Quantum Ballistic Evolution in Quantum Mechanics: Application to Quantum Computers

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Abstract

Quantum computers are important examples of processes whose evolution can be described in terms of iterations of single step operators or their adjoints. Based on this, Hamiltonian evolution of processes with associated step operators $T$ is investigated here. The main limitation of this paper is to processes which evolve quantum ballistically, i.e. motion restricted to a collection of nonintersecting or distinct paths on an arbitrary basis. The main goal of this paper is proof of a theorem which gives necessary and sufficient conditions that $T$ must satisfy so that there exists a Hamiltonian description of quantum ballistic evolution for the process, namely, that $T$ is a partial isometry and is orthogonality preserving and stable on some basis. Simple examples of quantum ballistic evolution for quantum Turing machines with one and with more than one type of elementary step are discussed. It is seen that for nondeterministic machines the basis set can be quite complex with much entanglement present. It is also proved that, given a step operator $T$ for an arbitrary deterministic quantum Turing machine, it is decidable if $T$ is stable and orthogonality preserving, and if quantum ballistic evolution is possible. The proof fails if $T$ is a step operator for a nondeterministic machine. It is an open question if such a decision procedure exists for nondeterministic machines. This problem does not occur in classical mechanics. Also the definition of quantum Turing machines used here is compared with that used by other authors.

I. INTRODUCTION

There are many processes in physics which can be described in terms of a sequence of steps. The computation process furnishes many examples. Each computer program is a collection of elementary steps which the physical system (computer) undergoes. Computation using a program on a given input consists of iteration of the program steps where the particular elementary steps carried out at the n+1st iteration depend on the system state and the available elementary steps. Each elementary step is local in the sense that changes in a space region depend on conditions in the region and not on far distant conditions.
Each computation by a given program on a specified input yields a sequence or path of distinct computation states. A computation state is a complete global specification of the states of all relevant degrees of freedom of the system carrying out the computation. For a Turing machine a computation state specifies the string of bits or numbers on the computation tape and the internal state and position of the scanning head. For networks of gates a computation state is a complete specification of the states of the systems moving in the wires and the states of the gates in the network.

The collection of all paths generated by the given program acting on all possible inputs is a collection of finite and infinite paths of computation states. The collection of paths depends on the computer program being considered as it is different for different programs. In many computational models, paths representing halting or nonhalting computations are finite or infinite respectively. In other models all paths are infinite with halting computations specified by a system flag.

As is well known computations can be reversible or irreversible. Irreversible computations are those for which each computation state has at most one successor but may have more than one predecessor. Computation states in reversible computations have at most one successor and one predecessor.

Since the interest here is in Hamiltonian models of process such as computation, consideration is limited to reversible computations only. As Bennett has shown, this is not a limitation in that for each Turing machine computation (reversible or irreversible) there is an equivalent reversible computation which is slower and has more relevant degrees of freedom (history and copying degrees) than the original computation.

This work, which showed that computation could be performed by reversible or information preserving steps only, along with that of Landauer formed the basis for early work on quantum mechanical Hamiltonian models of computers as Turing machines. This work, along with that of Feynman and Deutsch, formed the basis for the recent blossoming of the field. Recent work includes that of Lloyd on the halting problem for quantum computers, and Lloyd and DiVincenzo and others on the universality of 2-bit quantum gates for quantum circuit computation. The work of Shor, showing that the integer factoring problem could be solved in polynomial time on a quantum computer, has provided much of the impetus for the recent work.

Work has also been proceeding on developing physical models of quantum computers. As is well known proper functioning of a quantum computer requires that phase relations be maintained between the component states of all the degrees of freedom in the model. Landauer has repeatedly emphasized the problem of physical realization of quantum computation in that environmental noise and decoherence cause degradation of performance. Additional work on the effects of decoherence on quantum computation has been done by Unruh and others. Recent work on quantum error correcting codes gives hope that the effects of noise and decoherence can be minimized. It is also clear that it is advantageous to minimize the number of degrees of freedom needed to carry out a quantum computation since fewer degrees involved means less effort is needed to minimize environmental influences.

The work of this paper is based on a translation of step processes such as reversible computation into quantum mechanics. To each process is associated a bounded linear operator $T$, called a "step operator" for the process such that iteration of powers of $T$ (or its adjoint
model successive steps forward (or backward) of the process. Note that no association of a finite time interval with a step is assumed. As a result step operators can be used directly in the construction of Hamiltonians. Additional discussion is provided in the next section.

The states of the model process system can be represented as states in some basis. For the purposes of this paper it is not necessary that \( T \) be equal to a sum of elementary step operators. However, if the process consists of a set of elementary steps, such as a model of a computer program, then it is useful to write \( T \) as a sum of corresponding elementary step operators.

The procedure used here differs from that used by Deutsch [6] and Bernstein and Vazirani [19] in their description of quantum computation. They assumed that the step operator is unitary, spatially local, and associated with a finite time interval. In this case a Hamiltonian can be defined by \( T = e^{-iHt} \).

Because of problems with this approach, such as the nonexistence of a Hamiltonian which is simple and local, this approach is not used here. Instead a step operator \( T \) for a process such as quantum computation is associated with an infinitesimal time interval. As a result, it can be used to construct a Hamiltonian \( H(T) \) which describes the unitary time evolution of the process. The Hamiltonian is time independent, selfadjoint, and has the complexity of \( T \) and not of all steps of the process. The step operator \( T \) associated with a process need not be unitary, selfadjoint, or even normal. More details on a comparison between this approach and that of Deutsch and Bernstein and Vazirani [6,19] will be discussed later on.

In earlier work [20,21] unitary step operators for quantum Turing machines were constructed. However the work was limited to deterministic computations only. In addition the unitarity was artificial in that it held only for the subspace of states defined by all iterations of the step operator and its adjoint. In general (e.g. for universal machines) this subspace cannot be defined effectively. Also on the larger space of all states (which can be effectively defined) the step operator was not unitary and its properties on the larger space were not considered.

In this paper much attention is given to conditions that a step operator \( T \) must satisfy such that iteration of \( T \) or its adjoint on the states in some basis generates a collection of paths in the basis. A path is a finite or infinite sequence of distinct states in a basis. A basis is a set of pairwise orthogonal, normalized states which span a Hilbert space. The idea is that if the model process system is in any state in a path, then successive states in the path represent successive steps of the process.

An additional requirement is that the model process step operator be distinct path generating in some basis. This follows the restriction made for reversible classical computations [2]. This means that if the process is started on different input states, the paths generated by successive steps of the process must be distinct and have no overlap. Otherwise computations started on distinct inputs would overlap and one would not know which input was associated with the output.

In general an arbitrary operator as a candidate model step operator may not have any of these desired properties. Iteration of the operator may not generate a path in any basis in that orthogonality of states is not preserved under iteration. Or the operator may generate paths which branch and join into a network of interconnected paths in all bases. Note that in order to ensure that no paths join or branch it is necessary that the states in all the paths be in the same basis. For example if each of two different paths were in different bases,
Then the overlap of states in the different bases would destroy the distinctness of the paths. If there were no overlap between the states in the two paths, then another basis, which includes the states in both of the paths, would be a suitable basis for the requirement of distinct path generation.

The main goal of this paper is to give necessary and sufficient conditions that an arbitrary model process step operator must have in order that there exist a quantum mechanical Hamiltonian which describes quantum ballistic evolution of the process. Quantum ballistic evolution refers to the "motion" of the model process system along paths of states and is limited to step operators which are distinct path generating. The paths are defined by iteration of the process step operator or its adjoint on states in the basis. Under this type of evolution any wave packet of states on a path moves along the path, spreading out as it moves.

It is important to note that full advantage is taken here of the fact that in quantum mechanics there exist many inequivalent basis sets. In classical mechanics there is only one\(^1\). In particular nondeterministic computations, which allow arbitrary bit transformations (such as \(|i\rangle \to \alpha|0\rangle + \beta|1\rangle\) for \(i = 0, 1\)), and deterministic computations, which limit bit transformations to \(0 \to 1, 1 \to 0\) only, are included. This is done by allowing basis sets, with respect to which the paths are defined and quantum ballistic evolution occurs, to be arbitrarily complex with entanglements between the component model systems.

Another goal of this paper is to determine if there exists an effective decision procedure to decide if a model step operator for an arbitrary process is distinct path generating and thus if a Hamiltonian description of quantum ballistic evolution exists. It will be seen that in general such a decision procedure does not exist. However, for models of computation, this problem exists only for nondeterministic computations. An effective decision procedure is shown to exist for deterministic models.

In the next section there is more discussion on paths, distinct path generation by process step operators, and quantum ballistic evolution for partial isometries. Feynman’s prescription of construction of a Hamiltonian from process step operators is introduced.

In Section \(\text{II}\) definitions of stability and orthogonality preserving for operators are introduced. Some theorems are stated and proved including the result that stability plus orthogonality preservation are equivalent to distinct path generation. Section \(\text{V}\) introduces power partial isometries and gives some of their main properties of interest here. The equivalence between complete orthogonality preservation and power partial isometry is proved.

Section \(\text{V}\) contains the main result. It is proved that necessary and sufficient conditions for the existence of a Hamiltonian description of quantum ballistic evolution on some basis for a process step operator \(T\) is that \(T\) is a partial isometry which is orthogonality preserving and stable. Canonical eigenfunctions and eigenvalues are given for the Feynman Hamiltonian (Eq. \(\text{II}\)).

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\(^1\)This distinction between classical and quantum mechanics follows from the fact that bases are in 1-1 correspondence with maximally fine resolutions of the identity (i.e. those in which all the projection operators are one dimensional). In quantum mechanics there are many maximally fine resolutions which do not commute. In classical mechanics there is only one. Here inequivalent bases are defined to be those for which the corresponding resolutions of the identity do not commute.
Sections [VI] and [VII] give illustrative examples and a definition of the step operators for Turing machine models of quantum computation. The existence of nondeterministic quantum Turing machines which evolve quantum ballistically is shown by explicit example construction. Following is a discussion of effective determination of the existence of a Hamiltonian description of quantum ballistic evolution for a process with associated step operator \( T \). Some other aspects, including a discussion of the approach used here and that of Deutsch and Bernstein and Vazirani [6,19], are included in Section [IX].

II. QUANTUM BALLISTIC EVOLUTION

As noted the interest here is in step operators \( T \) which are distinct path generating. That is

**Definition 1** A step operator \( T \) and its adjoint are distinct path generating on a basis \( B \) if iterations of \( T \) and \( T^\dagger \), started at any state in \( B \), generate paths in \( B \) that are distinct in that they do not intersect or join one another.

In more precise terms this definition means that \( T \) and its adjoint are distinct path generating if for all states \( |p_j\rangle \) in a basis \( B \), if \( T|p_j\rangle \neq 0 \), then there exists a unique state \( |p_k\rangle \) in \( B \) such that \( T|p_j\rangle = |p_k\rangle \) and \( T^\dagger |p_k\rangle = |p_j\rangle \). A similar statement holds with \( T^\dagger \) replacing \( T \). Note that distinct path generation is defined here for norm preserving motion only. In future work this restriction will be removed from the definition by allowing \( T|p_j\rangle = \alpha_{jk}|p_k\rangle \) where \( \alpha_{jk} \) can be different from 1.

The purpose of this definition is to get rid of paths which join, branch or intersect. Note that paths of 0 length are included. (i.e. for some \( |p_j\rangle, T|p_j\rangle = T^\dagger |p_j\rangle = 0 \). Also it is clear that any \( T \) satisfying the definition is a partial isometry. An operator is a partial isometry if both \( T^\dagger T \) and \( TT^\dagger \) are projection operators.

Step operators \( T \) which are distinct path generating on some basis can be used to model the evolution of some system whose elementary steps are modelled by \( T \) and \( T^\dagger \). The adjoint is used instead of the inverse as \( T \) may not have an inverse. A state of the system on a path consists of a wave packet of states on a path. In general such a wave packet has the form

\[
\Psi(t) = \sum_{n=0}^{M} c_n(t)T^n|0\rangle + \sum_{n=1}^{L} c_{-n}(t)(T^\dagger)^n|0\rangle.
\]  

The time development is shown in Eq. [1] by the explicit time dependence of the coefficients \( c_n(t) \).

