Ground State Quantum Computation

Ari Mizel, M. W. Mitchell, and Marvin L. Cohen

Department of Physics, University of California at Berkeley, Berkeley, CA 94720, USA, and Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA.

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We formulate a novel ground state quantum computation approach that requires no unitary evolution of qubits in time: the qubits are fixed in stationary states of the Hamiltonian. This formulation supplies a completely time-independent approach to realizing quantum computers. We give a concrete suggestion for a ground state quantum computer involving linked quantum dots.

The discovery of efficient quantum mechanical factoring and database searching algorithms has fueled tremendous research interest in the field of quantum computing. Much recent effort has been dedicated to the problem of realizing a quantum computer in the laboratory. This problem is technically challenging, in part because it requires overcoming the decoherence of quantum mechanical variables as a result of interactions with the environment. Several experimental systems have been proposed as candidates for quantum computers, and progress has been exciting, but fundamental obstacles still stand in the way of creating viable computers. In this letter, we formulate a novel approach to quantum computing that circumvents the problem of decoherence, which motivates new directions for quantum computer design. Our scheme works exclusively with quantum mechanical ground states, completely obviating the need for time-dependent control of a system. While researchers have considered using quantum mechanical ground states to perform classical computations, the idea of executing quantum algorithms using a ground state computer is an exciting unexplored possibility.

In traditional quantum computation, one examines the development in time of a collection of quantum mechanical “qubits” under controlled unitary evolutions. Each qubit is a two-state system, described by inner products of the quantum mechanical state $|\psi(t)\rangle$ with basis states $|0\rangle$ and $|1\rangle$ associated with the 0 and 1 bit values. As an $N$-step quantum computation proceeds, the 0 and 1 states remain fixed. The state of the system progresses as $|\psi(t)\rangle = U_i |\psi(t_{i-1})\rangle$, $i = 1$ to $N$, where $U_i$ is a unitary operator. The progress of the computation is described by the 2($N+1$) inner products $\langle 0 | \psi(t_i) \rangle$ and $\langle 1 | \psi(t_i) \rangle$, which evolve according to the matrix equation

$$
\begin{bmatrix}
\langle 0 | \psi(t_i) \\
\langle 1 | \psi(t_i)
\end{bmatrix}
= U_i
\begin{bmatrix}
\langle 0 | \psi(t_{i-1}) \\
\langle 1 | \psi(t_{i-1})
\end{bmatrix}.
$$

In our method, the qubits do not change in time; they are fixed in their ground states. The steps in the computation correspond, not to evolution between time points, but rather to development of the ground state between connected parts of the Hilbert space. Here a “qubit” is a single system with 2($N+1$) available states, grouped into ($N+1$) two-state subspaces $\{ |0_i\rangle, |1_i\rangle \}$ one for each stage of the calculation. The ground state of the qubit is a superposition containing at least one component of each subspace, $|\psi_g\rangle = \sum_i |0_i\rangle \langle 0_i | \psi_g \rangle + |1_i\rangle \langle 1_i | \psi_g \rangle$. The progress of the computation is then described in terms of the 2($N+1$) inner products $\langle 0_i | \psi_g \rangle$ and $\langle 1_i | \psi_g \rangle$. As demonstrated below, proper choice of the Hamiltonian leads to a sequence of these inner products according to equation (1), in exact analogy to traditional quantum computation.

Consider the example of a spin 1/2 particle acting as a qubit. In a traditional quantum computation scheme, the basis states $|0\rangle$ and $|1\rangle$ would correspond to states $|\downarrow\rangle$ and $|\uparrow\rangle$, respectively. The state of the particle at time $t_i$, $|\psi(t_i)\rangle$, would evolve from time step to time step by external manipulation of the direction of the particle’s spin. Computation steps would leave the spatial wavefunction of the particle fixed (and irrelevant to the computation). In our approach, the spin 1/2 particle might be contained in the ground state of a box, and this ground state would evolve only trivially in time. However, the Hamiltonian controlling the particles in the box would be designed so that its ground state $|\psi_g\rangle$ possessed a desired non-trivial relationship between spin variables and spatial variables. As a result, the spin of the ground state would develop in a desired way through real space. We would set $|0_i\rangle = |x = x_i, \downarrow\rangle$ and $|1_i\rangle = |x = x_i, \uparrow\rangle$, where the $x_i$ denote successive spatial locations. The quantum computation would proceed via the development of $\langle 0_i | \psi_g \rangle$ and $\langle 1_i | \psi_g \rangle$ in space across the box.

