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GENERALIZED TURING QUANTUM MACHINE AND ITS ALTERNATIVE BULK NMR IMPLEMENTATION

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Abstract: The purpose of the present paper is twofold. First, we introduce the notion of a generalized version of both the classical and quantum Turing computational models, namely, Turing machine able to act in a single step on any finite continuous segment of its band. Second, we produce an alternative bulk NMR implementation of such a generalized Turing machine. The qualifier "alternative" denominates our new and greatly simplified bulk NMR technique of experimental quantum computational modeling which offers the possibility to work with nuclear magnetic resonance on macroscopic materials, either liquid or solid and as primitive as water or solid xenon.

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1. Two Challenges of Realistic Quantum Computing: Qubits and Architecture Implementation

The research on Quantum Information Processing (*QIP*), see [1], both in its theoretical and experimental dimensions, became today an engrossing, flourishing and extremely fruitful enterprise, even though an eventual justification of its most important inspirational sources and a realistic attainability of its ultimate double objective, a viable quantum computer and a both manageable and effective theory of quantum computations / Algorithms, remain almost as intriguing, remote and uncertain as ever : "*The most interesting thing that might come out of an attempt to build a quantum computer is the discovery that we can't do it*", see [3]. In more practical terms, we are still trying to "*understand origins of the fragility of quantum computers in theoretical and laboratory settings*" and to "*find ways to make quantum information processing robust against corruption both at the theoretical and experimental levels*", see [4].

The present paper is the first installment of the report on our study of a new promising theoretical and experimental approach exploiting the *Nuclear Magnetic Resonance* (*bulk NMR*) technology for the purpose of quantum computing.

In classical *bulk NMR* quantum computing techniques a suitable molecule is chosen as quantum computing processor, with parts of the molecule representing distinguishable qubits. The qubits interact by spin-spin couplings but qubits that are not connected directly have to interact via intermediate qubits. There is no real choice of architecture in such a quantum computer: once the molecule is chosen the architecture is fixed, see [2].

In the approach advanced by the present project, the material bearer of the quantum processor is a macroscopic cylinder of liquid (water) and, potentially, of solid material (frozen xenon), with a qubit being not a part of a molecule but rather a frequency range created by applying a gradient to the magnetic field. We present below the techniques of effective manipulation of individual qubits: the techniques of one argument quantum gates (*1-qugates*). We are researching now several ways for designing two and three arguments quantum gates (*2- and 3-qugates*), and we will report on our progress in this domain in coming installments of our report.

If and when such gates will be available, we will have a scalable quantum computer based on the principle that increasing the number of qubits is achieved by decreasing the different frequency ranges. This is in stark contrast with the

classical NMR method where increasing the number of qubits involves finding an entire new molecule. The main potential advantage of our approach is a greater than in the traditional bulk NMR computing freedom in the choice of computer architecture: as the qubits are linearly separated in frequency, the corresponding linear array could be furnished with an architecture of *generalized Turing quantum machine*, able to act in a single step both on individual qubits and on any finite continuous segment of its infinite (to the left, to the right, or in both directions) band.

2. Experimental and Theoretical Background of the NMR Experiment

The best known experimental quantum computing with five to seven qubits was obtained by bulk NMR on different types of molecules, see [2]. In NMR implementations of QIP, a qubit is defined by the resonance frequency of a nuclear spin in its local magnetic field i.e. the applied magnetic field B_0 corrected by a shield due to the surrounding electrons. The initial step of QIP is to define a pure quantum state which is masked by the fact that for bulk NMR the spin system is a statistical ensemble and the correct description of the system is given by the use of the density matrix formalism. The J coupling between two nuclear spins induces coherences of nuclear spin states revealing, via interference effects, the quantum nature of the system. The first demonstration of spinor character for spin $\frac{1}{2}$ nucleus via NMR interferometry using the J coupling was performed by M.E. Stoll et al using ^{13}C enriched sodium formate ($NaCHO_2$) dissolved in D_2O. In absence of a constant coupling between the spin states, spin interferences have been observed with a neutron beam interferometer in 1975. Already in 1950, N.F. Ramsey showed that two successive $\pi/2$ pulses can induce atomic state interferences, the so called Ramsey fringes. Recently it was shown that superconducting tunnel junction circuit displayed signatures of macroscopic quantum behavior as Ramsey fringes. Here we will show that such interference effects can be detected in bulk water at room temperature.