Quantum ballistic evolution refers to the time evolution of such packets along distinct paths in some basis. As these packets move under the action of some Hamiltonian they spread out along the paths. If a path is two way infinite, \( M = L = \infty \), motion continues with no momentum change. If a path is infinite in one direction only reflection occurs at the path end. If the path is finite with distinct ends, reflection occurs at both ends. For cyclic paths the packet moves around the cycle with interference occurring as the packet spreads over a distance greater than one cycle. Additional details on the packet spreading are given in [20,21].
A very simple example of quantum ballistic evolution would be free system motion in a collection of quantum wires, which do not intersect, branch or join, on a three dimensional space lattice. This includes straight or curved lines or line segments, closed loops such as circles, chains of closed loops, etc. For this example the basis $B$ is the set $\{ |x, y, z \rangle \}$ of position vectors on the lattice. In this paper the basis set is not fixed in advance, and the character of $B$ on which quantum ballistic evolution occurs, if it is possible, is determined by the properties of the operator $T$.

A schematic representation of wave packets on infinite paths is shown in Figure 1. Here the states in some basis are represented as points in space. Two paths, shown by dotted lines are shown. Path A is nonterminating and path B has a terminus T. Two wave packets, $\psi_1(t)$ and $\psi_2(t)$ are shown. For each the time dependent coefficients are represented schematically by $c(t) = r(t)e^{i\theta(t)}$. The basis state dependence of the coefficients is also indicated.

Quantum ballistic evolution can also be used to describe motion for an initial state which is a linear superposition of wave packets in many different paths. By linearity the packets in each path evolve independently of the others. However, this can lead to great entanglement among the different degrees of freedom in the system being modelled. How much entanglement, if any, depends on the basis set used and the system being modelled. In quantum computation use of linear superpositions in this manner is referred to as computation by quantum parallelism \[6\]. For example, a linear combination of the two packet states shown in Figure 1 would evolve in parallel.

A Hamiltonian description of quantum ballistic evolution can be obtained by use of Feynman’s prescription \[5\]. That is, given an arbitrary step operator $T$ for a process (which may or may not be distinct path generating) define the corresponding $H$ by

$$H = K(2 - T - T^\dagger)$$

This Hamiltonian has the advantage that it is simple. That is, it has a complexity of the order of $T$. In particular, it does not have the complexity of all paths generated by iteration of $T$ or its adjoint. In the case that $T$ models a quantum computation, $H$ has the complexity of the computer program. This is especially desirable in the case that $T$ models a universal Turing machine.

In general for an arbitrary step operator, the Hamiltonian given above does not describe quantum ballistic evolution. If $T$ is a step operator for a collection of paths that intersect or join, then $e^{-iHt}$ will describe the unitary evolution of some process. But it may be a different process from that obtained by iteration of $T$. This is especially the case if iteration of $T$ describes an irreversible process. For example, there are operators $T = T_1 + T_2$ such that the Hamiltonian of Eq. \[2\] describes the evolution of a different process, namely, that with the step operator $X = T_1 + T_2^\dagger$.

If $T$ is distinct path generating, then the Hamiltonian of Eq. \[2\] describes quantum ballistic evolution. To see this, consider the power series expansion of $e^{iKt(T + T^\dagger)}$ where $e^{-iHt} = e^{-2iKt}e^{iKt(T + T^\dagger)}$. Each term in the expansion has the form $\cdots (T^\dagger)^m T^n (T^\dagger)^m T^n$ where the $m_i$ are nonnegative integers. Because $T$ is distinct path generating, the term will describe motion back and forth along each path. For finite paths of length $n$, terms for which $m_i \leq n$ for some $i$, will give 0 operating on any state in the path. If $\psi$ is a state not on any path of $T$ then $e^{-iHt}\psi = e^{-2Kt}\psi$ which shows no change occurs.

This is clearly a description of quantum ballistic evolution as motion is restricted to be
in either direction along the distinct paths. No motion occurs on states outside the paths. Conversely if \( H \) is an arbitrary Hamiltonian describing quantum ballistic evolution on some basis \( B \) then a step operator \( T \) which is distinct path generating can be associated with \( H \). Details of the construction will be given later on.

As noted earlier a step operator associated with a process is defined to be that operator \( T \) such that iteration of \( T \) (or \( T^\dagger \)) defines forward (or backward) motion of the process on each of the paths. Note that there is an arbitrariness which is decided by convention: namely, that \( T \) and not \( T^\dagger \) is associated with the forward direction for the process on each path. Also \( T \) is defined to be a step operator if there exists some basis \( B \) (the step basis) such that for each state \( \psi \) in \( B \), \( T\psi \) and \( T^\dagger \psi \) are orthogonal to \( \psi \).

For processes such as computations, the step operator \( T \) is a sum of time ordered products of noncommuting operators for which the time interval is 0 but the noncommutativity and thus the time ordering remains. Computer programs have this property in that they are sums of elementary program elements each of which is a product of time ordered spatially local actions. Because there is no finite time interval associated with \( T \) it can be used directly to construct Hamiltonians such as the Feynman Hamiltonian of Eq. 2.

Another desirable feature is that for many models of processes, \( H \) can be separated into kinetic and potential energy parts. This is the case for models of quantum Turing machines which will be modelled as motion of a head on a one dimensional space lattice of qubits. For these models, \( H = KE + PE \) where \( KE = K(2 - U - U^\dagger) \) and \( PE = K(U - T + U^\dagger - T^\dagger) \). \( U \) denotes free motion along the lattice. In this case \( KE \) represents the (symmetrized) lattice equivalent of the second derivative \( Kd^2/dx^2 \) and \( PE \) is the interaction potential between the head and lattice systems. In this form \( H \) is seen to be similar to that used in the tight binding model (with off-diagonal potentials) to describe one dimensional particle motion in solids \[22\]. This similarity will be exploited in future work.

From the above it is clear that it is important to be able to determine if an operator \( T \) is distinct path generating. This appears difficult since it appears necessary to examine the properties of all powers of \( T \) and its adjoint, or instead examine the action of \( T \) and its adjoint on all states in the basis. It is desirable to investigate other properties of operators which can be proved equivalent to distinct path generating and for which effective decision procedures may exist. The next section is concerned with two candidate properties, orthogonality preservation and stability.

**III. ORTHOGONALITY PRESERVATION, STABILITY**

As was noted in the introduction the work of Bennett and Landauer \[2,1\] showed that an irreversible computation could be made reversible by addition of history degrees of freedom. The expanded process was reversible in that distinct states remained distinct with no overlap as the process evolved. From a quantum mechanical viewpoint an important part of this work is the preservation of orthogonality relative to some basis. These considerations suggest the following definition: Let \( \{|p_i\} \) denote a basis set for a finite or separable Hilbert space \( \mathcal{H} \) and \( T \) be a bounded linear operator over \( \mathcal{H} \):

**Definition 2** An operator \( T \) is weakly orthogonality preserving in the basis \( \{|p_i\} \) if for all \( i, j \), \( \langle p_i | p_j \rangle = 0 \implies \langle Tp_i | Tp_j \rangle = 0 \).
Note that the definition applies to all states including those for which either \(|T p_i\rangle = 0\) or \(|T p_j\rangle = 0\). It also says nothing about the value of \(\langle T p_i|T p_i\rangle\) if \(|T p_i\rangle \neq 0\).

There are many operators which preserve orthogonality weakly in some basis. This includes all normal operators which preserve orthogonality weakly in their eigenfunction (or spectral measure) basis. The two dimensional operator given by the matrix

\[
\frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 \\ 1 & 1 \end{pmatrix}
\]

does not weakly preserve orthogonality in the basis \(|1\rangle, |0\rangle\) as it converts \(|1\rangle\) to \(1/\sqrt{2}|0\rangle\) but leaves \(|0\rangle\) unchanged (other than normalization). However, it preserves orthogonality weakly in the basis \(|+\rangle, |−\rangle\) where \(|±\rangle = 1/\sqrt{2}(|1\rangle ± |0\rangle)\). The projection operator \(P_0\) on the state \(|0\rangle\) preserves orthogonality weakly in the basis \(|0\rangle, |1\rangle\). It does not preserve orthogonality weakly in the basis \(|+\rangle, |−\rangle\). This would be applicable for instance to binary bits represented by the states \(|+\rangle, |−\rangle\). These simple examples show the basis dependence of weak orthogonality preservation in quantum mechanics.

These two operators appear equivalent as far as the definition is concerned. Yet one feels intuitively that there is a difference. The relevant difference is seen by considering the adjoints. The adjoint of the first example preserves orthogonality weakly in a different basis, namely. \(|1\rangle, |0\rangle\), whereas the adjoint of the projection operator preserves orthogonality weakly in the same basis.

From these and other examples, such as the Turing Machine examples studied in [24], the relevant distinction is between operators for which both \(T\) and \(T^\dagger\) preserve orthogonality weakly on a common basis and those for which the basis is different for \(T\) than for \(T^\dagger\). This suggests the following definition:

**Definition 3** An operator \(T\) is orthogonality preserving if both \(T\) and its adjoint \(T^\dagger\) are weakly orthogonality preserving on the same basis.

Based on this definition, one has the following Theorem:

**Theorem 1** An operator \(T\) and its adjoint are orthogonality preserving if and only if \(T^\dagger T\) and \(T T^\dagger\) commute.

The proof of this theorem, which is straightforward, is given in Appendix A.

It is an immediate consequence of this theorem that there is a common spectral measure which is a common refinement of those for \(T^\dagger T\) and \(T T^\dagger\). By the spectral theorem [23] spectral measures exist for these two operators as they are both selfadjoint. By the above theorem a common refinement exists for \(T^\dagger T\) and \(T T^\dagger\). If physicists license of usage is allowed, the theorem guarantees the existence of an eigenfunction expansion which is common to both \(T^\dagger T\) and \(T T^\dagger\). The eigenfunctions are the basis set referred to in the theorem.

It also follows from this that if any of the spectral subspaces in the common refinement has dimension \(n\) with \(n > 1\), there exists an uncountable infinity of inequivalent bases for which \(T\) is orthogonality preserving. To see this take any basis in the subspace and change
the basis using any unitary operator in $U(n)$. $T$ will also be orthogonality preserving for the new basis.

For the purposes of this paper the requirement that a model operator $T$ be orthogonality preserving for a common basis is necessary but not sufficient. To see this recall that the interest here is in constructing Hamiltonians whose time evolution gives states representing evolution along trajectories of successive steps of the process. Since 1 step of the process is represented by the model operator $T$, $n$ steps are represented by $T^n$. If the Hamiltonian is to properly represent the process evolution, then it is necessary that all positive powers of $T$ and $T^\dagger$ be orthogonality preserving.

This requirement is still not sufficient because, by the definition of orthogonality preservation, it means that for each $n$, there is a basis set $\{|p_i^n\rangle : i = 0, 1, \cdots\}$ which preserves orthogonality for $T^n$ and $(T^\dagger)^n$. However, the basis set which satisfies the definition may depend on $n$.

To avoid this dependence it is required here that there exist a common basis for which orthogonality is preserved by all powers of $T$ and its adjoint. More precisely:

**Definition 4** An operator $T$ and its adjoint are completely orthogonality preserving if there exists a basis set $\{|p_i\rangle : i = 0, 1, \cdots\}$ such that for all $i, j$, $\langle p_i | p_j \rangle = 0 \implies \langle T^n p_i | T^n p_j \rangle = 0$ and $\langle (T^\dagger)^n p_i | (T^\dagger)^n p_j \rangle = 0$ for $n = 1, 2, \cdots$.

It is clear from the definition that complete orthogonality preservation implies orthogonality preservation, but not the converse. Existence of specific examples which are orthogonality preserving but not completely orthogonality preserving follow from the results in the next sections.

Note that for any operator $T$, the set of discrete eigenfunctions (if any) of $T$ are completely orthogonality preserving on the subspace spanned by the eigenfunctions. This basis is not of interest here as it is stationary with respect to iterations of $T$. It is also easy to see that all normal operators ($T$ is normal if $T^\dagger T = TT^\dagger$) are completely orthogonality preserving. However, the main interest here is in operators $T$ which are not normal.

