PAPER Special Issue on Integrated Electronics and New System Paradigms

Analog Computation Using Coupled-Quantum-Dot Spin Glass

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SUMMARY A novel analog-computation system using quantum-dot spin glass is proposed. Analog computation is a processing method that solves a mathematical problem by applying an analogy of a physical system to the problem. A 2D array of quantum dots is constructed by mixing two-dot (antiferromagnetic interaction) and three-dot (ferromagnetic interaction) systems. The simulation results show that the array shows spin-glass-like behavior. We then mapped two combinatorial optimization problems onto the quantum-dot spin glasses, and found their optimal solutions. The results demonstrate that quantum-dot spin glass can perform analog computation and solve a complex mathematical problem.

key words: *analog computation, spin glass, quantum dot, spin, combinatorial optimization problem*

1. Introduction

One of the challenges in nanoelectronics is to develop information processing systems that utilize quantum mechanical effects. To construct such systems, we must employ a computing paradigm that is suitable for a quantum structure system. Some proposals for quantum devices that have been advanced try to represent a binary signal and perform Boolean logic operations under a Neumann-type computing architecture [1]–[3]. But, these proposals shared some serious problems such as that the input bits cannot be pipelined [4]. In contrast, analog computation using quantum structures is a promising architecture for information processing in nanoelectronics. This paper proposes an analog-computation system using coupled-quantum-dot spin glass.

Analog computation is a processing method for solving a mathematical problem by applying an analogy of a physical system to the problem [5]. To implement analog computation, we must prepare an appropriate physical system and use its physical quantities to represent all the problem variables. If the mathematical relationships between the physical quantities are analogous to those of the problem, then we can find the solution to the problem by operating the physical system and measuring the quantities. Analog computation has the following features. 1) It is based on properties of a physical system and not on symbolic operations. 2) Computation is parallel and instantaneous, because the changes in the physical quantities occur simultaneously when the physical system is operated. Thus, analog computation is one approach to avoiding the Neumann bottleneck and solving complex problems in a short time.

Spin glass is a kind of ferromagnetic-antiferromagnetic mixture [6]. The ferromagnetic and antiferromagnetic interactions distribute spatially in the spin glass and there is competition between them. The ferromagnetic interaction makes the spins at all lattice points parallel, while the antiferromagnetic interaction makes the spins at two neighboring lattice point antiparallel. The result is that no single configuration of the spins is uniquely favored by both kinds of interactions. This phenomenon is commonly called "frustration." Spin glass is the most complex kind of condensed state encountered so far in solid-state physics. Finding the ground state of a spin glass is analogous to solving some combinatorial optimization problems. This may therefore allow us to construct an analog computation system that solves such problems.

In this paper we propose a novel analog-computation system using *coupled-quantum-dot spin glass*. In the following sections we first describe the spin-glass-like behavior in a two-dimensional (2D) array of coupled-quantum dots (Sect. 2), and then apply an analogy of the quantum-dot spin glass to combinatorial optimization problems (Sect. 3). We demonstrate that the spin glass can perform analog computation. We also discuss issues related to the physical implementation (Sect. 4). Finally, we summarize the main results (Sect. 5).

2. Coupled-Quantum-Dot Spin Glass

2.1 Model

Technological progress has enabled us to fabricate an array of quantum dots. If the array is designed well and the quantum dots are occupied by an appropriate number of single electrons, we can expect magnetic order states in the electron system due to strong correlation

Manuscript received January 27, 1999.
Manuscript revised March 25, 1999.

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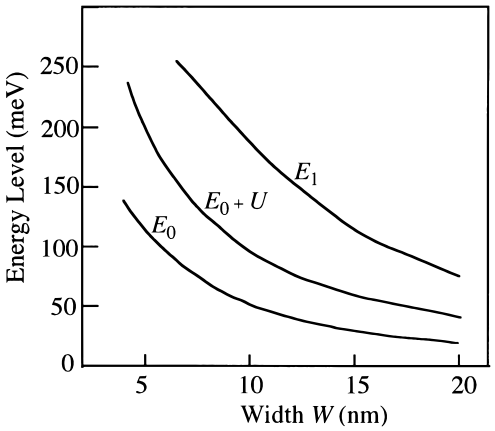

Fig. 1 Dependence of the ground state level E_0 and the 1st excited state level E_1 on the width of the box-shaped dot. The Coulomb repulsion energy U is also given.

