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АНСАМБЛЕВЫЕ ЯМР КВАНТОВЫЕ КОМПЬЮТЕРЫ НА КРЕМНИИ

THE ISOTOPIC EFFECT

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As an ensemble scheme of solid-state NMR quantum computers the scheme based on the array of ^{31}P donor atoms which are spaced lengthwise of the strip gates is considered. The possible planar topology of such ensemble quantum computer is suggested. The estimation of the output NMR signal is performed and it is shown that for the number $N \geq 10^5$ of ensemble elements involving $L \sim 10^3$ qubits each, the standard NMR methods are usable. As main mechanisms of decoherence for low temperature (< 0.1 K), the adiabatic processes of random modulation of qubit resonance frequency determined by secular part of nuclear spin hyperfine interaction with electron magnetic moment of basic atom and dipole-dipole interaction with nuclear moments of neighboring impurity atoms was considered, Estimations of allowed concentrations of magnetic impurities and of spin temperature whereby the required decoherence suppression are obtained. Semiclassical decoherence model of two qubit entangled states is also presented.

Introduction

Atomic nuclei with spin quantum number $I = 1/2$ are the *natural candidates* for qubits in quantum computers. The early approach to NMR quantum computers was suggested in 1997 [1,2] and then confirmed in experiments [3,4]. In this search several diamagnetic organic liquids whose individual molecules, having a number of interacting non-equivalent nuclear spin-qubits with I=1/2 and being nearly independent on one another where used. They act in parallel as an ensemble of *almost independent* quantum molecule-microcomputers. In so doing the nuclear spins of an individual molecule are described by mixed state density matrix of *reduced quantum ensemble. Initialization* of the nuclear spin states in this case means the transformation of mixed state into so called, effective or *pseudo-pure* state [1,2,4,5].

The access to individual qubits in a liquid sample is replaced by simultaneous access to related qubits in all molecules of a bulk ensemble. Computers of this type are called *bulk-ensemble* quantum computers. The liquid-based quantum computer can operate at *room temperature*. For control and measurements of qubit states the standard NMR technique is used.

The principle one-coil scheme of experiment and some notations are shown in Fig. 1. The sample is placed in the constant external magnetic field **B** and in the alternating (say, linearly polarized) field **b**(t), produced by RF voltage $V_\omega(t)$:

$$\mathbf{B}(t) = \mathbf{B} + \mathbf{b}(t) = B\mathbf{k} + 2b\cos(\omega t + \varphi)\mathbf{i}, \tag{1}$$

where **i** and **k** are unit vectors along the axes x and z.

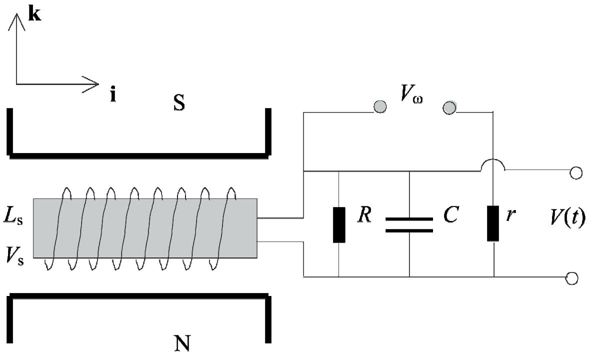

Fig. 1. The principle one-coil scheme of NMR measurement

Let the sample represent an ensemble of N molecule–microcomputers with L qubits each at temperature $T = 300$ K, in the external magnetic fields $B = 1$-10 T. The resonance nuclear spin frequency is $\omega_A/2\pi \sim \gamma_I B/2\pi < 150$ MHz, γ_I is gyromagnetic ratio of nuclear spin ($\gamma_I \sim \gamma_N = 95.8$ radMHz/T), $\hbar\omega_A/kT < 10^{-5}$.

The output oscillating voltage $V(t)$ is

$$V(t) = QKd\Phi(t)/dt = \mu_0 QKAdM_x(t)/dt\,, \tag{2}$$

where $\Phi(t) = \int_A \mu_0 M_x(t)dydz$ is magnetic flux produced by resonant spins in the coil ($\mu_0 = 4\pi\cdot 10^{-1}$T^{2}cm^3/J, $L_s = \mu_0\,(KA)^2/V_s$ is solenoid inductance of the resonance contour, V_s is volume of the solenoid, K is the number and A is area of coil turns, $Q = R/(\omega_A L_s) > 10^2$ is the *quality factor* of resonance contour for parallel connected resistance R (Fig. 1). For resonance condition: $\omega = \omega_A = (L_sC)^{-1/2}$.

The maximum nuclear spin read-out magnetization M_{xmax} (the liquid sample is considered here to be a continuous medium and to have volume $V \sim V_s$) at *optimum resonance condition* is defined by the amplitude of RF field $b = 1/(\gamma_I\sqrt{T_{\perp I}T_{\|I}})$ [6] (see also (20) below):

$$M_{xmax} = M_{zm}\sqrt{T_{\perp I}/T_{\|I}}\,/2 \approx \gamma_I\hbar/2\cdot(N/V_s)\cdot\varepsilon(L)/2\,, \tag{3}$$

where M_{zm} is maximum equilibrium nuclear magnetization, $T_{\perp I}$ and $T_{\|I}$ are effective transverse and longitudinal relaxation times, N is number of resonant nuclear spins (one in a molecule) in volume V_s. Parameter $\varepsilon(L)$ is the maximum probability of the full nuclear polarization in pseudo-pure state $P_I = 1$ [7]. It may be estimated by the difference of equilibrium population between the lowest and the highest energy states. For nearly homonuclear L-spin system [7] it is:

$$\varepsilon(L) = \frac{2\sinh(L\hbar\omega_A/2kT)}{2^L\cosh^L(\hbar\omega_A/2kT)}\,. \tag{4}$$

In the high temperature limit $\hbar\omega_A/(kT) \ll 1$ we have $\varepsilon(L) = L2^{-L}\,\hbar\omega_A/(kT)$, that is, the signal amplitude *exponentially drops* with the number of qubits, but it *does not* drop for $\hbar\omega_A/(kT) \gg 1$ when $\varepsilon(L) = 1$ (the pure ground nuclear spin quantum state).

The maximum NMR signal intensity S is defined by amplitude

$$S = |V_{max}| = (\mu_0/4)QKA(N/V_s)\gamma_I \hbar\omega_A \varepsilon(L)\,, \tag{5}$$

where the product KA can also be expressed as

$$KA = (L_s V_s/\mu_0)^{1/2} = (RV_s/(\mu_0 Q\omega_A))^{1/2}\,. \tag{6}$$

For the root-mean square noise voltage in the measurement circuit we write

$$V_N = \sqrt{4kTR\Delta\nu}\,, \tag{7}$$

where as a rule the amplifier bandwidth is $\Delta\nu \sim 1$ Hz.

