A model for ensemble NMR quantum computer using antiferromagnetic structure

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Abstract

The one-dimensional homonuclear periodic array of nuclear spins I = 1/2, owing to hyperfine interaction of nuclear spins with electronic magnetic moments in antiferromagnetic structure, is considered. The neighbor nuclear spins in such array are opposite oriented and have resonant frequencies determined by hyperfine interaction constant, applied magnetic field value and interaction with the left and right nuclear neighbor spins. The resonant frequencies difference of nuclear spins, when the neighbor spins have different and the same states, is used to control the spin dynamics by means of selective resonant RF-pulses both for single nuclear spins and for ensemble of nuclear spins with the same resonant frequency.

A model for the NMR quantum computer of cellular-automata type based on an one-dimensional homonuclear periodic array of spins is proposed. This model may be generalized to a large ensemble of parallel working one-dimensional arrays and to two-dimensional and three-dimensional structures.

Introduction

The fundamental obstacle, preventing experimentalists from extending the number of qubits to $L \gg 1$ in an individual molecule of the liquid-state NMR quantum computer, is the difficulty of distinguishing L unique set of two-state cells. To remove this obstacle it was already proposed several models for solid-state quantum computers with both *individual* and *ensemble* control of qubits. One of such potentially realizable model based on a onedimensional cellular automaton, using an one-dimensional periodic array ABCABC... of *three types* of two-state quantum-mechanical cells (they may be heteronuclear system of spins I = 1/2) with distinct resonant frequencies and local interaction between near neighbors, was first considered by S.Lloyd [1]. The effect of the interaction contains in a shift of the each cell energy levels depending on states of its neighbors. After using the resonant π -pulse all cells of type A, for instance, invert their state if, and only if, the left neighbor C is in ground state and the B on its right is in excited state. In [1], it was represented algorithm, which was applied globally to all cells, so that there is no need to address cells individually. This model was recently developed by S.Lloyd [2]. The more general model of a solid state ensemble NMR quantum computer was described in [3], where it was considered periodic structure of ABCABCABC... type in two or three dimensions with the nuclear spins 1/2 only of three distinguish types A, B, C. It was supposed that the nuclei are embedded in a crystal lattice of some solid state compound with spinless nuclei and all spins are initialized to the ground state $|0\rangle$. Each ABC-unit of this superlattice can be used to store quantum information by setting one of spin up or down. This information can be moved around via some quantum cellular state shifting mechanism. Cascading unitary quantum SWAP operations of $A \Leftrightarrow B, B \Leftrightarrow C, C \Leftrightarrow A, A \Leftrightarrow B, \ldots$ is used for this process. An ancillary dopand nucleus D with spin 1/2 in the proximity of an A-site can serve as the input/output port. A local environment region near dopand nucleus provides a large quantum system with a wealth of qubits and only three types of nuclear spins. Therefore impurity doping may induce large-scale quantum automata in a single crystal and the whole crystal contains a huge ensemble of such identical NMR quantum computers — large artificial "molecules".

One-dimensional scheme that was based only on two different A and B types of cell in a periodic array without the ability to distinguish the left neighbor from the right was described in [4]. Each two-state cell of the scheme has ground $|\downarrow\rangle$ and excited $|\uparrow\rangle$ internal eigenstates and can represent any quantum superposition of these states. All cells are initially in the same ground states $|\downarrow\rangle$ and the state of the all array is $|\downarrow\downarrow\downarrow\downarrow\dots\downarrow\rangle$, similar to an one-dimensional two-sublattice ferromagnetic. Each qubit of quantum information in the state is represented by four consecutive units: the qubit basis state "0" is represented by unit $|\uparrow\uparrow\downarrow\downarrow\downarrow\rangle$, whilst the state "1" is represented by $|\downarrow\downarrow\downarrow\uparrow\uparrow\rangle$.

The model of array described below could be realized by using a linear artificial "molecule" with A and B cells alternating along its length in antiferromagnetic-type structure. As the cells in this array are used only identical nuclear spins I = 1/2. The neighbor nuclear spins in the ground state of antiferromagnetic structure are opposite orientated and have distinct resonant frequencies determined by hyperfine interaction constant, by applied magnetic field value and by interaction with the left and right nuclear neighbor spins. The major advantage of this variant over the ferromagnetic structure is that the antiferromagnet doesn't have the total spontaneous magnetization and the nuclear resonance frequency doesn't depend on the sample shape.

