Hamiltonian Models of Quantum Computers which Evolve Quantum Ballistically

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Quantum computation is a subject of much recent interest. In much of the work in the literature [1] quantum computers are described as built up from a sequence of unitary operators where each unitary operator carries out a stage of the overall quantum computation. The sequence and connection of the different unitary operators is provided presumably by some external agent which governs the overall process. However there is no description of a an overall Hamiltonian needed to give the actual quantum dynamics of the computation process.

In this talk, earlier work by the author [2] is followed in that simple, time independent Hamiltonians are used to describe quantum computation, and the Schrodinger evolution of the computation system is considered to be quantum ballistic [3, 4]. However, the definition of quantum ballistic evolution used here is more general than that used in the earlier work. In particular, the requirement that the step operator T associated with a process be a partial isometry, used in [4], is relaxed to require that T be a contraction operator. (An operator T is a partial isometry if the selfadjoint operators $T^\dagger T$ and $TT^\dagger$ are also projection operators. T is a contraction operator if $\| T \| \leq 1$.)

The main purpose of this talk is to investigate some consequences for quantum computation under this weaker requirement. It will be seen that system motion along discrete paths in a basis still occurs. However the motion occurs in the presence of potentials whose height and distribution along the path depends on T and the path states.

The time development of a quantum computation will be taken here to be generated by Hamiltonians constructed from step operators T following the prescription of Feynman [5]:

$$H = K(2 - T - T^\dagger). \tag{1}$$

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In general a step operator for a process is a bounded linear operator T over some separable Hilbert space $\mathcal{H}$ which describes the elementary steps of the process. Successive iterations of T (or $T^\dagger$) on a process system state in $\mathcal{H}$ describe states corresponding to successive steps of the process in the forward (or backward) time direction. Of course Schrodinger evolution with H defined by Eq. 1 is smooth in that the wave function evolves continuously from one step state to the next.

The explicit model for quantum computation used here is the Turing Machine model. In this model a head in any one of a finite number of internal states, l, moves along a two way infinite one dimensional lattice of qubits. The head scans one qubit at a time. The action taken depends on the head state l and the qubit state s. Possible elementary step actions are, changing the head internal state, head motion one site to the right or left, and changing the scanned qubit state. All these changes need not be present in each elementary step operator.

The computation basis is the set of states $\{|j,l,S\rangle\}$ where j and l are the position and internal state label of the head and $|S\rangle = \otimes_{j=-\infty}^{\infty}|S(j)\rangle$ where S is any function from the integers to the set $\{s\}$ of qubit state labels which also satisfies a tail condition. Although qubits which can assume any one of a finite number of states (such as a spin J system) can be used, it is convenient to limit the qubits to be binary systems. In this case the set $\{s\} = \{0,1\}$. A tail condition is needed to keep the number of basis states denumerable. Here the function S is restricted to be such that $S(j) \neq 0$ for at most a finite number of sites. This condition, denoted the 0 state tail condition, is one of a infinite number of possible conditions which could be chosen.

Paths are finite or infinite sequences of states in the computation basis. Each step operator T has a unique collection of paths associated with it in that the paths can be generated by iteration of T or its adjoint on the states in the computation basis. Paths terminate at states annihilated by T or $T^\dagger$.

For a lattice model such as the one used here, the Hamiltonian of Eq. 1 can be written as

$$H = KE + PE \tag{2}$$

where the lattice kinetic and potential energy terms are given by $KE = K(2 - U - U^\dagger)$ and $PE = K(U - T + U^\dagger - T^\dagger)$. U is a bilateral shift which moves the head one site to the right along the lattice. The kinetic energy term is the symmetrized lattice version of the second derivative $-((\hbar)^2/2m)d^2/(dx)^2$.

The form of Eq. 2 shows H with T a step operator for a QTM is equivalent to a 1D tight binding Hamiltonian with off- diagonal potentials. Tight binding models of particle motion in one dimensional solids have been much studied [6] and continue to be studied [7]. This similarity will be exploited here to examine the use the transfer matrix formalism and Landauer resistance [8] as a measure of the probability of a quantum computation to arrive at the Nth

step, with N arbitrary. The usefulness of this derives from the fact that for the generalized definition of quantum ballistic evolution used here, motion of a QTM state along a path in the computation basis with potentials present at some path sites is equivalent to both tunnelling through and partial reflection from barriers provided by the potentials.