So for *signal to noise ratio* we obtain

$$(S/N) \equiv |V_{max}|/V_N \cong \frac{1}{8}\sqrt{\frac{\mu_0 \hbar Q h\omega_A}{\Delta\nu V_s kT}}\gamma_I N\varepsilon(L) \sim 0.2\sqrt{(Q/V_s)\cdot(\hbar\omega_A/kT)}N\varepsilon(L)\cdot 10^{-9}\,, \tag{8}$$

(here V_s in cm^3). For example, for two qubit molecules ($L = 2$), with, $\varepsilon(L) = \hbar\omega_A/(2kT) \sim 10^{-5}$, we can make an estimation

$$(S/N) \sim (Q/V_s)^{1/2} N\cdot 10^{-16}\,. \tag{9}$$

Thus, to keep the value $(S/N) > 1$, the number of resonant nuclear spins for two qubit liquid ensemble at room temperature, $V_s \sim 1$ cm^3 and $Q \sim 10^3$, is bound to be $N > 10^{16}$.

In the case of *paramagnetic liquids*, one would expect that the number of polarized nuclei may be increased with dynamic polarization (say, Overhauser effect). Assuming electron and nuclear gyromagnetic ratio $\gamma_e/\gamma_I \sim 10^3$ we obtain that in the probability $\varepsilon(L)$ for a L-qubits single state the value $\hbar\omega_A/(kT)$ in (8) should be replaced by $10^3\,\hbar\omega_A/(kT)$. Therefore, for the same value $\varepsilon(L)$ and number of molecules N, the allowed number of qubits L approximately will be estimated from

$$L2^{-L} > 10^{-3}\,, \tag{10}$$

whence it follows that $L < 12$ qubits.

An additional increase of read-out NMR signal may be obtained in paramagnetic liquids using the ENDOR technique. It is generally believed that for the liquid bulk-ensemble quantum computers a *limiting value* is $L < 20$-30 [7].

There are five basic criteria for realization of a *large-scale NMR quantum computer*, which can outperform all traditional classical computers [8]:

1. For any physical system, which presents large-scale quantum register, the necessary number of qubits in quantum register must be $L > 10^3$.
   One such example of this register is solid-state homonuclear system in which identical atoms containing nuclear spins are housed at regular intervals in a natural or an artificial solid-state structure.
2. There is a need to provide the conditions for preparation of initial basic quantum register state. For a many-qubit solid-state NMR quantum computer the quantum register state initializing can be obtained by going to *extra-low nuclear spin temperature* (<1 mK at fields of order of several Tesla).
3. The decoherence time of qubit states T_d should be at least up to 10^4 times longer than the 'clock time', that is value of order of several seconds for NMR quantum computers. *The decoherence suppression is one of the important problems* in realization of a large-scale quantum computers.
4. There is a need to perform during a decoherence time a set of quantum logic operations determined by a logic unitary transformation. This set should contain certain set of the one-qubit and two-qubit operations witch are shielded from random errors. The electromagnetic pulses that control the quantum operation should be performed with an accuracy of better than 10^{-4}–10^{-5}.
5. There is a need to provide *accurate and sensitive read-out measurements of the qubit states*. This is another one of the important and hard problems.

The design of solid-state NMR quantum computers was proposed by B. Kane in [9,10]. It was suggested to use a semiconductor MOS structure on a ^{28}Si spinless substrate, in a near-surface layer where stable phosphorus isotopes ^{31}P, acting as donors, are implanted in the form of a regular chain. These donors have a nuclear spin $I = 1/2$ and substitute silicon atoms at the lattice sites, producing shallow impurity states. The number of donors or the qubit number L in such a quasi-one-dimensional *artificial 'molecule'* may be arbitrary large. It is suggested an *individual* nuclear spin-qubit electrical control and measurement of qubit states with the use of special gate structures. The experimental implementation of Kane's scheme is undertaken now in Australian Centre for Quantum Computer Technology [11,12].

However, there are four essential difficulties in implementing this quantum computer:

1. First of all, signal from the spin of an individual atom is very small and *high sensitive single-spin measurements* are required.
2. It is required for initialization of nuclear spin states to use *very low nuclear spin temperature* (~ mK).
3. It is required to use regular donors and gates arrangement with high precision in *nanometer scale*.
4. It is necessary to suppress the quantum states *decoherence* defined by *fluctuations* of gate voltage.

As an alternative, we proposed the variant of *an ensemble silicon-based quantum computer* [13,14]. One would expect that with the ensemble approach, where many independent 'molecules' of Kane's type work simultaneously, the measurements would be greatly simplified. Here we will give some further development of this scheme.

1. The silicon structure with regular system of strip gates

In this case, unlike the structure suggested in [9], gates **A** and **J** form a chain of narrow ($l_A \sim 10$ nm) and long strips along which donor atoms at l_y distant from each other are placed (Fig. 2). Thus, they form a *regular* structure of the planar silicon topology type.

The separation between neighboring donor atoms in Si, as in Kane's scheme, must be $l_x \le 20$ nm. In this case, the interqubit interaction is controlled by gates **J**. The depth of donor d is ~ 20 nm. For $l_y \gg l_x$ the exchange spin interaction between electrons of donor atoms disposed along the strip gates (y-axis) is negligibly small. Hence, such a system breaks down into an ensemble of near-independent Kane's artificial 'molecule', whose electronic spins at temperature $T \le 0.1$ K are initially fully aligned with the field of several Tesla ($\gamma_e \hbar B/kT \gg 1$). As in case of liquids, the nuclear spin states of individual Kane's chain-'molecule' will be described by density matrix of reduced quantum ensemble. Access to individual qubits will be replaced by simultaneous access to related qubits in all 'molecules' of ensemble.

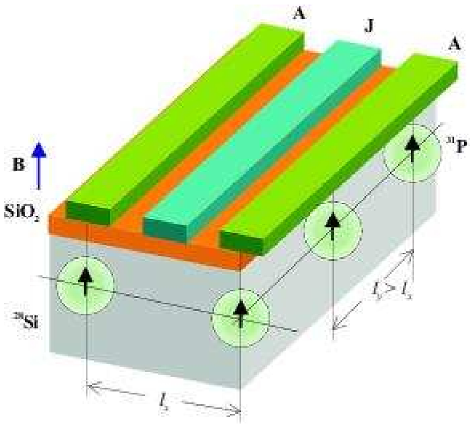

Fig. 2. The structure of two qubit cells for three-ensemble component

The linear qubit density in the artificial 'molecules' is ~50 qubits on micrometer. For the realization of considered structure, as well as of the Kane's scheme, *the nanotechnology* with resolution of the order of ~ 1 nm is also needed.

For *the initializing* of all nuclear spin-qubit quantum states (fully polarized nuclear spins) there is a need to attain, for the time being, nuclear spin temperature $T \le 10^{-3}$ K. An output signal in this system, as in liquids, will be proportional to the number of 'molecules' or donor atoms N (component number of our ensemble) in the chain along axis y. In the following, the lower value of N will be estimated.