It is easy to show by means of specific examples that if an operator $T$ is completely orthogonality preserving in a basis $B$, this does not imply that for states $|p_i\rangle$ in $B$, that the states $T^n|p_i\rangle$ remain in $B$. This is the case for most unitary operators which are completely orthogonality preserving in all bases. To avoid this the additional requirement that a step operator be stable in an orthogonality preserving basis will be used.

**Definition 5** $T$ and $T^\dagger$ are stable for some basis if there exists a basis $B$ such that for all $|p_i\rangle$ in $B$, if $T|p_i\rangle \neq 0$, then $T|p_i\rangle = \alpha_{k,i}|p_k\rangle$ for some $|p_k\rangle$ in $B$. $\alpha_{k,i}$ is a constant $\neq 0$. A similar statement holds for $T^\dagger$ for the basis $B$.

In other words $T$ and its adjoint are stable for some basis $B$ if $T$ and $T^\dagger$ map some (or all) states of $B$ into states which, except for normalization, are states in $B$ and annihilate the others. In particular $T$ and its adjoint do not map states of $B$ into linear sums of states in $B$.

The utility of stability is shown by the next two theorems.
Theorem 2  An operator $T$ (and its adjoint) are orthogonality preserving and stable for some basis $B$ if and only if $T$ (and its adjoint) are completely orthogonality preserving and stable in $B$.

The proof depends on the fact that if $T$ and its adjoint are orthogonality preserving and stable on some basis $B$, then one can use an inductive argument to show that all powers of $T$ and $T^\dagger$ are orthogonality preserving on $B$, which is equivalent to complete orthogonality preservation and stability on $B$. The proof in the other direction is immediate.

Theorem 3  A partial isometry $T$ is orthogonality preserving and stable in some basis $B$ if and only if $T$ is distinct path generating in $B$.

The proof of this theorem is given in Appendix A.

It follows from these theorems that if $T$ is required to be stable on some basis, then orthogonality preservation and complete orthogonality preservation on the same basis are equivalent. This raises the question of the need for complete orthogonality preservation, since it appears superfluous. For the purposes of this paper, this question can be explored by asking how far can one go, assuming that an operator is completely orthogonality preserving without using the assumption of stability? The answer is, "a long way". This will become clear in the following sections. It will also be seen that the eigenfunctions and eigenvalues have a canonical form for the Hamiltonian of Eq. 2 where $T$ is a partial isometry, which is stable and orthogonality preserving in some basis.

From now on the operator $T$ will be limited to be a partial isometry. Recall that $T$ is a partial isometry if and only if $T^\dagger$ is. Model operators for many processes can be constructed which are partial isometries. This includes models of quantum computers as (deterministic or nondeterministic) Turing machines (Section VII).

IV. POWER PARTIAL ISOMETRIES

At this point it is necessary to introduce power partial isometries. A partial isometry $T$ is a power partial isometry if all positive powers of $T$ and its adjoint are partial isometries.

Power partial isometries (PPI)s were first described by Halmos and Wallen [23] and further developed by others [28,29,27,31]. Related work on partial isometries and semigroups of partial isometries includes that of [28–30]. Halmos and Wallen have given the main properties of PPIs and proved a structure or decomposition theorem. The relevant mathematical results are summarized here. For details the literature should be consulted. For any partial isometry $T$ the projection operators $I = T^\dagger T$ and $F = TT^\dagger$ define the respective domain and range spaces for $T$ and $T^\dagger$. That is, $T = TI = FT$ and $T^\dagger = T^\dagger F = IT^\dagger$.

Let $W$ and $V$ be two partial isometries. The product $WV$ is a partial isometry if and only if $VV^\dagger$ commutes with $W^\dagger W$. This will be referred to as the ”H-W lemma” in Appendix A.

There are many partial isometries that are not power partial isometries. Halmos and Wallen [23] have given a method of explicit construction of an operator $U$ such that the distribution of values of $n$ for which $U^n$ is or is not a partial isometry is arbitrary. Their construction is as follows: Let $U_1$ denote any contraction operator which is not a partial
isometry, for example $U_1 = a(\sigma_x - i\sigma_y)$ where the $\sigma$s are the Pauli spin operators and $|a| < 1/2$. For any operator $T$ define the operator $D_T = (1 - TT^\dagger)^{1/2}$ (positive square root implied) and the matrix operator $M(A)$ by

$$M(A) = \begin{pmatrix} A & DA \\ 0 & 0 \end{pmatrix}$$

For each $n$ the operator $U_n$ is defined inductively for $n = 2, 3, \cdots$ by $U_n = M(U_{n-1})$. For any $k$ where $1 \leq k < n$, $U_k^n$ is a partial isometry, $U_k^n$ is not, and $U_k^{n+1} = 0$.

Let $s$ be any infinite sequence of 0’s and 1’s. The desired operator is defined by $U = \bigoplus_{n=1}^{\infty} U_n \delta_{1,s(n)}$. Here $\bigoplus$ denotes the direct sum and $\delta$ the Kronecker delta. This result is quite remarkable and has the consequence that one has to be very careful to avoid making unwarranted assumptions about operators modelling processes such as quantum computations.

Let $T$ be a power partial isometry. For each $n = 0, 1, 2, \cdots$ define the operators $I_n$ and $F_n$ by

$$I_n = (T \dagger)^n T^n$$
$$F_n = T^n (T \dagger)^n.$$  \hfill (3)
$$\hfill (4)$$

Since $T$ is a PPI, all the $I_n$ and $F_n$ are projection operators. The $I_n$ and $F_n$ form nonincreasing sequences. That is, for all positive $n$ $I_n \geq I_{n+1}$ and $F_n \geq F_{n+1}$. Also all the $I$’s and all the $F$’s commute among themselves and with each other. That is, for all nonnegative $m, n$ $[I_m, I_n] = [F_m, F_n] = [I_m, F_n] = 0$. One also has that $T I_n = I_{n-1} T$ and $TF_{n-1} = F_n T$.

Define $I_\infty$ and $F_\infty$ to be the respective projections on the subspaces $\bigcap_{n=0}^{\infty} I_n \mathcal{H}$ and $\bigcap_{n=0}^{\infty} F_n \mathcal{H}$. $I_\infty$ and $F_\infty$ commute with each other and all the $I_n$ and $F_n$.

The main property of interest here is the decomposition theorem of Halmos and Wallen [23] which states that every power partial isometry has a unique decomposition into a direct sum of operators with nonoverlapping domain and range spaces (i.e. which reduce $T$) given by

$$T = T_1 + T_2 + T_3 + \sum_n T_{4n}. $$  \hfill (5)

Here $T_1$ is a unitary operator on the range space of $I_\infty F_\infty$, $T_2$ is a pure isometry (i.e. $T \dagger T = 1$ on $\text{ran} I_\infty - I_\infty F_\infty$, $T_3$ is a pure coisometry (i.e. $TT \dagger = 1$) on $\text{ran} F_\infty - I_\infty F_\infty$, and for each $n$, $T_{4n}$ is a truncated shift of index $n$ on the range space of $P_n$.

A truncated shift of index $n$ is an operator defined on the sum of $n$ copies of a Hilbert space which takes any state in the $l$th copy to the same state in the $l+1$st copy and annihilates states in the $n$th copy. That is $T_{4n} < \psi_1, \psi_2, \cdots, \psi_{n-1}, \psi_n > = < 0, \psi_1, \psi_2, \cdots, \psi_{n-1} >$. For the decomposition theorem the $l$th copy (for $l = 1, \cdots, n$) is the range space of the projection operator $P_{n,l} = (F_{l-1} - F_l)(I_{n-1} - I_{n-l+1})$. The projection operator $P_n$ is defined by $P_n = \sum_{l=1}^{n} P_{n,l}$.

A pure isometry is an isometry which is unitarily equivalent to a direct sum of copies of the unilateral shift. It acts like a truncated shift of index $\infty$ except that there is no state annihilation at any index. In the above decomposition the domain of $T_2$ is given by $\sum_{l=1}^{\infty} P_{\infty l} = \sum_{l=1}^{\infty} (F_{l-1} - F_l)I_{\infty}$. It is easy to see that $P_{\infty l} P_{\infty m} = P_{\infty l} \delta_{l,m}$ and $T_2 P_{\infty l} = P_{\infty l+1}$. 
Theorem 4 Let $T$ be a partial isometry. Then $T$ and $T^\dagger$ are completely orthogonality preserving if and only if $T$ is a power partial isometry.

The proof of this theorem is given in Appendix A.

V. QUANTUM BALLISTIC EVOLUTION AND ORTHOGONALITY PRESERVATION

The material presented so far is sufficient to give a proof of a main point of this paper, which is stated in the following theorem. The proof is summarized here with details left to the reader.

Theorem 5 A necessary and sufficient condition that there exists a Hamiltonian description of quantum ballistic evolution of a process is that there exists a process step operator $T$ and a basis $B$ such that $T$ is a partial isometry and is stable and orthogonality preserving in $B$.

Sufficiency: Assume $T$ is a partial isometry and is orthogonality preserving and stable with respect to a basis $B$. By Theorem 3, $T$ and $T^\dagger$ are distinct path generating. The collection of paths can be determined by iteration of $T$ and its adjoint on states of $B$. Use Eq. 2 to define a Hamiltonian $H = K(2 - T - T^\dagger)$.

The time evolution is given by $e^{-iHt}$. A general term in the power series expansion of $e^{iK(t+T^t)}$ where $e^{-iHt} = e^{-2iKt}e^{iK(t+T^t)}$ has the form $\cdots (T^\dagger)^m T^n (T^\dagger)^l$ where $m, n, k, l$ are nonnegative integers. Since $T$ is distinct path generating this term describes $l$ steps forward (i.e. the $T$ direction), $k$ steps backward, $n$ steps forward, $m$ steps backward, etc., along any of the paths generated by $T$ or its adjoint. All of these terms in the expansion except the first give 0 when applied to any states of $B$ not in a path. When applied to any state in $B$ in a path, many of the terms give another state of $B$ in the path. Since all terms in the expansion are of this form, it is clear that $H$ describes quantum ballistic evolution.

Necessity: Assume the existence of a Hamiltonian which describes quantum ballistic evolution on a basis $B$. $B$ is clearly not a basis of eigenfunctions for $H$. The Hamiltonian can be used to construct paths as follows: For any pair $|a\rangle, |b\rangle$ of distinct states in $B$ (i.e. $\langle a|b\rangle = 0$), $|a\rangle, |b\rangle$ are on the same path if there exists an $n$ such that $\langle b|H^n|a\rangle \neq 0$. $|a\rangle, |b\rangle$ are not on the same path if $\langle b|H^n|a\rangle = 0$ for all $n$. Since $H$ describes quantum ballistic evolution, if $|a\rangle, |b\rangle$ with the two states distinct are on the same path, there is a least $n$ such that $\langle b|H^n|a\rangle \neq 0$. Denote the least $n$ by $n_{ba}$. Note that $n_{ba} = n_{ab}$.
A pair of distinct states $|a\rangle, |b\rangle$ are adjacent if $n_{ab} = 1$. In general a state can have $0,1,2,\cdots$ adjacent states. Since $H$ describes ballistic evolution, motion is restricted to distinct paths only. Thus, at most, 2 states can be adjacent to a given state in $B$. A state with 0, 1, 2 states adjacent is on no path (or a path of length 0), is a terminal state of a path, or is an interior state of a path respectively. Note also by the definition of quantum ballistic evolution, for any pair $|a\rangle, |b\rangle$ of distinct states in $B$, $\langle b|H|a\rangle \neq 0 \Rightarrow \langle b|H|a\rangle = c$ where $c$ is a constant independent of $|a\rangle, |b\rangle$.