1 The one-dimensional antiferromagnetic model on atoms ³¹P.

In [5, 6] it was suggested a bulk-ensemble generalization of the silicon quantum computer model proposed by Kane previously [7]. In ensemble case, unlike the individual Kane's model, two-type electrodes **A** and **J** form a set of narrow ($l_{\rm A} \sim 10 \,\mathrm{nm}$) and long (several micrometers) strips. The distance between neighbors **A** gates was assumed $l_{\rm x} \sim l_{\rm A}$. Along the gates **A**, donor ³¹P atoms $l_{\rm y}$ distant from each other are placed. If exchange interaction constant for localized electronic spins along the strip gates is more than for electronic spins between neighboring strips and more than Zeeman energy $J(l_{\rm y}) \gg J(l_{\rm x}), 2\mu_{\rm B}B$ (*B* is the induction of the applied magnetic field), it produces an artificial one-dimensional antiferromagnetically ordered state of electronic spins. At the temperatures well below the critical temperature (Neel temperature) $T_{\rm NS} \sim J(l_{\rm y})/k$ (k — the Boltzmann constant) we will have a pure macroscopic electronic ground quantum state. Due to hyperfine interaction nuclear spins will be oriented according to the electronic spin direction in the resultant field and will form array with the alternating orientation of nuclear spins. Note, this state is not the true pure nuclear antiferromagnetic state so as long as the phases of distinct nuclear spins at macroscopic distances are not correlated at temperature of order or higher then critical temperature of nuclear magnetic dipole ordering, that is $T > T_{\rm NI} \sim (10^{-6} - 10^{-7})K$ [8]. However, the phase correlations of near neighbor nuclear spins of course exist.

The nuclear resonant frequencies $\nu_{A,B}$ of neighbor nuclear spins are different for each of the magnetic quasi-one-dimensional subarrays A and B in the chain and depend on the states of neighboring spins. We will take it in the form:

$$\nu_{\rm A,B}(m_{<}+m_{>}) \approx |g_{\rm N}\mu_{\rm N}B \pm A/2 - I_{\rm n}(m_{<}+m_{>})|/2\pi\hbar,$$
(1)

where $\mu_{\rm N} = 5.05 \cdot 10^{-27} \,\text{J/T}$ is the nuclear magneton, A is hyperfine interaction constant, (for ³¹P: $g_{\rm N} = 2.26$, $A = 7.76 \cdot 10^{-26} \,\text{J}$), $I_{\rm n}$ — the constant of two neighbor nuclear indirect spin-spin interaction, $m_{<}$ and $m_{>}$ are the magnetic quantum numbers for the left and right spins. The nonsecular part of interaction is neglected here taking in to account that $g_{\rm N}\mu_{\rm N}B$, $A/2 \gg I_{\rm n}$.

Thus we have the one-dimensional homonuclear periodic array of nuclear spins I = 1/2, formed in the one-dimensional antiferromagnet at the applied magnetic field, owing to hyperfine interaction of nuclear spins with the electronic magnetic moments. At magnetic fields $B \ge A/2g_{\rm N}\mu_{\rm N} \sim 3.5 \,\mathrm{T}$ and at temperatures $T \sim 10^{-3} \,\mathrm{K}$ the nuclear spins ³¹P have in each subarray almost 100% orientation $(2\pi\hbar\nu_{\rm A,B}/kT \le 1)$, that is they are *in ground* state. Note, that the using of dynamic methods, such as optical pumping, makes possible the high orientation of nuclear spins also at more large temperatures.

We will estimate here the exchange interaction constant $J > 2\mu_{\rm B}B \sim 6.5 \cdot 10^{-23}$ J, the critical temperature $T_{\rm NS} \sim J/k \sim 4.5$ K and the nuclear spin critical temperature, that is due mainly to the Suhl-Nakamura indirect spin-spin interaction, $T_{\rm NI} \sim I_{\rm n}/k \sim A^2/Jk \sim 10^{-5}$ K.

Here we shall use for the organization of logic operations the addressing to spin states and qubits, analogously to consideration [4]. We shall consider at first the simple one-dimensional model of the antiferromagnet, in which each cell is represented by the magnetic atom and has one electronic and one nuclear spin 1/2 with hyperfine interaction, similar to the mentioned above artificial molecule of antiferromagnetically ordered donors ${}^{31}P$ in silicon substrate.

