Quantum Computing, NP-complete Problems
and
Chaotic Dynamics

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Abstract

An approach to the solution of NP-complete problems based on quantum computing and chaotic dynamics is proposed. We consider the satisfiability problem and argue that the problem, in principle, can be solved in polynomial time if we combine the quantum computer with the chaotic dynamics amplifier based on the logistic map. We discuss a possible implementation of such a chaotic quantum computation by using the atomic quantum computer with quantum gates described by the Hartree-Fock equations. In this case, in principle, one can build not only standard linear quantum gates but also nonlinear gates and moreover they obey to Fermi statistics. This new type of entaglement related with Fermi statistics can be interesting also for quantum communication theory.

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1 Introduction

There are important problems such as the napsack problem, the traveling salesman problem, the integer programming problem, the subgraph isomorphism problem, the satisfiability problem that have been studied for decades and for which all known algorithms have a running time that is exponential in the length of the input. These five problems and many other problems belong to the set of NP-complete problems. Any problem that can be solved in polynomial time on a nondeterministic Turing machine is polynomially transformed to an NP-complete problem [1].

Many NP-complete problems have been identified, and it seems that such problems are very difficult and probably exponential. If so, solutions are still needed, and in this paper we consider an approach to these problems based on quantum computers and chaotic dynamics.

It is widely believed that quantum computers are more efficient than classical computers. In particular Shor [2] gave a remarkable quantum polynomial-time algorithm for the factoring problem. However, it is unknown whether this problem is NP-complete.

The computational power of quantum computers has been explored in a number of papers. Bernstein and Vazirani [3] proved that BPP⊆BQP⊆PSpace. Here BPP stands for the class of problems efficiently solvable in the classical sense, i.e., the class of problems that can be solved in polynomial time by probabilistic Turing machines with error probability bounded by 1/3 for all inputs. The quantum analogue of the class BPP is the class BQP which is the class of languages that can be solved in polynomial time by quantum Turing machines with error probability bounded by 1/3 for all inputs.

The question whether NP⊆BQP, i.e., can quantum computers solve NP-complete problems in polynomial time, was considered in [4]. It was proved in [4] that relative to an oracle chosen uniformly at random, with probability 1, the class NP can not be solved on a quantum Turing machine in time \(o(2^{n/2})\). An oracle is a special subroutine call whose invocation only costs unit time. This result does not rule out the possibility that NP⊆BQP but it does establish that there is no black-box approach to solving NP-complete problems in polynomial time on quantum Turing machines. We would like to mention that these results are not immediately applicable to the chaotic quantum computer which we consider in this paper.

For a recent discussion of computational complexity in quantum comput-
ing see [5, 6, 7]. Mathematical features of quantum computing and quantum information theory are summarized in [8]. A possibility to exploit nonlinear quantum mechanics so that the class of problems \( \text{NP} \) may be solved in polynomial time has been considered by Abrams and Lloyd in [9]. It is mentioned in [9] that such nonlinearity is purely hypothetical; all known experiments confirm the linearity of quantum mechanics.

The satisfiability problem (SAT), which is \( \text{NP} \)-complete problem, has been considered in quantum computing in [10]. It was shown in [10] that the SAT problem can be solved in polynomial time by using a quantum computer under the assumption that a special superposition of two orthogonal vectors can be physically detected. The problem one has to overcome here is that the output of computations could be a very small number and one needs to amplify it to a reasonable large quantity.

In this paper we propose that chaotic dynamics plays a constructive role in computations. Chaos and quantum decoherence are considered normally as the degrading effects which lead to an unwelcome increase of the error rate with the input size. However, in this paper we argue that under some circumstances chaos can play a constructive role in computer science. In particular we propose to combine quantum computer with the chaotic dynamics amplifier. We will argue, by using the consideration from [10], that such a chaotic quantum computer can solve the SAT problem in polynomial time.

As a possible specific implementation of chaotic quantum computations we discuss the recently proposed atomic quantum computer [11]. It is proposed in [11] to use a single atom as a quantum computer. One can implement a single qubit in atom as a one-particle electron state in the self-consistent field approximation and multi-qubit states as the corresponding multi-electron states represented by the Slater determinant.