A step operator can be defined as follows: Choose states of $B$ until a pair $|a\rangle, |b\rangle$ of adjacent distinct states are found. Set $T|a\rangle = |b\rangle$ and $T^\dagger|b\rangle = |a\rangle$. Continue searching $B$ for states adjacent to and distinct from either $|a\rangle$ or $|b\rangle$. If a state $|d\rangle$ adjacent to $|b\rangle$ is found, set $T|b\rangle = |d\rangle$ and $T^\dagger|d\rangle = |b\rangle$. If no state adjacent to $|b\rangle$, other than $|a\rangle$ is found, set $T|b\rangle = 0$. The same construction applies for a state, if any, adjacent to $|a\rangle$ with $T^\dagger$ exchanged for $T$. If no states are both distinct from and adjacent to $|a\rangle$, set $T|a\rangle = 0$.

Continuing in this manner by searching through all states of $B$ defines all paths of $H$ and an associated step operator $T$ which is a partial isometry. Since $T$ is distinct path generating, by Theorem 3, $T$ is orthogonality preserving and stable on $B$, and the theorem is proved.

The necessity proof of the theorem has an arbitrariness in the choice of directions on each path for $T$ and $T^\dagger$. This can be seen by exchanging $T$ for $T^\dagger$ on one or more paths. From this one sees that for a given quantum ballistic Hamiltonian that describes motion on $n$ distinct paths, there are $2^n$ possible choices for the associated step operator $T$.

This arbitrariness is equivalent to the possibility of construction of wave packets which can move in either of two directions on each path. However if $H$ describes quantum ballistic evolution for some process with a defined “forward” direction with increasing time, then one of the possible choices of $T$ will be the step operator for the process. Which one is chosen will depend on external conditions, such as the choice of possible initial states. This is case for quantum computations, including reversible ones, where there are well defined forward and backward directions. The choice of whether $T$ or $T^\dagger$ is associated with the forward direction for all the paths is chosen by convention.

It should be noted that on any basis for which $T$ is orthogonality preserving, the Hamiltonian generating quantum ballistic evolution for $T$ is not orthogonality preserving on the basis. Since Hamiltonians are selfadjoint and thereby normal, they are completely orthogonality preserving on some basis. However they are not even orthogonality preserving on any quantum ballistic basis for $T$. For example, $T + T^\dagger$, which is in essence the Hamiltonian of Eq. 13 is not orthogonality preserving on any quantum ballistic basis for $T$. On the other hand, any unitary operator, such as $e^{-iHT}$, is completely orthogonality preserving on all basis sets. In fact unitary operators are the only ones with this property.

It is of interest to examine the effect of replacing in Theorem 5 stability and orthogonality preservation with complete orthogonality preservation. It is clear that necessity still holds but sufficiency fails. However sufficiency almost works at least if $T$ is a partial isometry. To see this note that if $T$ is a partial isometry and is completely orthogonality preserving, it is a power partial isometry and the decomposition theorem applies. All components of the decomposition are distinct path generating, except for those components in the unitary part which are not equivalent to (copies of) the bilateral shift or to cyclic orbits on a basis. For these components sufficiency fails. This is the sense in which complete orthogonality
preservation without the separate assumption of stability "almost works".

This can be said in another way by noting that if $T$ is a power partial isometry, then $H$ defined by Eq. 3 is partially quantum ballistic. This concept, which will be used later, means that on some of the reducing subspaces $H$ is quantum ballistic and on others it is not. If $T$ is a PPI then $H$ is quantum ballistic except possibly on components in the unitary part that are not equivalent to the bilateral shift or finite cyclic shifts.

It is of interest to examine the eigenfunctions and eigenvalues of the Hamiltonian given by Eq. 3 in the case that $T$ satisfies the conditions of Theorem 5. In this case $T$ is a power partial isometry which models some process which evolves quantum ballistically on $B$. For any such $T$, the eigenfunctions and eigenvalues of the Hamiltonian given by Eq. 3 all have the same form.

To see this it is sufficient to consider the unitary, isometric, coisometric, and truncated shift components separately. Paths in each part are defined by a basis set $\{|n,l\rangle\}$ where $T|n,l\rangle = |n+1,l\rangle$ and $T^\dagger|n,l\rangle = |n-1,l\rangle$. The label $l$ stands for the fact that $T$ may be a direct sum of PPIs and for the fact that the subspaces in the direct sum for the truncated shift can be multidimensional. The basis state labels are kept simple for the sake of clarity.

Eigenfunctions and eigenvalues for $H$ can be determined by writing the eigenfunction in the general form \[\Psi_k = \sum_{n=-L}^{M} (A e^{ikn} + B e^{-ikn}) |n\rangle\] (6)

where $T|M\rangle = T^\dagger|-L\rangle = 0$. Here $k$ denotes a momentum. The values of $M, N$ depend on the part being considered. Eigenvalues and eigenfunctions are obtained by writing $(E-H)\Psi_k = 0$, equating coefficients of each basis state to 0, and solving the system of linear equations so obtained. For all parts eigenvalues are given by \[E_k = 2K(1 - \cos k)\] (7)

where $k$ ranges from $-\pi$ to $\pi$.

For the unitary part there are two type of paths to consider, two way infinite and finite cycles or orbits. Eigenfunctions are obtained from Eq. 3 by setting $B = 0$. For the infinite paths, $M = L = \infty$ and

\[\Psi_k = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} e^{ikn} |n\rangle\] (8)

The momentum $k$ can assume all values. For the orbits, $L = 0$ and $M$ is finite with $T|n,l\rangle = |n+1,l\rangle$ if $n < M$ and $T|M,l\rangle = |0,l\rangle$. $T^\dagger$ moves along the orbit in the opposite direction. The eigenfunctions, which are also eigenfunctions of $T$ and $T^\dagger$ separately, are given by

\[2\text{In mathematical language the basis ranging over all } l \text{ for a fixed value of } n \text{ span a wandering subspace for the part being considered.}\]
\[ \Psi_k = \frac{1}{\sqrt{M+1}} \sum_{n=0}^{M} e^{ikn} |n\rangle \]  \hspace{1cm} (9)

where \( k \) is discrete with \( k = 2\pi m / (M + 1) \) with \( m = 1, 2, \ldots, M + 1 \).

For the pure isometric part which is a direct sum of copies of the unilateral shift, \( L = 0, M = \infty \), and the eigenfunctions have the form (the index \( l \) is suppressed)

\[ \Psi_{k, \geq 0} = C' \sum_{n=0}^{\infty} \sin k(n + 1) |n\rangle. \]  \hspace{1cm} (10)

For the coisometric part \( L = -\infty, M = 0 \) and

\[ \Psi_{k, \leq 0} = C' \sum_{n=-\infty}^{0} \sin k(n - 1) |n\rangle. \]  \hspace{1cm} (11)

For both these cases \( k \) can assume any value between \( -\pi \) and \( \pi \). \( C' \) is a normalization constant. The isometric and coisometric eigenfunctions represent standing waves for complete reflection from a barrier at state \( |0\rangle \) which defines the beginning or terminus (for \( T \)) of a path.

For a truncated shift of index \( N, L = 0, M = N - 1 \) and the eigenstates are given by

\[ \Psi_k = \frac{1}{(N)^{1/2}} \sum_{n=0}^{N-1} \sin k(n - N) |n\rangle \]  \hspace{1cm} (12)

The eigenvalues, given by Eq. 7, are discrete with \( k = m\pi / (N + 1) \) and \( m \) takes on integral values from 1 to \( N \). The value \( m = 0 \) is excluded as the eigenfunction is identically 0 for this case. The eigenfunctions are 0 at \( n = -1 \) and \( n = N + 1 \) and correspond to bound states in a square well with completely reflecting walls at \( n = -1 \) and \( n = N + 1 \).

The above shows that \( H \) given by Eq. 2 has the eigenvalues and eigenfunctions corresponding to quantum ballistic evolution on basis state paths. The types of paths correspond to the types of shifts in the decomposition of \( T \). Furthermore any wave packet state along a path defined by Eq. 1 moves along the path spreading out as it moves.

The reason for presenting a description of eigenvalues and eigenfunctions and wave packet spreading is that it gives a complete description of eigenvalue and eigenfunction structure for all processes modelled in quantum mechanics by step operators \( T \) which are partial isometries and are stable and orthogonality preserving on some basis. The differences in individual processes show up in the multiplicities and in the complexity and description of basis states in the paths. Examples which illustrate this are given next.

**VI. EXAMPLES**

Some simple examples will be considered to illustrate aspects of the preceding. The physical model considered will be that appropriate for discussion of Turing machines. To this end the model consists of a two way infinite one dimensional lattice of qubits represented as spin \( 1/2 \) systems fixed at the lattice points. A head moves along the lattice interacting locally with spins. For the simple examples considered the head is spinless. For Turing
machines, the head has a large but finite number of internal states, such as the $2L + 1$ spin projection states for a particle with spin $L$.

The above description gives an uncountable infinity of lattice spin basis states which can be written in the form $|s⟩ = \otimes_{j=-\infty}^{\infty} |s(j)⟩$ where $s$ is any function $s : Z → \{0, 1\}$. $Z$ is the set of integers. In order to work with a separable Hilbert space $s$ is limited to be any function with at most a finite number of values different from 0. The resulting Hilbert space $H_{00}$ for the lattice spins is spanned by all spin states with tails of 0 in both directions.

The overall model (separable) Hilbert space is spanned by vectors of the form $|l, j, s⟩$ where $l$ is the internal head state, $j$ is the head lattice position and $|s⟩$ is limited to 0 tail states. Here each of the lattice systems and the head are taken to be distinguishable particles to avoid the complications of antisymmetrization which are not relevant here. Also the direction of quantization is taken to be along the $z$-axis for each of the spins.

A. Motion in the Presence of 0s

In this example the (spinless) head moves along the lattice only at spin 0 lattice sites. The operator $T$ and its adjoint are defined by

$$T = \sum_{j=-\infty}^{\infty} P_{0,j} U P_j \tag{13}$$

$$T^\dagger = \sum_{j=-\infty}^{\infty} P_{0,j} P_j U^\dagger. \tag{14}$$

Here $P_{i,j}$ is the projection operator for finding the site $j$ lattice spin in state $|i⟩$ with $i = 0$ or $i = 1$, $P_j$ is the projection operator for the head at site $j$, and $U$ is the unitary operator shifting the head one site to the right ($UP_j = P_{j+1}U$). The sum is over all lattice sites. The lattice spin projectors commutute over all lattice sites.

It is easy to verify that $T$ is a power partial isometry. In particular $I_n$ and $F_n$, Eqs. [3] and [4], given by

$$I_n = \sum_{j=-\infty}^{\infty} P_{0,j+n-1} P_{0,j+n-2} \cdots P_{0,j} P_j \tag{15}$$

$$F_n = \sum_{j=-\infty}^{\infty} P_{0,j+n-1} P_{0,j+n-2} \cdots P_{0,j} P_{j+n} \tag{16}$$

are projection operators. Also the $I_n$ and $F_n$ commute among themselves and with each other.

It follows from Theorem 4 that $T$ and $T^\dagger$ are completely orthogonality preserving. The common basis set is the set of all $|j, s⟩$ as defined above. It is also clear by inspection of the definition of $T$ and its adjoint that $T$ and $T^\dagger$ are stable in this basis. $T$ also has pieces in each of the components given by the decomposition theorem. The component subspaces are defined by properties of the spin lattice. The unitary part of $T$ acts in the subspace which is spanned by $|j, s⟩$ where $s$ is the constant 0 sequence. On this space $T$ is the bilateral shift.
The other component subspaces are characterized by those sequences $s$ which contain a finite positive number of 1’s. Let $m_u$ and $m_l$ be the greatest and least integer respectively such that $s(m_u) = s(m_l) = 1$. Then $T$ restricted to the subspace spanned by $\{|j, s\rangle : j \geq m_u + 1\}$ is an isometry in that it is a unilateral shift. Note that $T^{|m_u + 1, s\rangle} = 0$. Similarly, $T$ restricted to the subspace spanned by $\{|j, s\rangle : j \leq m_l\}$ is a coisometry in that $T^\dagger$ is a unilateral shift. Note that $T^{|m_l, s\rangle} = 0$.

