MASTER THESIS

Time Evolution of
Quantum Computer

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論 文 要 旨
（和 文）

（論文題目）

量子計算機の時間発展シミュレーション

（内容の要旨）

　量子計算機は、１９８５年に Deutsch によって明確に定式化された、量子力学の原理に基づく全く新しい計算機の概念である。古典力学に従う従来の計算機では、０または１のどちらかのみの状態をとるビットを基本の計算要素としている。量子計算機では、古典計算機の０にあたるビットを２準位系の基底状態、１にあたるものを第一励起状態と対応させ、０と１の重ね合わせ状態に拡張したビットを用いる。このビットは qubit と呼ばれている。また量子計算機ではその計算にあたる操作を、ユニタリー変換による量子状態の遷移として行う。このとき初期状態としてお互いに量子的な相関を持つ qubit を複数用意することによって、同時に重ね合わせ状態を並列計算できることが量子計算機の利点である。

　この概念を利用した量子計算機の実現にあたっては、量子的な重ね合わせ状態を良質に維持するために、環境系との相互作用によるデコヒーレンス時間が長いことが必要となる。この要求に対する新しい方法が１９９８年にKane によって提案された。それはシリコン中にドープした ^{31}P の核スピンをqubit として用いることにより、qubit が環境系と相互作用することによる緩和を防ぐものである。この提案におけるゲート操作は NMR で行われている方法と同様に外部磁場によって誘起されたゼーマン分裂に、共鳴した高周波磁場を照射することによって行う。

　本研究では、Kane の提案した半導体量子コンピュータのゲート操作を数値的に再現することを試みた。これを行う方法として、まず半導体デバイス中にドープされた ^{31}P は水素類似原子であると仮定した。z 軸方向の静磁場中における核-電子系のスピンハミルトニアンに、高周波磁場を時間に依存する摂動として加え、エネルギー準位間の遷移確率を求めた。

Graduate College of Science and Engineering, Aoyama Gakuin University

Master Thesis

Time evolution of quantum computer

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Deutsch formulated in 1985 a new computer based on the quantum mechanics. In quantum computers, the ones and zeros of classical digital computers are replaced by the quantum state of a two-level system which is named qubit. Computation, i.e., a sequence of unitary transformations, simultaneously affects each element of the superposition, generating a massive parallel data processing, albeit within one piece of quantum hardware.

Practical of quantum computer, requires preventing decoherence (uncontrolled interaction of a quantum system with its surrounding environment) in order to maintain the superposition. In 1998, Kane proposed the scheme of implementing a quantum computer on an array of nuclear spins lacated on donors in silicon. Because nuclear spins are extremely well isolated from environment, operations on nuclear-spin qubits could have low error rates. Quantum logic gate is performed by transitions between the different energy levels of the electron-nuclear spin states, which is induced by a radio-frequency magnetic field B applied at a frequency resonant with the energy level difference.

In this study, we numerically simulated the quantum logic gate of Kane's quantum computer, In by neglecting, the complications generated from the band structure in Si. For the calculation of the time evolution of the quantum logic gate, we obtain the transition probabirity between the energy levels of electron-nuclear spin states under the influence of a time-dependent perturbation $\hat{V}(r,t)$.

MASTER THESIS
Time evolution of quantum computation

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Abstract

Deutsch formulated in 1985 a new computer based on quantum mechanics. In quantum computers, the ones and zeros of classical digital computers are replaced by the quantum state of a two-level system which is named qubit. Computation, i.e., a sequence of unitary transformations, simultaneously affects each element of the superposition, generating a massive parallel data processing, albeit within one piece of quantum hardware.

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In this study, we numerically simulated the quantum logic gate of Kane's quantum computer, by neglecting the complications generated from the band structure in Si. For the calculation of the time evolution of the quantum logic gate, we compute the transition probability between the energy levels of electron-nuclear spin states under the influence of a time-dependent perturbation.

Contents

1   Introduction

The concepts of information and computation can be properly formulated only in the context of a physical theory—information is stored, transmitted, and processed always by *physical* means. When quantum effects become important, at the level of single atoms and photons, existing, purely abstract classical theory of computation becomes fundamentally inadequate. Entirely new modes of computation and information processing become possible. Phenomena such as quantum interference and quantum entanglement can be exploited for computations.

The idea of a quantum computer has been developed theoretically over several decades to elucidate fundamental questions concerning the capabilities and limitations of mechanics in which information is treated quantum mechanically. Specifically, in quantum computers the ones and zeros of classical digital computers are replaced by the quantum state of a two-level system, namely a qubit. Computation, i.e., a sequence of unitary transformations simultaneously affects each element of the superposition, generating a massive parallel data processing, albeit within one piece of quantum hardware. Consequently, quantum computers can efficiently solve some problems that are believed to be intractable on any classical computer.

Quantum computation can, in principle, only occur in system that are almost completely isolated from their environment and which consequently must dissipate no energy during the process of computation, conditions that are extraordinarily difficult to fulfill in practice. Interest in quantum computation has increased dramatically in the past years because of two important insights: first, quantum algorithms (most notably for prime factorization[1] and for exhaustive search[2]) have been developed that outperform the best known algorithms doing the same tasks on the classical computer. These algorithms require that the internal state of the quantum computer be controlled with extraordinary precision, so that the coherent quantum state upon which the quantum algorithms rely is not destroyed. Because completely preventing decoherence (uncontrolled interaction of a quantum system with its surrounding environment) is impossible, the existence of quantum algorithms does not prove that they can ever be implemented in a real machine. The second critical insight has been the discovery of quantum error-correcting codes[3, 4] that enable quantum computers to operate despite some degree of decoherence and which may make quantum computers experimentally realizable.

The variety of physical system is proposed. The state of spin 1/2 particles that are two-level systems can potentially be used for quantum computation. Nuclear spins have been incorporated into several quantum computer proposals, because they are extremely well isolated from environment and so operations on nuclear-spin qubits could have low error rates. The primary challenge using nuclear spins in quantum computers lies in measuring the spins. The bulk spin resonance approach to quantum computation circumvents the single-spin detection problem essentially by performing quantum calculation in parallel in a large number of molecules and determining the result from macroscopic magnetization measurements. The measurable signal decreases with the number of qubits, however, and scaling this approach above about ten qubits will be technically demanding. To attain the goal of large number qubits quantum computer, Kane proposed a scheme for implementing a quantum computer on an array of nuclear spins located on donors in silicon. Logical operations and measurements can in principle be performed independently and in parallel on each spin in the array. Here in order to analyze the principles of Kane's quantum computer, we simulate numerically the time evolution of the Hamiltonian with the Kane's quantum computer.