In order to maximize clarity and keep things as simple as possible this talk will restrict consideration to QTMs with associated step operators T such that the potentials along the paths on the computation basis are finite square barriers of a fixed height. The locations, widths, and number of barriers can vary from path to path. The ends of paths correspond to the presence of infinite reflecting barriers.

This will be done by requiring T to have the form

$$T = \sum_{j=-\infty}^{\infty} (A_{j,0}P_{j,0} + \gamma A_{j,1}P_{j,1})P_j. \tag{3}$$

Here $P_{j,s}$ and P_j are the respective projection operators for finding the site j qubit in state $|s\rangle$ and the head at site j, and γ is a constant between 0 and 1. $A_{j,s}$ is a sum of all elementary actions associated with the site j qubit in state $|s\rangle$. It is the factor which is different for different QTMs. It is convenient but not necessary to require that the form of $A_{j,s}$ be independent of j. Recall that $s = 0, 1$.

$A_{j,s}$ can be expanded as an operator matrix over the head states. That is $A_{j,s} = \sum_{l,m=0}^{L} \langle m|A_{j,s}|l\rangle$ where

$$\langle m|A_{j,s}|l\rangle = d_{m,l}|m\rangle\langle l|v_{l,s}U_{l,s}. \tag{4}$$

Here $d_{l,m}$ is a constant which assumes the values 0 or 1; $|m\rangle\langle l|$ is the transition operator from head states $|l\rangle$ to $|m\rangle$. $v_{l,s}$ is an arbitrary unitary operator in $U(2)$ which acts on the site j qubit. $U_{l,s}$ is the unitary head shift operator which assumes the values $U, U^\dagger, I$ corresponding to moving one site to the right, to the left, or no motion. U is the bilateral shift on the lattice. The dependence of both $v_{l,s}$ and $U_{l,s}$ on l, s is shown explicitly. L is the number of head states.

The requirement that T be quantum ballistic on the computation basis imposes conditions on $A_{j,s}$. It was shown elsewhere [4] that it is necessary and sufficient that T and $T^\dagger$ be orthogonality preserving and stable on B. These conditions are discussed in detail in [4]. It follows from these conditions that for each value of l $d_{m,l} \neq 0$ for at most one value of m and that $v_{l,s}$ be restricted to be either the identity or the qubit $0-1$ state exchange operator. (For spin 1/2 qubits this is the Pauli operator σ_x for z-axis quantization).

For the most part this corresponds to requiring that T be limited to describing deterministic QTMs only. A limited special class of nondeterministic machines is included (see [4] for an example) but this is of no concern here.

Deterministic machines in the computation basis, are limited to qubit transformations which are the identity or $0-1$ exchanges. Unitary transformations which take qubit states $|0\rangle$ or $|1\rangle$ into linear combinations of these states are excluded. Of course this limitation and definition of determinism can be extended to any arbitrary rotated qubit basis $v|0\rangle, |1\rangle$ by limiting transformations in T to the identity and $v\sigma_x v^\dagger$.

The limitation used here corresponds to association of a potential determined by the constant γ, Eqs. 3 and 4, with just those elementary step operations which correspond to reading a 1 at the qubit site scanned by the head. This corresponds to association of a potential of height $V = 2K(1-\gamma)$ with all computation basis path states for which such operations are active.

It is hoped to analyze some simple examples of these QTMs in the talk and give an analysis of the motion of a quantum computation state as it progresses through potential barriers. This includes calculation of the Landauer resistance [8], which is the ratio of the reflection coefficient to the transmission coefficient, as a function of overall system energy or momentum for these examples.

The property of the Landauer resistance to decrease rapidly from extremely high values, at energies corresponding to forbidden energy regions in appropriate infinite structures, to high values at energies corresponding to allowed energy bands, and even to small values of order unity over *extremely* narrow regions of energy or momentum has been shown by other authors [9], to hold for some distributions of potentials. These include periodic distributions and substitution dynamic distributions.

The usefulness of the Landauer resistance as a measure of the probability for a QTM to complete at least N steps will be examined. For the simple examples for which the Landauer resistance decreases to values of order unity, the usefulness of this as a measure of the completion probability for N steps of the computation will be discussed. Problems associated with the extremely narrow momentum range over which the Landauer resistence is of order unity will be discussed.

1 Acknowledgements

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