Those $s$ with one solid block of 1’s surrounded on both sides by 0’s extending to infinity, are included in the pure isometric and pure coisometric subspaces of $T$ only. Those $s$ with one or more groups of 0’s separated by 1’s on both sides, $T$ also has truncated shift components in addition to the terminal isometric and coisometric components. For example let $s$ be such that all lattice spins are down except at locations $N$, and $N + W + 1$. Figure 2 shows details. Here $T$ is a truncated shift of index $W + 1$ on the subspace spanned by $\{|j, s\rangle : N + 1 \leq j \leq N + W + 1\}$.

The eigenfunctions and eigenvalues for the Hamiltonian of Eq. 4 are included in the results of the previous section. The Hamiltonian has a rich eigenfunction structure in that it corresponds to a collection of many different Hamiltonians, one for each lattice state $|s\rangle$, each describing head motion on a one dimensional lattice in the potential environment given by $|s\rangle$.

For the unitary component the head eigenfunctions, $\psi_k$, are given by Eq. 8. Eigenvalues are given by Eq. 9 with all values of the momentum $k$ between $-\pi$ and $\pi$ allowed. For the example shown in Figure 2, the isometric and coisometric eigenfunctions describe respectively righthand standing waves reflecting off the 1 at site $N + W + 1$ and lefthand standing waves reflecting off the site at location $N + 1$. These are given by

$$\psi_k = C' \sum_{n=N+W+1}^{\infty} \sin(k(n - N - W - 1)) |n,\rangle. \tag{17}$$

for the righthand state and

$$\psi_k = C' \sum_{n=-\infty}^{N+1} \sin(k(n - N - 1)) |n\rangle \tag{18}$$

for the lefthand head state. These equations are obtained from Eqs. 10 and 11.

There is an assymetry in the barrier locations in that for the isometry the barrier is at the position of the 1 whereas for the coisometry it is displaced one site to the right of the 1 position. This is a consequence of the assymetry implicit in the definition of $T$ and its adjoint. $T$ reads the location from which the head moves and $T^\dagger$ reads the location to which the head moves. The same displacement effect for the bound states is shown in Fig. 2.

For the regions of 0’s in between the 1’s the bound state eigenstates are given by

$$\psi_k = \frac{1}{(W + 1)^{1/2}} \sum_{n=N}^{N+W+2} \sin k(n - N - W - 2) |n\rangle \tag{19}$$

for the region of 0’s between sites $N$ and $N + W + 1$, Fig. 2. The eigenvalues are given by Eq. 6 where $k = m\pi/(W + 2)$ and $m$ takes on integral values from 1 to $W + 1$.

These results hold for all values of $W \geq 2$. For $W = 1$ there is just one 0 between the two 1s. In this case there are two eigenvalues, $k = 0$ with $E = K$ and $k = \pi$ with $E = 3K$. 17
It is also clear that any region of one or more 1’s acts as a completely reflecting barrier with no communication between states on either side. Thus states on both sides of the barrier are completely independent of one another.

The bound state components correspond to infinite square wells in the limit of 0 lattice spacing. To see this let $d$ denote the lattice spacing. From Eq. 4 one has that $\langle H \rangle = E = 2K$ for any head state in spin-up lattice regions. Since $K$ is proportional to $d^{-2}$ one has that $E \rightarrow \infty$ as $d \rightarrow 0$. If the potential width is given by $D = (W + 2)d$, Eq. 7 gives in the limit $d \rightarrow 0$ with $K = c/d^2$, $E = K(m\pi/(W + 2))^2 = c(m\pi/D)^2$. This corresponds to the usual continuum limit [33].

These results extend to more complex expressions on the tape. For example, let $|s\rangle$ contain $M$ bands of $m_1, m_2, \cdots, m_M$ 0s separated by bands of 1s. Each band of 0s is equivalent to a square well with $m_1 - 1, m_2 - 1, \cdots, m_M - 1$ eigenstates of the form of Eq. 19 with eigenvalues given by Eq. 7 with $W = m_1, m_2, \cdots, m_M$. Linear superpositions of eigenstates from different wells are also eigenstates, but only for component eigenstates with equal energy eigenvalues.

The above shows how the one simple Hamiltonian in this example combining all lattice spin states which are products of $|1\rangle$ or $|0\rangle$ spin projection states to generate all possible distributions of completely reflecting barriers and the lattice equivalent of infinitely high square wells for particle motion on a one dimensional lattice.

Except for the unitary part, each of these components in the decomposition is of infinite multiplicity in that there are an infinite number of different 0 – 1 spin distributions contributing to each component. Each lattice spin state $|s\rangle$ with at least one 1 contributes to the isometric and coisometric parts. Each $|s\rangle$ with $n$ 0s between 1s contributes to the truncated shift of index $n$ part. Thus the general definition of path given in Section II applies here. Only one distribution, that with 0s only, contributes to the unitary part.

In many aspects the properties of this first example are obvious or straightforward. No bit transformations are involved. These are introduced in the next example.

**B. Arbitrary Bit Transformation**

As will be seen in the next section, elementary program elements of Turing computations consists of two types: those in which the head state changes after one iteration and those in which the head state is fixed. An example of an operator which models the latter type is given by

$$T = \sum_{j=-\infty}^{\infty} v_j P_{0,j} UP_j \quad (20)$$

Here $v_j$ is any unitary operator in $U(2)$ which transforms the site $j$ lattice spin state. An example is the "Fourier" transformation $[33,34]$ $v_{00} = 1/\sqrt{2}(\sigma_x + \sigma_z)$ which has been used in quantum computation $[34,35]$.

For Turing machine steps, $v_j$ is independent of $j$. However the following discussion for this example remains valid if $v_j$ depends on $j$. For deterministic computations $v_j$ is either 1 or $\sigma_{x,j}$. For nondeterministic computations $v_j$ is not restricted. However it has been shown by Deutsch $[3]$ and Bernstein and Vazirani $[13]$ that it is sufficient to limit $v_j$ to the
deterministic operators plus a rotation by an irrational multiple of $\pi$. This limitation will not be used here.

It is easy to see that $T$ is a power partial isometry and is completely orthogonality preserving. It is quite similar to the previous example in that all parts of the Halmos-Wallen decomposition are present except the unitary and coisometric parts. For each component of the decomposition which is present, eigenfunctions and eigenvalues have exactly the same form and values as those for the previous example.

The main difference is in the stable basis to which they refer. Here the basis consists of states of the form $|j, S_j\rangle$ where

$$|j, S_j\rangle = |j\rangle \otimes |S_{<j}^M\rangle \otimes |S_{\geq j}\rangle$$

(21)

where $j$ denotes the head lattice position and $M$ is any integer $\leq j$.

For all nonempty parts in the Halmos-Wallen decomposition $|S_{<j}^M\rangle$ is given by

$$|S_{<j}^M\rangle = \otimes_{k=M}^{j-1} v_k |0\rangle_k \otimes v_{M-1} |1\rangle_{M-1} \otimes \psi_{<M-1}$$

(22)

where $M \leq j$. The state $\psi_{<M-1}$ denotes an arbitrary state in the spin space for lattice spins at positions $< M-1$ and represents the fact that any basis set over this lattice spin subspace consistent with the tail condition is allowed. The dimension of this subspace is countably infinite. The arbitrariness is possible because no state in the basis of Eq. 21 has the head in this region. Orthogonality is guaranteed because for a fixed $j$ and $L \neq M$, $\langle S_{<j}^L | S_{<j}^M \rangle = 0$ independent of the tail states. This arises because the factor $\langle 1 | v^\dagger v | 0 \rangle = 0$ at sites $L$ or $M$ if $M < L$ or $L < M$.

For the isometric part $|S_{\geq j}\rangle = \otimes_{k=j}^{\infty} |0\rangle_k$. For the truncated shifts,

$$|S_{\geq j}\rangle = \otimes_{k=j}^{N-1} |0\rangle_k \otimes |1\rangle_N \otimes \psi_{>N}$$

(23)

where $N \geq j$. The argument given above for $\psi_{<M-1}$ applies to $\psi_{>N}$ with $T$ replacing $T^\dagger$.

The reason there are no unitary or coisometric parts is that the state $S_{<j}^M$ with $M = -\infty$ is orthogonal to any state consistent with the 0 tail condition. Cyclic orbits cannot occur because of the different bases used for the bits to the right and to the left of the head position.

It is left to the reader to see that $T$ is stable and orthogonality preserving with respect to this basis. Theorem 5 gives the result that the Hamiltonian of Eq. 2 [5] describes quantum ballistic evolution on this complex basis. For this and the previous examples, arguments given earlier show that complete orthogonality preservation is equivalent to orthogonality preservation and stability on the described basis.

These considerations emphasize how orthogonality preservation and stability depend on the basis set chosen. For the first example, $T = \sum_j P_{0,j} U P_j$ is orthogonality preserving and stable in the 0,1 computation basis. However it is not orthogonality preserving in the $v|0\rangle, v|1\rangle$ basis since for most $v$, $\langle 1 | v^\dagger P_0 v | 0 \rangle \neq 0$.

For this example, eigenfunctions and eigenvalues can be easily found for the Hamiltonian of Eq. 2. It is left to the reader to see that they are the same as those for the isometric and truncated shift parts of the previous example. The main difference between this example and the previous one is the complexity of the basis for which $T$ is orthogonality preserving. In this basis the head motion becomes entangled with changes in the spin projections on the lattice. Also the lack of unitary and coisometric components is a result of the 0 tail condition.
VII. QUANTUM COMPUTERS: TURING MACHINES

Step operators for quantum Turing machines (QTM)s can be defined based on the physical model given earlier. To this end let \( f, d, v \) be three functions with a common domain \( D \subseteq [0, N] \times [0, 1] \) and respective ranges in \([0, N],[1, \dagger],U(2)\). Here \([0, N]\) is a finite set of whole numbers from 0 to \( N \) representing the spin states of the head, \([0, 1]\) denotes the two states of each qubit or lattice spin in whatever basis is chosen as the computation basis, and \( U(2) \) denotes the set of 2 dimensional unitary operators. Each quantum Turing machine is represented by a triple \( f, d, v \) of such functions with the model operator \( T_{f,d,v} \) given by

\[
T_{f,d,v} = \sum_{l,s \in D} T_{ls}^{f,d,v}
\]

as a finite sum over program element operators. \( l \) and \( s \) denote elements of \([0, N],[0, 1]\). From now on the superscript ” \( f, d, v \)” will be suppressed.

The program element operators have the form

\[
T_{ls} = \sum_{j=\pm} u^{f(l,s)}Q_0(u^\dagger)v_{lsjP^s,j}P_j U_{ls}(d(l,s)P_j)
\]

where \( Q_l \) is the projection operator for finding the head in state \( |l\rangle \), \( u \) is the unitary operator which shifts the head state up by one unit, \( uQ_l = Q_{l\dagger}u \mod N \), and \( v_{lsj} \) is a unitary operator which changes the state of the site \( j \) lattice spin. The action of \( v_{lsj} \) on the site \( j \) spin is the same for all values of \( j \). The other operators are as previously defined.

This definition uses the work of Bernstein and Vazirani [19] which shows that any QTM with program elements with no head motion can be replaced by an equivalent machine with program elements in which the head moves either one cell to the left or to the right.

Both deterministic and nondeterministic QTMs are included. In the usual basis with lattice spins up or down, a deterministic quantum Turing computation is one for which the spin change operators \( v_{lsj} \) in each of the program elements (Eq. 25) in the sum over \( l, s \) (Eq. 24) are restricted to be either the identity or the spin flip operator \( \sigma_z \). By use of suitable unitary transformations this definition can be applied to any lattice spin bit basis chosen as the computation basis.

The program element operators of Eq. 25 are of two types depending on whether \( f(l, s) \neq l \) or \( f(l, s) = l \). In the first case it is easy to verify that \( T_{ls}^2 = (T_{ls})^2 \) = 0 and \( T_{ls} \) is a partial isometry. For the case where \( f(l, s) = l \) a straightforward calculation gives (Eqs. 26 and 27)

\[
I_{ls} = Q_l \sum_{j=\pm} \prod_{h=0}^{n-1} P_{s,j\pm(h)P_j}
\]

\[
F_{ls} = Q_l \sum_{j=\pm} \prod_{h=0}^{n-1} v_{lsj\pm h}P_{s,j\pm h}v_{lsj\pm h}^\dagger P_{j\pm n}
\]

Here ” \( \pm \)” denotes + if \( d(l, s) = 1 \) and \( - \) if \( d(l, s) = \dagger \).