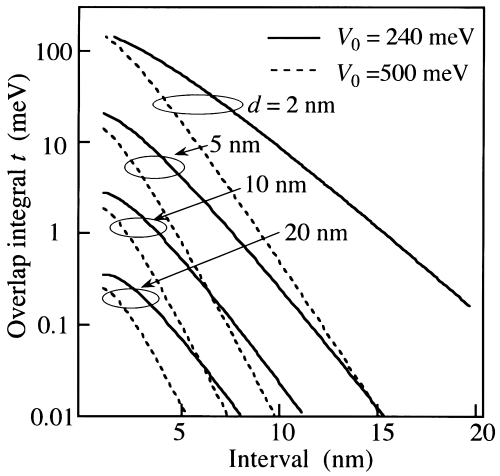

Fig. 2 Dependence of the overlap integral t on the interval and barrier height between the coupled dots for two barrier heights: 240 and 500 meV. Here d is the width of the quantum dot.

interaction. We first clarify the magnetic properties of the array and then demonstrate that the array can show a spin-glass-like behavior. In the following, we use a GaAs/AlGaAs quantum dot as an analytic model.

We can neglect the valence-band and core electrons in our analysis because these electrons in any dot are highly localized and their wave functions do not overlap with each other. Furthermore, because the energy of an electron confined in a quantum dot is strongly quantized, the energy spectrum of the electron is discrete. A time-independent Schrodinger equation is solved numerically for the ground state level E_0 and the first excited state level E_1 in a box-shaped quantum dot. The energy U of Coulomb repulsion between two electrons sited on the same dot can also be calculated by $U = q^2/4\pi\varepsilon_0\varepsilon_r(w/3)$ [2]. The result is shown in Fig. 1. The difference between the levels E_0 and E_1 decreases with dot width w. The excited level E_1 is larger than $E_0 + U$. Thus, when the number of electrons is less than twice the number of quantum dots in the array, we can use the one-band extended Hubbard model [2], [7] to analyze the magnetic properties of the quantum dot array. The Hubbard-type Hamiltonian is given by

$$H = \sum_{k,j,\sigma} t_{kj} c^+_{k,\sigma} c_{j,\sigma} + \frac{1}{2} \sum_{k,j,\sigma} U_{kj} n_{k,\sigma} n_{j,-\sigma} + \frac{1}{2} \sum_{k,\sigma} U n_{k,\sigma} n_{k,-\sigma}, \quad (1)$$

where $c^+_{k,\sigma}(c_{k,\sigma})$ is the creation (annihilation) operator for an electron at quantum dot k with spin σ; $n_{k,\sigma}$ is the number operator of this electron; t_{kj} is the overlap integral that represents the interdot coupling between two quantum dots k and j; E_0 is the ground state level in a quantum dot; and U_{kj} is the Coulomb repulsion between the electrons at the k- and j-th dots.

2.2 Ferromagnetic and Antiferromagnetic States

First we clarify quantitatively how the overlap integral t depends on the interval and barrier height between two nearest-neighbor dots. It depends on physical factors such as the dot size and both the interval and the barrier height. When ψ_1 (ψ_2) is the electron wave function at dot 1 (dot 2), it is given by

$$t = \int \psi_1 \{V(x) + E_0\} \psi_2 dx, \quad (2)$$

where $V(x)$ is the potential profile of the coupled quantum dots. Figure 2 shows the calculated dependence of the overlap integral t on barrier height and interval for different widths of quantum dots. To investigate its dependence on the barrier height, in addition to a barrier height of 240 meV (GaAs/AlGaAs quantum dot), we also used a barrier height of 500 meV to calculate t. The electron effective mass m^* was taken to be $0.067\,m_0$ and the dielectric coefficient was 10. The overlap integral t decreased from 100 to 0.01 meV with increasing interval between the coupled quantum dots. When the interval was constant, t for a barrier height of 240 meV was more than that for 500 meV.

