger)^{-m}\psi_1\}$ for integral m, n where $n \geq 0$, $m < 0$ represents a path of states. The ordering of the states in a path is conveniently expressed by the notation $|k, i\rangle \sim T^k\psi_1$ for integral $k \geq 0$ and $|k, i\rangle \sim (T^\dagger)^{-k}\psi_1$ for $k < 0$. The relation $\sim$ means equality up to normalization. The path label is denoted by i where $|0, i\rangle = \psi_1$ and k denotes the path position of the state.

The state $T^n\psi_1$ for $n \geq 0$ is a terminal state if $T^{n+1}\psi_1 = 0$. Similarly $(T^\dagger)^{-m}\psi_1$ for $m < 0$ is terminal if $(T^\dagger)^{-m+1}\psi_1 = 0$. Paths are two way infinite or cyclic if they have no terminal states, one way infinite if they have one terminal state, and finite with distinct ends if they have two terminal states.

The goal of the above definitions of paths is to satisfy the condition that iterations of T or $T^\dagger$ on states describe successive steps of a quantum computation in the forward or backward direction respectively. So far this requirement is not satisfied because any state $|k, i\rangle$ in a path may have nonzero overlap with other states $|j, i\rangle$ in the path. Thus state $|k, i\rangle$ which is supposed to correspond to completion of the kth step may also correspond to completion of the jth and other steps.

To remove this possibility it is required that all the states in any path must be pairwise orthogonal. If this condition is satisfied then the state $|k, i\rangle$ represents unambiguously the

completion of the kth step in the forward direction for $k \geq 0$ and in the backward direction for $k < 0$. Another condition that must be satisfied is that for each $n \geq 0$ and $m < 0$, $T^\dagger T^{n+1}\psi_1 = T^n\psi_1$ and $T(T^\dagger)^{-m}\psi_1 = (T^\dagger)^{-m-1}\psi_1$. This condition expresses the requirement that motion one step backwards from the state corresponding to completion of the $n+1st$ step should give the state corresponding to completion of the nth step. Also motion one step forward from the $-mth$ step in the backward direction should give the state corresponding to the $-m-1st$ backward step (recall that $m < 0$).

A third condition is that if ψ_2 is a state that is orthogonal to all states in the path defined above for ψ_1, denoted from now on as path 1, then all states in path 2, generated as defined above with ψ_2 replacing ψ_1, should be orthogonal to all states in path 1. By convention ψ_2 is in no path if $T\psi_2 = T^\dagger\psi_2 = 0$. This expresses the intuitive requirement that computations started out on initial states that are orthogonal must maintain the orthogonality through all steps, forward and backward, of the computation. Otherwise one could not associate an outcome with a specific input.

Mathematically these conditions are expressed by requiring that T be distinct path generating. That is there must exist some basis B such that for each $|b\rangle$ in B if $T|b\rangle \neq 0$ then, up to normalization, $T|b\rangle$ is a state in B. Similarly if $T^\dagger|b \neq 0$, then, up to normalization, $T^\dagger|b\rangle$ is in B. It follows from this condition that all states in a path are pairwise orthogonal or both T and $T^\dagger$ are the identity on some $|b\rangle$. Up to normalization means that the normalized state $T|b\rangle/|\langle b|T^\dagger T|b\rangle|^{1/2}$ is in B. A similar condition holds for $T^\dagger$.

The above condition of pairwise orthogonality of states within a path combined with the condition of orthogonality of all states in one path with those in another path can be expressed by $\langle j, i|k, i'\rangle = 0$ unless $j = k$ and $i = i'$. Here $|k, i\rangle$ and$|j, i'\rangle$ are states in B. The condition that states generated by iteration of T and $T^\dagger$ remain within a path is expressed by $T|k, i\rangle \neq 0 \rightarrow T|k, i\rangle \sim |k+1, i\rangle$ and $T^\dagger|k, i\rangle \neq 0 \rightarrow T^\dagger|k, i\rangle \sim |k-1, i\rangle$.

These conditions for distinct path generation can be combined into one condition. This is that T must be such that there exists a basis B for which each row and each column of the matrix of T in B contains at most one nonzero element. If this condition is satisfied, it is always possible to choose B so that the matrix elements of T are positive real numbers. In addition the matrix elements are bounded from above, since T is bounded, and from below, for technical reasons (noted in the next section).

It is convenient to let B_T denote any basis for which T (and $T^\dagger$) is distinct path generating. In general if T is distinct path generating, there are a great many bases for which T is distinct path generating. This may be the case if there is more than one copy of paths of the same type (two way infinite, finite of the same length, etc.,) present. For the models of quantum computers considered here there are either no copies or infinitely many copies of the same type present. This is a consequence of the spatial homogeneity of T.

A. Basis Independent Description of Distinct Path Generation

The above description of distinct path generation is basis dependent as it is given in terms of matrix elements of T in some basis. An equivalent basis independent operator theoretic description is also possible. It has been shown elsewhere [8,12] that the conditions given above for distinct path generation are equivalent to the requirement that T is a direct sum of weighted shifts [25]. That is

$$T = UD = \oplus_i U_i D_i \tag{10}$$

where for each i U_i is either a bilateral shift, a unilateral shift, the complement of a unilateral shift, a finite shift or a cyclic shift. Many copies of each type can be present and some types may be absent. The types of paths associated with each of these shift types are shown in Figure 1. Note that the only shifts that are unitary are the bilateral and cyclic shifts.

This follows from the decomposition theorem for power partial isometries [26] since U is a power partial isometry and D is a diagonal operator [25]. The i sum corresponds to a sum over distinct path subspaces $\mathcal{H}_i$ where $\mathcal{H}_i$ is spanned by the basis states in the path generated by U_i and its adjoint. That is if $|j,i\rangle$ is such a state in $\mathcal{H}_i$ then either $|j,i\rangle$ is terminal for U or $U|j,i\rangle = U_i|j,i\rangle = |j+1,i\rangle$. A similar condition holds for $U^\dagger$. Here the set of states $\{|j,i\rangle\}$ (plus any additional basis states that span the null space for T, if such a space exists) form a distinct path generating basis for T.

It should be noted that the converse implication does not hold. That is if U is a power partial isometry, it does not follow that U is distinct path generating in some basis. The reason is that the unitary component of the decomposition may not be distinct path generating in any basis [8]. Distinct path generation does follow if the unitary component of U in the decomposition is either empty or is a bilateral or cyclic shift.