It is straightforward to show that for all \( m, n \) \( I_{ls} \) and \( F_{ls} \) are projection operators and that \( [I_{ls}, F_{ls}] = 0 \). So all \( T_{ls} \) as defined by Eq. 25 are power partial isometries.

This result, although of interest, is not sufficient since one is interested in the overall computation process operator \( T \), not just the program elements. Iteration of \( T \) leads to
interaction among the different program elements. In the interest of simplicity it is assumed here any history recording steps can be added by additional steps on a 1-tape machine. In this fashion $T$ with or without any history has the form of Eq. 24 with all individual elements given by Eq. 27. This requirement that $T$ be a one tape machine is not essential, as the arguments can be extended to apply to machines with more than one tape.

The definition of $T$ given above for quantum Turing machines is quite general. For example step operators for irreversible Turing computers are included as are many $T$ which are not partial isometries or do not describe ballistic evolution. It is thus of interest to relate the necessary and sufficient conditions for quantum ballistic evolution, given in the previous sections, to detailed properties of QTM step operators as defined by Eqs. 24 and 25 and used in the Hamiltonian of Eq. 2.

By definition $T$ is a partial isometry if and only if $I_1, F_1$, defined by Eqs. 9 and 10, are projection operators. That is they satisfy $I_1^2 = I_1$ and $F_1^2 = F_1$. $I_1, F_1$ are given by

$$I_1 = \sum_{(ls),(l's')} T_{ls}^\dagger T_{l's'}$$

$$F_1 = \sum_{ls} T_{ls} T_{ls}^\dagger$$

$$= \sum_{ls} F_{ls1}$$

From the definition of $T$ one sees that all nondiagonal elements vanish in the definition of $F_1$.

A straightforward calculation using the above shows that

$$I_1^2 = \sum_{(ls),(l's'),(mt)} T_{ls}^\dagger F_{l's'1} T_{mt} = I_1 + \sum_{(ls)(mt)} \sum_{(l's') \neq (ls),(mt)} T_{ls}^\dagger F_{l's'1} T_{mt}.$$  \hfill (31)

So $I_1^2$ is a projection operator if and only if the righthand double sum in Eq. 31 equals 0. Carrying out a similar calculation for $F_1$ shows that $F_1$ is a projection operator if and only if

$$\sum_{(ls) \neq (l's')} F_{ls} F_{l's'} = 0.$$  \hfill (32)

Although these conditions are necessary and sufficient for determining if $T$ is a partial isometry, they are abstract. It would be good to have more concrete conditions related to the detailed properties of the computation. To this end note that a sufficient condition for $T$ to be a partial isometry is that $I_1 = \sum_{ls} I_{ls1}$, that is, all nondiagonal terms $T_{ls}^\dagger T_{mt}$ with $(ls) \neq (mt)$ equal 0. (An equivalent expression of this is that the terms in the sum of Eq. 24 are pairwise orthogonal on the left.)

This condition is the quantum mechanical equivalent of the classical requirement that no pair of program elements takes two different computation states into the same state. That is, in the reverse computation at most one elementary step is active at each stage. The already existing condition that nondiagonal terms equal 0 in $F_1$ ensure that in the forward computation at most one elementary step is active at each stage. In quantum mechanics where nondeterminism and quantum parallelism occur, more than one elementary term $T_{ls}$ can be active in a stage.
A sufficient condition for the validity of $I_1 = \sum_{ls} I_{ls1}$ is that the function $f$ in Eq. $24$ be $1 - 1$ on $D$. A less restrictive condition is the following: For all $(ls), (mt)$ in $D$ if $(ls) \neq (mt)$ and $f(ls) = f(mt)$, then $d(ls) = d(mt)$ and for each $j$, $P_{sj} v_{l}^{j} v_{mtj} P_{j} = 0$. Here $P_{s}, P_{t}$ are projection operators for single lattice spin states $s, t$. This condition, called here condition X, follows from the properties of the factors in

$$ T_{ls} T_{mt} = u^{f} Q_{0} u^{f(ls) - f(mt)} Q_{0} (u^{f})^{m} \sum_{j,k} P_{s} v_{l}^{j} v_{mtk} P_{k} (U) d(l) U d(mt) P_{k} $$

(33)

From this equation it can be seen that Condition X is equivalent to the condition that the nondiagonal terms $T_{ls} T_{mt} = 0$ individually. It is thus a sufficient but not necessary condition for $T$ to be a partial isometry.

It remains to show that the requirement of quantum ballistic evolution is not empty for nondeterministic QTMs. It is first shown that there exist step operators for nondeterministic QTMs which are partially quantum ballistic. That is, they are quantum ballistic on some subspaces but not on other subspaces. To this end consider the following example step operator and its adjoint:

$$ T = Q_{0} \sum_{j} v_{00j} P_{0j} U P_{j} + u Q_{0} \sum_{j} P_{1j} U^{\dagger} P_{j} + Q_{1} \sum_{j} P_{1j} U^{\dagger} P_{j} $$

(34)

$$ T^{\dagger} = Q_{0} \sum_{j} P_{0j} v_{00j}^{\dagger} P_{j} U^{\dagger} + Q_{0} u^{\dagger} \sum_{j} P_{1j} U P_{j} + Q_{1} \sum_{j} P_{1j} U^{\dagger} P_{j} $$

(35)

$T$ is a sum of three elementary steps: the head in internal state 0 moves to the right and carries out $v_{00}$ on 0 bits only (term 1); if a 1 bit is encountered, change head state to 1 and move one step to left (term 2); with the head in state 1 shift to the left and flip the encountered bit if and only if it is a 1 (term 3).

For most $v_{00}$ in $U(2)$, $T$ is nondeterministic. $T$ is also a partial isometry (Condition X holds) and it is orthogonality preserving. A comparison of $T$ with the example of section [VTB] shows that with the head in state 0 the first term of $T$ is identical with the example. Thus $T$ is quantum ballistic on all subspaces in which term 1 only is active and term 2 is never activated. These correspond to the isometric subspaces of the example in section [VTB].

$T$ is also quantum ballistic on subspaces in which term 2 only is active or term 3 only is active. All paths in the subspaces on which term 2 only is active are of length 1 (i.e. contain two states). This is an example of the term type with $f(ls) \neq l$.

However, $T$ does not appear to be quantum ballistic on the computation subspace in which all three terms are active. To see this consider the subspace of states $|0 \rangle |l \rangle |S_{<l} \rangle |S_{>l} \rangle$ with $|S_{<l} \rangle |S_{>l} \rangle$ given by Eqs. [22] and [23]. (The $M$ superscript is suppressed.) This state describes the head at position $l$ and in internal state $|0 \rangle$ with the spin lattice transformed to the left of $l$ and in the $0 - 1$ spin basis to the right of $l$. Under the action of term 1, Eq. [34], the head moves ballistically to the right until the 1 at site $M - 1$ is encountered. Then term 2 moves the head back to position $M - 1$ and changes the head state to $|1 \rangle$. Term 3 now becomes active. However it is active only when it sees a 1 on the transformed component; it annihilates the state when it sees a 0 in the transformed component. The amplitudes per step for following these choices are given by $\langle 1 | v_{00} | 0 \rangle$ and $\langle 0 | v_{00} | 0 \rangle$ respectively.

This can be stated in another way. Suppose term 1 is active for $n$ steps before a 1 is encountered where $v_{00} |0 \rangle = a |0 \rangle + b |1 \rangle$ with $|a|^{2} + |b|^{2} = 1$. At the end of $n$ steps the lattice
spin state for the \( n \) spins can be expanded as a sum over the \( 2^n \) paths (as \( 0 - 1 \) strings of length \( n \)) in the computation basis, \( \sum_p c(p) \bigotimes_{l=0}^{n} |p(l)\rangle \), with amplitudes \( c(p) \) given by \( n \) fold products of \( a, b \). Iteration of term 3 describes head motion back along each path. As long as 1 are encountered the head moves back to the left along each path ballistically until the first 0 is encountered. At this point the next iteration of term 3 gives 0, thereby removing the path state with its corresponding amplitude from the overall system state.

This shows that repeated iterations of \( T \) generate at some point states whose norm starts decreasing below 1. This is a result of the removal of paths at each step at which term 3 is active. As the process of iteration of \( T \) continues, the amplitude of the remaining state continually decreases.

It must be emphasized that removal of paths and decrease of overall state amplitude refers only to the effect of iterations of \( T \) or its adjoint. It does not refer to the actual time evolution of the system. Since the evolution operator \( e^{-iHt} \) is unitary no paths are removed and the overall state normalization is preserved. Instead paths which are removed by iterations of \( T \) correspond to halting paths of the process. If for some path state \( \psi, T\psi = 0 \), then \( \psi \) is the final or halting state for the particular path. Dynamically these halting states will be seen in future work to act like partially reflecting barriers under the action of \( e^{-iHt} \).

The loss of overall state amplitude under iteration of \( T \) or \( T^\dagger \) shows that for this subspace and \( T \) given by Eq. 34, the evolution does not proceed quantum ballistically. As defined here quantum ballistic evolution describes either norm preserving motion under iteration of \( T \) or \( T^\dagger \) or simultaneous removal of all paths at the same step. It does not describe motion in which different paths are removed at different stages.

The above suggests that in order for a nondeterministic \( T \) to be quantum ballistic, for a given input string state, all paths in the computation basis must be of the same length. This can be achieved by either adding ballast type evolution to each path to ensure all paths are infinite, or that all paths are of the same finite length. A simple example of a nondeterministic \( T \) with all paths of the same finite length is given in Appendix B.

It is to be emphasized that the restriction to paths of the same length applies only to paths generated as a result of properties of \( H \). It is not a restriction on the properties of the input state. For example, the input state can be a linear superposition of different inputs to the computation, (i.e. quantum parallel computation [6]). Computation paths for each of the component inputs can be of different length without affecting the ballistic evolution. This is a consequence of the fact that, because the paths on different inputs are distinct, the requirement of ballistic evolution applies to each input separately.

VIII. EFFECTIVE DETERMINATION OF QUANTUM BALLISTIC EVOLUTION

As has been shown in earlier sections, an arbitrary QTM step operator defined by Eqs. 24 and 25 may not be a step operator for a quantum ballistic computation. In general \( T \) may be quantum ballistic on some subspace, or not on any subspace, or on the whole Hilbert space. The question arises of how one determines if \( T \) and the associated Hamiltonian of Eq. 3 describe a quantum ballistic computation at least on the subspaces of the computation. This problem applies to step operators for arbitrary process, not just quantum Turing machines.

Theorem 5 shows that this question is equivalent to that of the existence of an effective decision procedure for determining if a step operator is a partial isometry and is stable and
orthogonality preserving for some basis. The examples of Section VI, and many of QTM step operators, show that step operators exist which satisfy these requirements.

By “effective procedure” is meant a decision process for determining whether or not there exists a basis for which a step operator \( T \) is orthogonality preserving and stable where the number of steps in the decision process is finite. If a numerical measure of the complexity of \( T \) is available, it is then desirable that the number of steps in an effective procedure is of the order of a polynomial in the complexity of \( T \). If \( T \) is a quantum Turing machine step operator, then for the purposes of this paper, the complexity of \( T \) is of the order of the (finite) number of elementary step operators in \( T \).

In particular a decision process is not effective if it requires raising \( T \) and \( T^\dagger \) to all positive powers in order to make the determination. The reason is that such a process has an infinite number of steps.

It is clear that for QTMs, one can determine effectively if \( T \) (and its adjoint) is a partial isometry and is orthogonality preserving. This follows from Theorem 1, Eq. 25, and the fact that determination if \( T^\dagger T \) and \( TT^\dagger \) commute and are equal to their squares requires a number of steps of the order of the fourth power of the number of elementary steps in \( T \).