In section 2, we describe the quantum computation with a P array in silicon. The transition probability which describes the time evolution of the quantum logic gate is explained in section 3. In section 4 we discuss the implementation of the 'single spin rotation' with a P atom in a magnetic field B_z, and the 'two-qubit controlled rotation' is discussed in section 5. In section 6, we described the measurement of individual nuclear-spin states.

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2 Quantum computation with a P array in silicon

In this section, we describe a scheme of implementation of silicon-based quantum computer. The basic requirement and performing of the quantum gate is described.

2.1 Basic requirements for semiconductor

Recently, Kane proposed[5] a new implementation of a solid-state quantum computer. Kane's idea is to use a semiconductor MOS structure on a ^{28}P spinless substrate into a thin layer of which ^{31}P stable phosphorus isotopes, acting as donors, are implanted. An important requirement for a quantum computer is to isolate the qubits from any degrees of freedom that may lead to decoherence. If the qubits are spins on a donor in a semiconductor, nuclear spins in the host are a large reservoir with which the donor spins can interact. Consequently, the host should contain only nuclei with spin $I = 0$. This simple requirement unfortunately eliminates all III-V semiconductors as host candidates, because none of their constituent elements possesses stable $I = 0$ isotopes[6]. Group IV semiconductors are composed primarily of $I = 0$ isotopes and can in principle be purified to contain only $I = 0$ isotopes.

The only $I = 1/2$ shallow (Group V) donor in Si is ^{31}P. At sufficiently low ^{31}P concentrations at temperature $T = 1.5$K, the electron spin relaxation time is thousands of seconds and the ^{31}P nuclear spin relaxation time exceeds ten hours. It is likely that at millikelvin temperature the phonon-limited ^{31}P relaxation time is of the order of 10^{18} seconds[7], making this system ideal for quantum computation.

2.2 Gate operation of electron-nuclear spin system of a donor

The quantum computer proposed by Kane comprises an array of such donors positioned beneath the surface of a semiconductor host (Fig.1). Quantum calculation proceeds by the control of three external parameters: (1) A-gates above the donors control the strength of the hyperfine interactions and hence the resonance frequency of the nuclear spins beneath them; (2) J-gates between the donors turn on and off electron-mediated coupling between the
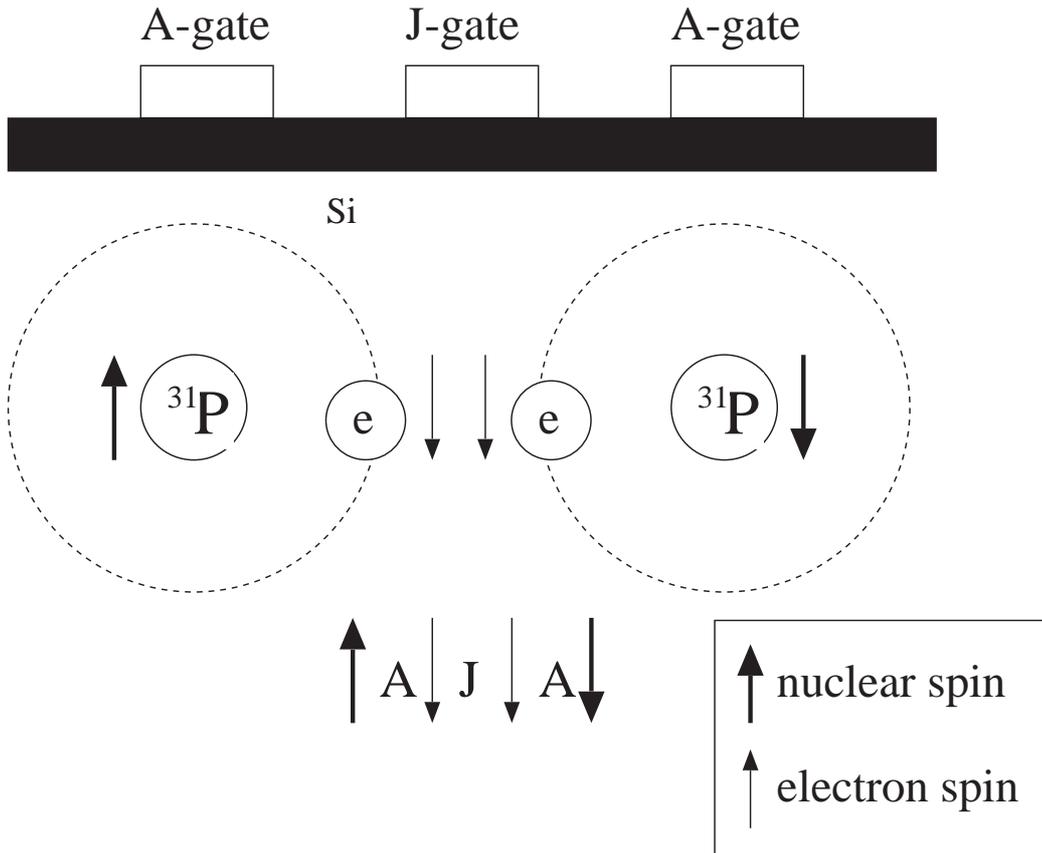
Figure 1: Two ^{31}P donors in silicon. The nuclear spins are coupled to the outer electrons by the hyperfine interactions A, which can be controlled by the A-gates. The electrons are mutually coupled via an exchange interaction J, which can be controlled by the J-gate.

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nuclear spins; (3) a globally applied magnetic field B_{ac} flips nuclear spins at resonance.