2. The states of insulated donor atoms in magnetic fields

The electron-nuclear spin Hamiltonian for a donor atom ^{31}P has the form

$$H = \gamma_e \hbar \mathbf{BS} - \gamma_I \hbar \mathbf{BI} + A\mathbf{IS}\,, \tag{11}$$

four energy levels of which are given by the well-known Breit-Rabi formula. For $I = 1/2$, $S = 1/2$ (the z-axis is parallel to **B**) this formula is written as

$$E(F, m_F) = -\frac{A}{4} - \gamma_I \hbar B m_F - (-1)^F \,\mathrm{sign}(1 + m_F X)\,\frac{A}{2}\sqrt{1 + 2m_F X + X^2}\,, \tag{12}$$

where constant of hyperfine interaction $A/(2\pi\hbar) = 116$ MHz [15], $X = (\gamma_e + \gamma_I)\hbar B/A \approx \gamma_e \hbar B/A \gg 1$, $F = I \pm 1/2 = 1,0$, and $m_F = M + m = \pm 1,0$, if $F = 1$ or $m_F = 0$, if $F = 0$ (Here $M = \pm 1/2$ and $m = \pm 1/2$ are z-projections of electron and nuclear spins accordingly). The energy level scheme is shown in Fig. 3. For the energy of the ground spin state, $F = 0$ and $m_F = 0$, hence, we obtain

$$E(0,0) = -A/4 - (A/2)\sqrt{1 + X^2}\,. \tag{13}$$

For the next, excited energy state, $F = 1$, $m_F = -1$ we have

$$E(1,-1) = A/4 - (\gamma_e - \gamma_I)\hbar B/2\,. \tag{14}$$

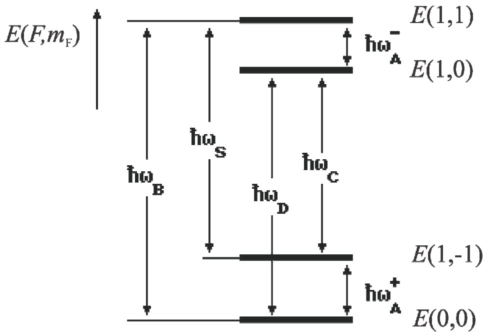

Fig. 3. Energy levels of an individual donor atom in magnetic field

Thus, the energy difference between the two lower states of the nuclear spin (the resonant qubit frequency), that interacts with an electron, whose state remains unchanged, is described in simple terms ($\gamma_e \gg \gamma_I$ for $X \approx \gamma_e \hbar B/A \gg 1$):

$$\begin{aligned} \hbar\omega_A^+ &= E(1,-1) - E(0,0) = A/2 + (\gamma_I - \gamma_e)\hbar B/2 + \frac{A}{2}\sqrt{1 + X^2} \approx \gamma_I \hbar B + \frac{A}{2} + \frac{A^2}{4\gamma_e \hbar B}, \\ \hbar\omega_A^- &= E(1,1) - E(1,0) \approx -\gamma_I \hbar B + \frac{A}{2} + \frac{A^2}{4\gamma_e \hbar B}. \end{aligned} \tag{15}$$

For ^{31}P donor atoms: $\gamma_e = 176.08$ radGHz/T, $\gamma_I = 1.13\gamma_N = 108$ radMHz/T, $\gamma_e / \gamma_I = 1.62 \cdot 10^3$. In magnetic field $B = 1$ T: $\omega_A^+/2\pi = 75\,\mathrm{MHz}$, $\omega_A^-/2\pi = 41\,\mathrm{MHz}$.

The frequencies ω_S, ω_B, ω_C, ω_D are in microwave, $\omega_A^\pm$ – in the RF ranges of frequencies. The transitions with frequencies ω_S in the first approximation are *forbidden*.

The states $|F, m_F\rangle$ in M,m basis are

$$\left.\begin{array}{l} |1,1\rangle = |1/2,1/2\rangle \\ |1,-1\rangle = |-1/2,-1/2\rangle \\ |1,0\rangle = (1-\alpha)^{1/2}|1/2,-1/2\rangle + \alpha^{1/2}|-1/2,1/2\rangle \\ |0,0\rangle = (1-\alpha)^{1/2}|-1/2,1/2\rangle - \alpha^{1/2}|1/2,-1/2\rangle \end{array}\right\}. \tag{16}$$

$$\alpha = \frac{1}{2}\left(1 - \frac{X}{\sqrt{1+X^2}}\right) \approx 1/(4X^2) << 1$$

The diagonal matrix elements of nuclear magnetization M_z per one donor atom for two lower energy states will be determined by

$$\begin{aligned} \langle 0,0|M_z|0,0\rangle &= \langle 0,0|I_z|0,0\rangle \gamma_I \hbar = \frac{X}{\sqrt{1+X^2}}\gamma_I \hbar/2 \approx \gamma_I \hbar/2, \\ \langle 1,-1|M_z|1,-1\rangle &= \langle 1,-1|I_z|1,-1\rangle \gamma_I \hbar = -\gamma_I \hbar/2. \end{aligned} \tag{17}$$

The probabilities of the L-qubit lowest and highest energy fully filling states for the same electron spin state $M = -1/2$, which correspond, as noted above, to the maximum probability of the nuclear polarization in pseudo-pure state, are:

$$\begin{aligned} p^L(1,-1) &= \frac{\exp(-L\hbar\omega_A^+/2kT)}{(\exp(\hbar\omega_A^+/2kT) + \exp(-\hbar\omega_A^+/2kT))^L}, \\ p^L(0,0) &= \frac{\exp(L\hbar\omega_A^+/2kT)}{(\exp(\hbar\omega_A^+/2kT) + \exp(-\hbar\omega_A^+/2kT))^L}. \end{aligned} \tag{18}$$

The possible maximum nuclear magnetization M_{zm} (the populations of states $|1,1\rangle$ and $|1,0\rangle$ are negligible for $\omega_S, \omega_B, \omega_C \gg \omega_A^{\pm}$) is

$$\begin{aligned} M_{zm} = \gamma_I \hbar/2 \cdot (N/V_c) & \left(\frac{\exp(L\hbar\omega_A^+/2kT)}{(\exp(\hbar\omega_A^+/2kT) + \exp(-\hbar\omega_A^+/2kT))^L} - \right. \\ & \left. - \frac{\exp(-L\hbar\omega_A^+/2kT)}{(\exp(\hbar\omega_A^+/2kT) + \exp(-\hbar\omega_A^+/2kT))^L} \right) = \gamma_I \hbar/2 \cdot (N/V_c)\varepsilon(L) \end{aligned}. \tag{19}$$

For $L\hbar\omega_A^+/2kT \ll 1$ and $X \gg 1$ we obtain (compare with (3))

$$M_{zm} \approx \gamma_I \hbar/2 \cdot (N/V_c) \cdot 2^{-L} L(\hbar\omega_A^+/kT). \tag{20}$$

But for very low temperatures ($\hbar\omega_A^+/2kT \gg 1$) we have the *full nuclear polarization* $M_{zm} \approx \gamma_I \hbar/2 \cdot (N/V_c)$ and $\varepsilon(L) = 1$.