The theoretical description of a system considers a macroscopic amount of N identical spins $I = \frac{1}{2}$ immersed in a static B_0 magnetic field for a long time:

$$\mathfrak{H} = -\mu \cdot B_0 = \gamma \cdot I \cdot B_0, \tag{1}$$

where γ is the gyromagnetic ratio of the spin I. The magnetic field direction is the most natural quantum axis along which one can define two eigenvectors

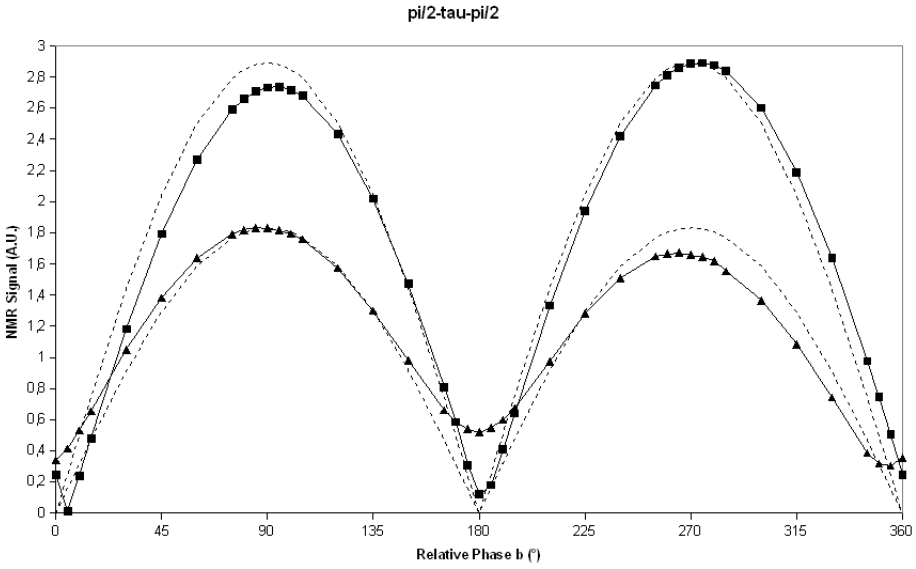

Figure 1: Amplitude of the NMR signal of $10m$ml of water after two $\pi/2$ pulses versus the relative phase β of the two pulses. Continuous line (■ NMR_1) is obtained in a high a homogeneous magnetic field, large dashed (▲ NMR_2) line in a less homogeneous field. Fine dashed lines correspond to $f(\beta) = G\,|\sin\beta|$ normalized to the maximum NMR signal in each case.

$|-\rangle$ and $|+\rangle$ of respective energies:

$$E_- = -\frac{1}{2}\gamma \cdot B_0 = -\frac{\omega_0}{2}\,, \quad E_+ = \frac{1}{2}\gamma \cdot B_0 = \frac{\omega_0}{2}, \tag{2}$$

where $\omega_0 = \gamma \cdot B_0$ is the angular frequency of the allowed transition between $|-\rangle$ and $|+\rangle$. As there is a statistical ensemble of N nuclear spins, one has to consider the density matrix of the system. If one applies two $\pi/2$ pulses with a relative phase β of the second pulse versus the phase of the first pulse separated by a delay τ, one can calculate the transverse magnetisation M_x using the density matrix formalism:

$$M_x = \frac{d}{2}\sin\omega_0\tau\sin\beta, \tag{3}$$

where d is the Boltzmann factor $\Delta E/kT$. One can easily see that in absence of free evolution, i.e. $\tau = 0$, there is no signal. This is due to the fact that in the $\tau = 0$ case, the $\pi/2 - \tau - \pi/2$ sequence corresponds to a single π pulse on the

sample which gives no signal.