The spin Hamiltonian for the nucleus-electron system in SI:P with magnetic field B_z is

$$\mathcal{H}_{en} = \mu_B B_z \sigma_z^e - g_n \mu_n B_z \sigma_z^n + A \vec{\sigma}^e \cdot \vec{\sigma}^n, \tag{1}$$

where $\vec{\sigma}$ denotes the Pauli spin matrices (with eigenvalues ± 1), $\mu_B = 9.27 \times 10^{-24}$[J/T] and $\mu_n = 5.05 \times 10^{-27}$[J/T] are respectively the Bohr and nuclear magneton, g_n is the nuclear g-factor (=1.13 for ^{31}P), and

$$A = \frac{8}{3} \pi \mu_B g_n \mu_n |\Psi(0)|^2$$

is the contact hyperfine interaction energy, with $|\Psi(0)|^2$ the probability density of the electron wave function evaluated at the nucleus[8]. Application of the field B_z leads to evolution of the states as first the electron and then the nuclear Zeeman energies exceed.

Transitions between the different energy levels are induced by a radio frequency magnetic field B_{ac} applied at a frequency resonant with the energy-level difference. The spin Hamiltonian for the electron-donor system with an electric field E and a magnetic field B_{ac} is

$$\mathcal{H}_{en} = \mu_B \vec{B} \cdot \vec{\sigma}^e - g_n \mu_n \vec{B} \cdot \vec{\sigma}^n + \tilde{A}(E) \vec{\sigma}^e \cdot \vec{\sigma}^n, \tag{2}$$

where

$$\vec{B} = B_z \hat{z} + B_{ac}(\hat{x} \cos \omega t + \hat{y} \sin \omega t),$$

and $\tilde{A}(E)$ is the contact hyperfine interaction energy affected by the external electric field E induced by the A-gate. A donor nuclear-spin-electron system close to an 'A-gate' functions as a voltage-controlled oscillator. The precession frequency of the nuclear spin is controllable externally and spins can be selectively brought into resonance with B_{ac}, allowing arbitrary rotations to be performed on each nuclear spin.

Quantum computation requires, in addition to single spin rotations, the SWAP operation of quantum logic, in which the spin quantum numbers of two qubits are interchanged. The SWAP operation in combination with the single-spin rotation can be used as the primitive operation of a universal quantum computer[10]. The Hamiltonian of two coupled donor nucleus-electron systems is

$$\mathcal{H} = \mathcal{H}(B) + A_1 \vec{\sigma}^{1e} \cdot \vec{\sigma}^{1n} + A_2 \vec{\sigma}^{2e} \cdot \vec{\sigma}^{2n} + J \vec{\sigma}^{1e} \cdot \vec{\sigma}^{2e}, \tag{3}$$

where

$$\mathcal{H}(B) = \mu_B \vec{B} \cdot \vec{\sigma}^{1e} - g_n \mu_n \vec{B} \cdot \vec{\sigma}^{1n} + \mu_B \vec{B} \cdot \vec{\sigma}^{2e} - g_n \mu_n \vec{B} \cdot \vec{\sigma}^{2n},$$

contains the magnetic field interaction terms for the spins. The coefficients A_1 and A_2 are the hyperfine interaction energies of the respective nucleus-electron system, while J is the exchange energy of the two electrons, which depends on the overlap of the electron wave functions. Two-qubit operations are performed by lowering the potential barrier between donor sites with the J-gate and turning on the exchange coupling between the donors. Electron-mediated nuclear-spin exchange will then occur between the donor nuclei.

3 Transition probability

In this section, we describe the calculation of the transition probability. We represent the time evolution of the quantum logic gates with the transition probability.

For the calculation of the transition probabilities from one state ψ_m to another state ψ_n under the influence of a time-dependent perturbation $\hat{V}(\vec{r}, t)$, we must solve the Schrödinger equation with $\hat{V}(\vec{r}, t)$. General predictions can only be made if the transition is caused by weak influences, i.e. weak potential $\hat{V}(\vec{r}, t)$. The Schrödinger equation with the perturbation is

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{\mathcal{H}}_0 \psi + \hat{V}(\vec{r}, t)\psi, \tag{4}$$

where $\hat{\mathcal{H}}_0$ is the operator for the total energy of the system without the perturbation (the index 0 stands for the time independence) and $\hat{V}(\vec{r}, t)$ is the perturbation.

Assume that the stationary part of the normalized wave function satisfies the equation

$$\hat{\mathcal{H}}_0 \psi_k(\vec{r}) = E_k \psi_k(\vec{r}).$$

Then the time-dependent functions

$$\tilde{\psi}_k(\vec{r}, t) = \psi_k(\vec{r}) e^{-\frac{i}{\hbar} E_k t}$$

are the solution of the unperturbed system. They form a complete set of functions and the solution of Eq.(4) can be expanded in terms of these functions, i.e.

$$\psi(\vec{r}, t) = \sum_k a_k(t)\psi(\vec{r})e^{-\frac{i}{\hbar}E_k t} \tag{5}$$

Inserting this into Eq.(4) leads to

$$i\hbar\frac{\partial a_m}{\partial t} = \sum_k a_k(t)V_{mk}(t)e^{i\omega_{mk}t}, \tag{6}$$

where

$$V_{mk}(t) = \langle\psi_m|\hat{V}(t)|\psi_k\rangle \quad and \quad \omega_{mk} = \frac{E_m - E_k}{\hbar}.$$

By defining

$$\vec{a} \equiv \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix}, \qquad A(t) \equiv \begin{pmatrix} V_{11} & V_{12}e^{i\omega_{12}t} & \cdots \\ V_{21}e^{i\omega_{21}t} & V_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix},$$

we rewrite Eq.(6) as

$$\frac{d\vec{a}}{dt} = \frac{A(t)}{i\hbar}\vec{a}. \tag{7}$$

This is the basic coupled differential equation that must be solved in order to obtain the probability of finding ψ_m as a function of t.