Nuclear spins of identical atoms at $g_N \mu_N B < A/2$ are oriented according to the electronic spin direction in the resultant field and will form a periodic ground state array of ABAB... type: $\uparrow \downarrow \uparrow \downarrow \ldots$, where \uparrow marks the ground state of nuclear spin in an A-site and \downarrow — the ground state of nuclear spin in a B-site, that is we have here *homonuclear system of spins* at two distinct ground states. Each nuclear spin in A-site of this scheme, has two internal eigenstates — ground $|\uparrow\rangle$ and excited $|\downarrow\rangle$ and in B-site, accordingly, — $|\downarrow\rangle$ and $|\uparrow\rangle$. We take into account that the life time (the longitudinal or spin-lattice relaxation time T_1) of excited states at low temperatures is very long. Each qubit of quantum information in this state will be represented here, similar to [4], by the *four* consecutive cells: the logical qubit basis state "0" will be represented by unit $|\downarrow\uparrow\uparrow\downarrow\downarrow\rangle$, whilst the state "1" — by $|\uparrow\downarrow\downarrow\downarrow\uparrow\rangle$. It is important here that the resonant frequencies of nuclear spins depend on neighbor spins states.

The input and output of the information in the array of ground states spins could be performed at the ends of the array, where the nuclear spin (say in A-site at the left end) has only one neighbor spin and distinguishing resonant frequency $\nu_{A,-1/2}$ ($m_{<} + m_{>} = -1/2$). The corresponding selective resonance RF $\pi_{A,-1/2}$ -pulse inverts only one nuclear spin (in A-site) at the end of array and doesn't influence on any ones. Then the new selective RF $\pi_{B,0}$ -pulse will invert next nuclear spin (in B-site), which has the opposite orientation of ground and exited neighbor nuclear spins ($m_{<} + m_{>} = 0$ in A-site) and consequently the new resonant frequency, distinguished from the frequency of spins with the neighbor nuclear spin in ground states ($m_{<} + m_{>} = 1$). Thus the qubit state "0", that is $| \downarrow \uparrow \uparrow \downarrow \rangle$, is formed in the following way (the pulses act on underlined spins):

The qubit state "1" at the edge of array is formed by means of still three pulses: at first $\pi_{A,0}$, then $\pi_{A,-1/2}$ and $\pi_{B,0}$ -pulses:

$$\overline{\Downarrow}_{AB-B}^{\pi_{A,0}-\text{pulse}} \uparrow \dots \xrightarrow{\pi_{A,0}-\text{pulse}} \downarrow \overline{\uparrow}_{--}^{\pi_{A,-1/2}-\text{pulse}} \uparrow \overline{\downarrow}_{--}^{\pi_{A,-1/2}-\text{pulse}} \downarrow \overline{\downarrow}_{--}^{\pi_{$$

The states $|\overline{\uparrow \downarrow \downarrow \uparrow}\rangle$ and $|\overline{\downarrow \uparrow \uparrow \downarrow}\rangle$ may be called as the reversed states relative to the states $|\overline{\uparrow \downarrow \downarrow \uparrow}\rangle$ and $|\overline{\downarrow \uparrow \uparrow \downarrow}\rangle$.

Note that a random inversion of only one spin will result in completely destruction of the qubit. However, to form, for example, the error of "0" \Rightarrow "1" type in the coding of stored quantum information it is essential to invert simultaneously four spins. Therefore, it may be concluded that the considered way of qubit coding ensures a better fault-tolerance with respect to this type of errors.

Authors of [9] have considered also another scheme of the four-spin encoding two logical qubits, which are represented by the two zero-total states of four spins, generated by the pairs respectively of the singlet and triplet states. This scheme leads in the collective decoherence conditions to the fault-tolerant implementation of quantum computations. The collective decoherence conditions can be attained in coupled spins at very low temperatures, where all collective but the longest wavelength acoustic phonon modes are quenched.

The further shift-loading of qubit states into the array is implemented by means of pulse sequence $\pi_{A,0}$, $\pi_{B,0}$, $\pi_{A,0}$, $\pi_{B,0}$, ..., which is represented by following SWAP operation:

$$\begin{array}{c} \underbrace{\overset{"1"}}{\uparrow\downarrow\downarrow\uparrow\uparrow\uparrow} \\ AB-B \end{array} \uparrow \dots \xrightarrow{\pi_{A,0}-\text{pulse}} \uparrow \overline{\downarrow\uparrow\uparrow\uparrow\downarrow} \downarrow \dots \xrightarrow{\pi_{B,0}-\text{pulse}} \uparrow \downarrow \overline{\uparrow\downarrow\downarrow\downarrow\uparrow\uparrow} \dots \xrightarrow{\pi_{A,0}-\text{pulse}} \\ \Rightarrow \uparrow \downarrow \uparrow \overline{\downarrow\uparrow\uparrow\downarrow\downarrow} \downarrow \dots \xrightarrow{\pi_{B,0}-\text{pulse}} \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \overline{\uparrow\downarrow\downarrow\downarrow\uparrow\uparrow} \dots \xrightarrow{\pi_{A,0}-\text{pulse}} \\ \Rightarrow \uparrow \downarrow \uparrow \overline{\downarrow\uparrow\uparrow\downarrow\downarrow} \downarrow \dots \xrightarrow{\pi_{B,0}-\text{pulse}} \uparrow \downarrow \uparrow \downarrow \uparrow \downarrow \overline{\uparrow\downarrow\downarrow\downarrow\uparrow\uparrow} \uparrow \downarrow \dots$$

and so on.