A possible realization of the standard quantum gates in the atomic quantum computer by using the electron spin resonance has been discussed in [11]. In this paper we argue that in the atomic quantum computer one can build also nonlinear quantum gates because the dynamics of the multi-electron atom in the very good approximation is described by nonlinear Hartree-Fock equations.

The tensor product structure of states is very important for computations and the multielectron atom admits such a structure. More exactly, instead of the standard tensor product used in quantum computing we have to use the Slater determinant to take into account the Fermi statistics. The standard computational basis in quantum computing does not have Bose or Fermi
symmetry. In the atomic case we have to make an appropriate modification of quantum gates to take into account Fermi statistics and this leads to a new type of entanglement related with Fermi statistics.

Such Fermi or Bose entanglement could be interesting also for quantum communication theory, in particular for quantum teleportation [22, 23].

2 SAT Problem

Let \( \{x_1, \ldots, x_n\} \) be a set of Boolean variables, \( x_i = 0 \) or \( 1 \). Then the set of the Boolean variables \( \{x_1, \overline{x}_1, \ldots, x_n, \overline{x}_n\} \) with or without complementation is called the set of literals. A formula, which is the product (AND) of disjunctions (OR) of literals is said to be in the product of sums (POS) form. For example, the formula

\[
(x_1 \lor \overline{x}_2) (\overline{x}_1) (x_2 \lor \overline{x}_3)
\]

is in POS form. The disjunctions \( (x_1 \lor \overline{x}_2), (\overline{x}_1), (x_2 \lor \overline{x}_3) \) here are called clauses. A formula in POS form is said to be satisfiable if there is an assignment of values to variables so that the formula has value 1. The preceding formula is satisfiable when \( x_1 = 0 \), \( x_2 = 0 \), \( x_3 = 0 \).

**Definition (SAT Problem).** The satisfiability problem (SAT) is to determine whether or not a formula in POS form is satisfiable.

The following analytical formulation of SAT problem is useful. We define a family of Boolean polynomials \( f_\alpha \), indexed by the following data. One \( \alpha \) is a set

\[
\alpha = \{S_1, \ldots, S_N, T_1, \ldots, T_N\},
\]

where \( S_i, T_i \subseteq \{1, \ldots, n\} \), and \( f_\alpha \) is defined as

\[
f_\alpha(x_1, \ldots, x_n) = \prod_{i=1}^{N} \left( 1 + \prod_{a \in S_i} (1 + x_a) \prod_{b \in T_i} x_b \right).
\]

We assume here the addition modulo 2. The SAT problem now is to determine whether or not there exists a value of \( x = (x_1, \ldots, x_n) \) such that \( f_\alpha(x) = 1 \).
3 Quantum Algorithm

We will work in the \((n + 1)\)-tuple tensor product Hilbert space \(\mathcal{H} \equiv \otimes_{1}^{n+1} \mathbb{C}^{2}\) with the computational basis

\[ |x_1, \ldots, x_n, y \rangle = \otimes_{i=1}^{n} |x_i \rangle \otimes |y \rangle \]

where \(x_1, \ldots, x_n, y = 0 \) or \(1\). We denote \(|x_1, \ldots, x_n, y \rangle = |x, y \rangle\). The quantum version of the function \(f(x) = f_\alpha(x)\) is given by the unitary operator \(U_f |x, y \rangle = |x, y + f(x) \rangle\). We assume that the unitary matrix \(U_f\) can be built in the polynomial time, see [10]. Now let us use the usual quantum algorithm:

(i) By using the Fourier transform produce from \(|0,0 \rangle\) the superposition

\[ |v \rangle = \frac{1}{\sqrt{2^n}} \sum_{x} |x, 0 \rangle. \]

(ii) Use the unitary matrix \(U_f\) to calculate \(f(x)\):

\[ |v_f \rangle = U_f |v \rangle = \frac{1}{\sqrt{2^n}} \sum_{x} |x, f(x) \rangle. \]

Now if we measure the last qubit, i.e., apply the projector \(P = I \otimes |1 \rangle \langle 1|\) to the state \(|v_f \rangle\), then we obtain that the probability to find the result \(f(x) = 1\) is \(\|P |v_f \rangle\|^2 = r/2^n\) where \(r\) is the number of roots of the equation \(f(x) = 1\). For small \(r\) the probability is very small and this means we in fact don’t get an information about the existence of the solution of the equation \(f(x) = 1\).