Next we calculated the low-energy eigenstates of two electrons in a two-dot system using Hamiltonian (1). As is well known, the two electrons in the coupled quantum dots can be described by singlet and triplet orbital states. We diagonalized the Hamiltonian numerically to calculate all the eigenstates using the four underlying basis vectors. Figure 3 shows the dependence of the ground state and the first excited state levels on the ratio of the Coulomb repulsion U to the integral t. The ground state of the two-dot system corresponds to the singlet (antiferromagnetic) state, in which each dot is occupied by one electron and the spins of the two

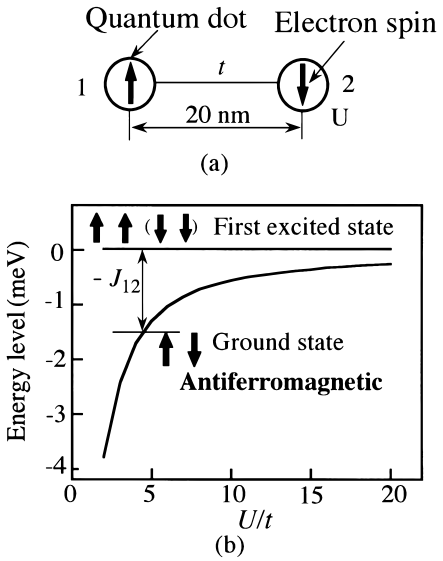

Fig. 3 (a) The two electrons and two nearest-neighbor quantum dots and (b) the levels of the low-energy singlet and triplet states as a function of U/t. $J_{12}(< 0)$ is the spin interaction coefficient.

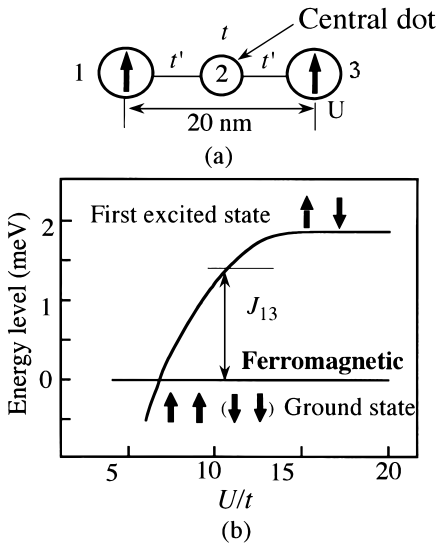

Fig. 4 (a) The two electrons and three neighbor quantum dots and (b) the levels of the low-energy singlet and triplet states as a function of U/t. $J_{13}(> 0)$ is the spin interaction coefficient when U/t is larger than 7.

electrons are antiparallel, as shown in Fig. 3(a). The excited state is the triplet state in which the spins of the two electrons are parallel.

We also calculated the low-energy eigenstates of two electrons in a three-dot system in the same manner. Figure 4 shows the dependence of the ground state and the first excited state on U/t. In the case of the three-dot system, owing to the Coulomb repulsion, the two electrons preferentially occupied the two dots on the left and right sides. The ground state of the two electrons in the three-dot system corresponds to the

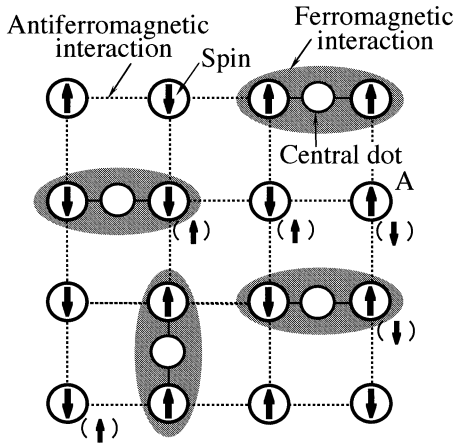

Fig. 5 Simulated ground state of a 2D quantum-dot array consisting of 20 quantum dots and 16 electrons. The arrow represents the spin polarization. It shows spin-glass-like behavior.

triplet (ferromagnetic) state, in which the spins of the two electrons are parallel (when U/t is larger than 7). The excited state is the singlet state. Although the central dot in the three-dot system is not occupied by an electron, it plays an important role in the ferromagnetic interaction.