The role of the atoms at array ends can play here, as it was discussed in [3], also dopand nuclei D at the certain place of the array with distinct resonant frequency or a defect that modifies the resonant frequency of the nearest nuclear spin in the array. Starting from the perfectly initialized states inputting the information can be performed by setting the dopant D-spin to desired state by means of pulse at his resonant frequency. The nuclear spin state of cell nearest to the dopand is created by SWAP operation mentioned above. After the required information is loaded, D-spin is reset to the ground state $|0\rangle$. Upon completion of computation, the state of any qubits can be measured by moving it to the A-site nearest to D, then swapping $A \Leftrightarrow D$ and finally measuring the state of D-spin.

2 One-qubit operations in one dimension

As in [4], we introduce still $\pi_{A,1}$ and $\pi_{B,-1}$ -pulses and operators $U_{A,1}$ and $U_{B,-1}$. The last means, that each spin in A- and B-site is subjected to a unitary transform U, which acts on spins in A- and B-sites with resonant frequency corresponding to the both neighbor nuclear spin in the *same excited* states ($m_{<} + m_{>} = \pm 1$, sign "+" is for excited neighbor spins in B-sites $| \Uparrow \rangle$, and sign "-" — for A-sites $| \Downarrow \rangle$, see Table). Note, that when operator U is a simple inversion, the actions of $U_{A,1}$ and $U_{B,-1}$ are identical to $\pi_{A,1}$ and $\pi_{B,-1}$ -pulse.

Table. The π -pulses for spins in A- and B-sites

Neighbor spin states. A-site	$\uparrow\downarrow$	↓↑↓	↓↑↑	↑↑↓	↑↑↑
Resonance frequency	$\nu_{\rm A}(-1/2)$	$\nu_{\rm A}(-1)$	$\nu_{\rm A}^{\rm A}(0)$	$\nu_{\rm A}^{ m A}(0)$	$\nu_{\rm A}^{\rm A}(1)$
π -pulses	$\pi_{\mathrm{A},-1/2}$	$\pi_{\mathrm{A},-1}$	$\pi_{\mathrm{A},0}$	$\pi_{\mathrm{A},0}$	$\pi_{\mathrm{A},1}$
Neighbor spin states. B-site	$\downarrow \uparrow$ B	$\uparrow \downarrow \uparrow$	1↓↓ B	$\downarrow \downarrow \uparrow$	\Downarrow_{B}
Resonance frequency	$\nu_{\rm B}(1/2)$	$\nu_{\rm B}(1)$	$\nu_{\rm B}(0)$	$\nu_{\rm B}(0)$	$\nu_{\rm B}(-1)$
$\pi-$ pulses	$\pi_{\mathrm{B},1/2}$	$\pi_{\mathrm{B},1}$	$\pi_{\mathrm{B},0}$	$\pi_{\mathrm{B},0}$	$\pi_{\mathrm{B},-1}$

Let us construct now the logical gates of quantum computer. At first we shall investigate at first the scheme for one-qubit gate. The considered section of the array (Fig. 1) contains three qubits in states "1", "0" and "1", each being separated by number multiple four of spacer cells -nuclear spins in ground state. Therefore each qubit requires a total of eight physical spins in the array (four for the encoding plus four spacers) (Fig. 1). As it was made in [1, 4], we will also introduce here *one control unit*, (not to be confused with *control qubit* in case of CNOT gates), which is represented here by *six* consecutive cells in the pattern $\overline{\uparrow \Downarrow \downarrow \uparrow \uparrow \Downarrow}$. The control unit (CU) exists only in one place along the array and is separated by odd number of spacer cells — spins (the scheme at Fig. 1 has three).





Fig. 1. The scheme of the SWAP update pulse sequence.

The applying SWAP update sequence of pulses $\pi_{A,0}$, $\pi_{B,0}$, $\pi_{A,0}$, $\pi_{B,0}$, $\pi_{A,0}$... moves the qubits to the right and CU to the left relative to the qubits, yet the form of the qubits and the CU are *preserved*. The CU passes through qubit in state "1" and "0", leaving it unchanged and continues further (Fig. 1).