3. The gain effect for NMR signal

Transitions between two lower states are induced by a RF magnetic field, applied at a resonant frequency ω_A^+. The Rabi resonance frequency Ω, which is defined by matrix elements of the Hamiltonian of the spin interaction with the external RF field $\mathbf{b}(t)$

$$H_{rf}(t) = (\gamma_e S_x - \gamma_I I_x)\hbar b_x(t), \qquad b_x(t) = 2b\cos(\omega_A^+ t) \tag{21}$$

can be found from

$$\Omega = \gamma_I b_{eff}(X) = 2\left|\langle 0,0|H_{rf}(0)|1,-1\rangle\right|/\hbar. \tag{22}$$

For the amplitude of effective RF field, acting on nuclear spin, $b_{eff}(X)$ we obtain

$$b_{eff}(X) = b\left(\alpha^{1/2}(\gamma_e/\gamma_I) + (1-\alpha)^{1/2}\right) \tag{23}$$

where b is the amplitude of circularly polarized field component.

The Rabi frequency has the maximum value for $X = 0$ ($\alpha = 1/2$) and monotonically reduces to value for the insulated nuclear spin ($\alpha \Rightarrow 0$), $\gamma_I b_{eff}(X \gg 1) = \gamma_I b$. From the rate of quantum operation standpoint it is desirable to operate in relatively weak fields [10], at which $\gamma_e/\gamma_I \gg X \approx \gamma_e \hbar B/A \gg 1$ or $3.5\,\mathrm{T} > B \gg 3.9 \cdot 10^{-3}\,\mathrm{T}$.

In this case from (23) we will obtain

$$b_{eff} = (1+\eta)b \gg b, \tag{24}$$

where $\eta = A/(2\gamma_I \hbar B) \gg 1$ is the *gain factor*. Under these conditions, RF field operates through the transverse component of electronic polarization. For magnetic fields $B = 1$ T we have the value $b_{eff} = 4.4b$, and for $B = 0.01$ T we have the value $b_{eff} = 338b$. The gain effect involves an increase of NMR signal and Rabi frequency. This effect was indicated previously by K. Valiev in [16].

In the pulse technique, this effect makes it possible *to decrease the length of pulse* and along with it the times of logic operation performing. Moreover, the computer operations, owing to this effect, can be performed at lower RF fields. At last, it permits to *reduce the RF field influence* on the operation of neighboring semiconductor devices.

To describe the nuclear dynamics for the two low-lying level systems being discussed ($X \gg 1$), we can write the following Bloch-type equation with only two effective relaxation times:

$$\frac{d\mathbf{M}}{dt} = \gamma_I [\mathbf{M} \times \mathbf{B}_{eff}] - \frac{M_x \mathbf{i} + M_y \mathbf{j}}{T_{\perp I}} - \frac{(M_z - M_{zm})\mathbf{k}}{T_{\parallel I}}, \qquad (25)$$

where **i**, **j**, **k** are orthogonal unit vectors (Fig. 1), M_{zm} is defined as (19),

$$\mathbf{B}_{eff} = (\omega_A / \gamma_I)\mathbf{k} + 2b_{eff} \cos(\omega t)\mathbf{i}. \qquad (26)$$

It follows from it that the value of maximum nuclear read-out magnetization in NMR signal $M_{xmax} = M_{zm}\sqrt{T_{\perp I} / T_{\parallel I}} / 2$ can be obtained for $b_{eff}(X) = 1/(\gamma_I \sqrt{T_{\perp I} T_{\parallel I}})$. Hence, the read-out *NMR signal cannot be increased* through the gain effect over its maximum value, that corresponds to $M_{zm}\sqrt{T_{\perp I} / T_{\parallel I}} / 2$.

4. The signal to noise ratio for an ensemble silicon quantum computer

For the realization of an ensemble silicon quantum register, we propose a variant of planar scheme [17], that, as an example, contains $n \cdot p$ in parallel acting identical blocks, and each block has N_0 in parallel connected L-qubit Kane's linear 'molecules'. This scheme is schematically depicted in Fig. 4.

Let the sample be the silicon (^{28}Si) plate of thickness 0.1 cm. For the full number of computer-'molecules' in ensemble $N = p \cdot N_0 \cdot n$, the volume of sample and of solenoid is $V_s \approx \delta \cdot l_x \cdot l_y \cdot L \cdot N$ (the filling factor is assumed for simplicity to be one).

The read-out signal from such *ensemble in parallel acting* chains, as distinct from liquid prototype, for full nuclear polarization or, what is the same, for nuclear spin temperatures $T_I \leq 10^{-3}$ K has instead of the small factor in intensity of the NMR signal of type $\varepsilon(L) = 2^{-L} L \cdot \hbar\omega_A/(kT)$ the factor $\varepsilon(L) = 1$. The NMR signal from our sample within a non-essential factor is the same as from macroscopic sample [17]. Therefore, with the expressions (4) and (8), $\hbar\omega_A/(kT_I) < 1$ ($T_I < 1$ mK) and $\varepsilon = 1$ we will obtain as an estimation for maximum signal to noise ratio

$$(S/N) \approx \sqrt{Q\hbar\omega_A/(kTV_s)} \cdot N \cdot 10^{-9} \approx \sqrt{QN/(\delta l_x l_y L)} \cdot 10^{-10}. \qquad (27)$$

It is believed that for low temperatures $Q \sim 10^6$. Taking info account that the effective volume of one 'molecule' for $l_x = 20$ nm, $l_y = 50$ nm, $L = 10^3$, $V_s = \delta l_x l_y L = 10^{-9}$ cm^3 we receive that the read-out signal in our scheme may be *available for standard NMR technique*, if the number of 'molecules' in ensemble is of about $N \geq 10^5$. High-sensitive devices for measurement of individual spin-states are not needed.

To estimate the values n, p let us consider the square plate with $50N_0 p = 20 \cdot 10^3 n$ and $N_0 = 100$. As a result, we receive $n \approx 16$ and $p \approx 63$. The area of the structure without passive regions is $\sim 315 \times 315$ μm^2. This size is sufficiently small for sample to be housed in the gap between the magnet poles of a standard NMR spectrometer. Real plate may have considerably more area and correspondingly more number of 'molecules' N.