The main problem is the effective determination of stability for a given step operator. For deterministic QTM step operators such a procedure exists. This follows from the fact that the only spin transformations allowed in the terms of the step operator \( T \) are lattice spin flips or changes of the spin projections of the head with respect to a fixed quantization axis. Simple inspection of each of the elementary step terms of the step operator \( T \) is sufficient to determine if this is the case. Furthermore step operators for deterministic QTMs are usually constructed so that the usual computation basis is stable for \( T \).

It follows that for deterministic QTM there exists an effective decision procedure for deciding if \( T \) is orthogonality preserving and stable for some basis.

For nondeterministic QTMs the above proof fails because there does not appear to be a way to determine effectively from properties of \( T_i s \), Eq. 25 if \( T \) is stable for some basis. This can be seen from the arguments of the last section, that show for a given input string state, a search must be carried out through on all state paths in the computation basis generated by successive iteration of \( T \) and \( T^\dagger \) on the input state. If two paths of different length are encountered, the computation is not quantum ballistic on the given input. However all iterative powers must be searched before one can conclude a computation is quantum ballistic.

It is thus concluded that an effective decision procedure exists for determining for the step operator for an arbitrary deterministic quantum Turing machine if a simple Hamiltonian description of quantum ballistic evolution exists for the computation. It is an open question if such a procedure exists for the step operator of a nondeterministic quantum Turing machine.

Note that, given a step operator for a nondeterministic QTM, one can use some prescription such as that provided by Bennett [2] to add history and copying degrees of freedom. The problem is to determine for each input to the computation, if there exists a basis for which the expanded step operator \( T \) is stable on the computation subspace (the subspace spanned by the states obtained by all iterations of \( T \) and \( T^\dagger \) on the input state. As noted before an effective procedure exists for determining if \( T \) is orthogonality preserving.

It is of interest to consider the case in which a process step operator \( T \) is a power partial isometry and has no unitary components, (except possibly for bilateral shifts and cyclic finite
orbits). In this case the main theorem, Theorem 5, holds with orthogonality preservation and stability replaced by complete orthogonality preservation. In this case the decision process involves determining if a step operator $T$ is a partial isometry and is completely orthogonality preserving (Theorem 4).

It is easy to determine effectively if $T$ is a partial isometry: one needs only to determine if $I_1$ and $F_1$ are projection operators (i.e. if $(I_1)^2 = I_1$ and $(F_1)^2 = F_1$). The problem is to determine effectively if $T$ is completely orthogonality preserving.

The nonexistence of an effective decision procedure for complete orthogonality preservation follows from the Halmos-Wallen counterexample. It shows that one cannot conclude complete orthogonality preservation from orthogonality preservation and that all positive powers of $T$ and its adjoint would have to be inspected. In particular it shows that operators exist for which all powers up to some arbitrarily large $n$ are orthogonality preserving, but the $n + 1$st is not.

**IX. DISCUSSION**

Several aspects of the material presented so far in this paper should be stressed. First, it is important to emphasize the distinction between the reversibility and ballistic properties of a step operator $T$ and those of the associated Feynman Hamiltonian $H = K(2 - T - T^\dagger)$. In general $T$, including those defined for QTM\s by Eqs. 24 and 25 do not even describe reversible processes. Or they may describe reversible processes which do not evolve ballistically. An example of the latter would be any unitary $T$ which is not stable on any basis (Theorem 5).

An example of the former is the erasure operator $T = \sum_{j=-\infty}^{\infty} (P_{0,j} + \sigma_{x,j} P_{1,j}) U P_j$, which describes resetting of all 1’s in a string to 0’s. This process is not reversible as iteration of $T$ describes paths which join. As Landauer [1] has emphasized, information is destroyed. In this case the Hamiltonian of Eq. 2 will describe evolution of another process which is reversible and not that associated with iteration of $T$.

The definition of quantum Turing machines used here (Section VII) differs from that proposed by Deutsch [3] and Bernstein and Vazirani [19] and which is often quoted in the literature. These authors restrict $T$ to be unitary and local in the computation basis and to apply to a finite time. That is, $T = e^{-iHt}$ for some finite time interval $t$.

As was noted earlier in this paper, it is impossible to satisfy these requirements with a Hamiltonian which is local and is simple in that it has the complexity of $T$ and not of all powers of $T$ and $T^\dagger$. This suggests that one combine the two approaches by restricting $T$ to be unitary and to refer to infinitesimal time steps only. In this way the Feynman Hamiltonian [5], Eq. 2 constructed from unitary $T$ is local and is simple.

There are some problems with this approach. The main problem is that it is unnecessarily restrictive to require $T$ to be unitary. Step operators constructed as sums of local step or program elements used in algorithms are not likely to be unitary. The definition given here in which $T$ is not even required to be normal is more general and it corresponds more closely to what one actually does in construction of algorithms as sums of local step or program elements. As an example consider Simon’s algorithm [34] for a quantum computation. This consists of two “Fourier transforms” separated by the computation of a function $f$:
\[ \{0, 1\}^n \Rightarrow \{0, 1\}^m \text{ with } m \geq n \text{ to generate the state } \sum_p c(p) |p\rangle \otimes |f(p)\rangle. \]

The sum is over all \( 2^n 0-1 \) strings \( p \) of length \( n \). It is clear that any step operator \( T \), which corresponds to a sum of local steps for computation of the function and generation of \( |p\rangle \otimes |f(p)\rangle \) from \( |p\rangle \) is not likely to be unitary.

Another way around this problem might be to consider any step operator \( T \) for a QTM as defined here such that \( T \) is a partial isometry and is orthogonality preserving on some basis. Then dilate \( T \) to a unitary operator on the whole Hilbert space by suitable extension of the definition of \( T \) to the null subspace. One problem with this is that there is no way to effectively define either the null subspace or the subspace on which \( T \) is unitary.

This problem was already mentioned for earlier work [20,21]. In particular, the null (or unitary) subspace consists of all states in some basis which are not (or are) reached at some stage of the computation on some input. If \( T \) is the step operator for a (deterministic) universal Turing machine, an effective definition of the null or unitary subspaces would require solution of the halting problem which is impossible.

Another problem with this approach is that even if the dilation is unitary, powers of the dilation would not correspond to powers of the original \( T \). This was examined elsewhere [24] where minimal unitary power dilations \( V^T \) of step operators were constructed. It was seen that the construction added an extra degree of freedom and that history was generated automatically when needed.

However examples of deterministic Turing machine step operators showed that \( T \) needed to be expanded by addition of history and copy degrees of freedom prior to unitary power dilation. This was needed to avoid most of the state amplitude going into history components. This suggests that, at least for deterministic QTMs, unitary power dilation with the addition of another degree of freedom is not needed. It is not known if unitary power dilation of step operators for nondeterministic QTMs has any advantages.

Another problem with expansion of a process step operator into a unitary operator by addition of degrees of freedom is that all degrees of freedom need to be kept isolated from the environment so that coherence between phases of the states of all degrees of freedom are maintained. This is especially important for constructing quantum mechanical computers as their operation (for example, Shor’s algorithm [12]) depends on maintaining phase relations among the different components.

This suggests that it is important to minimize the number of degrees of freedom to be added. In this way effects of the environment, such as decoherence, etc. [14,16,18] make it useful to minimize the number of additional degrees of freedom that need to be protected.

The results of this paper suggest that to ensure quantum ballistic evolution, it is sufficient to add just enough additional degrees of freedom so that a step operator \( T \) for the expanded process is a partial isometry, preserves orthogonality, and is stable for some basis. In particular, it is not necessary to add even more degrees of freedom to ensure that the expanded operator is unitary. If \( T \) is stable and orthogonality preserving in some basis, then (Theorem 5) for such processes there always exists a simple time independent Hamiltonian (for example that of Eq. 2) which correctly models quantum ballistic evolution a simple

\[ \text{Theorem 5: } \]

\( \text{For such processes there always exists a simple time independent Hamiltonian which correctly models quantum ballistic evolution.} \)

---

\[ \text{3 Here oracle presentation of } f \text{ is replaced by computation of } f \text{ to obtain a physically meaningful procedure.} \]
time independent Hamiltonian (for example that of Eq. 2) which correctly models quantum ballistic evolution. It is, however, an open question how one can effectively determine the minimal number of degrees of freedom needed to guarantee reversible or quantum ballistic evolution. was limited here to quantum Turing machines. It also applies to other models of quantum computation such as quantum circuits. Specifically, any quantum circuit which can be modelled by a step operator and for which quantum ballistic evolution is a satisfactory description of the computation, is included.

X. FUTURE WORK

Much of the concern of this paper was with necessary and sufficient conditions for a step operator $T$ to generate quantum ballistic evolution for a process. It was seen that if $T$ was a partial isometry, orthogonality preservation and stability gave for the Feynman Hamiltonian, Eq. 2 a canonical form for both the eigenvalues and eigenfunctions and the description of quantum ballistic evolution.

As was seen there are many processes which fit these requirements. However there are also many processes in physics with associated step operators which are reversible but do not evolve quantum ballistically. The work of this paper needs to be generalized to accomodate these. Also the consequences of orthogonality preservation and stability for step operators which are not partial isometries needs to be investigated.

Also it was shown that it is an open question if there exists an effective decision procedure to determine if a step operator for a process such as a nondeterministic QTM describes quantum ballistic evolution. This open question needs to be closed, either by giving an effective decision procedure or by proof that the question is effectively undecidable.

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APPENDIX A

Theorem 1 An operator $T$ and its adjoint are orthogonality preserving if and only if $T^\dagger T$ and $TT^\dagger$ commute.

Proof: Let $\{|n\rangle: n = 0, 1, \cdots \}$ denote a common basis set for which both $T$ and $T^\dagger$ are weakly orthogonality preserving. Then

$$\langle n| T^\dagger TT^\dagger - TT^\dagger T|m \rangle = \sum_j[\langle n| T^\dagger T|j \rangle \langle j| TT^\dagger|m \rangle - \langle n| TT^\dagger|j \rangle \langle j| T^\dagger T|m \rangle].$$

By the definition of weak orthogonality preservation the component matrix elements are different from 0 only if $j = m$ and $j = n$. This is impossible if $m \neq n$.

Conversely suppose $T^\dagger T$ commutes with $TT^\dagger$. Since both these operators are self adjoint, by the spectral theorem, there exist two spectral measures, $E$ and $F$ such that

$$T^\dagger T = \int \lambda dE_\lambda,$$

$$TT^\dagger = \int \lambda dF_\lambda.$$

Since $T^\dagger T$ and $TT^\dagger$ commute, there exists another spectral measure $G$ which is a common refinement or product of $E$ and $F$. Let $\{|r\rangle: r \in $ spectrum of $T^\dagger T$ or $TT^\dagger\}$ be a basis set of continuous or discrete eigenfunctions defined by $G$. Here physicists license is being used to speak of continuous eigenfunctions. In case of degeneracy, extra basis labels are implicitly assumed.

By construction it is clear that if $r \in $ spectrum of $T^\dagger T$, then $E_{s}|r \rangle = |r \rangle [0]$ if $s > r$ [$s \leq r$]. If $r$ is not in the spectrum of $T^\dagger T$, then $E_{s}|r \rangle = 0$ for all $s$. Similar relations hold for $F$ and $TT^\dagger$.

It follows that if $r \neq s$ then $\langle s| T^\dagger T|r \rangle = \langle s| TT^\dagger|r \rangle = 0$, which proves the theorem.

Theorem 3 A partial isometry $T$ is orthogonality preserving and stable in some basis $B$ if and only if $T$ is distinct path generating in $B$.

Proof: $\implies$: If $T$ and $T^\dagger$ are orthogonality preserving and stable in a basis $B$ then iteration of $T$ or its adjoint generates paths in $B$. This follows from the definition of stability and bases as $T|p_i \rangle$ is in $B$ if $|p_i \rangle$ is in $B$ and $T|p_i \rangle \neq 0$.

To show that $T$ and $T^\dagger$ are distinct path generating suppose that two states $|p_i \rangle$ and $|p_j \rangle$ are in different paths as generated by iterations of $T$ or its adjoint and that there exist smallest values $m, n$ such that $\langle T^m p_i | T^n p_i \rangle \neq 0$. That is starting from $|p_i \rangle$ and $|p_j \rangle$, the paths first intersect after $m$ and $n$ iterations of $T$ respectively. By assumption $\langle T^{n-1} p_j | T^{m-1} p_i \rangle = 0$. But orthogonality preservation and stability implies that $\langle T^n p_j | T^m p_i \rangle = \langle T(T^{n-1}) p_j | T(T^{m-1}) p_i \rangle = 0$ which is a contradiction. Thus $T$ is distinct path generating. Repetition of the above for $T^\dagger$ proves the implication.