To implement the one-qubit logical gate the additional computing updates six pulse sequence π_{A1} , π_{B1} , π_{B0} , π_{A1} , π_{B0} , $U_{A,1}$ is applied when CU reaches the mid-way through passing the qubit Y ("1" or "0", marked * and ** at Fig. 1). The effect of the additional sequence is to apply a unitary transform U only to the spin representing the qubit Y: t = UY (Fig. 2). The scheme of the additional computing update pulse sequence after stage * is shown at Fig. 2. The scheme of sequence after stage ** is shown in Appendix A1.

Fig. 2. The scheme of the additional computing update pulse sequence after stage *

Let us take now the one-cell unitary operation at the end of additional sequence:

$$U_{A,1}|\uparrow\rangle = a|\uparrow\rangle + b|\Downarrow\rangle, |a|^2 + |b|^2 = 1.$$
(2)

Re-applying the update pulses after unitary operation in reverse order the CU moves away from transformed cell and is returned to its initial state (see Appendix A2). We will have in the result the superposition of states:

$$|\psi\rangle = a|\overline{\uparrow\downarrow\downarrow\downarrow\uparrow\uparrow}\rangle + b|\overline{\downarrow\uparrow\uparrow\downarrow}\rangle. \tag{3}$$

The CU and additional computing updates pulse sequence together ensure the computing operations with qubits. Note, such one-qubit gate requires seventeen elementary pulses.

Not let us consider the state of quantum register, shown at the first line on Fig. 1 and apply after stage marked ** the pulse $\pi_{A,1}$. The result is presented on Fig. 3.

Fig. 3. The result of the SWAP pulse sequence finished by pulse $\pi_{A,1}$.

We see that the CU moves transparently past the qubit "1" and continues until mid-way through passing qubit "0". Now the CU itself is subject to a transformation: it is altered from $\overline{\uparrow \downarrow \downarrow \uparrow \downarrow \uparrow}$ to $\overline{\downarrow \uparrow \downarrow \uparrow \downarrow \uparrow}$ (only for passing the qubit "0"!) and qubit "0" itself will be destroyed (Fig. 3).

Now we will apply again the SWAP pulse sequence and will become:



Fig. 4. The scheme of the SWAP pulse sequence following sequence Fig. 3.

We see here, that by passing qubit "1" the altered CU is preserved his form.

3 Two-qubit operations in one dimension

To implement the two-qubit gate such as CNOT it should be applied the another update pulse sequence.

Let now the qubit "0" will be as *control qubit* of CNOT gate. The CU transforms in altered form by passing the control qubit and then we extend the sequence Fig. 5 after stage marked ***** by following pulses with the end inversion pulse $U_{A,1} \equiv \pi_{A,1}$:

$$\pi_{A,1}, \pi_{B,1}, \pi_{B,0}, \pi_{A,0}, \pi_{A,1}, \pi_{B,0}, \pi_{A,0}, \pi_{B,1}, \pi_{A,1}.$$
(4)

We will obtain:





The last inversion operation *doesn't have effect* on target qubit "1", as it must be for CNOT gate. The reverse sequence returns CU and qubits to their initial states.

Let us return then to sequence Fig. 1 and continue it after stages marked **, when CU passes mid-way through qubit "1" by following sequence:







The scheme of the update pulse sequences after stage **** when CU also passes the qubit "1" is shown in Appendix A3.

We see, that the last inversion operation has effect on target qubit, as it must be for CNOT gate only when the control qubit is "1".

We can consider a large set of quasi-one-dimensional antiferromagnetically ordered weakly coupled at $J(l_y) \gg J(l_x)$ arrays donors ³¹P in silicon substrate as an ensemble of artificial molecules. In this case, there is no need to address qubits individually. We suppose that for the determination of nuclear spin states in ensemble of those identical artificial molecules, as in liquid-state bulk-ensemble quantum computer [9, 10], there are no need to fulfill the electrical measurements and consequently any electrodes. Since the read-out signal in this case will be proportional to the numbers of artificial molecule in the ensemble, it may be used the NMR or fluorescence techniques for ensemble measurement of spin states.

4 Two- and three-dimensional antiferromagnetic structures

Instead of generalization to the parallel model employing "sub-computers" with one-dimensional structure, which was considered in [4], our approach allows to use also two and threedimensional structures. The coupled antiferromagnetically ordered chains model can be extended to a two-dimensional antiferromagnetic chess-type ordering. Let the electronic spins of the neighboring chains are setting for $J(l_y) \neq J(l_x) > 2\mu_B B$. The electronic spins of two neighbor chains will be in the singlet ground state. The subarray of nuclear spins will have the opposite orientation of nuclear spins relative to the subarray of neighboring chain. The electron subsystem of two neighbor chains is in antiphase state, that is have the half period shift of antiferromagnetically ordered electronic spins in the one chain relative to the other. The nuclear subsystem of the both chains becomes corresponding chess-type ordering (Fig. 7).