The operator D is self adjoint and bounded with eigenstates $|j,i\rangle$. That is $D|j,i\rangle = D_i|j,i\rangle = d_{j,i}|j,i\rangle$ where $d_{j,i}$ is a positive real number. For technical reasons it is useful to require that $d_{j,i} > \epsilon > 0$ for all j,i [25]. This avoids such functions as $d_{j,i} = 1/j$ on infinite paths. Note that the operator D accounts for the possible loss of normalization referred to for T. Additional details on U are given in [26,8].

B. Eigenfunctions, Spectrum of H

If T is distinct path generating the eigenfunctions and energy spectrum of the Hamiltonian of Eq. 3 all correspond to one dimensional motion on a path of states in B_T. If $T = \sum_i U_i$ with $D = 1$ the motion is free except for the possible presence of infintely high potential walls located adjacent to terminal path states. Details are given in [8]. If no walls are present (path a in Figure 1) the eigenfunctions are given by $\psi_k = \sum_{j=-\infty}^{\infty} e^{ikj}|j,i\rangle$ where k is the momentum. The B_T path state $|j,i\rangle$ is defined at the beginning of section V. The energy eigenvalues are given by $E = 2K(1-\cos k)$ where k can take any value between $-\pi$ and π.

If one wall is present the eigenstates describe standing waves reflected off the potential wall. For reflection to the left (path b in Figure 1) eigenstates are given by $\psi_k = \sum_{j=-\infty}^{b} \sin k(b-j)|j,i\rangle$ where b is the wall location ($T|b-1,i\rangle = 0$). For reflection to the right (path c in Figure 1) $\psi_k = \sum_{j=a}^{\infty} \sin k(j-a)|j,i\rangle$ where a is the wall location ($T^\dagger|a+1,i\rangle = 0$). The eigenvalues are the same as for the free case above.

For finite paths (path d in Figure 1) the eigenstates describe bound state motion between two reflecting walls. For the walls located at a and b with $a < b$ the eigenstates are given by $\psi_k = \sum_{j=0}^{b-a} \sin k(b-a-j)|a+j,i\rangle$. The energy is given by $E = 2K(1-\cos k)$ where $k = 2\pi m/(b-a)$ with $m = 1,2,\cdots,b-a-1$. A similar expression holds for cyclic paths.

For the case in which $D \neq 1$ finite potentials of different heights and widths can be present in addition to the reflecting walls at path terminal states. The eigenstates and

spectra of H are much more complex in that reflections and transmissions occur at the path locations of the potentials [11]. A specific example analyzed elsewhere [12,13,20] showed a complex band structure for the spectrum of H.

C. Sum Over Paths Representation

It is of interest to examine a sum over paths representation of the unitary evolution operator e^{-iHt} to show the relation between the paths defined by iteration of T and $T^\dagger$ and those in the path sum. T is assumed to be distinct path generating. The representation is based on a straightforward power series expansion of e^{-iHt}. In the context of this paper, representation as a sum or integral over action weighted paths [27] is not used as it appears to require more development.

The time development of the state of a QTM under the action of a Hamiltonian H can be expressed in any basis B by

$$\Psi(t) = \sum_{b',b\epsilon B} |b'\rangle\langle b'|e^{-iHt}|b\rangle\langle b|\Psi(0)\rangle. \tag{11}$$

Here $\Psi(t)$ and $\Psi(0)$ are the system states at times t and 0 and $\langle b'|e^{-iHt}|b\rangle$ is the amplitude that a QTM in state $|b\rangle$ is in state $|b'$ after a time interval t.

Use of the power series expansion gives

$$\langle b'|e^{-iHt}|b\rangle = \sum_{n=0}^{\infty} \frac{(-it)^n}{n!}\langle b'|H^n|b\rangle. \tag{12}$$

Expansion of the matrix element by inserting a complete set of B states between each H factor gives

$$\langle b'|H^n|b\rangle = \sum_{b_1,b_2,\cdots b_{n-1}} \langle b'|H|b_{n-1}\rangle\cdots\langle b_2|H|b_1\rangle\langle b_1|H|b\rangle. \tag{13}$$

This is equivalent to a sum over paths p of states in B of length $n+1$ that begin with $|b\rangle$ and end with $|b'\rangle$:

$$\langle b'|H^n|b\rangle = \sum_{p}{}' \langle p(n+1)|H|p(n)\rangle\cdots\langle p(3)|H|p(2)\rangle\langle p(2)|H|p(1)\rangle. \tag{14}$$

The prime on the sum means the sum is restricted to length $n+1$ paths with the initial and terminal restrictions noted above.

The equations hold for arbitrary Hamiltonians H and bases B. If H is given by Eq. 3 and T is distinct path generating in B (i.e. $B = B_T$) the matrix element $\langle b'|H^n|b\rangle = 0$ for all n unless $|b'\rangle$ and $|b\rangle$ are in the same T path. T paths are the paths defined earlier by iteration of powers of T and $T^\dagger$ on states of B_T.

If $|b'\rangle$ and $|b\rangle$ are in the same T path, the above shows that $\langle b'|e^{-iHt}|b\rangle$ is equal to a sum of path amplitudes over paths of all lengths within the T path containing $|b'\rangle$ and $|b\rangle$. Each path in the sum describes 1-D motion within the T path. This includes motion in both directions with reflections from any terminal states or potentials encountered [12].

D. Effective Determination of Distinct Path Generation

The question can be asked if there is any effective way to determine if a step operator T that satisfies Eqs. 1 and 2 is distinct path generating in some basis B_T. That is, does there exist any algorithm or computation which can decide in a finite number of steps for any T that satisfies Eqs. 1 and 2 whether T is or is not distinct path generating?

The first step is to note that if T is distinct path generating in the computation basis B_C, then this can be decided effectively. To see this note that if T satisfies Eqs. 1 and 2, then, because of space homogeneity, it is sufficient to search through the matrix elements of $\tilde{T}$ with j set at a fixed value, say $j = 0$. The search involves deciding if each row and column of the matrix for $\tilde{T}$ has at most one nonzero element. Since for fixed j the matrix is finite dimensional, this can be effectively decided provided there is an effective procedure for determining if the matrix elements of $\tilde{T}$ are zero or nonzero.

The more general situation in which T is distinct path generating in a basis B_T different from B_C was examined elsewhere [8]. There it was shown using the operator theoretic description that in general no effective procedure exists. For the matrix description of T one would need to examine the states $T^n|l,0,s\rangle$, $(T^\dagger)^m|l,0,s\rangle$ for all m,n and all l,s to see if the resulting states can be organized into a basis for which T is distinct path generataing. This procedure is not effective as there are an infinite number of values of n,m.

