Nuclear Spin Network Quantum Computers

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1 Quantum Computation

Quantum computation is a radical paradigm of information processing in which genuine quantum effects such as superposition, entanglement, and interference are utilized to drastically speed up solution finding. The striking power of quantum computation is best demonstrated by Shor's factoring algorithm[1] which may break the public key cryptography widely used in today's information society. However the demonstration is so far only in theory and experimental realization is regarded as one of the most challenging goals in physics of the next century.

A building block of a quantum computer is a quantum bit (qubit) which allows superposition of 0 and 1 and also allows interaction with other qubits for unitary operations. Quantum algorithms are very fast because they can explore exponentially large number (2^n for n-qubits) of possibilities simultaneously by quantum parallelism of superposition state and unitary operations, and then enhance the success probability by quantum interference.

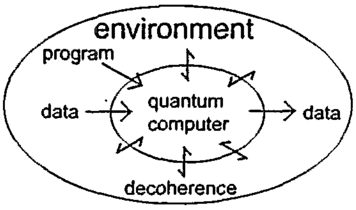

Figure 1: Quantum computer and environment

The major difficulty comes from inability of maintaining quantum coherence over a macroscopic object like a computer during a whole computation process. The decoherence arises from interactions with environment. Therefore the quantum computer must be isolated from the environment in order to avoid decoherence. On the other hand, it must be interfaced to the macroscopic world for users to feed program and data and read the results as shown in Fig.1. These two requirements often contradict.

Various physical implementations[2] of quantum computation have been proposed and some of them have been studied experimentally.

2 Quantum Computer in a Molecule

Nuclear spin is one of the most promising candidates for qubit because of relatively long coherence time and suitable couplings for quantum operations between qubits. Nuclei with spin 1/2 (Fig.2), such as ^{1}H, ^{19}F, ^{31}P, ^{13}C, or ^{15}N can be used as qubit and manipulated by nuclear magnetic resonance (NMR) technique. Quantum computation using nuclear spins in solution molecule was proposed in 1996[3,4] and demonstrated in 1998.[5] In this scheme, a molecule (for example, Fig. 3) in a static magnetic field works as a quantum computer. Each qubit is addressed by its magnetic resonance frequency. Any single qubit operation can be realized as rotation(s) of spin by resonant RF magnetic field pulse(s). Two qubit operation can be performed using J- (or scalar) coupling between nuclear spins. J-coupling results in quantum operation called controlled-rotation which rotates one qubit depending on the state of the other qubit and *vice versa.* Any unitary operation can be realized by combination of these two operations.

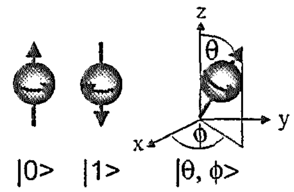

Figure 2: Spin $\frac{1}{2}$ as a qubit

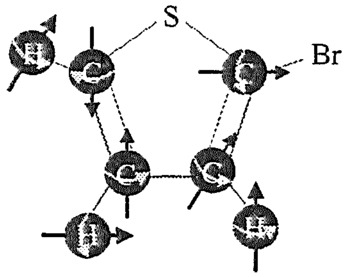

Figure 3: Molecule as a quantum computer

3 More Qubits for Quantum Computation

Quantum algorithms have been so far demonstrated in very small molecules with only a few qubits of nuclear spins. IBM has recently reported 5-qubit quantum computer[6] using molecule.

However, increasing the number of qubits by increasing the size of molecules is not at all straightforward since resonant frequencies get closer or degenerated, couplings get sparser, decoherences get faster, and signals get exponentially weaker. We discuss these problems in the following subsections. It is widely recognized that the current form of NMR quantum computation lacks scalability and will not go beyond 10-qubit.[3,4,7,8] Our research goal is to challenge this limit and seek the way towards scalable quantum computer.

3.1 Quantum Circuit

When the number of qubits is increased, frequency separations between qubits decrease because available spectral resource is limited. To control each qubit independently, pulse lengths must be increased roughly in proportion to the number of qubits. This leads to slower operations. Also it is very difficult to find a molecule with many distinguishable qubits.

In a small molecule with up to several qubits, all qubits may be directly connected with each other by J-couplings and two-qubit operation on any pair may be performed easily. As the number of qubits increases, couplings between separated qubits get weaker or disappear. This leads to slower operations. It also requires different strategy for implementing quantum circuit on sparse network of qubits.

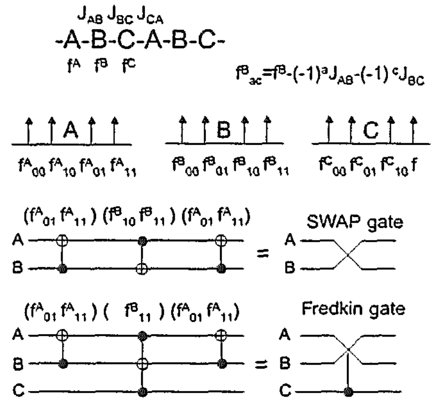

Figure 4: Polymer Quantum Circuit

One dimensional polymer with $(ABC)_n$ structure was proposed as a possible architecture of quantum computer with only nearest neighbor couplings.[9] By applying line selective π pulses, SWAP gate and controlled-SWAP gate (Fredkin gate) can be constructed as shown in Fig. 4. Only limited number of frequencies are needed regardless of the number of qubits. Experimental demonstration of the architecture is one of our research goals.

3.2 Initialization

The initial state of NMR quantum computer is so far thermal equilibrium at room temperature. Since the thermal energy is much (5 orders of magnitude) larger than Zeeman energy, every state is almost equally populated with a population 2^{-n}. The number of molecules with a specific initial state decreases exponentially with the number of qubits n and so does the signal strength. Therefore NMR quantum computation with more than 10-qubit seems hopeless unless nuclear spins are initialized by some physical means. Initialization of nuclear spins is the most important subject of our research.

4 Our Project

Our project consists of four groups. 1) Molecular Quantum Computer group, 2) Crystal Quantum Computer group, 3) Photonic Quantum Computer group, and 4) Quantum Computation Theory group. Molecular Quantum Computer group is mainly working on molecular quantum circuits and initialization of nuclear spins in molecules. Crystal Quantum Computer group is working on materials and NMR technique including initialization for quantum computer using nuclear spins in crystal.[10] Photonic Quantum Computer group is working on complimentary experiments such as quantum error correction[11] using linear optics.[12] Quantum Computation Theory group is working on the theoretical aspects of quantum computation.

5 Summary

We work on many-qubit quantum computers which utilize regularly aligned nuclear spins and their coupling network in polymers or crystals with the emphases on large-scale quantum circuit synthesis, material search and development, and physical initialization of nuclear spins.

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