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Nuclear magnetic resonance spectrum of ^{31}P donors in silicon quantum computer

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Abstract. The influence of an electric field created by a gate potential of the silicon quantum computer on the hyperfine interaction constant (HIC) is obtained. The errors due to technological inaccuracy of location of donor atoms under a gate are evaluated. The energy spectra of electron-nuclear spin system of two interacting donor atoms with various values of HIC are calculated. The presence of two pairs of anticrossing levels in the ground electronic state is shown. Parameters of the structure at which errors rate can be greatly minimized are found.

Introduction

One of the most perspective ideas on experimental realization of the quantum computer is the possibility of creating artificial multispin systems. Such an approach, not yet realized, was offered by Kane [1] and was studied further in [2–4]. The special feature of this variant consists in the realization of the individual addressing to separate spins-qubits. For this purpose it is supposed to use a silicon structure of the MOS type, where donor atoms of stable isotope of phosphorum ^{31}P replacing silicon atoms in the knots of a crystalline lattice are introduced into the thin layer of the spinfree silicon ^{28}Si isotope. Such a donor has nuclear spin with $I = 1/2$ and states which are characterized by a high value of an effective Bohr radius. In the considered approach it is necessary to use rather low temperatures so that the electrons of donor atoms occupied only the lower spin state in the magnetic field, that is $T \ll 2\mu_B B/k$, where $\mu_B = 9.27 \times 10^{-24}$ J/T is Bohr magneton, B is induction of the external constant magnetic field, $k = 1.38 \cdot 10^{-23}$ J/K is Boltsman constant. At fields $B > 2$ T it corresponds to temperatures $T < 0.1$ K, which are much lower, than the temperature of freezing out the donors electronic state. Therefore, the donors will remain in the neutral ground orbital S-state.

Each donor atom with its nuclear spin in a semiconductor structure is supposed to be arranged regularly with an adequate accuracy under "its" own control metal gate (gate A), separated from the surface of silicon by a thin dielectric. The gates A form a linear chain of any length with the period l. The variation of the electrical potential of gates J, located between gates A, allows to control a degree of overlapping of electrons' wave functions located on the adjacent donors a and b and the constant of their exchange interaction J as well as the constant of scalar interaction of their nuclear spins I_{ab}.

This is achieved by redistribution of electronic density between adjacent donor atoms. It is supposed that with the help of electrical field created by gates A it is possible to change distribution of an electronic density near the nucleus in the main state by adjusting, respectively, individual resonance frequency of a nuclear spin of each donor atom, which is determined by hyperfine interaction between the atom and electronic spin. It allows to realize quantum operations by selective influence of resonance radio-frequent impulses on nuclear spins of certain donors.

Thus, for the development of a variant of the semiconductor quantum computer proposed in [1], it is important to have a detail information about properties of a donor atom energy spectrum hyperfine structure.

1. Dependence of the hyperfine interaction constant on the electrical field

The spin Hamiltonian of hyperfine interaction is:

$$\hat{H}_{IS} = A\left(\hat{\vec{I}}\hat{\vec{S}}\right), \tag{1}$$

where $\hat{\vec{I}}$ and $\hat{\vec{S}}$ are nuclear and electron spins respectively,

$$A(V) = \frac{8\pi}{3}|\Psi_0(0, V)|^2 2\mu_B g_N \mu_N \frac{\mu_0}{4\pi}, \tag{2}$$

$\mu_N = 5.05 \cdot 10^{-27}$ J/T is nuclear magneton, $\mu_0 = 4\pi \cdot 10^{-1}$ T^{2}cm^3/J, $g_N = 2.26$ is Lande's factor of ^{31}P, $\mu_B = 9.27 \cdot 10^{-24}$ J/T is Bohr's magneton, $\Psi_0(0, V)$ is the wave function of the electron near nucleus. Taking into account the existing electric field the Schrödinger equation for this wave function should be supplemented by an perturbation operator $\Delta\hat{H} = e\phi(\rho', z')$ ($e = 1.6 \cdot 10^{-19}$ C, $\rho'^2 = x'^2 + y'^2$) [2], where the potential ϕ is induced by the gate which has the form of round disk of radius $a = l_A/2$. By factorizing this potential and taking as undisturbed wave functions hydrogen-like functions, we calculate matrix elements of transitions necessary for calculation of error corrections for the wave function within the framework of the theory of perturbations. Limiting ourselves by the second order of the perturbations theory and conducting necessary number substitutions, we shall receive the following expression for a relative error correction of the donor atom hyperfine interaction constant (with $c = 2a = 10$ nm, V is expressed in volts):

$$\frac{\Delta A(V)}{A} = 0.55V - 0.09V^2. \tag{3}$$

Let us consider the case, when gates A have the form of endlessly long strips with the breadth of $2a = l_A$ located at distance D from the conducting substrate, from which the potential of a gate is accounted. Conducting similar operations, we shall receive for a relative error correction of the donor atom HIC the following expression (with $c = 2a = 10$ nm, $D/a = 100$):

$$\frac{\Delta A(V)}{A} = -0.063V^2. \tag{4}$$

The voltage in (4) is expressed, similar to the above, in volts.