For implementation of two-qubit logic operation it is required the controlled by gates **J** interqubit indirect interaction with characteristic frequency $\nu \sim 100$ kHz $\ll \omega_A \sim 100$ MHz. To bring about fault-tolerant quantum computations on large-scale quantum computers the relative error for single logic operation must be no more than $\sim 10^{-5}$ [17]. Hence it follows that a *resolution* bound of the NMR spectrometer must be of the order of $\sim 100\,\text{kHz} \cdot 10^{-5} \sim 1$ Hz, that is consistent with the usual requirements. It is significant that such high precision is needed only for performing the logic quantum operation, but it is not needed for read-out measurements.

The read-out signal may be more increased by means of an electron-nuclear double resonance (ENDOR) methods [18] of observing the electron resonance at transitions with frequencies ω_B and ω_C (Fig. 3).

Consequently, by the use of standard NMR and additionally

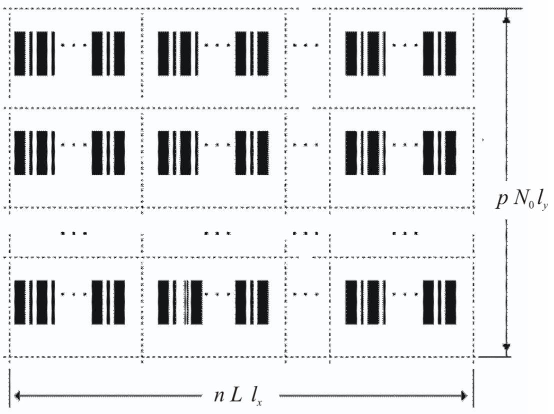

Fig. 4. The scheme of the proposed planar silicon topology with p·n parallel connected blocks of the ensemble L-qubit quantum computers (the connections are not shown here). The broad and narrow lines denote the ***A*** *and* ***J*** *gates*

of ENDOR techniques *the first main difficulty* of Kane's scheme can be overcome.

5. The cooling of nuclear spin system and nuclear state initialization by means of dynamic polarization

The electron and nuclear *longitudinal relaxation times* for the *allowed* transitions in four energy level system of phosphorus-doped silicon have been extensively investigated experimentally in [18, 19]. For the allowed transitions with frequencies ω_B and ω_C (Fig. 3) electron longitudinal relaxation times $\tau_{\|B} \approx \tau_{\|C}$ were found to be exceedingly long at low temperatures. They are of the order of *one hour* at $T = 1.25$ K, $B \sim 0.3$ T, are independent of phosphorus concentration below $C \sim 10^{16}\mathrm{cm}^{-3}$ (mean distance between phosphorus atoms is of the order of 45 nm) and are approximately inversely proportional to the lattice temperature *T*. The nuclear longitudinal relaxation time $T_{\|}$ at the frequency ω_A^+ was found to be equal to 10 hours.

The relaxation time for transition with frequency ω_D, which involves a simultaneous electron-nuclear spin flip-flop, at $T = 1.25$ K, $C \sim 10^{16}$ cm^{-3} and $B \sim 0.3$ T was $\tau_{\|D} \sim 30 \text{ hours} \gg \tau_{\|B}, \tau_{\|C}$.

The *extremely long relaxation times* of the electron and nuclear spins imply that the required initializing of nuclear quantum states (full nuclear *nonequilibrium polarizations*) can be attained by deep cooling of short duration of *only nuclear spin system* to $T_I \le 1$ mK without deep cooling of the lattice. There is the possibility to reach it at the *indirect cooling* of nuclear spin system by means of *dynamic nuclear spin polarization techniques* [19].

One such method of dynamic nuclear spin polarization for donor atoms is based on the saturation by *the microwave pumping of the forbidden transition* (frequency ω_S in Fig. 3), that is designated as the Abragam's *solid state effect* [6,19].

Let us consider this effect as applied to the ensemble of ^{31}P atoms. The polarization of electrons $P_S = 2\langle S_z\rangle$ and of nuclei $P_I = 2\langle I_z\rangle$ may be for the sake of simplicity expressed as

$$\begin{aligned} P_S &= p(1,1) + p(1,0) - p(1,-1) - p(0,0) \\ P_I &= p(1,1) + p(0,0) - p(1,0) - p(1,-1) \end{aligned}, \tag{28}$$

where $p(F, m_F)$ are the populations of states $\left|F, m_F\right\rangle$ (Fig. 3). They also fulfill the requirement

$$p(1,1) + p(1,0) + p(1,-1) + p(0,0) = 1. \tag{29}$$

The rate equations for the populations are (it is assumed, that the relaxation rates for transitions at frequencies $\omega_A^{\pm}$ are equal to $T_{\|A}$):

$$\begin{aligned} \frac{dp(0,0)}{dt} &= (p(1,1) - p(0,0)r_B)/\tau_{\|B} + (p(1,0) - p(0,0)r_D)/\tau_{\|D} + (p(1,-1) - p(0,0)r_A^+)/T_{\|A} \\ \frac{dp(1,-1)}{dt} &= (p(1,0) - p(1,-1)r_C)/\tau_{\|C} + (p(1,1) - p(1,-1))W_e + (p(0,0)r_A^+ - p(1,-1))/T_{\|A} \\ \frac{dp(1,0)}{dt} &= (p(1,-1)r_C - p(1,0))/\tau_{\|C} + p(0,0)r_D - p(1,0) + (p(1,1) - p(1,0)r_A^-)/T_{\|A} \\ \frac{dp(1,1)}{dt} &= (p(0,0)r_B - p(1,1))/\tau_{\|B} + (p(1,-1) - p(1,1))W_e + (p(1,0)r_A^- - p(1,1))/T_{\|A}, \end{aligned} \tag{30}$$

where parameters $r_{B,C,D,A} = \exp(-\hbar\omega_{B,C,D,A}/kT)$ are ratios of rates for the up and down thermal transitions. For values $\hbar\omega_{B,C,D}/kT \gg 1$, $\hbar\omega_A^{\pm}/kT \ll 1$ ($T \le 0.1$ K) there are the thermal electron $P_{S0} \approx -1$ and nuclear $P_{I0} = \hbar\omega_A^+/kT \ll 1$ polarizations.