Let us simplify our notations. After the step (ii) the quantum computer will be in the state

\[ |v_f \rangle = \sqrt{1 - q^2} |\varphi_0 \rangle \otimes |0 \rangle + q |\varphi_1 \rangle \otimes |1 \rangle \]

where \(|\varphi_1 \rangle\) and \(|\varphi_0 \rangle\) are normalized \(n\) qubit states and \(q = \sqrt{r/2^n}\). Effectively our problem is reduced to the following 1 qubit problem. We have the state

\[ |\psi \rangle = \sqrt{1 - q^2} |0 \rangle + q |1 \rangle \]

and we want to distinguish between the cases \(q = 0\) (i.e. very small \(q\)) and \(q > 0\). To this end we propose to employ chaotic dynamics.
4 Chaotic Dynamics

Various aspects of classical and quantum chaos have been the subject of numerous studies, see \[12\] and ref’s therein. The investigation of quantum chaos by using quantum computers has been proposed in \[13, 14, 15\]. Here we will argue that chaos can play a constructive role in computations.

Chaotic behaviour in a classical system usually is considered as an exponential sensitivity to initial conditions. It is this sensitivity we would like to use to distinguish between the cases $q = 0$ and $q > 0$ from the previous section.

Consider the so called logistic map which is given by the equation

$$x_{n+1} = ax_n(1 - x_n), \quad x_n \in [0, 1].$$

The properties of the map depend on the parameter $a$. If we take, for example, $a = 3.71$, then the Lyapunov exponent is positive, the trajectory is very sensitive to the initial value and one has the chaotic behaviour \[12\]. It is important to notice that if the initial value $x_0 = 0$, then $x_n = 0$ for all $n$.

\[
\begin{array}{c}
\text{Fig.1. Change of } x_n \text{ w.r.t. time } n
\end{array}
\]

It is known \[13\] that any classical algorithm can be implemented on quantum computer. Our stochastic quantum computer will be consisting from two blocks. One block is the ordinary quantum computer performing computations with the output $|\psi\rangle = \sqrt{1 - q^2} |0\rangle + q |1\rangle$. The second block is a quantum computer performing computations of the classical logistic map.
This two blocks should be connected in such a way that the state $|\psi\rangle$ first be transformed into the density matrix of the form

$$\rho = q^2 P_1 + \left(1 - q^2\right) P_0$$

where $P_1$ and $P_0$ are projectors to the states $|1\rangle$ and $|0\rangle$. This connection is in fact nontrivial and actually it should be considered as the third block. One has to notice that $P_1$ and $P_0$ generate an Abelian algebra which can be considered as a classical system. In the second block the density matrix $\rho$ above is interpreted as the initial data $\rho_0$ for the logistic map

$$\rho_{n+1} = a \rho_n (1 - \rho_n)$$

After one step, the state $\rho_1$ becomes

$$\rho_1 = a q^2 (1 - q^2) I,$$

where $I$ is the identity matrix on $\mathbb{C}^2$. In particular, if one has $q = 0$ then $\rho_0 = P_0$ and we obtain $\rho_n = P_0$ for all $n$. Otherwise the stochastic dynamics leads to the amplification of the small magnitude $q$ in such a way that it can be detected. As is seen in Fig.1, we can easily amplify the small $q$ in several steps, i.e., within about ten times measurements as in Shor’s algorithm. The transition from $\rho_n$ to $\rho_{n+1}$ is nonlinear and can be considered as a discrete Heisenberg evolution of the variable $x_n$.

One can think about various possible implementations of the idea of using chaotic dynamics for computations. Below we discuss how one can realize nonlinear quantum gates on atomic quantum computer.

## 5 Atomic Quantum Computer

Many current proposals for the realization of quantum computer such as NMR, quantum dots and trapped ions are based on the using of an atom or an ion as one qubit, see [17, 18, 19, 20]. In these proposals a quantum computer consists from several atoms, and the coupling between them provides the coupling between qubits necessary for a quantum gate. It was proposed in [11] that a single atom can be used as a quantum computer. One can implement a single qubit in atom as a one-particle electron state in the self-consistent field approximation and multi-qubit states as the corresponding multi-electron states represented by the Slater determinant. So, to represent
10 qubits one can use an atom with 10 electrons and to represent 50 qubits one has to control only around 50 levels in an atom with 50 electrons.