This approach completely eliminates the need for time-dependent control of quantum mechanical variables. Instead, we face the different challenges involved in designing and realizing a tunable static Hamiltonian. While it has been shown that time-dependent quantum computation can be performed with a static “cursor Hamiltonian,” such an approach requires complicated many-particle interactions and time-dependent state preparation and measurement. Our scheme is time-independent in both the Hamiltonian and the state of the computer, and requires only two-particle interactions.
We now propose a more detailed implementation of a ground state quantum computer in the form of an array of quantum dots. A single qubit is realized by a chain of linked quantum dots, as depicted in Fig. 1. At each stage i in the chain, the state \(|i\rangle\) (\(|1\rangle\)) describes an electron localized on the left (right) dot and represents a 0 (1) value for that qubit. This state can be expressed in terms of a creation operator \(c^\dagger_{i0}\) \((c^\dagger_{i1})\), where \(|i\rangle = c^\dagger_{i0} |\text{vac}\rangle\) \((|1\rangle = c^\dagger_{11} |\text{vac}\rangle\)). It is convenient to group creation operators together into \(C^i = [c^\dagger_{i0}\ c^\dagger_{i1}]\).

For the quantum computation, we will design the Hamiltonian to have a twofold degenerate ground state. In particular, the ground states \(|\psi_{g0}\rangle\), \(|\psi_{g1}\rangle\) can be established such that \((1_0|\psi_{g0}\rangle = (0_0|\psi_{g1}\rangle = 0\), while \((0_0|\psi_{g0}\rangle\) and \((1_0|\psi_{g1}\rangle\) are nonzero. These states correspond to input bit values of 0 and 1, respectively.

To implement a particular computation, \(|\psi_{g0}\rangle\) and \(|\psi_{g1}\rangle\) can be designed to develop as required by the algorithm. The algorithm consists of a sequence of unitary transformations \(U_i\), \(i = 1\) to \(N\). In the ground state quantum computer, this transformation requires that the amplitudes of the components of the ground state \(|\psi_{g0}\rangle\) satisfy

\[
\begin{bmatrix}
|0_1|\psi_{g0}\rangle \\
|1_1|\psi_{g0}\rangle
\end{bmatrix} = U_i \begin{bmatrix}
|0_1|\psi_{g0}\rangle \\
|1_1|\psi_{g0}\rangle
\end{bmatrix},
\]

where \((1_0|\psi_{g0}\rangle = 0\). For \(|\psi_{g1}\rangle\) the transformations are analogous but start with \((0_1|\psi_{g1}\rangle = 0\).

For what follows, it is convenient to describe how a ground state with the desired development can be built up row by row. Suppose we already have a single qubit computer consisting of the \(j\) rows 0 to \(j-1\) which implements the first \(j-1\) unitary operations of an algorithm. Denote the ground states of this computer by \(|\psi_{g0}^{j-1}\rangle\)

and \(|\psi_{g1}^{j-1}\rangle\). If we add an additional row \(j\) (yielding \(j+1\) total) to the computer so that the qubit undergoes an additional unitary operation \(U_j\), then the new ground state \(|\psi^j_{g0}\rangle\) is, by equation (2)

\[
|\psi^j_{g0}\rangle = (1 + C^j U_j C^j_{j-1}) \ |\psi^{j-1}_{g0}\rangle
\]

and similarly for \(|\psi^j_{g1}\rangle\). Here and throughout this letter the uninteresting constant factors which maintain normalization of the states have been omitted.

There are many positive semi-definite Hamiltonians that satisfy \(H |\psi_{g0}\rangle = H |\psi_{g1}\rangle = 0\), thus possessing the desired degenerate ground states. For an \(N+1\) row qubit, a particularly convenient Hamiltonian is \(H = \sum_{i=1}^{N} h^i(U_i)\) where

\[
h^i(U) \equiv \epsilon \left[ C^i_{i-1} C_{i-1} + C^i C_i - (C^i U C_{i-1} + \text{h.c.}) \right]
\]

and the constant energy \(\epsilon\) defines the energy scale of the Hamiltonian. This Hamiltonian has an appealing modular character: the unitary matrix \(U_i\) only enters the Hamiltonian through matrix elements between states on rows \(i-1\) and \(i\).