The fact that there is no effective proceedure for general T does not prevent one from studying many examples for which distinct path generation on bases different from B_C can be demonstrated. For these examples one method of proving that T is distinct path generating is to prove that T is a power partial isometry or direct sum of shifts. Another method that is sometimes useful is the direct construction of the states in B_T. Use of these methods will be seen in the following examples.

VI. EXAMPLES

One goal of studying examples is to show the large diversity of QTMs with step operators T that are distinct path generating for bases B_T that are different from B_C. All examples discussed here have this property. The second example is chosen to emphasize this property. It also is an example where the activity or sequence of steps carried out on each computation path in the computation basis is different for the different paths. It is a computation of the form $|\underline{0}\rangle \rightarrow \sum_{s=0}^{2^n-1} c_s|\underline{s}\rangle \rightarrow \sum_{s=0}^{2^n-1} c_s|\underline{f(s)}\rangle$. Here $\underline{s}$ and $s = \sum_{l=1}^{n} \underline{s}(l)2^{l-1}$ denote a length n binary sequence and the corresponding number. The constant 0 sequence is denoted by $\underline{0}$. The computed function f is the simple one-one function "add 1 mod 2^n" where n is arbitrary.

Another goal is the study of the structure of the graphs obtained by expansion of the states in the B_T paths as superpositions of states in a reference basis such as B_C. Many of the graphs for the above example have the form of finite binary trees that may be iterated by appending other trees to the terminal branch lines from the preceeding tree. These graphs have the property that they are open in that they contain no closed loops.

The third example (actually two examples) was chosen to illustrate a closed loop graph with one input and one output line. The graph structure of paths of states in B_T, when expanded in terms of states in B_C, is that of an interferometer in coordinate space. For

these examples the emphasis is on the graph structure and not on computation. The first example is very simple with identical activity occurring in the two arms. The second example is slightly more complex in that the activity is different in each of the two arms. However, differences in path states resulting from these activity differences must be removed coherently before the interferometer is closed. This corresponds to bringing the two arms together in coordinate space interferometers.

The main purpose of the first example is to show that some step operators have different properties than they appear to have at first glance. For this example the step operator appears to describe an irreversible process of erasure in a string of qubits. However it describes a quite different reversible process for which T is distinct path generating.

A. The Erasure? Operator

Let the step operator T be defined by

$$T = \sum_{j=-\infty}^{\infty} \frac{\sigma_x P_{1,j} + P_{0,j}}{\sqrt{2}} u P_j. \tag{15}$$

The Pauli operator σ_x satisfies $\sigma_x P_{i,j} = P_{i\oplus 1,j}\sigma_x$ where $i \oplus 1$ denotes addition mod 2. The operator u is a shift operator for the head on the lattice, $uP_j = P_{j+1}u$. No internal head states are needed.

Iteration of this operator on a computation basis state moves the head from left to right on the lattice converting each qubit state $|1\rangle$ to $(1/\sqrt{2})|0\rangle$ and leaving $|0\rangle$ alone other than changing the normalization to $(1/\sqrt{2})|0\rangle$. Thus iteration of T appears at first glance to describe an irreversible erasure along the lattice of qubits changing all $1s$ to 0 and leaving 0 alone.

Appearances are deceiving, though, because T is in fact distinct path generating on a basis $B_T \neq B_C$. This is the reason for the question mark in the subsection title. This can be seen by rewriting T in the form

$$T = \sum_{j=-\infty}^{\infty} \sqrt{2} P_{0,j} P_{+,j} u P_j. \tag{16}$$

This follows from the fact that $(1+\sigma_x)/2$ is the projection operator P_+ on the state $|+\rangle = 1/\sqrt{2}(|0\rangle + |1\rangle)$.

It is straightforward to see that T and $T^\dagger$ are power partial isometries [26,8]. This follows from the fact that for each $n = 1, 2, \cdots$, $(T^\dagger)^n T^n$ and $T^n (T^\dagger)^n$ given by

$$\begin{aligned} (T^\dagger)^n T^n &= \sum_{j=-\infty}^{\infty} \prod_{k=0}^{n-1} P_{0,j+k} P_j \\ T^n (T^\dagger)^n &= \sum_{j=-\infty}^{\infty} \prod_{k=1}^{n} P_{+,j-k} P_j \end{aligned} \tag{17}$$

are projection operators. Also for each m, n the operators $(T^\dagger)^n T^n$ and $T^m (T^\dagger)^m$ commute [26,8].

The direct sum decomposition of T, Eq. 10 into shifts (as $D = 1$) contains no unitary components. All paths are either finite or one way infinite from the left. The operators U_i are either a complement of a unilateral shift (a coisometry) or a finite shift. The absence of unilateral shifts or bilateral shifts is a consequence of the 0 state tail condition in the definition of $\mathcal{H}$. The eigenstates and eigenvalues are as described in subsection V B.

For the one way infinite path the path states in B_T have the form

$$|n, i\rangle = |n\rangle \otimes \theta_n \tag{18}$$

Here $|n\rangle$ denotes the head at site n. The state of the lattice qubits θ_n is given by

$$\theta_n = |\underline{0}_{\leq n}\rangle \otimes_{j=n+1}^{b-1} |+\rangle_j \otimes |-\rangle_b \otimes \alpha_{>b}. \tag{19}$$

Here $|\underline{0}_{\leq n}\rangle$ denotes the constant 0 sequence for all lattice sites $\leq n$ and $|\pm\rangle_j$ denotes the state $(1/\sqrt{2})(|0\rangle \pm |-\rangle)$ for the site j qubit. The path state $|b, i\rangle$ is terminal for T. The value of b is arbitrary. The state $\alpha_{>b}$ denotes any state of the qubits at sites $> b$ consistent with the 0 state tail condition. The arbitrariness in $\alpha_{>b}$ is possible because the head never enters the lattice region to the right of site b.