The solution of Eq.(7) is given by

$$\begin{aligned} \vec{a}(t) &= e^{\frac{1}{i\hbar}\int_0^t A(t')dt'}\vec{a}(0) \\ &\cong e^{\frac{\Delta t}{i\hbar}A(\frac{2n-1}{2}\Delta t)}\ldots\ldots e^{\frac{\Delta t}{i\hbar}A(\frac{3}{2}\Delta t)}e^{\frac{\Delta t}{i\hbar}A(\frac{\Delta t}{2})}\vec{a}(0) \end{aligned} \tag{8}$$

By diagonalizing $A(t)$ as

$$A(t) = U(t)\begin{pmatrix} \lambda_1(t) & & & \\ & \lambda_2(t) & & \\ & & \ddots & \\ & & & \lambda_n(t) \end{pmatrix}U^\dagger(t),$$

we obtain

$$\vec{a}(t) = U(\frac{2n-1}{2}\Delta t)\begin{pmatrix} e^{\frac{\Delta t}{i\hbar}\lambda_1(\frac{2n-1}{2}\Delta t)} & & \\ & e^{\frac{\Delta t}{i\hbar}\lambda_2(\frac{2n-1}{2}\Delta t)} & \\ & & \ddots \end{pmatrix}U^\dagger(\frac{2n-1}{2}\Delta t)\cdots$$

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$$\times U(\frac{3}{2}\Delta t) \begin{pmatrix} e^{\frac{\Delta t}{i\hbar}\lambda_1(\frac{3}{2}\Delta t)} & & \\ & e^{\frac{\Delta t}{i\hbar}\lambda_2(\frac{3}{2}\Delta t)} & \\ & & \ddots \end{pmatrix} U^\dagger(\frac{3}{2}\Delta t)$$

$$\times U(\frac{\Delta t}{2}) \begin{pmatrix} e^{\frac{\Delta t}{i\hbar}\lambda_1(\frac{\Delta t}{2})} & & \\ & e^{\frac{\Delta t}{i\hbar}\lambda_2(\frac{\Delta t}{2})} & \\ & & \ddots \end{pmatrix} U^\dagger(\frac{\Delta t}{2}) \quad . \tag{9}$$

The probability of finding ψ_m is obtained by evaluating $|a_m(t)|^2$.

4 Electron-nuclear spin system of a donor in a magnetic field

In this section, we discuss the electron-nuclear spin system of a donor. One-qubit unitary transformation is discussed in this section.

In order to solve Eq.(1), we use the basis set

$$| \uparrow\uparrow\rangle, \qquad | \uparrow\downarrow\rangle, \qquad | \downarrow\uparrow\rangle, \qquad | \downarrow\downarrow\rangle,$$

where $| \ \rangle$ stands for a ket vector that represents

$$|\text{electron spin state, nuclear spin state}\rangle.$$

The Hamiltonian (1) can readily be solved exactly with this basis set. The energy levels for Si:P are shown in Fig.2(a) as a function of B_z. (The contact hyperfine interaction A is fixed to $A_0 = 7.62 \times 10^{-26}$[J].) For $B_z = 0$, the energy eigenstates of (1) are also the eigenstates of the spin-exchange operator. The ground state is the singlet $| \uparrow\downarrow\rangle - | \downarrow\uparrow\rangle$, lying $4A$ below the threefold-degenerate triplet excited states. The energy difference between the electron-nucleus spin states is shown in Fig.2(b). As the magnetic field B_z is increased, the singlet makes a transition to the state $| \downarrow\uparrow\rangle$ (Fig.3). Thus the transition between the states $| \downarrow\downarrow\rangle$ and $| \downarrow\uparrow\rangle$, i.e., a rotation of the nuclear spin can be performed with the radio frequency magnetic field B_{ac}.

In order to obtain the transition probability between the singlet and the triplets, we represent the time-dependent perturbation $\hat{V}$ in the form of the

4×4 matrix

$$
\hat{V} = \begin{pmatrix}
0 & -g_n\mu_B B_{\mathrm{ac}}e^{-i\omega t} & \mu_B B_{\mathrm{ac}}e^{-i\omega t} & 0 \\
-g_n\mu_n B_{\mathrm{ac}}e^{i\omega t} & 0 & 0 & \mu_B B_{\mathrm{ac}}e^{-i\omega t} \\
\mu_B B_{\mathrm{ac}}e^{i\omega t} & 0 & 0 & -g_n\mu_n B_{\mathrm{ac}}e^{-i\omega t} \\
0 & \mu_B B_{\mathrm{ac}}e^{i\omega t} & -g_n\mu_n B_{\mathrm{ac}}e^{i\omega t} & 0
\end{pmatrix} .(10)
$$

Calculating the matrix elements V_{mk} with the eigenvectors and inserting them into Eq.(7), we obtain the transition probability $a(t)$ (Fig.4). The initial state is $|\downarrow\uparrow\rangle$. The transition probabilities to the states $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ are nearly zero. In this calculation, we obtained the result that one-qubit unitary transformation need to be controlled of the order 10^{-6}[sec], when the magnetic field are fixed to $B_{\mathrm{z}} = 1$[T] and $B_{\mathrm{ac}} = 0.001$[T].

Nuclear spins must be selectively brought into resonance with B_{ac}, allowing arbitrary rotations to be performed on each nuclear spins. A donor nuclear-spin electron system close to an 'A-gate' functions as a voltage-controlled oscillator. The precession frequency of the nuclear spin is controlled by changing the electric field E, and thereby changing the parameter $A(E)$. The energy level differences determined by the $A(E)$ are also changed.