A possible realization of the standard quantum gates in the atomic quantum computer by using the electron spin resonance has been discussed in [11]. In this paper we propose that in the atomic quantum computer one can build also nonlinear quantum gates because the dynamics of the multi-electron atom in the very good approximation is described by nonlinear Hartree-Fock equations. Therefore it follows from [11] and the considerations in this paper that the atomic quantum computer can solve the SAT problem in polynomial time.

It is well known that in atomic physics the concept of the individual state of an electron in an atom is accepted and one proceeds from the Hartree-Fock self-consistent field approximation, see for example [21]. The state of an atom is determined by the set of the states of the electrons. Each state of the electron is characterized by a definite value of its orbital angular momentum \( l \), by the principal quantum number \( n \) and by the values of the projections of the orbital angular momentum \( m_l \) and of the spin \( m_s \) on the \( z \)-axis. In the Hartree-Fock central field approximation the energy of an atom is completely determined by the assignment of the electron configuration, i.e., by the assignment of the values of \( n \) and \( l \) for all the electrons.

The tensor product structure of states is very important for computations. Fortunately a multielectron atom admits such a structure. More exactly, instead of the standard tensor product used in quantum computing we have to use the Slater determinant to take into account the Fermi statistics. The standard computational basis in quantum computing does not have Bose or Fermi symmetry. In the atomic case we have to make an appropriate modification of quantum gates to take into account Fermi statistics and this leads to a new type of entanglement related with Fermi statistics.

An application of the electron spin resonance (ESR) to process the information encoded in the hyperfine splitting of atomic energy levels and to build standard linear quantum gates has been considered in [11]. In this paper we suggest that in atomic quantum computer one can build also nonlinear quantum gates described by the Hartree-Fock equations.

The Hamiltonian for the \( N \)-particle system has the form

\[
H = \sum_{i=1}^{N} \left( -\frac{\nabla_i^2}{2m_i} + v(r_i) \right) + \sum_{i<j} V(r_{ij})
\]
In the Hartree-Fock method one takes the $N$-particle wave function in the form of the Slater determinant

$$\Psi(t, r_1, ..., r_N) = \text{Antisym}(\Phi_1(t, r_1) ... \Phi_N(t, r_N))$$

Here the one-particle wave functions $\Phi_i(t, r_i)$ satisfy the nonlinear Hartree-Fock equations which have the form of nonlinear Schrödinger equation

$$i \frac{\partial \Phi_i(t, r)}{\partial t} = H(\Phi) \Phi_i(t, r)$$

where

$$H(\Phi) \Phi_i(t, r) = \left( -\frac{\nabla^2}{2m_i} + v(r) + U_i(t, r) \right) \Phi_i(t, r) - \int \text{d}r' \mathcal{W}(t, r', r) \Phi_i(t, r')$$

and

$$U_i(t, r) = \sum_{j \neq i} \int \text{d}r' \Phi_j^*(t, r') V(r', r) \Phi_j(t, r')$$

$$\mathcal{W}(t, r', r) = \sum_j \Phi_j^*(t, r') V(r', r) \Phi_j(t, r)$$

If we consider only the spin dependent part of the wave function of the one-electron state

$$\varphi = \left( \begin{array}{c} \varphi_0(t) \\ \varphi_1(t) \end{array} \right),$$

then one can get the nonlinear equation of the form

$$i \frac{\partial \varphi}{\partial t} = A\varphi + B(\varphi) \varphi.$$

Here $A$ is a $2 \times 2$ matrix and the matrix $B$ depends on $\varphi$. By using this equation one can describe nonlinear quantum gate. The nonlinearity can be tuned by means of magnetic field.

6 Conclusion

The complexity of the quantum algorithm for the SAT problem has been considered in [10] where it was shown that one can build the unitary matrix
$U_f$ in the polynomial time. We have also to consider the number of steps in the classical algorithm for the logistic map performed on quantum computer. It is the probabilistic part of the construction and one has to repeat computations several times to be able to distinguish the cases $q = 0$ and $q > 0$. Thus it seems that the chaotic quantum computer can solve the SAT problem in polynomial time.

In conclusion, in this paper the chaotic quantum computer is proposed. It combines the ordinary quantum computer with quantum chaotic dynamics amplifier which can be implemented by using the atomic quantum computer. We argued that such a device can be powerful enough to solve the NP-complete problem in polynomial time.

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