For finite paths between and including lattice sites a and b, the path states in B_T have the same form as in Eq. 18 with $a \leq n \leq b$. The state of the lattice qubits θ_n is given by

$$\theta_n = \alpha_{\leq a-2} \otimes |1\rangle_{a-1} \otimes |\underline{0}_{[a,n]}\rangle \otimes_{j=n+1}^{b-1} |+\rangle_j \otimes |-\rangle_b \otimes \alpha_{\geq b+1}. \tag{20}$$

Here $|\underline{0}_{[a,n]}\rangle$ denotes the constant 0 state for qubits on sites between a and n, $\alpha_{\geq b+1}$ is as defined before, and $\alpha_{\leq a-2}$ is an arbitrary state of the qubits on lattice sites $\leq a - 2$ consistent with the 0 state tail condition. The head never moves outside the lattice region $[a, b]$ as $T|b, i\rangle = T^\dagger|a, i\rangle = 0$.

B. General Product Qubit Transformation and Add 1

This example is given to show that step operators that are distinct path generating include computations in which linear superpositions of input states each corresponding to a different numerical input are generated. In addition the computation activity, such as the number and actions of the elementary steps, depends on the numerical input.

The QTM considered here moves down a string of qubits each in state $|0\rangle$ between two markers carrying out an arbitrary but fixed unitary transformation v on each qubit to generate the lattice qubit state $\Psi = \otimes_j v|0_j\rangle$ for all the qubits between the markers. Next the QTM adds 1 mod 2^n to each length n state $|\underline{s}\rangle$ in the superposition Ψ. For each $|\underline{s}\rangle$ the computation begins with the head moving toward the marker region and ends with the head moving away from the marker region with no further changes in the lattice. The number n is determined by the separation of the two markers.

In order to accomodate marker states each qubit is assumed to be a ternary system with a basis $|i\rangle$, $i = 0, 1, 2$ spanning the Hilbert space of each qubit. In this case the two dimensional unitary operator v is expanded to be the identity when acting on $|2\rangle$ or $v \to P_2 \oplus v$ where P_2 is the projection operator for the state $|2\rangle$. In the following v is assumed to be so expanded.

A step operator T that implements this model is the sum of 9 terms. It is given by

$$T = \sum_{j=-\infty}^{\infty} \Bigg[\underset{1}{Q_0 P_{0,j} u} + \underset{2}{w Q_0 P_{2,j} u} + \underset{3}{Q_1 v_j P_{0,j} u} + \underset{4}{w Q_1 P_{2,j} u^\dagger} + \underset{5}{Q_2 \sigma_{x,j} P_{1,j} u^\dagger} + \underset{6}{w Q_2 \sigma_{x,j} P_{0,j} u} + \underset{7}{w Q_2 P_{2,j} u} + \underset{8}{Q_3 P_{0,j} u} + \underset{9}{w Q_3 P_{2,j} u} \Bigg] P_j. \tag{21}$$

In the above sum for T Q_i with $i = 0, 1, 2, 3$ is the projection operator for the head in state $|i\rangle$ and w shifts the head state by 1 mod 4. That is $wQ_i = Q_{i+1}w \bmod 4$. The projection operator P_j for the head at site j is at the end of the expression and v_j is the expanded unitary operator described above for the site j qubit.

The numbers under each term denote the term number for each of the 9 terms. They are present to facilitate discussion of the action of T and $T^\dagger$. $T^\dagger$ is given by

$$T^\dagger = \sum_{j=-\infty}^{\infty} \Bigg[\underset{1^\dagger}{Q_0 P_{0,j} P_j u^\dagger} + \underset{2^\dagger}{Q_0 w^\dagger P_{2,j} P_j u^\dagger} + \underset{3^\dagger}{Q_1 P_{0,j} v_j^\dagger P_j u^\dagger} + \underset{4^\dagger}{Q_1 w^\dagger P_{2,j} P_j u} + \underset{5^\dagger}{Q_2 P_{1,j} \sigma_{x,j} P_j u} + \underset{6^\dagger}{Q_2 w^\dagger P_{0,j} \sigma_{x,j} P_j u^\dagger} + \underset{7^\dagger}{Q_2 w^\dagger P_{2,j} P_j u^\dagger} + \underset{8^\dagger}{Q_3 P_{0,j} P_j u^\dagger} + \underset{9^\dagger}{Q_3 w^\dagger P_{2,j} P_j u^\dagger} \Bigg]. \tag{22}$$

The operators $I = T^\dagger T = \sum_{i=1}^{9} i^\dagger i$ and $F = TT^\dagger = \sum_{i=1}^{9} i i^\dagger$ where i is the term number are given by

$$I = \sum_{j=-\infty}^{\infty} [(Q_0 + Q_1 + Q_3)(P_{0,j} + P_{2,j})] + Q_2 \tag{23}$$

$$F = \sum_{j=-\infty}^{\infty} [(Q_0(P_{0,j} + P_{2,j}) + Q_1(P_{2,j} + v_j P_{0,j} v_j^\dagger))P_{j+1} + Q_2(P_{0,j} + P_{2,j})P_{j-1}] + Q_3. \tag{24}$$

Since I and F are projection operators T and $T^\dagger$ are partial isometries with I and F projection operators on the domain and range space of T. The role of I and F is reversed for $T^\dagger$ in that F and I are the respective domain and range space projection operators for $T^\dagger$. The i sums over terms show that only the diagonal terms contribute, that is $i^\dagger j = i j^\dagger = 0$ if and only if $i \neq j$.

The action of T can be shown by consideration of an initial lattice qubit state $|\underline{s}\rangle$ with qubits at sites 0 and $n+1$ in the state $|2\rangle$ and in the state $|0\rangle$ at all other sites. Start with an initial state of the form $|0, -m, \underline{s}\rangle$ with the head in state $|0\rangle$ and at position $-m$. Iteration of T moves the head up to position 0 by the actions of term 1. The state of the head and qubit lattice at this point is shown in Figure 2. Term 2 acts once to give the state $|1, 1, \underline{s}\rangle$. Term 3 takes over to give the state $|1, n+1\rangle \Pi_{j=0}^{n} v_j \underline{s}\rangle$ after n iterations of T. At this point the lattice qubit state is a linear superposition of 2^n states in the computation basis with the coefficients depending on v. If $v = (\sigma_z + \sigma_x)/\sqrt{2}$ then the above iteration of T carries out the Hadamard transformation on the n qubits.

Note that so far, and in the following, at most one term of T is active at any iteration. This is shown by Eqs. 23 and 24 where only the diagonal terms contribute. In fact T was constructed so that it has this property as it greatly lessens the complication of path determination during iteration of T and $T^\dagger$.

The next iteration (term 4) gives the head state $|2, n\rangle$ with no change in the lattice qubit state. Terms 5 and 6, which implement the "add 1" operation, now become active.

