«ФИЗИКА ЭЛЕМЕНТАРНЫХ ЧАСТИЦ И АТОМНОГО ЯДРА»
2000, ТОМ 31, ВЫП. 7А

УДК 517.92.87

ATOMIC QUANTUM COMPUTER

I.V.Volovich

V.A.Steklov Mathematical Institute, Moscow, Russia

The 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. In these proposals a quantum computer consists of several atoms and the coupling between them provides the coupling between qubits necessary for a quantum gate. We discuss whether a *single* atom can be used as a quantum computer. One can implement a single qubit in atom as a one-particle electron state and multi-qubit states as multi-particle states. Spin-orbit and spin-spin interactions provide the coupling between qubits. In particular one can use the electron spin resonance (ESR) to process the information encoded in the hyperfine splitting of atomic energy levels. By using quantum state engineering one can manipulate the internal states of the natural or artificial (quantum dot) atom to make quantum computations.

Quantum computers [1–5] have an information processing capability much greater than the classical computers. Considerable progress in quantum computing has been made in recent years. A number of quantum algorithms have been developed [6, 7] and experimental implementations of small quantum computers have been achieved [8–10]. In particular such realizations of quantum computers as NMR [8, 9], ion traps [12], cavity QED [13] and quantum dots [14] have been proposed.

The proposed technologies for realization of quantum computer have serious intrinsic limitations [15]. In particular NMR devices suffer from an exponential attenuation of signal to noise as the number of qubits increase and an ion trap computer is limited by the frequencies of the vibrational modes in the trap. In this note we discuss a possible realization of quantum computer which perhaps can help to avoid these limitations.

Basic elements of quantum computer are qubits and logic elements (quantum gates). A qubit is a two-state quantum system with a prescribed computational basis. The current proposals for the experimental realization of quantum computer are based on the implementation of the qubit as a two-state atom or an ion. Quantum computer in these schemes is a *molecular machine* because it is built up from a number of coupled atoms or quantum dots. Here we propose to do quantum computations using a *single* atom. In this scheme the atomic quantum computer is a single atom. It is interesting to study such an *atomic machine* theoretically but it could have also some advantages for the practical realization with respect to the molecular machines.

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 self-consistent field approximation, see for example [16]. 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.

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-particle states represented by the Slater determinant.

Almost all real spectra can be systematized with respect to LS or jj coupling schemes. Every stationary state of the atom in the LS coupling approximation is characterized by a definite value of the orbital angular momentum L and the total spin S of the electrons. Under the action of the relativistic effects a degenerate level with given L and S is split into a number of distinct levels (the fine structure of the level), which differ in the value of the total angular momentum J. The relativistic terms in the Hamiltonian of an atom include the spin-orbit and spin-spin interaction. There is also the further splitting of atomic energy levels as a result of the interaction of electrons with the spin of the nucleus. This is the hyperfine structure of the levels.

One can use these interactions to build quantum logic gates.

As a simple example let us discuss how the hyperfine splitting can be used to do quantum computations on a single atom. Let us consider the Hamiltonian which includes both nucleus and electron for a case of quenched orbital angular momentum. If one assumes that the electron spin Zeeman energy is much bigger than the hyperfine coupling energy then one gets an approximate Hamiltonian [17]

$$\mathcal{H} = g\beta H S_z - \gamma_n \hbar H I_z + A S_z I_z.$$

Here S_z and I_z are the electron and nuclear spin operators, H is the magnetic field which is parallel to the z-axis, β is the Bohr magneton, γ_n is the nuclear gyromagnetic ratio, A is the hyperfine coupling energy and g is the g-factor.

Let us consider the simplest case of nuclear and electron spins of 1/2. Then a single qubit is a nuclear spin $|m_I>$ and electron spin $|m_S>$ function, where m_I and m_S stand for eigenvalues of I_z and S_z. The two-qubit states are the eigenfunctions of the Hamiltonian $\mathcal{H}$ and they are given by the product of the nuclear spin and electron spin functions

$$|m_I, m_S> = |m_I> |m_S> .$$

The coupling used to produce magnetic resonances is an alternating magnetic field applied perpendicular to the static field. The possible transitions produced by an

alternating field are found by considering a perturbing term in the Hamiltonian

$$\mathcal{H}_m(t) = (\gamma_e \hbar S_x - \gamma_n \hbar I_x) H_x \cos \omega t.$$

Many of the basic principles of nuclear magnetic resonance apply to electron magnetic resonance (ESR). However there are some special features of spin echoes that arise for electron spin resonance which are not encountered in nuclear magnetic resonance. This is because in many cases the nuclear quantization direction depends on the electron spin orientation.

It is well known that any quantum algorithm can be implemented with one-qubit rotations and two-qubit controlled-NOT gate, see [4, 5, 18]. The implementation of the controlled-NOT gate by using pulse sequences is well known in NMR [8–10]. For example it can be represented as a network which includes one qubit Hadamard gates and a 4×4 matrix which can be implemented as the following pulse sequence

$$(90^\circ I_z)(90^\circ S_z)(-90^\circ 2 I_z S_z).$$

Two-qubite realizations of the Deusch–Jozsa algorithm and the Grover algorithm have been accomplished using NMR spectroscopy of spin 1/2 nuclei of appropriate molecules in solution [8–10]. One can use the similar technique in the case of ESR.

If computers are to become much smaller in the future, the miniaturization might lead to the atomic quantum computer. One of the advantages of the atomic quantum computer is that quantum state of a single atom can be stable against decoherence, for a discussion of the decoherence problem in quantum computing see [5, 15, 19] and references therein. Recent experimental and theoretical advances on quantum state engineering with a natural and artificial (quantum dots) atoms [20–24] and the development of methods for completely determining the quantum state of an atom [25] show that quantum computations with a single atom should be possible.

To summarize, I propose using a single atom to do quantum computations. Such an atom can be also used, of course, as a part of a computational network. I discussed the simple realization of the two-qubit atomic quantum computer based on ESR and hyperfine splitting. However the idea of atomic quantum computer is more general. To build a multi-qubit atomic quantum computer one has to use the fine and hyperfine splitting of energy levels to process the information encoded in the multielectron states. In principle one can build an atomic quantum computer based on a natural or artificial (quantum dot) atom.

Recently, the atomic quantum computer and stochastic dynamics have been used to investigate NP-complete problems [26].

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