2.3 Coupled-Quantum-Dot Spin Glass

The two electrons in two-dot and three-dot systems showed the antiferro- and ferromagnetic states, respectively. Here we consider how to design a 2D array of quantum dots by mixing two-dot (antiferromagnetic interaction) and three-dot (ferromagnetic interaction) systems. Figure 5 gives an example of such a 2D array consisting of 20 quantum dots and 16 electrons. The distance between the two dots at the left and right sides in the three-dot system is equal to that between the two quantum dots in the two-dot system. It is difficult to diagonalize the Hamiltonian to calculate all the eigenstates since the number of underlying basis vectors is too large (about 10^{17}). We used Monte-Carlo simulation method, as described in Ref. [7], to calculate the spin polarization for the ground state. The simulated ground state of the quantum-dot array is shown in Fig. 5. There is competition between the ferromagnetic and antiferromagnetic interactions in the quantum-dot array. As a result of this competition, no single configuration of the spins is uniquely favored by all the interactions. For example, the energy of the array does not change even if quantum dot A takes the spin polarization represented by the arrow placed in parentheses. This is called as "frustration." This result indicates that the quantum-dot array shows spin-glass-like behavior.

In the case of strong electronic correlations ($U/t \gg 1$), Hubbard model is transformed into the Heisenberg-type model [8].

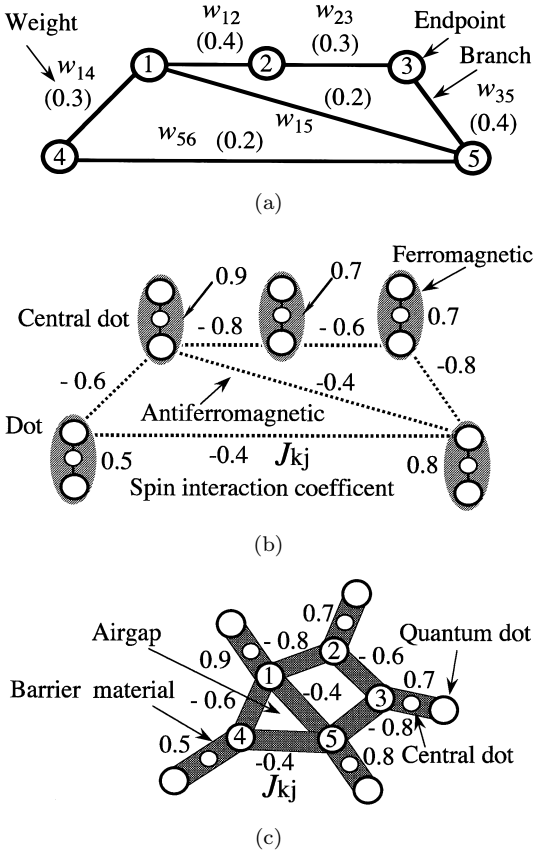

Fig. 6 (a) Example of a max cut problem with five endpoints and (b) a corresponding quantum-dot spin glass and (c) a possible layout of the quantum-dot spin glass.