At this point which term is active and the sequence of actions is different for the different components in the superposition of the n qubit states. Iteration of term 5 moves the head back along a string of $1s$ changing the qubit state $|1\rangle$ to $|0\rangle$ until a qubit in state $|0\rangle$ is encountered. Term 6 then changes the qubit to state $|1\rangle$, which completes the "add 1" operation in that component state. On all component states in which the site n qubit is in state $|0\rangle$, term 5 never acts and term 6 acts just once. Note that the site n qubit corresponds to the least significant (units) position with significance increasing as n decreases to 0, the most significant position.

At this point the computation is completed. Terms 7,8, and 9 which move the head to the right without stopping and no further qubit state changes, now become active. The final state, when "add 1" is just completed in all components, has the following form:

$$\Psi_{3n+4} = \sum_{j=0}^{n}[(1-\delta_{j,n})\langle 0|v|0\rangle + \delta_{j,n}](\langle 1|v|0\rangle)^j \\ \times |0, 3n+2-2j\rangle v|0_1\rangle v|0_2\rangle \cdots v|0_{n-1-j}\rangle|1_{n-j}\rangle|0_{n-j+1}\cdots|0_n\rangle|\underline{s}_{\neq[1,n]}\rangle. \qquad (25)$$

In this state $\langle i|v|i'\rangle$ is the v matrix element between the qubit states $|i\rangle$, $|i'\rangle$ where $i, i' = 0, 1$, and $|0, 3n+2-2j\rangle$ denotes the head in state $|0\rangle$ at lattice position $3n+2-2j$. $|\underline{s}_{\neq[1,n]}\rangle$ is the state of all qubits not at sites $1, 2, \cdots, n$. The states of these qubits are unchanged by the action of T or $T^\dagger$.

The state Ψ_{3n+4} is the state obtained by $3n+4$ iterations of T on the initial state $|0, 0, \underline{s}\rangle$ with $\underline{s}$ given by Figure 2. That is $\Psi_{3n+4} = T^{3n+4}|0, 0, \underline{s}\rangle$. All 2^n components in the computation basis are included even though there are only $n+1$ terms in the j-sum. The reason is that each term in the j-sum corresponds to "add 1" to all 2^{n-1-j} components with j consecutive $1s$ at sites $n, n-1, \cdots, n-j+1$ and a 0 at site $n-j$. (For $j = n$ $2^{n-1-j} = 1$.)

It is of interest to schematically expand the states along the computation path as superpositions of states in B_C. To this end let the state Ψ_m denote the path state obtained by m iterations of T or $T^\dagger$ on the state $|0, 0, \underline{s}\rangle$. That is

$$\Psi_m = \begin{cases} T^m|0, 0, \underline{s}\rangle & \text{if } m \geq 0 \\ (T^\dagger)^{-m}|0, 0, \underline{s}\rangle & \text{if } m < 0 \end{cases} \qquad (26)$$

The expansion of Ψ_m as a superposition of states in B_C for increasing m shows an initial line branching into an n stage binary tree (generated by n iterations of term 3 in Eq. 21) with each of the 2^n lines continuing. This is shown in Figure 3 which shows the tree development by successive iterations of T starting from the initial state shown in Figure 2.

The above construction can be extended to initial lattice qubit states with more than two qubits in state $|2\rangle$. For example let $|\underline{s}\rangle$ be such that qubits at sites $0, n_1, n_2, n_3$ with $0 < n_1 < n_2 < n_3$ are in states $|2\rangle$ and are in state $|0\rangle$ everywhere else. Let the number of $|0\rangle$ state sites between the $|2\rangle$ sites be given by $n = n_1 - 1, p = n_2 - 1 - n_1, m = n_3 - 1 - n_2$.

In this case the structure of T is such that "add 1" is carried out on the n and m qubits in the first and third regions. Iteration of T for states where the head is in the second region of p qubits just moves the head along with no changes in the head or lattice qubit state until the head arrives at site n_2. Note that in Eq. 25 the head position is different in each of the n components in the j sum. As a result the iteration number or arrival time for the head at n_2 is different for each of the n components.

The final states with the head to the right of n_3 describe the completed "add 1" in both regions. The structure of the final state corresponding to Eq. 25 is complex as it contains a double sum $\sum_{j,k}$ with $j = 0, 1, \cdots, n$ and $k = 0, 1, \cdots, m$. Also the head position is different for each term in the sum as it depends on both j and k. Each component in the double sum is a product of lattice qubit states of the form given in Eq. 25 for $j = j$ and for $j = k$. For $j = k$ the lattice qubit state describes the qubits in the region between sites n_2 and n_3. Adjustments in qubit state indices that label the qubit location and for the possibility that $m \neq n$ must be made. Details are left to the reader.

Expansion of the final states as superpositions of states in B_C gives a double binary tree structure with a binary tree of m stages attached to each terminal branch of an n stage tree. The length of the line (corresponding to the number of T iterations) between the last branching in the first tree and the beginning of branching in the second tree depends on the lattice distance $n_2 - n_1$ and to which component in the j sum of Eq. 25 a particular branch corresponds. The structure can be visualized by attaching an m stage binary tree like that shown in Figure 3 to each of the 2^n output paths of the tree shown in the figure. The second tree would begin about $n_2 - n_1$ path states from the solid triangles shown in the output paths.

For initial lattice qubit states with an even number $2h$ of qubits in state $|2\rangle$ with regions of $0s$ in between the above attachment of binary trees to the end branches of a preceeding tree is iterated h times. The lengths of the lines betweeen the last branching of the kth tree and the beginning of the $k + 1st$ tree for $k = 1, 2, \cdots h - 1$ follow a pattern similar to that described above for the two trees $h = 1$.

The terminal tree structure is different for initial qubit states that contain an odd number of qubits in state $|2\rangle$. to see this it is sufficient to consider the case with the site 0 qubit the only one in state $|2\rangle$ and all other qubits in state $|0\rangle$. In this case only the first three terms of T are active. Iteration of T moves the head in state $|1\rangle$ to the right without stopping. As it moves it converts each qubit from state $|0\rangle$ to $v|0\rangle$.

Expansion of the path states in terms of the basis B_C shows a nonterminating binary tree. The branching begins when term 3 of Eq. 21 becomes and remains permanently active. For initial states with an odd number $2h + 1$ of qubits in state $|2\rangle$ separated by regions of $0s$. There are h iterations of finite stage binary trees attached as described above for the even number of $2s$ in the initial state. In addition a nonterminating binary tree is attached to each terminal branch of the last (hth) tree in the iteration.