We simulate the transition probability for the contact hyperfine interaction energy $A(E)$ different from $A_0 = 7.62 \times 10^{-26}$[J] (Fig.5). In this calculation, we obtained the result that the transition time depends on A. It is possible to perform the nuclear-spin rotation selectively.
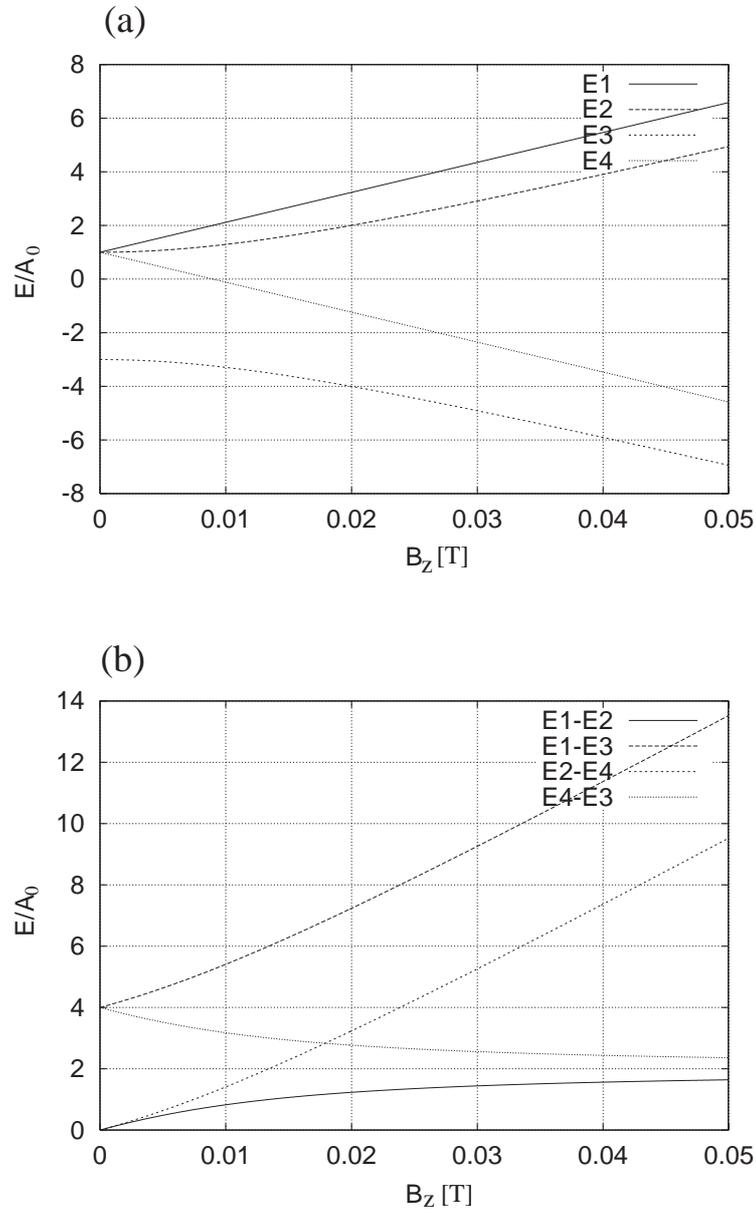
(a)

(b)

Figure 2: (a) The spin energy levels of a ^{31}P donor in Si. The spin states of the energy E1, E2 and E4 is the triplet and E3 is the singlet. (b) the energy differences of the levels as a function of the applied magnetic field B_z.
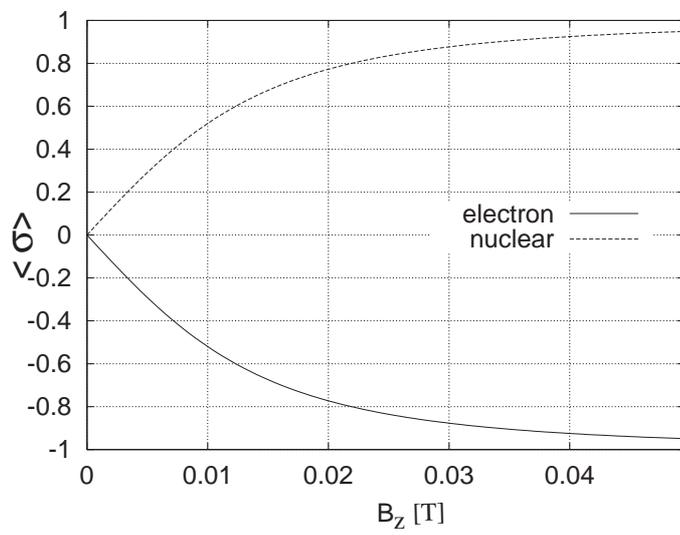
Figure 3: The expectation values of the electron and nuclear spin state as a function of B_z.
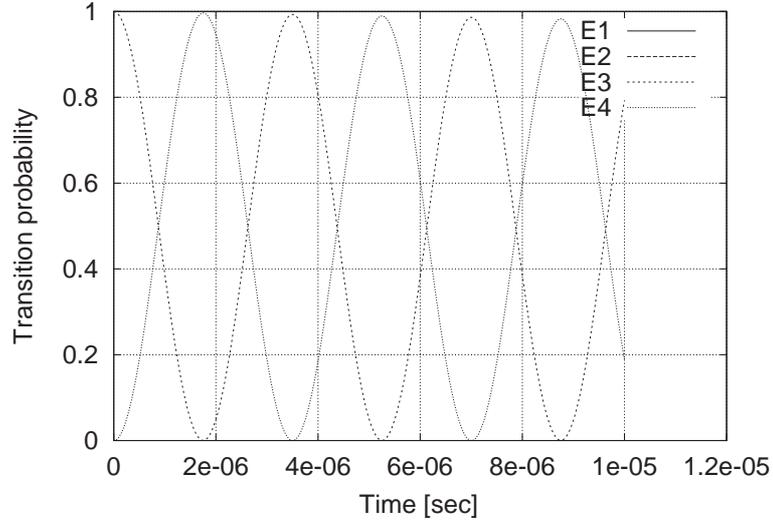
Figure 4: The transition probability between the state $| \downarrow\downarrow \rangle$ (the energy E4) and the state $| \downarrow\uparrow \rangle$ (the energy E3) with the parameter $A = A_0 = 7.62 \times 10^{-26}$[J]. The energy E1 is of the state $| \uparrow\uparrow \rangle$ and the energy E2 is of the state $| \uparrow\downarrow \rangle$. The transition probabilities to these states are nearly zero. The magnetic fields are fixed to $B_z = 1$[T] and $B_{ac} = 0.001$[T]. The frequency is fixed to $\omega_0 = \frac{E4-E3}{\hbar} = 1.81 \times 10^9$(Hz).
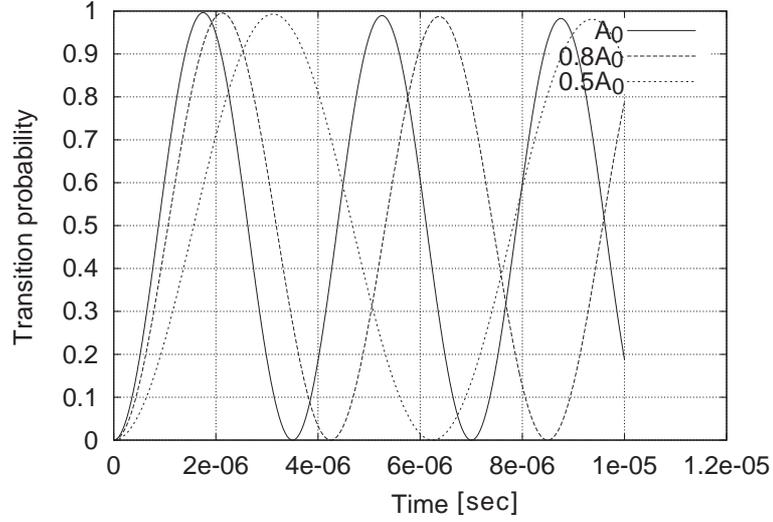
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Figure 5: The transition probability of the state $| \uparrow \downarrow \rangle$ with the parameter A changed from $A_0 = 7.62 \times 10^{-26}$[J]. The frequency is also changed from $\omega_0 = 1.81 \times 10^9$(Hz) as a function of A. The parameter A is fixed to the $0.8A_0$, then the frequency is $\omega = 1.49 \times 10^9$(Hz). The parameter A is fixed to the $0.5A_0$, then the frequency is $\omega = 1.01 \times 10^9$(Hz). The magnetic fields are the same as in Fig.4.