2. Influence of the technological location spread of donor atoms on the HIC. Voltage error on a gate

Technological inaccuracies of a donor atom location under a gate in respect of the position of $x = 0$, $z = c$ shall be designated by δx and δz. We resrtict ourselves here to the consideration of only the case of a strip gate. Factorizing the electric field strength and its gradient along axes x and z to degrees δx and δz, we receive a resultant expression for a relative error of the HIC:

$$\frac{\delta A}{A} = \delta z\left\{0.063V^2\frac{2c}{a^2 + c^2}\right\} + (\delta x)^2\left\{0.063V^2\frac{2c^2 - a^2}{\left(a^2 + c^2\right)^2} - 0.085V\frac{2c^4 - a^4}{2c^2\left(a^2 + c^2\right)^2}\right\} \tag{5}$$

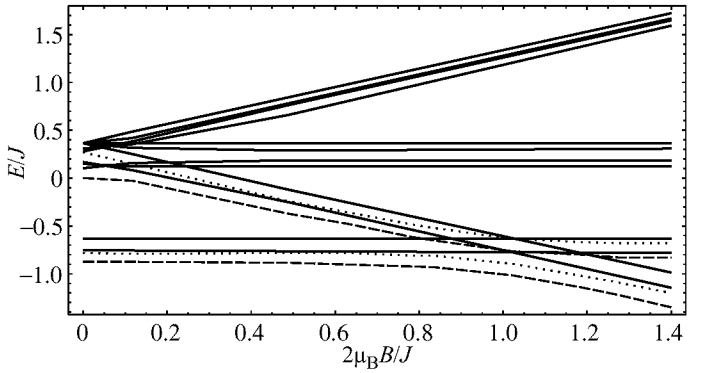

Fig. 1. Levels of energy of spins for a system of two atoms ^{31}P in a magnetic field ($A_a/J = 0.3$; $A_b/J = 0.4$).

The second item in (5) can be turned to zero with different values of a, c and V. That is why by setting a required relative error, it is possible to determine parameters of structure a and c and voltage V at which the required accuracy will be realized. Permissible deviation of the donor atom along axis z connected with the technological inaccuracy of location in 2–3 nm corresponds to a 1% preset relative error of hyperfine interaction. Voltage error at a gate allowed for a correctly controlled quantum computing process can be determined from resultant expressions for changes of the hyperfine interaction constant. The bandwidth of resonance impulse frequencies should be, at least, one order less than the resonance frequency of nuclear spins which is equal to hundreds of kHz. Taking the value of the error for the hyperfine structure constant corresponding to the bandwidth of the resonance impulse $\delta(\Delta A) \sim 10^4$ Hz, we shall find the value of the error for the voltage at the gate being equal to 10^{-4}–10^{-3} V. Let us note, that in case of round disks gates because of the linear V summand in expression (4), there is a chosen voltage at which the allowable voltage error greatly increases.

3. Energy spectrum of an electronic-nuclear spin system of two interacting donor atoms

Let us consider two donor atoms being at a distance of l from each other. This distance should be such that constant J of the effective exchange interaction of electrons caused by partial overlapping of their wave functions, had the magnitude sufficient for organizing double qubit operations. The spin Hamiltonian of such a system looks as follows:

$$\hat{H} = 2\mu_B \vec{B}\left(\hat{\vec{S}}_a + \hat{\vec{S}}_b\right) + J\left(\hat{\vec{S}}_a \hat{\vec{S}}_b\right) - g_N \mu_N \vec{B}\left(\hat{\vec{I}}_a + \hat{\vec{I}}_b\right) + A_a\left(\hat{\vec{I}}_a \hat{\vec{S}}_a\right) + A_b\left(\hat{\vec{I}}_b \hat{\vec{S}}_b\right) \quad (6)$$

where, $\hat{\vec{S}}_a$, $\hat{\vec{I}}_a$, $\hat{\vec{S}}_b$, $\hat{\vec{I}}_b$ are spin operators of both an electron and a nucleus for the first and second atoms respectively, $\vec{B}$ is magnetic field (it is directed along the z axis), A_a and A_b are constants of hyperfine interaction depending on the potentials on gates, μ_B is Bohr magneton, μ_N is nuclear magneton, g_N is Lande's factor for ^{31}P. The eigen values of a Hamiltonian was accurately calculated. With the help of this matrix the energy levels were numerically established.

4. The conclusion

The proposed paper has a detailed analysis of the influence of the electric field created by gate A on the hyperfine interaction constant for two types of gates: in the form of a disk and in the form of a strip. A weaker dependence of the hyperfine interaction constant on the depth of the donors position under a gate as well as decreasing of its value as the distance between the gate and the substrate was increasing were noted. The conducted calculations with the two types of gates make it possible to conclude that there is a significant dependence of the hyperfine interaction constant on the form of a gate.

The obtained expressions enable to determine permissible values of technological inaccuracies δx and δz with the set value of the A constant error and working values of the V gate potential.

The paper contains calculation of the full energy spectrum of an electronic-nucleus spin system of two interacting donor atoms for different values of HIC. The presence of two pairs of anticrossing levels in the main electronic condition corresponding to the projection of full electronic and nuclear spins-1 (dotted line) and 0 (dashed line) is shown. For organizing computing and measuring process both pairs anticrossing levels can be used.

References

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