It remains to discuss the proof that T and $T^\dagger$ are distinct path generating. This is done by considering the path states Ψ_m defined above in Eq. 26. One has to show that for each $m \geq 0$ iteration of $T^\dagger$ on Ψ_m does not generate new states. That is for each $n < 0$ $(T^\dagger)^{-n}\Psi_m = \Psi_{m+n}$. Also for each $m < 0$ and each $n > 0$ $T^n\Psi_m = \Psi_{m+n}$. The critical step in the proof is to note that $T^\dagger$, acting on the state $\langle 0|v|0\rangle|3, j+1\rangle|1_j\rangle + \langle 1|v|0\rangle|2, j-1\rangle|0_j\rangle$, gives (terms $5^\dagger$, $6^\dagger$ active) the state $|2, j\rangle v|0_j\rangle$. Irrelevant parts of the state have been excluded for clarity. Additional details are left to the reader.

It is clear that this proof applies to initial states containing arbitrary distributions of $0s$ and $2s$ in the qubit state lattice and to arbitrary positions of the head in any one of the four internal states. For all of these states T is a direct sum of countable many copies of the bilateral shift and the restriction of T to these subspaces is unitary.

The proof is easily extended to cover initial states with one or more qubits in state $|1\rangle$.

Thus it is clear that T is distinct path generating in that it is a direct sum of copies of finite shifts, unilateral shifts, complements of unilateral shifts, and bilateral shifts.

C. QTMS with Interferometer Graph Structures

The above example shows that the restriction of T to be distinct path generating is sufficiently powerful to include quantum computations that generate branchings in B_C where the specific computation steps in each branch are different. The graph structure for a large number in intial lattice qubit states was seen to be that of iterated binary trees with or without a nonterminating terminal tree.

Here two examples of QTMs are given for which some paths in B_T correspond to graphs in B_C that have the structure of interferometers. It is of interest to note that use of coordinate space interferometers to factor integers has been described [28].

For the first example let T be given as an l, s sum, Eq. 5, by

$$T = \sum_{j=-\infty}^{\infty} [Q_0 P_{0,j} + w Q_0 P_{1,j} + (Q_1 + Q_2) P_{0,j} + Q_0 w^\dagger P_{1,j}] u P_j \tag{27}$$

Here w is a unitary operator that takes the head state $|0\rangle$ into the linear superposition $(1/\sqrt{2})(|1\rangle + |2\rangle)$ of head states $|1\rangle$ and $|2\rangle$. It is this linear superposition that creates the two branches of the interferometer. The interferometer is opened when the second term of T is active and closed when the last (righthand) term is active.

It is straightforward to prove that T is a power partial isometry with all types of noncyclic paths present in the decomposition into shifts. Note that any state of the form $|\phi, j, \underline{s}\rangle$ where ϕ is the head state $(1/\sqrt{2})(|1\rangle - |2\rangle$ and the site j qubit is in state $|1\rangle$ is a terminal B_T path state for T.

Iteration of T on any state of the form $|0, j, \underline{s}\rangle$ where $j < 1$ and $|\underline{s}\rangle$ has the form shown at the top of Figure 4, moves the head to the right until the state $|1\rangle$ qubit is encountered at site 1. The next iteration opens the interferometer with the two branches labelled by different head states. Continued iteration of T describes head motion along the lattice with the head in state $(1/\sqrt{2})(|1\rangle + |2\rangle)$. This state, which is a coherent sum of 2 B_C states, describes the two arms of the interferometer. The interferometer is closed when the second qubit in state $|1\rangle$ at site n is encountered. The bottom of Figure 4 shows the interferometer where paths of connected dots refer to paths of states in B_C. The branches labelled with 2 and 1 correspond to the two head states $|2\rangle$ and $|1\rangle$. Note that the positions of opening and closing of the interferometer correspond to the lattice positions of the qubit in state $|1\rangle$. This occurs because all terms of T show the head moving in the same direction.

This example is a very simple QTM in which the action in both branches of the interferometer is identical and no changes in the qubit lattice occur. The two arms are distinguished by different head states only. It is of interest to see if there exist QTMs for which different activities occur in the two arms and for which the step operators are distinct path generating. The answer is that such QTMs exist provided activities in each arm are such that all differences in the computation states in the two arms generated by iteration of T are removed at the step prior to coherent combination or closure of the arms. Also this must hold for all initial states.

An example of such a QTM is given by the following operator with 9 terms:

$$T = \sum_{j=-\infty}^{\infty} \Big[\underset{1}{Q_0 P_{0,j} u} + \underset{2}{w'_{12} Q_0 P_{1,j} u} + \underset{3}{w^2 Q_1 v P_{0,j} u^\dagger} + \underset{4}{w^2 Q_2 P_{0,j} u^\dagger} + \underset{5}{w^2 Q_3 P_{1,j} u} + \underset{6}{w^2 Q_4 P_{1,j} u} + \underset{7}{w^2 Q_5 P_{0,j} v^\dagger u} + \underset{8}{w^2 Q_6 P_{0,j} u} + \underset{9}{Q_0 (w'_{78})^\dagger P_{1,j} u} \Big] P_j \tag{28}$$

As before the term numbers are placed below the terms. Terms 3, 5, and 7 are active in one arm and terms 4, 6, and 8 are active in the other arm of the interferometer. Terms 2 and 9 open and close the interferometer.

There are 9 different head states with w the unitary shift shift operator on the head states defined by $wQ_h = Q_{h+1}w$ mod 9. The two unitary operators w'_{12}, w'_{78} satisfy $w'_{12}|0\rangle = 1/\sqrt{2}(|1\rangle + |2\rangle)$ and $w'_{78}|0\rangle = 1/\sqrt{7}(|1\rangle + |8\rangle)$. The two dimensional unitary operator v is arbitrary, and the head shift operator u is as defined in other examples.

The interferometer is opened by the action of term 2 where the head in state $|0\rangle$ is converted to state $1/\sqrt{2}(|1\rangle + |2\rangle)$. Terms 3,5,and 7 are active in succession in the arm with head state $|1\rangle$, and terms 4,6, and 8 are active in succession in the arm with head state $|2\rangle$. The interferometer is closed by the action of term 9. Each arm of the interferometer is a path containing just 4 states. This is a consequence of the fact that, except for the first term, each term of T in an iteration is active just once. This follows from the presence and properties of the head state change operators present in each term except the first.