5 Electron-nuclear spin system for two interacting donor atoms

In this section, we discuss two interacting donor atoms. The SWAP operation is discussed in this section.

Consider two donor atoms separated from each other by distance r. we use the basis set

$$
\begin{array}{cccc}
|\uparrow\uparrow\uparrow\uparrow\rangle & |\uparrow\downarrow\uparrow\uparrow\rangle & |\downarrow\uparrow\uparrow\uparrow\rangle & |\downarrow\downarrow\uparrow\uparrow\rangle \\
|\uparrow\uparrow\uparrow\downarrow\rangle & |\uparrow\downarrow\uparrow\downarrow\rangle & |\downarrow\uparrow\uparrow\downarrow\rangle & |\downarrow\downarrow\uparrow\downarrow\rangle \\
|\uparrow\uparrow\downarrow\uparrow\rangle & |\uparrow\downarrow\downarrow\uparrow\rangle & |\downarrow\uparrow\downarrow\uparrow\rangle & |\downarrow\downarrow\downarrow\uparrow\rangle \\
|\uparrow\uparrow\downarrow\downarrow\rangle & |\uparrow\downarrow\downarrow\downarrow\rangle & |\downarrow\uparrow\downarrow\downarrow\rangle & |\downarrow\downarrow\downarrow\downarrow\rangle,
\end{array}
$$

where $|\ \rangle$ stands for a ket vector that represents

|electron spin state in donor 1, electron spin state in donor 2,

nuclear spin state in donor 1, nuclear spin state in donor 2 $\rangle$.

The energy levels of the Hamiltonian (3) are shown in Fig.6 as a function of B_z. Tunneling of electrons between the two sites becomes possible, leading to an exchange interaction between the electron spins and also to an indirect (or electron-mediated) exchange interaction between the nuclear spins.

The magnitude of the exchange interaction J between the electron spins on donors as a function of their separation r can be approximated by equations derived for the case of well-separated H atoms[9],

$$
J(r) \cong 0.4 \frac{e^2}{\epsilon a_B} \left(\frac{r}{a_B} \right)^{\frac{5}{2}} \exp\left(\frac{-2r}{a_B} \right), \tag{11}
$$

where r is the distance between the donors, $\epsilon = 11.9\epsilon_0$ ($\epsilon_0 = 8.85 \times 10^{-12} [F \cdot m^{-1}]$) is the dielectric constant of the semiconductor, and $a_B = 30[\mathring{A}]$ is the semiconductor Bohr radius. This function, with values appropriate for Si is plotted in Fig.7. For two-electron systems, the exchange interaction lowers the energy of the electron singlet $|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$ with respect to the triplets.

In the magnetic field, however, the state $|\downarrow\downarrow\rangle$ is approximately the electron ground state for $J \ll \mu_B B$. When the two electron spins are in the state $|\downarrow\downarrow\rangle$ and are each coupled to the donor nuclear spins by the same
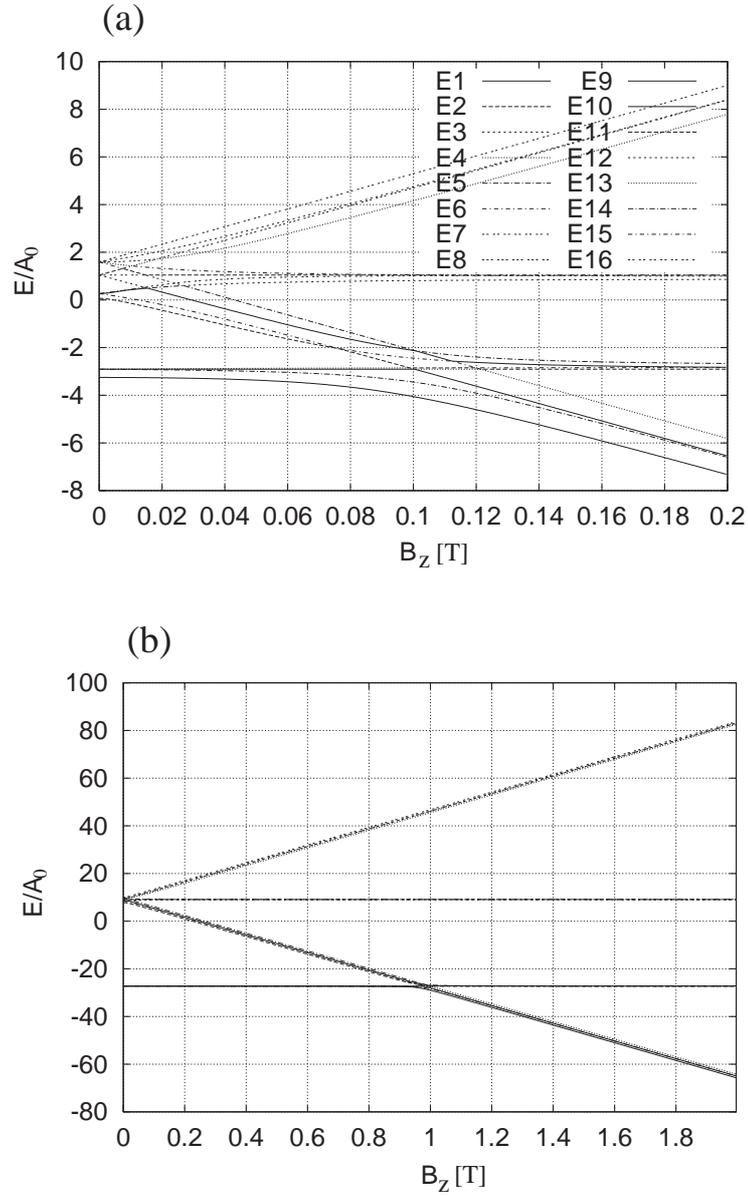
(a)