Let us assume next that the rate of *induced forbidden electron transitions* $\left|1,1\right\rangle \Rightarrow \left|1,-1\right\rangle$ at frequency ω_S, that is W_S and electron longitudinal relaxation times satisfy the conditions:

$$W_S^{-1} < \tau_{\|B} \approx \tau_{\|C} \ll T_{\|A}, \tau_{\|D}, \tau_{\|S} \tag{31}$$

where $\tau_{\|D}$, $\tau_{\|S}$ are the longitudinal relaxation times of electron spins for the forbidden transition. Hereafter we shall write

$$\begin{aligned} \frac{dp(0,0)}{dt} &= p(1,1)/\tau_{\|B} + (p(1,-1) - p(0,0))/T_{\|A} \\ \frac{dp(1,-1)}{dt} &= p(1,0)/\tau_{\|B} + ((p(1,1) - p(1,-1))\cdot W_e + (p(0,0) - p(1,-1))/T_{\|A} \\ \frac{dp(1,0)}{dt} &= -p(1,0)/\tau_{\|B} + (p(1,1) - p(1,0))/T_{\|A} \\ \frac{dp(1,1)}{dt} &= -p(1,1)/\tau_{\|B} + (p(1,-1) - p(1,1))\cdot W_e + (p(1,0) - p(1,1))/T_{\|A}. \end{aligned} \tag{32}$$

With equations (28),(29),(31) we can obtain the rate equations for P_s and P_I:

$$\begin{aligned} dP_S/dt &= -(P_S + P_I)\cdot W_e - (P_S + 1)/\tau_{\|B} \\ dP_I/dt &= -(P_S + P_I)\cdot W_e - P_I/T_{\|A} \end{aligned}. \tag{33}$$

The steady-state saturation condition ($W_e \gg 1/T_{\|A}$) of the transition $|1,1\rangle \Rightarrow |1,-1\rangle$ gives rise to the equalization of the populations $p(1,1) = p(1,-1)$ and to the *full nuclear spin polarization* respectively

$$P_I = -P_S = p(0,0) = 1\,. \tag{34}$$

It is obvious that this state is equivalent to the state with nuclear spin temperature $T_I < \hbar\omega_A/k \sim 10^{-3}$ K.

Hence, the initialization of nuclear states may be obtained by using ENDOR technique at the lattice temperature of the order of 0.1 K and by this means that *the second difficulty* of Kane's scheme can be overcome.

Notice here that there is also another possibility of ensemble NMR implementation, which does *not have the gate system*. The selectivity of nuclear resonance frequencies for individual qubit in the ensemble of Kane's chains can be achieved, rather than using the **A**-gate voltage, with the applying of the external magnetic field gradients along axis x. For neighboring qubits separated by ~ 20 nm it is required $dB_z/dx \sim 1$ T/cm (that is feasible now), which produce a resonance frequency difference ~ 100 Hz.

6. The decoherence of nuclear spin states due to the hyperfine interaction of nuclear and electron spins

The relaxation of nonequilibrium state of the nuclear spin system represented by the product of independent (nonentangled) one-qubit states, owing to the interaction with isotropic environment, shows two processes. One is a slow establishment of equilibrium state associated with dissipation of energy. For it, the diagonal elements of density matrix decay with characteristic longitudinal (spin-lattice) relaxation time $T_\|$. The decay of non-diagonal matrix elements called decoherence of quantum states is characterized by a decoherence time T_d or transverse (spin-spin) relaxation time $T_\perp$. The longitudinal relaxation times $T_\|$ in the case of nuclear spin of ^{31}P atoms as qubits is defined mainly by thermal modulation of qubit resonance frequency accompanied by spin flips. It is usual that for solids $T_\perp \ll T_\|$.

The *internal adiabatic decoherence* mechanisms due to a random modulation of qubit resonance frequency are produced by local fluctuating magnetic fields without spin flips. These fields are determined by secular parts of interactions of nuclear spins with electron spins of the basic phosphorus atoms, with impurity paramagnetic atoms and also with nuclear spins of impurity atoms. We have named this mechanism as *internal*. It seems to be the leading one.

The modulation of nuclear spin resonance frequency $\Delta\omega(t)$, which is determined by the secular part of hyperfine interaction, may be written as

$$\Delta\omega(t) = A(t)S_z(t) - A_0\langle S_z\rangle \approx A_0(S_z(t) - \langle S_z\rangle) - \Delta A(t)\langle S_z\rangle\,, \tag{35}$$

where $A(t) = A_0 + \Delta A(t)$, $\Delta A(t)$ is the modulation of hyperfine interaction constant, $A_0 = 725$ rad MHz. The influence of gate voltage noise on this frequency modulation was studied in [9,10,20] and it is not treated here (*external* decoherence process).

Another (internal) modulation mechanism of $A(t)$ is the interaction of donor atoms with acoustic phonons. It is our belief that for very low temperature this mechanism is not essential [21].

Let us consider now the first term in (35). We shall follow the semiclassical model of *adiabatic decoherence of one-qubit state* (Appendix). The correlation function of frequency modulation $\Delta\omega_S(t) = A_0\,(S_z(t) - \langle S_z\rangle)$ is determined by the fluctuations of electron spin polarization and depends on electron resonance frequency ω_S, longitudinal τ_1 (hours) and transverse τ_2 relaxation times. In adiabatic case $\omega_S = \gamma_S B > 1/\tau_2 \gg 1/\tau_1$ and we obtain:

$$\langle \Delta_S\omega(t)\Delta\omega_S(0)\rangle = \langle \Delta\omega_S^2\rangle \exp(-t/\tau_1) \tag{36}$$

where

$$\langle \Delta\omega_S^2\rangle = A_0^2\left(\langle S_z^2\rangle - \langle S_z\rangle^2\right) = A_0^2(1 - \tanh^2(\gamma_S\hbar B/2kT))/4\,. \tag{37}$$

Now, according to (62), for decoherence decrement we obtain

$$\Gamma(t) = \langle \Delta\omega_S^2\rangle \tau_1^2(t/\tau_1 - 1 + \exp(-t/\tau_1))\,. \tag{38}$$

For $\tau_1 \approx 10^4$s and $t \sim T_d = 1$s, $1 \ll \langle \Delta\omega_S^2\rangle \tau_1^2 < (\tau_1/T_d)^2$ we have the non-Markovian random process (slow dampening fluctuations). In this case

$$\Gamma(t) = \langle \Delta\omega_S^2\rangle t^2/2 \tag{39}$$

and the effective decoherence time can by estimated from $T_d \sim \langle \Delta\omega_S^2\rangle^{-1/2}$.

The necessary value of decoherence time for the NMR quantum computer clock time ~ 10^{-4} s should not exceed several seconds. Therefore, let us write the requirement for $\gamma_e\hbar B/kT \gg 1$ in the form

$$1/T_d^2 \approx A_0^2(1 - \tanh^2(\gamma_e\hbar B/2kT))/4 \approx 2A_0^2\exp(-\gamma_e\hbar B/kT) < 1\text{s}^{-2}\,, \tag{40}$$

from which we find that the decoherence suppression will be achieved only at *sufficiently large* $B/T > 30$ T/K. It corresponds to $B = 2$ T for lattice temperatures $T < 0.06$ K.

7. The adiabatic decoherence of nuclear spin states due to interaction with nuclear spins of impurity atoms

The paramagnetic impurity atoms having magnetic moments play also a role of environment for nuclear spins in solid state. However decoherence mechanism due to dipole-dipole interaction of their magnetic moments with nuclear spin-qubits is suppressed to a large extent at $B/T > 30$ T/K thanks to near-full electron spin polarization [21].