The activities in the two arms are different because of the presence of v and $v^\dagger$ in terms 3 and 7 but not in 4 and 6. Thus the middle two states in the arms differ by both the head states and the qubit states on which terms 3 and 5, and 4 and 6 act. These differences are shown in Figure 5 which shows explicitly the computation basis states in the interferometer arms for an initial state given by $|0,0\rangle|1_1,0_2,1_3\rangle|\underline{0}_{else}\rangle$. This state has the head in state $|0\rangle$ at lattice site 0 and the qubit lattice state with $0s$ everywhere except at sites 1 and 3. The states of the qubits at sites $1,2,3$ are shown explicitly.

The production of interferometers described above can be iterated by suitable choice of initial lattice qubit states. For example a string of n interferometers is generated for the initial state $|0,0,\underline{s}\rangle$ where $|\underline{s}\rangle$ contains n repetitions of the pattern $|1_j,0_{j+1},1_{j+2}\rangle$ for $j > 0$ with each repetition separated by one or more $0s$.

It is straight forward to prove that T is distinct path generating with all types of shifts present. One way to do this is to show that iteration of $T^\dagger$ on $T^n\psi$ for various n and different initial states does not generate new states (i.e. $(T^\dagger)^m T^n \psi = T^{n-m}\psi$ for $m \leq n$. Because of the structure of the terms of T it is sufficient to show this for values of $n = 0, 1, \cdots 7$ for suitably chosen states. The same demonstration is also needed for iterations in which the roles of T and $T^\dagger$ are interchanged.

As noted for this example the head motion is exactly the same for both arms of the interferometer. That is terms 3 and 4 move the head one site to the right. Terms 5,6,7, and 8 all move the head one site to the left. It is of interest to see what happens if this synchrony of head motion in the arms is broken. An example would be to change the definition of T by exchanging u and $u^\dagger$ in terms 4 and 6. In this case it is easy to show that the altered T is not distinct path generating. The reason is that under the alteration term 6 scans a different qubit in state $|1\rangle$ than does term 4. It is then easy to see that iteration of T on initial states of the form $|0,0\rangle|1_j\rangle|\underline{0}_{\neq j}\rangle$ for $j > 0$ generates terminal states in both arms of

the interferometer. However the path in the arm in which the altered term 6 is active is shorter than the path in the arm in which term 5 is active. Iteration of $T^\dagger$ on any state representing just one arm of the interferometer will not regenerate the initial state.

This example illustrates the fact that there are step operators T that are distinct path generating on some subspace of $\mathcal{H}$ even if they are not distinct path generating on the whole space. The above example showed states on which T is not distinct path generating. However this altered T is distinct path generating on lattice qubit states of the form $|1_j, 0_{j+1}, 1_{j+2}\rangle$ and 0 everywhere else with the head in state $|0, h\rangle$ with $h < j$. Besides these states there are many other types of initial states on which T is distinct path generating.

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FIGURE CAPTIONS

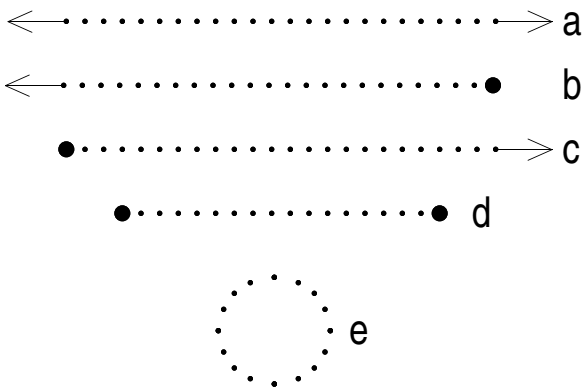
Figure 1. Different types of Possible Paths in a Basis B_T for which T is Distinct Path Generating. The small dots denote path states and the large dots path states that are terminal. Infinite paths are labelled by a, b, and c and finite paths by d and e. The corresponding shift types are a, bilateral (unitary); b, unilateral (isometry); c, adjoint of unilateral shift (coisometry); d, finite shift (noncyclic); and e, cyclic shift (unitary).

Figure 2. An Initial State for the "Add 1" Quantum Turing Machine. The vertical arrow with a 0 at site 0 denotes the head in state $|0\rangle$ at site 0. The two qubits in state $|2\rangle$ at sites 0 and $n+1$ are shown, with all other qubits in state $|0\rangle$.

Figure 3. The n Stage Binary Tree of Paths of States in B_C for the "Add 1" Quantum Turing Machine. Each dot denotes a state in B_C. The vertical arrow at the tree root denotes the computation basis state shown in Figure 2. The numbers at each vertex give the state of the qubit at the head location at each stage. The solid arrowheads denote the path state at which the "add 1" operation is complete and term 1 of T, Eq. 21 becomes active. The location of the arrowhead in each path depends on the number $1s$ before a 0 is reached. No arrowhead is shown for the uppermost path (all $1s$) as it occurs off the right edge of the figure at the path state $3n+4$ steps from the tree root state.

Figure 4. Initial Qubit Lattice State and Paths in B_C for the Interferometer Quantum Turing Machine. The initial latttice stae in the upper part of the figure shows qubits in state $|1\rangle$ at sites 1 and n and in state $|0\rangle$ elsewhwere. The lower part of the figure shows the interferometric structure of the B_C paths. The numbers $1, 2$ denote the two different head states that distinguish the two arms of the interferometer. The interferometer opens when the head is at site 1 and closes when the head is at site n. The number of states in the interferometer arms equals 1 plus the number of state $|0\rangle$ qubits between the $1s$ because all terms in T move the head in the same direction (from left to right).