(b)

Figure 6: The electron-nuclear spin energy levels for two interacting donor atoms as a function of the magnetic field B_z: (a) $0 \leq B_z \leq 0.2$; (b) $0 \leq B_z \leq 2.0$.
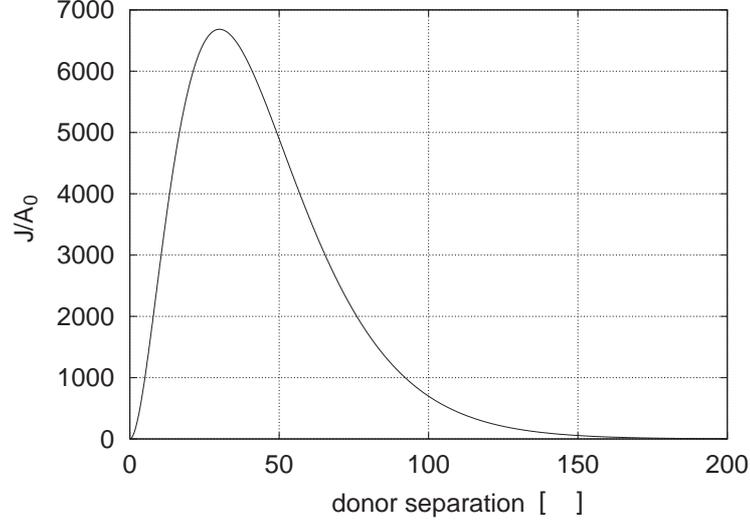
Figure 7: The strength of the electron exchange coupling between the donor sites, plotted as a function of their separation.

hyperfine interaction energy A, the nuclear spin exchange frequency ν_J is approximately[5] given by

$$h\nu_J = 2A^2\Big(\frac{1}{\mu_B B - 2J} - \frac{1}{\mu_B B}\Big),\tag{12}$$

where J is the electron-spin exchange energy and $2J \ll \mu_B B$ is assumed.

In order to perform the SWAP operation, we accomplish swapping the nuclear spin state between the state $|\downarrow\downarrow\uparrow\downarrow\rangle$ and the state $|\downarrow\downarrow\downarrow\uparrow\rangle$ in the following three-step processes:

(i) The positive voltage applied to the J-gate turns on the exchange interaction J between two donor nucleus-electron spin systems. As the exchange interaction J is increased ($J < \mu_B B$), the nuclear-electron spins make transitions to the state

$$
\begin{aligned}
|\downarrow\downarrow\uparrow\uparrow\rangle &\longrightarrow |\downarrow\downarrow\uparrow\uparrow\rangle, \\
|\downarrow\downarrow\uparrow\downarrow\rangle &\longrightarrow |\downarrow\downarrow\rangle(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)), \\
|\downarrow\downarrow\downarrow\uparrow\rangle &\longrightarrow |\downarrow\downarrow\rangle(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)), \\
|\downarrow\downarrow\downarrow\downarrow\rangle &\longrightarrow |\downarrow\downarrow\downarrow\downarrow\rangle;
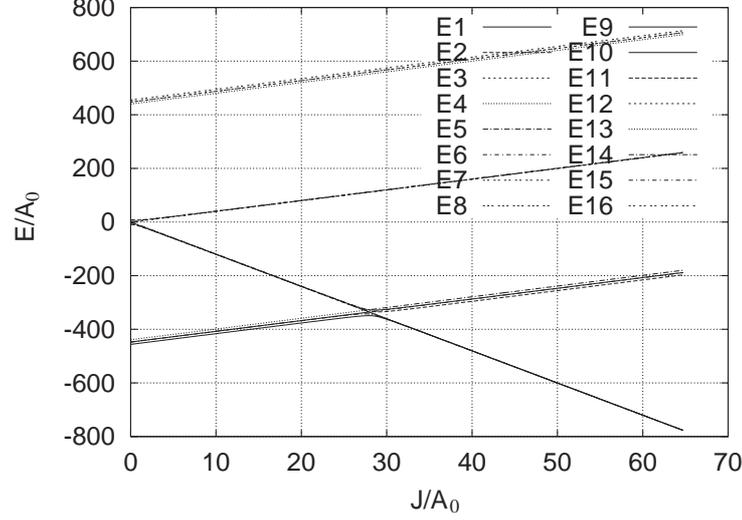\end{aligned}
$$

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Figure 8: The electron-nuclear spin energy levels for two interacting donor atoms as a function of J. In the ground state, the electrons are in the state $|\downarrow\downarrow\rangle$. The magnetic field is fixed to $B_z = 1[T]$.

(ii) We make a transition between the state $|\downarrow\downarrow\rangle(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ and the state $|\downarrow\downarrow\rangle(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ with the magnetic field B_{ac};

(iii) We turn off the positive voltage applied to the J-gate.

We must determine the appropriate value of J to split the states $|\downarrow\downarrow\rangle(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ and $|\downarrow\downarrow\rangle(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$. The energy-level splitting is shown in Fig.9 when B_z is $1[T]$ and two electron spin states is in the state $|\downarrow\downarrow\rangle$. Transition probability between the state $|\downarrow\downarrow\rangle(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ and the state $|\downarrow\downarrow\rangle(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ is shown in Fig.10 for $J/A_0 = 27$. The initial state is $|\downarrow\downarrow\rangle(\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$. The transition probabilities to the state $|\downarrow\downarrow\uparrow\uparrow\rangle$ and the state $|\downarrow\downarrow\downarrow\downarrow\rangle$ are nearly zero.