$\Longleftarrow$: Assume $T$ and $T^\dagger$ are distinct path generating in some basis $B$. From the definition of distinct path generation, stability in $B$ follows immediately. Orthogonality preservation also follows: to see this assume first that $|p_i \rangle, |p_j \rangle$ are distinct states in the same path for $T$. 

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By the definition of a path, either $T|p_i⟩ = 0$, $T|p_j⟩ = 0$ or both are different from 0 and are different states. In all these cases $⟨Tp_i|Tp_j⟩ = 0$.

If $|p_i⟩$ and $|p_j⟩$ are in different paths, then by assumption $T|p_i⟩$ and $T|p_j⟩$ are either 0 or are distinct. Thus $⟨Tp_i|Tp_j⟩ = 0$ which shows that $T$ is orthogonality preserving. Repetition the above for $T^\dagger$ completes proof of the theorem.

**Theorem 4** A partial isometry $T$ and its adjoint are completely orthogonality preserving if and only if $T$ is a power partial isometry.

Proof: $\implies$: For each $n$ let the operators $I_n$ and $F_n$ be defined by Eqs. 3 and 4. Since complete orthogonality preservation implies orthogonality preservation, Theorem 1 implies that for each $n$, $[I_n,F_n] = 0$.

Claim: for all $n,m$ with $n$ different from $m$, $[I_n,F_m] = 0$. To see this let $\{|p_j⟩\}$ be the common basis which preserves orthogonality for all powers of $T$ and its adjoint. By hypothesis and the definition of complete orthogonality preservation, such a basis exists. One also has

$$
⟨p_i|I_nF_m − F_mI_n|p_i⟩ = \sum_j⟨p_i|I_n|p_j⟩⟨p_j|F_m|p_i⟩ − ⟨p_i|F_m|p_j⟩⟨p_j|I_n|p_i⟩.
$$

Since $⟨p_i|I_n|p_j⟩$ and $⟨p_i|F_m|p_j⟩ = 0$ if $i \neq j$, the above expression is 0 since for $i \neq l$, $j$ cannot be equal to both $i$ and $l$. For $i = l$ the expression is clearly equal to 0. Thus $[I_n,F_m] = 0$.

The final step is by induction. One already has that $T$ and $T^2$ are partial isometries. Assume that $T^n$ and $T$ are partial isometries. Then $T^{n+1}$ is a partial isometry. This follows from the above proof that $[I_1,F_n] = 0$, and the H-W lemma.

$\impliedby$: Since $T$ is a power partial isometry, it can be decomposed [Halmos-Wallen] into a unitary operator on the subspace $H_1 = F_∞I_∞H$, an isometry on $H_2 = I_∞ − I_∞F_∞H$, a coisometry on $H_3 = F_∞ − I_∞F_∞H$, and for each $n$ a truncated shift of index $n$ on $H_{4,n} = P_nH$.

To prove the implication it is necessary to show the existence of a basis for each of the reducing components for which $T$ is completely orthogonality preserving. For the unitary part any selected basis will do because $T^\dagger T = TT^\dagger = 1$ on $H_1$. That is, for any basis on this subspace $\{|n⟩\}$, $n \neq m \implies ⟨T^\dagger n|T^\dagger m⟩ = ⟨⟨T^\dagger⟩^\dagger n|(⟨T^\dagger⟩^\dagger)m⟩ = 0$ for $l = 0,1,\cdots$.

For the isometric component use is made of the fact that any isometry is a direct sum of a unitary part and copies of unilateral shifts [32]. The unitary part is included above. For the unilateral shifts select for the basis the set $\{|n,k⟩\}$. Here $k$ is the index representing a term in the direct sum and $T|n,k⟩ = |n+1,k⟩$ for $n = 0,1,\cdots$. It is clear that complete orthogonality preservation occurs for this basis since, if $n \neq m$ then for all $j$, $⟨T^j n,k|T^j m,k⟩ = ⟨n+j,k|m+j,k⟩ = 0$ and $⟨⟨T^j⟩^\dagger n,k|(⟨T^j⟩^\dagger)m,k⟩ = ⟨n−j,k|m−j,k⟩ = 0$. The last equality for the adjoint of $T$ is trivially true for $n−j < 0, m−j < 0$.

For the coisometric component the above argument can be repeated by exchanging $T$ with its adjoint and letting $n$ range over the nonpositive integers.

For the truncated shifts of index $n$, the argument given for isometries can be repeated. That is, the operator $T_n$ which is the restriction of $T$ to the reducing subspace $H_{4,n} = P_nH$ can be written as a direct sum $\oplus_k T_{k,n}$ where $T_{k,n}$ is a truncated shift on the $k$th component of $H_{4,n}$.
Halmos and Wallen [23] (see also [26]) have shown that the projection operator \( P_n \) can be defined by the orthogonal sum

\[
P_n = \sum_{l=1}^{n} \Delta I_{n-l} \Delta F_l
\]

where \( \Delta I_{n-l} = I_{n-l} - I_{n-l+1} \) and \( \Delta F_l = F_{l-1} - F_l \). The \( I \) and \( F \) projection operators are defined by Eqs. 3 and 4.

Let \{\( |j,k\rangle \)\} represent a basis on \( \mathcal{H}_{4,n} \) such that for each \( l \),

\[
T^l|j,k\rangle = \begin{cases} 
|j+l,k\rangle & \text{if } j+l \leq n \\
0 & \text{if } j+l > n.
\end{cases}
\]

One also has

\[
(T^\dagger)^l|j,k\rangle = \begin{cases} 
|j-l,k\rangle & \text{if } j-l \geq 0 \\
0 & \text{if } j-l < 0.
\end{cases}
\]

It is clear from the above that \( T_n \) and its adjoint are completely orthogonality preserving on the defined basis. Since all cases of the decomposition of \( T \) are covered, the proof of the theorem is complete.
APPENDIX B

The goal here is to exhibit an example of a nondeterministic QTM step operator $T$ which is quantum ballistic. This is done by ensuring that for each input all computation paths are the same length. For the purposes of illustration the example will be made simple, with only one nondeterministic step.

Define a step operator $T$ by

$$T = Q_0 \sum_j P_0 j U P_j (1) + u Q_0 \sum_j v_j P_1 j U^\dagger P_j (2) + u Q_1 \sum_j P_0 j U P_j (3)$$

$$+ u Q_2 \sum_j P_0 j U P_j (4) + u^2 Q_2 \sum_j P_1 j U P_j (5)$$

(37)

The component operators are defined here as before. Recall that $v_j$ is any unitary operator in $U(2)$ and is the same for each $j$. The numbers in parentheses following each term are included for easy reference and are not part of the equation.

The first term moves the head in state 0 to the right along a string of lattice 0s. Term 2 carries out the only nondeterministic step by applying a $v$ transformation to the first 1 encountered, changing the head state to 1 and moving one step back. Term 3 moves the head back to the transformed bit, changing the head state to 2. The next two terms generate a path split in the computation basis by moving the head one step to the right and changing the head state to a 3 or a 4 if 0 or 1 is encountered respectively. The computation then stops after producing two paths, each of length 1, after the split. It is a straightforward but tedious exercise to show that $T$ is a power partial isometry. Note that it is sufficient to examine all powers of $T$ and $T^\dagger$ up to the fourth since all higher powers have the same structure as the fourth. Thus the Halmos-Wallen decomposition applies and $T$ can be decomposed into unitary, isometric, coisometric, and finite truncated shift components.

It remains to show that $T$ is stable on some basis. This will be done by explicit construction of the basis in the subspaces associated with each of the components. The unitary component is limited to the subspace spanned by the basis $|0,j,s\rangle$ for all $j$ where $|s\rangle = \bigotimes_{k=-\infty}^{\infty} |0\rangle_k$ is the constant 0 sequence on the lattice. On this subspace, the first term of $T$ in Eq. 37 is the only active term.

For most of the remaining components it suffices to consider a finite section of the lattice consisting of $n$ 0s terminated on both ends by 1s. That is $|s\rangle = |1\rangle_M \bigotimes_{k=M+1}^{L} |0\rangle_k \bigotimes |1\rangle_{L+1} = |s'\rangle \bigotimes |1\rangle_{L+1}$ where $L - M = n$. For all head positions $k$ between $M + 1$ and $L$ in the state $|0,k,s\rangle$, only term 1 is active in the iteration of $T$ or $T^\dagger$ moving the head to either end of the lattice segment. Terms 2 and 3 acting in succession convert the state $|0,L + 1,s\rangle$ into $|1,L,s\rangle v |1\rangle_{L+1}$ into $|2,L + 1,s'\rangle v |1\rangle_{L+1}$.

Both terms 4 and 5 are active in the next iteration of $T$. The state generated is $(a|3\rangle |0\rangle_{L+1} + b|4\rangle |1\rangle_{L+1}) |L + 2,s'\rangle$ where $a = \langle 0|v|1\rangle$, $b = \langle 1|v|1\rangle$. The state shows the

$$T^4 = 1111 + 2111 + 3211 + 4321 + 5321.$$

Here the single digits denote the term numbers in Eq. 37 and the order of the digits gives the order in which each of the $T$ terms appears. Higher powers of $T$ just add more “1” terms to the right of each of the 5 terms of $T^4$. 

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path split in the computation basis with the head state 3 correlated with a 0 bit at site $L+1$
and the head state 4 correlated with a 1 bit at the site.

The next iteration of $T$ annihilates both components of the above state giving the truncation at one end. Thus the two paths are of the same length. The states listed above along with similar ones obtained by iteration of $T^\dagger$ form a stable basis for a truncated shift of length $n+7$. Note that there are an infinite number of copies of this shift since there are an infinite number of basis states spanning the lattice region outside the interval $[M \geq n \geq L + 1]$. Also the $[M - L]$ interval can be shifted to any position on the lattice.

The above description, applied to each value of $n$, gives a description of the stable basis for all truncated shifts of length 8 or more. Setting $L = \infty$ or $M = -\infty$ gives the stable basis for the respective isometric and coisometric components. Stable basis states for the truncated shift components of length $< 8$ can also be easily described.

The above explicit description of a stable basis and the fact that $T$ is a power partial isometry show (Theorem 5) that the Hamiltonian of Eq. 2 describes quantum ballistic evolution for $T$ even though it is nondeterministic. In this case the fact that $T$ is a power partial isometry is sufficient proof since the unitary part is a bilateral shift.

For the step operator as defined each path has length 1 after the split. It is easy to extend the definition of $T$ so that the paths have length $n$ for any $n$. The definition can also be extended so that $T$ is quantum ballistic on some computation subspaces and not on others. This is the case if the terms $Q_3 \sum_j P_{1j} U P_j$ and $Q_4 \sum_j P_{0j} U P_j$ are added to $T$ defined by Eq. 37.
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FIGURE CAPTIONS

Figure 1. Schematic Representation of Quantum Ballistic Paths. The points (as solid circles) represent different basis states in a given basis. The coordinate distance and relative location of the points in the x-y plane has no meaning and is given for illustrative purposes only. Two infinite paths are shown with dashed lines. Path A shows no terminus and path B terminates at state T (no relation to the step operator T). The coefficients for each of two wave packets \( \psi_1(t), \psi_2(t) \) are shown as short vectors at each point on the paths. The coefficients \( c_n(t) \) (Eq. 1) are shown in the figure as \( c_n(t) = r(t)e^{i\theta(t)} \) where polar coordinates are used. The n-dependence of \( r(t) \) and \( \theta(t) \) are shown explicitly.

Figure 2. The Lattice State for Bound State Motion in the Presence of 0s, Section VI-A. The figure shows 1s at \( N \) and \( N+W+1 \) and 0s elsewhere. The solid vertical lines denote the positions at which the bound states are 0 (Eq. 19). As such they correspond to completely reflecting barriers.