Figure 5. Path States in B_C for the Quantum Turing Machine Interferometer with T given by Eq. 28. The states are shown explicitly. Normalization coefficients $(1/\sqrt{2})$ are excluded. For the middle two states the state of the site 2 qubit is different in the two arms.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b
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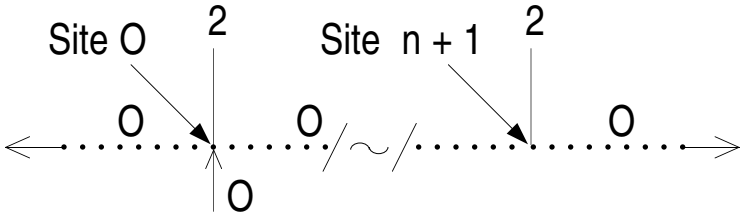
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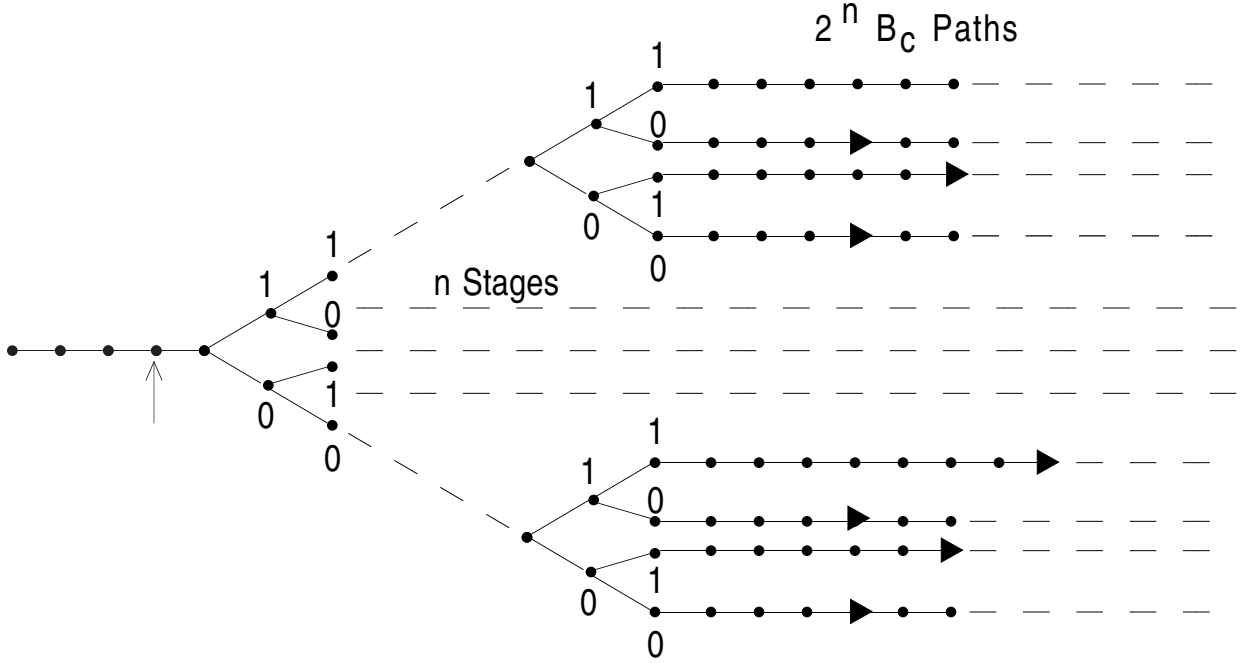
2
Site n + 1
2
O
O
O
O


2^n B_c Paths
n Stages
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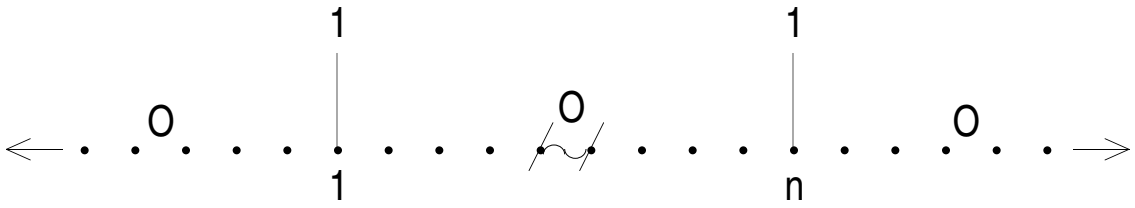
0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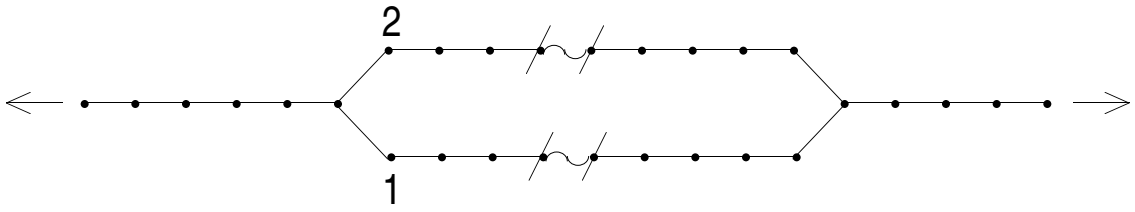
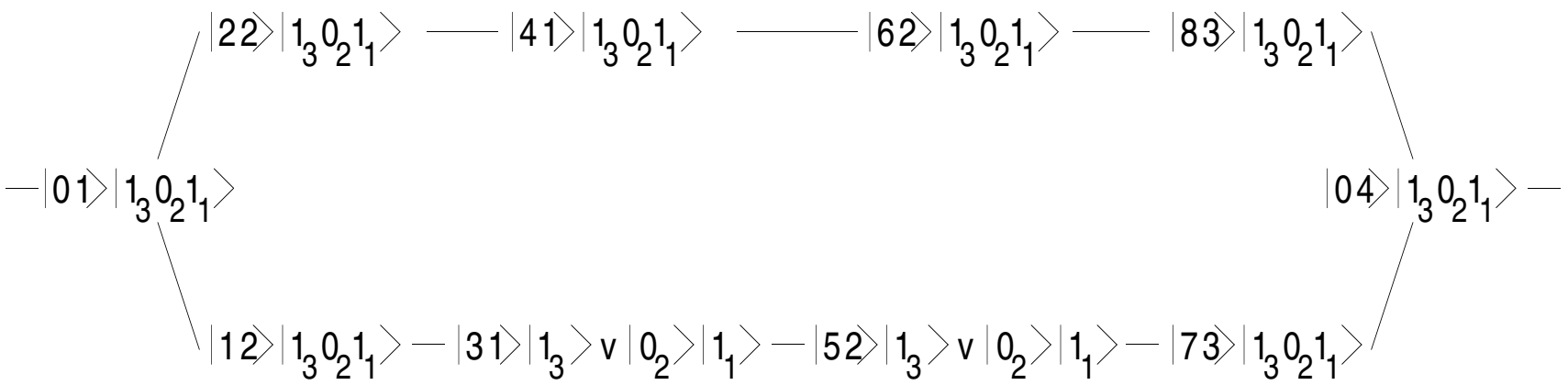
0
1
n


2
1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