3. Material and Methods

A sample of 10ml of degassed water was placed at room temperature in a wide-bore magnet with a magnetic field of 4.7T (Magnex). The NMR spectrometer (SMIS) allows a phase precision of the RF pulses of 0.25°. The RF pulses had a Gaussian shaped intensity with a duration of 600μs, a frequency $\omega_0/2\pi = 200,137$MHz, and half-width of 3000Hz. The inter pulse delay between the ends of the first and second pulse was $\tau = 1$ms. The NMR signal was detected in quadrature mode with a sample frequency of 5000Hz and 8K points. The intensity of the signal is obtained as the modulus of the 2 parts given by the quadrature detection mode. The homogeneity of the magnetic field was measured by the line width obtained by Fourier transform of the free induction decay (FID) acquired after a $\pi/2$ pulse. T1 measured by inversion-recovery sequence was 3.2s and T2 measured by a Carr-Purcell-Meiboom-Gill sequence was 1.8s slightly depending on the homogeneity of the magnetic field. NMR spectrum of pure water, as for all liquid sample with no J coupling, displays a very narrow line due to the motion averaging of the dipole-dipole coupling. Such a nuclear spin system is highly isolated from its surrounding and it is well-known that the relaxation time T1 which characterizes the energy exchange with the lattice and the inverse of the line width which measures the decoherence time are very long in high homogeneous magnetic field.

4. Results

Experimentally, it was impossible for us to tune τ at a time scale small enough to vary $\omega_0\tau$ over 2π. However, it is possible to ensure over typical experimental time (few minutes) an accurate stability of $\omega_0\tau$, i.e. the rms magnitude of the fluctuating part of this angle $\omega_0\tau$ remains much smaller than 2π. Under this last condition, one can then plot the NMR signal given by the $\pi/2 - \tau - \pi/2(\beta)$ sequence as a function of β, the relative phase of the two $\pi/2$ pulse fields and compare the results to that given by equation (3). If the experimental data match equation (3), then the nuclear spin interference term is revealed and also controlled.

The NMR signal (FID) after a single $\pi/2$ pulse is mainly dependent on the homogeneity of the magnetic field B_0. Figure 1 shows the amplitude of the

NMR signal at the beginning of the FID versus the relative phase β.

As seen in Figure 1, in the case of a highly homogeneous magnetic field ($\Delta B_0/B_0 = 2.0{\cdot}10^{-8}$), $f(\beta) = G\,|\sin\beta|$ (given by equation (3) for a well defined value of $\omega_0\tau$) fits the experimental data pretty well. The maximum relative deviation $\Delta s\,(\beta) = \frac{(\mathrm{NMR}_1(\beta) - f(\beta))}{\max(\mathrm{NMR}_1(\beta))}$ between the experimental curve $\mathrm{NMR}_1\,(\beta)$ and $f(\beta)$ is found to be $\Delta s(15^\circ) = 9.7\%$. In the case of a less homogeneous field ($\Delta B_0/B_0 = 2.7 \cdot 10^{-7}$), the fit is less good and the maximum relative deviation is found to be $\Delta s(18^\circ) = 28.3\%$.

5. Conclusion

We have shown here, that if the homogeneity of the static and RF magnetic fields are controlled at an enough high accuracy, we can control the nuclear spin interference term out the macroscopic sample of water molecules up to a maximum relative deviation of 9.7%. This number may certainly be decreased by giving additional care to the experimental set up. However, these results are a first step to manipulation of nuclear spin coherence of water molecules or any appropriate liquid molecules with negligible interactions with their environment.

The main application of this macroscopic quantum behavior is to use magnetic gradients to define several qubits by their frequencies in a specific magnetic environment rather than qubits defined by the chemical environment in a molecule. Such an approach could lead into a more scalable (see [1]) NMR computer than the use of chemical molecules. If the reported experiments involve only one qubit, by using a magnetic gradient along the direction of the tube contenting the water sample, it could be defined a linear arrangement of several qubits. The same setup could be used to create and manipulate up to thirty qubits arranged along a line, thus realizing one-dimensional (and thus rather sophisticated but not universal) quantum cellular automata on 30 qubits. We see no difficulties in extending our approach to two- and, possibly, three-dimensional settings implementing universal quantum cellular automata computers on at least as many qubits. Theses results on manipulation of nuclear spin coherence of water represent the first step in a radically new, scalable and easily reproducible approach to the field of quantum information processing based on liquid state NMR techniques, defying in particular some recent skepticism, lately partially reversed, on the viability of such techniques.

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