The Hamiltonian described thus far has been constructed to have a degenerate ground state: one state for each possible input value to the algorithm. The complete Hamiltonian for a calculation with a specific input value does not possess this degeneracy. Rather, the on-site energies of the 0th stage quantum dots differ by a small amount. Thus \(|\psi_{g0}\rangle\) or \(|\psi_{g1}\rangle\) is the sole ground state, corresponding to an input bit-value of 0 or 1, respectively. Physically, this can be accomplished by applying a voltage to one of the electrodes indicated in Fig. 1. With the system in its ground state, sensors near the \(N\)th stage quantum dots measure the results of the calculation, i.e., the location of the electron when it is at the output stage.

For generality, we have written the elements of the Hamiltonian in equation (4) in terms of arbitrary unitary transformations. For the case of a quantum-dot computer, tunneling matrix elements between dots can only be tuned to real values. (The tuning could be accomplished physically by placing intermediate quantum dots with controllable voltages in between the primary dots shown in Fig. 1. In this arrangement, the tunneling elements could be changed from run to run in order to implement varied algorithms.) Because the tunneling matrix elements will be real, only real unitary, i.e., orthogonal, transformations can appear in equation (3). Other implementations may not have this restriction. As we show below, the restriction does not impede the implementation of a nontrivial database search algorithm. This is because the matrix elements are real in important single qubit operations like NOT operations.
and rotations by $\pi/4$

$$U = R(\pi/4) = \begin{bmatrix} \cos \pi/4 & \sin \pi/4 \\ -\sin \pi/4 & \cos \pi/4 \end{bmatrix}. \tag{6}$$

However, for some computations, algorithm modifications may be necessary.

So far, we have described the behavior of a single qubit quantum computer. A general quantum computer has $M$ qubits each of which requires two columns of $(N+1)$ dots for an $N$-step computation. Suppose that, at the $j$th stage of the calculation, the algorithm specifies the $M$ qubit operation $U_j$ consisting of independent operations for each qubit. In analogy to equation (3), if $|\Psi^{j-1}_n\rangle$ is the ground state of a $j$ row quantum-dot computer with input $n$ then

$$|\Psi^j_n\rangle = \prod_{a=1}^{M}(1 + C_{a,j}^t U_{a,j} C_{a,j-1}) |\Psi^{j-1}_n\rangle. \tag{7}$$

$$|\Psi^j_n\rangle = \left(1 + c_{A,j,0}^t c_{A,j-1,0} + C_{B,j}^t C_{B,j-1,1} + c_{A,j,1}^t c_{A,j-1,1} + C_{B,j}^t N C_{B,j-1,1}\right) \prod_{a\neq A,B} (1 + C_{a,j}^t U_{a,j} C_{a,j-1}) |\Psi^{j-1}_n\rangle \tag{9}$$

where $N$ is the NOT operation matrix (5).

This state is the ground state of the enlarged quantum computer if the enlarged Hamiltonian is

$$H^j = H^{j-1} + h_{A,B}^j (\text{CNOT}) + \sum_{a=1, a\neq A,B}^M h_a^j (U_{a,j}) \tag{10}$$

where $h_{A,B}^j (\text{CNOT})$ is the addition to the Hamiltonian which effects the CNOT operation.

$$h_{A,B}^j (\text{CNOT}) = \epsilon C_{A,j-1}^t C_{A,j-1} C_{B,j}^t C_{B,j} + h_a^j (I) C_{B,j-1} C_{B,j-1} + c_{A,j,0}^t c_{A,j,0} h_a^j (I) + c_{A,j,1}^t c_{A,j,1} h_a^j (N). \tag{11}$$

The terms (11) and (12) ensure that it is only when the target qubit $B$ enters the gate, that the control qubit $A$ can pass through with an identity operation. If control qubit $A$ has value 0 once it passes through to row $j$, then $c_{A,j,0}^t c_{A,j,0}$ is non-zero and term (13) subjects qubit $B$ to an identity operation. Term (14) ensures that qubit $B$ is subjected to a NOT operation when qubit $A$ has value 1 at row $j$.

Here we have introduced an additional index $a$ on each operator in order to specify to which qubit it pertains. This relation has the property that if $P_j = \prod_a C_{a,j}^t C_{a,j}$ projects onto the subspace in which all electrons are in the $j$th row, then

$$P_j |\Psi^j_n\rangle = U_j A_{j,j-1} P_{j-1} |\Psi^{j-1}_n\rangle, \tag{8}$$

where $A_{j,k} = \prod_a C_{a,j}^t C_{a,k}$ simply moves the electrons from row $k$ to row $j$. In this way the development of the state reflects the unitary evolution of the algorithm. If the Hamiltonian describing the $j$ row computer (which accomplishes $j-1$ operations) is $H^{j-1}$, then the Hamiltonian for the $j+1$ row computer is $H^j = H^{j-1} + \sum_{a=1}^M h_a^j (U_{a,j})$.