Another mechanism of one qubit state decoherence is dipole-dipole interaction with not fully polarized nuclear spins $I \neq 0$ of impurity diamagnetic atoms having concentration $C_{I,imp}$. Isotope ^{29}Si with $\gamma_{I,imp} = -53$ rad MHz/T is one of such atoms. The random fluctuating local field, produced by nuclear spins of impurity atoms has the form

$$\Delta B_\alpha(t) = -\sum_{i,\beta}^{N} D_{\alpha,\beta}(\mathbf{r}_i)\left(I_{\beta,imp}(\mathbf{r}_i,t) - \left\langle I_{\beta,imp}(\mathbf{r}_i)\right\rangle\right), \tag{41}$$

where

$$D_{\alpha,\beta}(\mathbf{r}_i) = \frac{\mu_0}{4\pi}\frac{\gamma_I\gamma_{I,imp}}{r_i^3}\left(\delta_{\alpha\beta} - \frac{3r_{i\alpha}r_{i\beta}}{r_i^2}\right) \tag{42}$$

$\mathbf{r}_i$ is the distance-vector to *i*-th impurity nuclear spin.

In this case correlation function of frequency modulation

$$\left\langle \Delta\omega_S(t)\Delta\omega_S(0)\right\rangle = \gamma_I^2\left\langle B_z(t)B_z(0)\right\rangle = C_{I,imp}\int\sum_{\beta} D_{z,\beta}(\mathbf{r})(I_{\beta,imp}(\mathbf{r},t)I_{\beta,imp}(\mathbf{r}) - \rangle I_{\beta,imp}(\mathbf{r})\rangle^2)d\mathbf{r} \tag{43}$$

takes the form

$$\left\langle \Delta_S\omega(t)\Delta\omega_S(0)\right\rangle = \left\langle \Delta\omega^2\right\rangle \exp(-t/T_{\|,imp}), \tag{44}$$

where $T_{\|,imp} \approx 10^4$ s is impurity nuclear spin longitudinal relaxation time of isotope ^{29}Si at low temperature [18]. Taking $T_{\|,imp}$ to be much more than $T_d \sim 1$s, for the determination of allowable impurity concentration we obtain equation

$$1/T_d^2 \approx C_{I,imp}\frac{(\mu_0\gamma_I\gamma_{I,imp}\hbar)^2}{60\pi a^3}\left(1 - \tanh^2\left(\left|\gamma_{I,imp}\right|hB/2kT_I\right)\right), \tag{45}$$

where a is the minimal distance to impurity nuclear spin, and for Si a^{-3} is of the order of $5\cdot 10^{22}$cm^{-3}.

For $B/T > 30$ T/K and for spin temperature T_I at which there is near-full polarization of nuclear spins

$$\left|\gamma_{I,imp}\hbar B/kT_I\right| > 1 \tag{46}$$

or for $T_I < 0.8$ mK, we obtain that the allowed concentration of the isotope ^{29}Si is

$$C_{I,imp}\% < 4.5\cdot 10^{-2}\,\%. \tag{47}$$

This value can be increased due to the further decrease of nuclear spin temperature T_I. For comparison, natural abundance of isotope ^{29}Si in natural silicon is 4.7%. At present, the realized degree of cleaning ^{28}Si is 99.98%, which does *not fully suit* for our purposes yet.

8. Adiabatic decoherence of entangled two qubit states

In the processes of input of information and logic operation performance, some nonentangled initializing states of quantum register become entangled. The adiabatic process of transverse relaxation may be also the main decoherence mechanism of coherent entangled quantum states.

As a simple example let us consider here the adiabatic decoherence of the pure fully entangled two qubit triplet state of EPR-type $\left|\psi_{EPR}\right| = \sqrt{1/2}\left(\left|\uparrow\downarrow\right| + \left|\downarrow\uparrow\right|\right)$ with the zero projection of the total spin on the z-axis, which is described by density matrix

$$\rho_{EPR} = \left|\psi_{EPR}\right\rangle\left\langle\psi_{EPR}\right| = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{48}$$

The action of the environment on qubit states will be described quasiclassically as correlated random modulation of the qubit resonance frequencies $\Delta\omega_{1,2}(t)$ and of indirect spin-spin interaction parameter $\Delta\omega(t) = \Delta I_I(t)/2$. The secular part of Hamiltonian for interaction with the environment is represented by

$$\mathbf{H}(t) = -\Delta\omega_1(t)(\sigma_{1z}\otimes\mathbf{1})/2 - \Delta\omega_2(t)(\mathbf{1}\otimes\sigma_{2z})/2 + \Delta\omega_I(t)(\sigma_{1z}\otimes\sigma_{2z})/2, \tag{49}$$

where $\sigma_{1z,\,2z}$ are Pauli matrices.

The density matrix (48) under the action of random field in the rotating frame with resonance frequency ω_0 is described by expression

$$\rho_{EPR}(t) = \mathbf{U}(t)^{-1}\rho_{EPR}\mathbf{U}(t). \tag{50}$$

In the considered case, the unitary matrix 4×4 $\mathbf{U}(t)$ is ($\varphi_{1,2}(t) = \int_0^t \Delta\omega_{1,2}dt$, $\varphi_I(t) = \int_0^t \Delta\omega_I dt$):

$$\begin{aligned}\mathbf{U}(t) = &(\cos(\varphi_1(t)/2)\mathbf{1} + i\sin((\varphi_1(t)/2)\sigma_{1z}) \otimes (\cos(\varphi_2(t)/2)\mathbf{1} + i\sin((\varphi_2(t)/2)\sigma_{2z} \cdot \\ &\cdot(\cos\varphi_I(t)(\mathbf{1}\otimes\mathbf{1}) + i\sin\varphi_I(t)(\sigma_{1z}\otimes\sigma_{2z}))\end{aligned}. \tag{51}$$

For perturbed density matrix we obtain

$$\rho_{EPR}(t) = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & \exp(-i(\varphi_1(t)-\varphi_2(t))) & 0 \\ 0 & \exp(i(\varphi_1(t)-\varphi_2(t))) & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{52}$$

We see that the *modulation of spin-spin interaction has no effect* on density matrix of triplet EPR-state.