Let us suppose that an initial state containing some number of cells is loaded in the twodimensional structure of many coupled chains. The inputting the information into the cell nearest to dopant atoms D (D-spin) is performed by means of corresponding π -pulse: $\downarrow \Rightarrow \uparrow$ or $\uparrow \Rightarrow \downarrow$. Then, the resonant frequencies of neighbor spins in the same chain and of spins in neighbor chain is altered and another π -pulse will invert one of they or both according to the values I_1 and I_2 of indirect nuclear spins interaction inside and between the chains. Therefore, the excited nuclear spin states and accordingly the qubits may be passed to any place in all two-dimensional structure. We will suppose as before that the qubits state will be represented by four spin states in chains. The computing operation can be fulfilled analogous to the above-considered one-dimensional scheme.



Fig. 7. The scheme of two-dimensional nuclear spin ordering in antiferromagnetic structure. It is showed the different ways that connect the D-spin (marked \odot) and a certain qubit.

For everyone CU we have a two-dimensional section of array with *large enough number* of qubits and one dopant atom. It is defined as a single-domain antiferromagnetic sample. There are many ways that connect the D-spin and the qubit (Fig. 7). This section plays role of many-qubit artificial molecule and the whole structure represent a *large ensemble* of such molecules, which work simultaneously and ensure the parallelism of quantum operations.

The structures with two and three-dimensional antiferromagnetic and ferrimagnetic order may be found perhaps among the *natural rare earth* or *transition element* dielectric compounds.

The electron magnetization of a one subarray of antiferromagnet is defined by expression [12]:

$$2\mu_{\rm B}N\langle S_{\rm jz}\rangle = 2\mu_{\rm B}N(1-P(T)-\psi)/2,\tag{5}$$

where for low temperatures in *spin-wave approximation*

$$P(T) = \frac{1}{(2\pi)^{\mathrm{d}}} \int \frac{d^{\mathrm{d}}k}{\exp(\epsilon(k)/kT - 1)}$$
(6)

is the contribution of thermal and ψ — of quantum fluctuations, $\epsilon(k) = \sqrt{\epsilon_0^2 + (Jak)^2}$ — spin-wave spectrum, a — lattice period, Z — number of near neighbors, d — dimension of structure.

For antiferromagnetic state of *easy-axis* type, when the interaction Hamiltonian of two electron spin j and g for single-axis crystal has the form:

$$H_{j,g} = J\mathbf{S}_{j}\mathbf{S}_{g} - J_{A}(S_{jx}S_{gx} + S_{jy}S_{gy}),$$
(7)

where $J > J_A > 0$, J_A — anisotropy constant, the contribution of quantum fluctuation, as shown in [12], $\psi = 0$. In addition, for $k \Rightarrow 0$, $T \ll \epsilon_0$, where $\epsilon_0 \sim Z\sqrt{JJ_A}$,

$$P(T) \sim \text{Const} \cdot (kT\epsilon_0/J^2)^{d/2} \exp(-\epsilon_0/kT) \Rightarrow 0,$$
(8)

that is in this state the thermal fluctuations in electron system also are *not essential* for the ground electron spin states.

Note, that in the case of easy-flat state, $\psi \neq 0$, but the NMR resonance frequency depends on the neighbor nuclear states to a greater extent than in case of easy-axis state [13].

The quantum state decoherence at low temperatures is defined on the one hand by the active role of electron spin-wave effects [13]. They generate the fluctuated local field due to Raman process of the electron spin wave scattering on individual nuclear spins. The decoherence time or transverse relaxation time T_2 of NMR in antiferromagnet for the low temperatures ($\epsilon_0/kT \gg 1$) then is determined by expression [13]

$$1/T_2 \sim (A^2/J) \cdot (kT/J)^3 (\epsilon_0/kT) \exp(-\epsilon_0/kT)/\pi^2 \hbar \Rightarrow 0, \tag{9}$$

value T_2 rapidly grows.

On the other hand decoherence is defined by inhomogeneity of the local magnetic fields and spread in resonance frequencies. The nuclear spin-spin interaction in natural dielectric antiferromagnets is defined mainly by the Suhl-Nakamura indirect mechanism of interaction through exchange of spin waves and is typically greater than the value, determined by the direct nuclear spin-spin dipole interaction. This interaction of nuclear spins could play a large role in the case of high spin concentration. Both of these decoherence mechanisms can be, in principle, suppressed by some NMR many-pulse methods using the stroboscopic observation of spin dynamics [14, 15].