In addition to single-bit operations, a general quantum computer must perform multiple qubit operations such as the controlled-NOT operation (CNOT). Assume the algorithm specifies as the $j$th operation $U_j$ a CNOT of qubit B by qubit A and unitary operations $U_{a,j}$ on the other qubits $a \neq A, B$. Equation (8) still holds provided the state of the enlarged array is

$$\text{FIG. 2. Section of a two q-bit ground state quantum computer that implements a controlled NOT operation. Arrows mark conditional tunneling paths.}$$

In Fig. 2, we suggest how the controlled-NOT gate could be realized physically in a quantum-dot implementation. The connection (13)-(14) proceeds through two-body interactions, in which the electric field of the electron in the control qubit influences the tunneling matrix elements and on-site energies in the target qubit and vice versa.

The generalization of the state development and construction of the Hamiltonian to operations involving multiple simultaneous CNOT operations is straightforward. The incremental construction of the ground state and
the projection property of equation (8) guarantee that the state of the full quantum computer represents the full algorithm in that

\[ \Psi_n^N = U_N U_{N-1} \ldots U_1 A_{N,0} P_0 |\Psi_0^N\rangle. \]  

(15)

As in the single qubit computer, the initial state of the register \( P_0 |\Psi_0^N\rangle \) is selected physically by biasing one of the initial stage quantum dots for each qubit. This selects as input the binary representation of a number between 0 and \( 2^M - 1 \).

At this point, we have outlined a functioning quantum computer with both one and two qubit gates. For purposes of illustration, we now detail the specific implementation of a two-bit database search, developed by Grover \[4,5\] and described and implemented in an NMR system by Chuang, Gershenfeld, and Kubinec \[7\]. Following the description of reference \[4\], we note that the algorithm requires the operators \( W, C, \) and \( P, \) where \( W \) is a Walsh-Hadamard transform, \( C \) is a conditional sign flip, and \( P \) is a different conditional sign flip. These operators can be implemented in the following manner.

The operation \( W \) consists of a rotation by \( \pi/4 \) and a NOT for each qubit. To achieve these single bit operations, we add two rows to each qubit, one for the rotation and one for the NOT.

The operation \( C \) is a conditional sign flip which changes the sign of the state if and only if both qubits are in the 1 state. This operation can be implemented by rotating the second bit by \( \pi/4 \), doing a NOT of the second bit if the first bit has a value of 1, and then rotating the second bit by \( -\pi/4 \). Thus \( C \) requires that we add three more rows to each qubit.

The other conditional sign flip, \( P \), is achieved analogously. It requires an initial rotation of qubit \( a = 2 \) by \(-\pi/4\), a controlled-NOT in which qubit \( a = 2 \) suffers a NOT if qubit \( a = 1 \) has a 0 value, and then a final rotation of qubit \( a = 2 \) by \( \pi/4 \). Thus, like \( C \), \( P \) requires three rows in each qubit.

From our analysis of the operations \( W, C, \) and \( P, \) it follows that the most naive implementation of the full algorithm \( WPWCW \) will require 12 rows total, plus an initial input row. This number can be reduced by taking advantage of cancellations and other improvements.

In conclusion, we have presented a new ground state approach to quantum computation. With this scheme, many of the technical problems associated with realizing a traditional quantum computer are circumvented, while different challenges arise. Time-dependent or time-independent perturbations of the Hamiltonian could introduce errors into the calculation. Static perturbations due to imperfect implementation of the requisite Hamiltonian will adversely influence the ground state. Thus ground state quantum computation does not require time-dependent control of a system, but it does demand fine tunability of a static Hamiltonian. Time-dependent perturbations such as thermal fluctuations are capable of exciting the system out of the ground state. In a traditional quantum computation these fluctuations would lead to decoherence. To the extent that such excitations can be quenched by large energy level spacings and low temperatures, they do not disturb ground state quantum computation.

The implementation that we have proposed using quantum dot arrays may or may not be suitable for overcoming these sources of error. While the quantum-dot implementation may seem technically challenging, it is encouraging to note that a classical computation scheme using coupled quantum dots has been implemented \[2\]. Certainly, many other implementations could be envisioned; for example, the states \( |0\rangle \) and \( |1\rangle \) of a single qubit could take different locations in momentum space rather than different locations in real space.

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