Let us assume now that the random phases $\varphi_{1,2}(t)$ have mean value $\langle\varphi_{1,2}(t)\rangle = 0$ and belong to the reduced statistical ensemble, which is described by the *two-dimensional Gaussian distribution*:

$$w(\varphi_1(t),\varphi_2(t)) = \frac{1}{2\pi\sigma_1(t)\sigma_2(t)\sqrt{(1-\rho_{12}^2(t))}}\exp\left\{-\frac{1}{2(1-\rho_{12}^2(t))}\cdot\left(\frac{\varphi_1^2(t)}{\sigma_1^2(t)} - \frac{2\rho_{12}(t)\varphi_1(t)\varphi_2(t)}{\sigma_1(t)\sigma_2(t)} + \frac{\varphi_2^2(t)}{\sigma_2^2(t)}\right)\right\}. \tag{53}$$

Here

$$\sigma_{1,2}^2(t) = \left\langle\varphi_{1,2}^2(t)\right\rangle = 2\int_0^t (t-\tau)\, f_{1,2}(\tau)d\tau$$

are the variances and

$$\rho_{12}(t) = \frac{\left\langle\varphi_1(t)\varphi_2(t)\right\rangle\rangle\ \rangle}{\sigma_1(t)\sigma_2(t)} = \frac{2\int_0^t (t-\tau)\, f_{12}(\tau)d\tau}{\sigma_1(t)\sigma_2(t)}, \tag{54}$$

where

$$f_{1,2}(\tau) = \left\langle\Delta\omega_{1,2}(\tau)\Delta\omega_{1,2}(0)\right\rangle, \qquad f_{12}(\tau) = \left\langle\Delta\omega_1(\tau)\Delta\omega_2(0)\right\rangle. \tag{55}$$

The normalized mutual correlation function $\rho_{12}(t)$ takes values in interval $0 \le \rho_{12}(t) \le 1$.

After averaging (52) with (53) we have

$$\rho_{EPR}(t) = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & \exp(-\Gamma(t)) & 0 \\ 0 & \exp(-\Gamma(t)) & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{56}$$

where

$$\exp(-\Gamma(t)) = \int_{-\infty}^{\infty} d\varphi_1 \int_{-\infty}^{\infty} d\varphi_2 w(\varphi_1,\varphi_2)\exp(\pm i(\varphi_1-\varphi_2)) = \exp\{-(\sigma_1^2(t) - 2\sigma_1(t)\sigma_2(t)\rho_{12}(t) + \sigma_2^2(t)\} \tag{57}$$

In the absence of random field correlation $\rho_{12}(t) = 0$, the decrement $\Gamma(t)$ is equal to the *sum of decrements of two* one qubit states:

$$\Gamma(t) = (\sigma_1^2(t) + \sigma_2^2(t))/2 = 2\Gamma_1(t) \tag{58}$$

In the case of maximum correlation $\rho_{12}(t) = 1$ and $\varphi_1(t) = \varphi_2(t)$ (the same mode acts on both qubits), *adiabatic decoherence disappears*. The singlet EPR state has analogous properties.

We see here that decoherence of interacting qubit states may differ essentially from one qubit decoherence. Under the action of fully correlated random fields the coherence of two mentioned entangled states is not violated and they may be considered as the basis of decoherence-free substrate for logical qubits coding. Clearly, the pure nonfully entangled states $|\psi| = (\sqrt{1-\alpha}\,|\uparrow\downarrow| + \sqrt{\alpha}\,|\downarrow\uparrow|)$ have no such properties.

Adiabatic decoherence of other two-qubit fully entangled quantum Bell states $|\psi| = \sqrt{1/2}\left(|\uparrow\uparrow| \pm |\downarrow\downarrow|\right)$ under the action of fully correlated random fields with $\rho_{12}(t) = 1$ now does not disappear. Its decrement equals to $\Gamma(t) = (\sigma_1(t) + \sigma_2(t))^2/2 = 2\sigma_1^2 = 4\Gamma_1(t)$, that is *four times larger* than for one qubit decoherence.

Conclusion

1. The development of the large-scale ensemble NMR quantum computers has certain advantage over Kane's scheme. It consists in the possibility of employment of the standard NMR technique for the measurement of quantum states at output of computer, like in the liquid prototype.
2. Methods of dynamic polarization may be proposed for the initialization of nuclear spin states at temperature $T \sim 0.1$ K.
3. Analysis of proposed planar structure of ensemble silicon computer shows the possibility of realization of large-scale NMR quantum computer for ensemble component number $N \sim 10^5$.
4. The main reasons for the internal decoherence of one qubit states are the modulation of resonance qubit frequency due to hyperfine interaction with fluctuating electron spin and due to interaction with randomly distributed impurity diamagnetic atoms containing nuclear spins.
5. Analysis of different feasible ways for obtaining decoherence times large enough shows that the values, needed to perform the required number of quantum logic operations $\sim 10^5$ for large-scaled computations, can be achieved.

Appendix

Semiclassical model of adiabatic decoherence of one-qubit state

We will consider a long-living non-equilibrium qubit state when diagonal elements of density matrix may be treated as a constant.

The random modulation of resonance frequency $\Delta\omega(t)$ that causes the dephasing of a qubit state is determined by the random phase shifts

$$\varphi(t) = \int_0^t \Delta\omega(t)dt. \tag{59}$$

The one-qubit density matrix of pure state in the rotating frame with non-perturbed resonance circular frequency will be

$$\rho(t) = \frac{1}{2}\begin{bmatrix} 1+P_z & P_- \exp(i\varphi(t)) \\ P_+ \exp(-i\varphi(t)) & 1-P_z \end{bmatrix}, \tag{60}$$

where $P_\pm = P_x \pm iP_y$, P_x, P_y, P_z are Bloch vector components of length $P = \sqrt{P_x^2 + P_y^2 + P_z^2} = 1$.

By treating the resonance frequency modulation as Gaussian random process after averaging (60) over phase distribution with $\langle \varphi(t) \rangle = 0$ we obtain

$$\langle \rho(t) \rangle = \frac{1}{2}\begin{bmatrix} 1+P_z & P_- \exp(-\Gamma(t)) \\ P_+ \exp(-\Gamma(t)) & 1-P_z \end{bmatrix}, \tag{61}$$

where

$$\Gamma(t) = \frac{1}{2}\left\langle \left(\int_0^t \Delta\omega(t)dt \right)^2 \right\rangle = \int_0^t (t-\tau)\langle \Delta\omega(\tau)\Delta\omega(0) \rangle d\tau \tag{62}$$

$f(t) = \langle \Delta\omega(t)\Delta\omega(0) \rangle$ is the frequency correlation function of a random process, which is characterized by variance $\langle \Delta\omega(0)^2 \rangle$ and correlation time τ_C such that for $t > \tau_C$ $\langle \Delta\omega(t)\Delta\omega(0) \rangle \Rightarrow 0$. For $\Gamma(t) > 0$ the averaged density matrix presents a mixed quantum state with two non-zero eigenstates

$$1/2 \cdot \left(1 \pm \sqrt{1 - (P_x^2 + P_y^2)(1 - exp(-2\Gamma(t)))} \right) \tag{63}$$

and the populations of states $p_\pm = 1/2(1 \pm P_z(0))$ at $\Gamma(t) \Rightarrow \infty$.

Thus, the adiabatic decoherence problem is reduced to the determination of the function $\Gamma(t)$ or the correlation function of random frequency modulation.

In the case of an ensemble quantum register there is a need to average the one-qubit density matrix and correlation function over ensemble of independent equivalent spin-qubits.

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