Figure 10 shows that the SWAP operation needs to be controlled in the time scale of the order $10^{-6}[\sec]$, when the magnetic field are fixed to $B_z = 1[T]$ and $B_{ac} = 0.001[T]$.
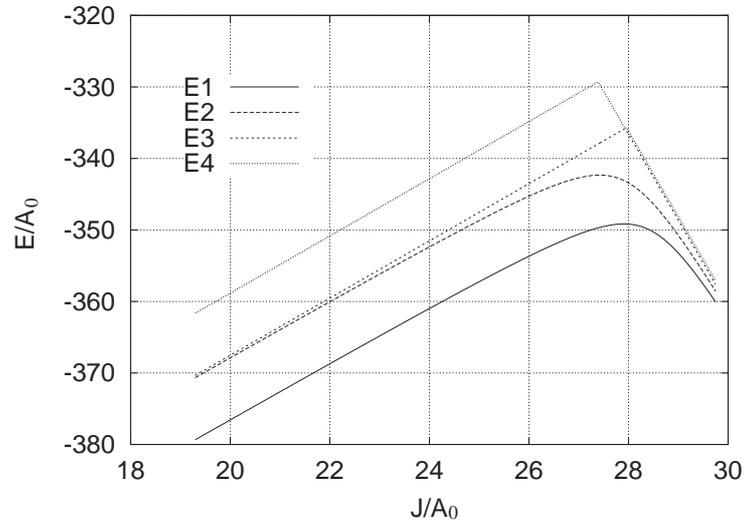
19

Figure 9: The electron-nuclear spin energy levels whose two electron spin states are $|\downarrow\downarrow\rangle$, as a function of J. The energy E2 is of the state $|\downarrow\downarrow\rangle(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ and E3 is of the state $|\downarrow\downarrow\rangle(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$. The energy E1 is of the state $|\downarrow\downarrow\uparrow\uparrow\rangle$ and the energy E4 is of the state $|\downarrow\downarrow\downarrow\downarrow\rangle$.
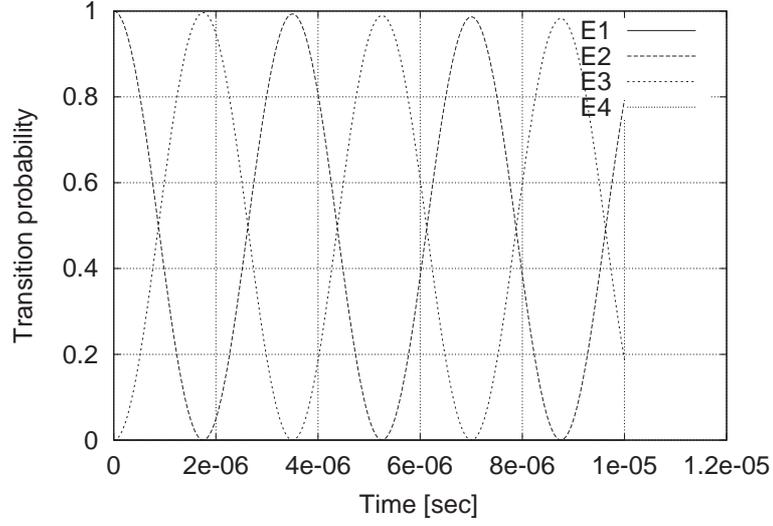
Figure 10: The transition probability between the state $\mid \downarrow\downarrow\rangle(\mid \uparrow\downarrow\rangle + \mid \downarrow\uparrow\rangle)$ (energy E3) and the state $\mid \downarrow\downarrow\rangle(\mid \uparrow\downarrow\rangle - \mid \downarrow\uparrow\rangle)$ (energy E2). The energy E1 is of the state $\mid \downarrow\downarrow\downarrow\downarrow\rangle$ and the energy E4 is of the state $\mid \downarrow\downarrow\uparrow\uparrow\rangle$. The transition probabilities to these states are nearly zero. The frequency is fixed to $\omega_0 = \frac{E3-E2}{\hbar} = 1.57 \times 10^9 (\text{Hz})$. The magnetic field are the same as in Fig.4

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6   Measurement of nuclear spin state

In this section, we describe the measurement of the nuclear spin states.

The nuclear-spin state is set for $J \ll 2\mu_B B$, where nuclear spins are handled by NMR methods by applying AC pulses of the resonance frequency. Suppose that after quantum computation at $J \ll 2\mu_B B$, two electrons, both on its donor atom, are initially in the triplet state, that is in the $|\downarrow\downarrow\rangle$ state. The whole electron-nuclear system is either in the state $|\downarrow\downarrow\rangle(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$ or in the state $|\downarrow\downarrow\rangle(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$.

By adiabatically increasing the exchange parameter to $J > 2\mu_B B$ in a process of the crossing point passage, we lead the electron-nuclear system transition from one antisymmetric state $|\downarrow\downarrow\rangle(\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ to another $(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)|\downarrow\downarrow\rangle$ at the same total spin projection and allow transfer the information from the nuclear to the electron spin subsystem.

In addition, if the bound energy for an electron at one neutral donor (it is usually small) is more than its energy of attraction to the neighboring ionized donor (D^+ state), the electron will be found near the neutral (D^- state or helium-like atom) and charge transfer from one donor to the other will occur. This may be reached also by the corresponding change of the A-gate electric potential. Therefore, a charge transfer from one donor to another takes place. It is supposed[5] that this process can be detected with highly sensitive single-electron capacitive techniques.

7   Conclusion

In Section 4, we obtained the transition probability between the state $|\downarrow\downarrow\rangle$ and the state $|\downarrow\uparrow\rangle$ of the order 10^{-6}[sec] using the perturbation $\hat{V}$ explained in Section 3. By appropriately modulating the transition time, we can obtain the superposition state $|\downarrow\downarrow\rangle + |\downarrow\uparrow\rangle$. To perform the nuclear-spin rotation selectively, we calculated the transition probability with the parameter A varied. We showed that the transition time depends on A. In Section 5, the full energy spectrum of the electron-nuclear spin system of two interacting donor atoms was calculated. To perform the transition between the state $|\downarrow\downarrow\downarrow\uparrow\rangle$ and the state $|\downarrow\downarrow\uparrow\downarrow\rangle$, we split the energy levels with an appropriate value of J. Then we observed the transition in the time scale of the order 10^{-6}[sec].

8 Acknowledgements

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