The general requirements for natural antiferromagnetic structures, required for the construction of NMR quantum computers, can be formulated in the following way:

1) The operating temperature T must correspond to the fully ordered antiferromagnet $T_{\rm NS} \gg T \gg T_{\rm NI}$ and to fully polarized nuclear spins $T_{\rm NS}A/J \sim A/k > T \gg T_{\rm NI}$. From where we will have the value $T \ge 10^{-3}$ K.

2) The two-dimensional and tree-dimensional magnetic structure must have chess-type order (see Fig. 7).

3) The magnetic structure must have the *easy-axis* state of antiferromagnetism in singleaxis crystals.

4) The atoms must have nuclear spins I = 1/2. Electron spins may be $S \le 1/2$.

There are the rare earth compounds of unique *thulium* stable isotope ¹⁶⁹Tm, that has nuclear spin I = 1/2, $g_N = 0.458$ and makes up 100% of naturally occurring elements with stable spinless isotopes of other elements. They can be: Tm₂O₃, TmSi₂, TmGe₂ and TmSe [16, 17]. The ground electronic state of magnetic ions Tm³⁺ corresponds to S = 1. The natural elements O, Si, Ge and Se have, accordingly, nuclear spin containing isotopes (in brackets it is shown the isotope occurrence) ¹⁷O I = 5/2 (0.04%), ²⁹Si I = 1/2 (4.7%), ⁷³Ge I = 9/2 (7.76%), ⁷⁷Se I = 1/2 (7.78%). For Yb₂O₃ $T_{\rm NS} \sim 2.3$ K, isotope ¹⁷¹Yb (14.31%) has I = 1/2 and S' = 1/2 (ground state is Kramers doublet). It is known, that compound TmSe has the critical temperature for antiferromagnetic transition $T_{\rm NS} \sim 2K$ [17]. The antiferromagnets with two different nuclear spin I = 1/2, for example FeF₂ with rutile-type and TmAg with CsCl-type structure, which have critical temperature 79 K and 9.5 K, may be also of interest to the considered questions. Isotopes ⁵⁷Fe (2.19%), ¹⁹F (100%), ¹⁰⁷⁺¹⁰⁹Ag (100%) have according values $g_N = 0.182$, $g_N = 5.26$ and $g_N = 0.24$.

In conclusion, we will point out the several advantages of the considered model: it uses the antiferromagnetic structure containing only one type of atoms with nuclear spin 1/2, it is not needed to have any gate electrodes, the decoherence associated with noise voltage is absent, the considered way of qubit coding ensures a better fault-tolerance with respect to the generation of wrong qubits, the model admits an ensemble address qubits, it may be used as base for development of bulk-ensembles three-dimensional solid-state NMR quantum computer.

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Appendixes

A1. The scheme of the additional computing update pulse sequence after stage ** at Fig. 1:

$$\begin{split} & \Pi_{\mathbf{B}, \mathbf{0}} \Rightarrow \dots \uparrow \downarrow \stackrel{\uparrow}{\uparrow} \downarrow \stackrel{\downarrow}{\downarrow} \stackrel{\uparrow}{\uparrow} \stackrel{\uparrow}{\downarrow} \stackrel{\downarrow}{\downarrow} \stackrel{\uparrow}{\downarrow} \stackrel{\uparrow}{\downarrow} \stackrel{\downarrow}{\downarrow} \stackrel{\uparrow}{\downarrow} \stackrel{\uparrow}{\downarrow} \stackrel{\downarrow}{\downarrow} \stackrel{\uparrow}{\downarrow} \stackrel{\uparrow}{\downarrow} \stackrel{\downarrow}{\downarrow} \stackrel{\uparrow}{\downarrow} \stackrel{\downarrow}{\downarrow} \stackrel{\uparrow}{\downarrow} \stackrel{\uparrow}{\downarrow} \stackrel{\downarrow}{\downarrow} \stackrel{\uparrow}{\downarrow} \stackrel{\uparrow}{\downarrow} \stackrel{\downarrow}{\downarrow} \stackrel{\uparrow}{\downarrow} \stackrel{\downarrow}{\downarrow} \stackrel{\uparrow}{\downarrow} \stackrel{\downarrow}{\downarrow} \stackrel{\uparrow}{\downarrow} \stackrel{\downarrow}{\downarrow} \stackrel{\downarrow}{\downarrow} \stackrel{\uparrow}{\downarrow} \stackrel{\downarrow}{\downarrow} \stackrel{\uparrow}{\downarrow} \stackrel{\downarrow}{\downarrow} \stackrel{\downarrow}{\downarrow} \stackrel{\uparrow}{\downarrow} \stackrel{\downarrow}{\downarrow} \stackrel{\uparrow}{\downarrow} \stackrel{\downarrow}{\downarrow} \stackrel{\uparrow}{\downarrow} \stackrel{\downarrow}{\downarrow} \stackrel{\uparrow}{\downarrow} \stackrel{\downarrow}{\downarrow} \stackrel{\downarrow}{\downarrow} \stackrel{\uparrow}{\downarrow} \stackrel{\downarrow}{\downarrow} \stackrel{\uparrow}{\downarrow} \stackrel{\downarrow}{\downarrow} \stackrel{\uparrow}{\downarrow} \stackrel{\downarrow}{\downarrow} \stackrel{\downarrow}{\downarrow} \stackrel{\downarrow}{\downarrow} \stackrel{\uparrow}{\downarrow} \stackrel{\downarrow}{\downarrow} \stackrel{\downarrow}{\downarrow} \stackrel{\downarrow}{\downarrow} \stackrel{\downarrow}{\downarrow} \stackrel{\uparrow}{\downarrow} \stackrel{\downarrow}{\downarrow} \stackrel{\downarrow}{\downarrow}$$

A2. The scheme of the reverse update pulse sequence after one-qubit operation $U_{A,1}$:





A3. The scheme of the update pulse sequences when CU passes the qubit "1" after stage ****:

References

- Lloyd, S., A Potentially Realizable Quantum Computer, Science, 1993, vol. 261, pp.1569–1571.
- [2] Lloyd, S., Programming Pulse Driven Quantum Computers. E-print LANL: quantph/9912086.

- [3] Wei, H., Xue, X. and Morgera, S.D., NMR Quantum Automata in Doped Crystals, 1998, E-print LANL: quant-ph/9805059.
- Benjamin, S.C., Schemes for Parallel Quantum Computation Without Local Control of Qubits, E-print LANL: quant-ph/9909007.
- [5] Valiev, K.A. and Kokin, A.A., Semiconductor NMR Quantum Computers with Individual and Ensemble Access to Qubits, *Microelektronika*, 1999, vol. 28, no. 5, pp. 326–337 (in Russian).
- [6] Valiev, K.A. and Kokin, A.A., Solid-State NMR Quantum Computer with Individual Access to Qubits and Some Their Ensemble Developments, E-print LANL: quantph/9909008.
- [7] Kane, B.E., A Silicon-Based Nuclear Spin Quantum Computer, *Nature*, (London), 1998, vol. 393, pp. 133-137.
- [8] Abragam, A. and Goldman, M., Nuclear Magnetism: Order and Disorder, Oxford: Clarendon Press, 1982.
- Bacon D., Kempe J., Lidar D.F. and Whalet K.B., Universal Fault-Tolerant Computation on Decoherence-Free Subspaces, E-print LANL: quant-ph/9909058.
- [10] Chuang, I.L., Gershenfeld, N., Kubinec, M.G., and Leung, D.W., Bulk Quantum Computation with Nuclear Magnetic Resonance: Theory and Experiment, *Proc. Roy. Soc. London*, 1998, vol. A454, no. 1969, pp. 447-467.
- [11] Cory, D.G., Price, M.D., and Havel, T.F., Nuclear Magnetic Resonance Spectroscopy: An Experimentally Accessible Paradigm for Quantum Computing, *Physica D*, 1997, vol. 120, no. 1-2, pp. 82–101.
- [12] Tyablikov, S.B., Metodi kvantovoi teorii magnetisma (Quantum methods in magnetism),
 Moscow: Nauka, 1975, 528p. (in Russian)
- [13] Turov, E.A. and Petrov, M.P., Jadernyi magnitnyi resonans v ferro- i antiferromagnetikakh (Nuclear magnetic resonance in ferro- and antiferromagnets), — Moscow: Nauka, 1969, 260p. (in Russian)
- [14] Haeberlen, U., High Resolution NMR in Solids: Selective Averaging; in Advances in Magnetic Resonance ed. by J.S.Waugh, — N.Y., Lond.: Acad. Press, 1976.
- [15] Slichter, C.P., Principles of Magnetic Resonance. Berl., Heidelb., N.Y., : Springer-Verlag, 1990.
- [16] Taylor, K.N.R. and Darby, M.I., Physics of Rare Earth Solids, Lond.: Chapman and Hall, 1972.
- [17] Nagaev, E.L., Fisika magnitnykh poluprovodnikov (Physics of Magnetic Semiconductors), — Moscow: Nauka, 1979, 432p. (in Russian)