$$H = -\sum_{k<j} J_{kj} \boldsymbol{S}_k \cdot \boldsymbol{S}_j - \sum_k J_{kk} \boldsymbol{S}_k, \tag{3}$$

where $\boldsymbol{S}_k$ and $\boldsymbol{S}_j$ are spin polarizations of the electrons at quantum dots k and j, and J_{kj} is the interaction coefficient between the spins of those electrons. The coefficient J_{kj} is defined as the energy difference between the antiferromagnetic and ferromagnetic states of the k and j electron spins, as shown in Figs. 3(b) and 4(b). If the system is ferromagnetic then $J_{kj} > 0$, otherwise $J_{kj} < 0$. J_{kk} is the bias interaction coefficient, such as the interaction between the electron spin and the local magnetic field. The spin interaction is a short-range phenomenon, so here we take into account only the interaction between the neighbor quantum dots. We will use model (3) to analyze the ground state of the spin glass using in the following.

3. Analog Computation

3.1 Relating Spin Glass to Combinatorial Optimization Problem

A combinatorial optimization problem is either a minimization problem or a maximization problem. Solving one amounts to finding the best optimal solution among a number of possible solutions. So far a wide variety of such problems have emerged from such diverse areas as economics, engineering, and VLSI design. However, there exists a class of combinatorial optimization problems of such inherent complexity that solving them requires a computational effort that grows exponentially with the size of the problem. It turns out that a number of combinatorial optimization problems share some of the essential features of spin glass such as frustration [6]. The spin glass mathematical models are analogous to some of the combinatorial optimization problems. Therefore spin glass can be used to map combinatorial optimization problems and solve them. To implement analog computation, an optimal problem is mapped onto a coupled-quantum-dot spin glass as follows. 1) Formulate the optimization problem as a binary variable 0-1 problem; 2) Use the spin polarization to represent the variable and define that "up" ("down") polarization of the dot spin as corresponding to the variable value "1" ("0"); 3) Design the interaction coefficient J between spins at quantum dots such that minimizing the energy function of the spin glass corresponds to minimizing (or maximizing) the cost function of the problem, i.e. the ground state of the spin configuration is mapped to the optimal solution of the problem. 4) Perform the computation. Because the spin configuration evolves toward its ground state spontaneously, performing the computation is equal to letting the spin glass settle down to its ground state after being given an initial spin configuration; 5) Find a optimal solution of the problem, i.e. detect the spin polarization at each dot. The analog computation of spin glass may provide the means to solve complex problems in a short time.

3.2 Implementing Combinatorial Optimization Problems

We will describe two optimization problems: the max cut problem and the independent set problem, and design the structures of the coupled-quantum-dot spin glasses for solving them. Figure 6(a) shows an example of a graph partitioning problem—the max cut problem. *Given a five-endpoint graph G with positive weights on six branches $w_{kj}(= w_{jk})$, the max cut problem is defined as the problem of finding a partition of the graph into two disjoint groups G_1 and G_2 such that the sum of the weights of the branches that have two endpoints in two groups, respectively, is maximal.* We use a variable x_k to represent the kth endpoint, and define $x_k = 1$ if the endpoint is in G_1, otherwise $x_k = 0$. Then the problem can be formulated as maximizing the cost function

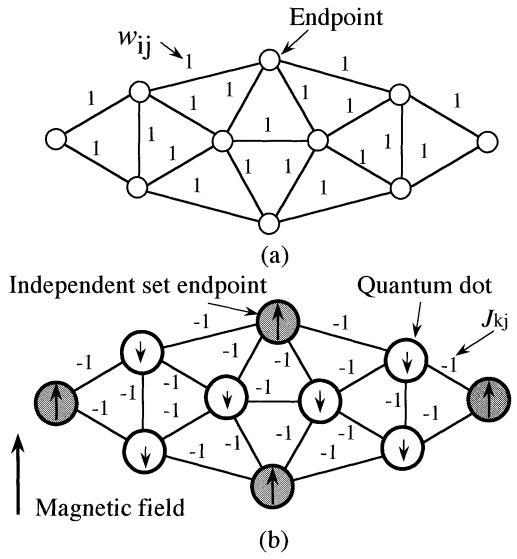

Fig. 7 (a) Example of an independent set problem with ten endpoints and (b) a corresponding quantum-dot spin glass to which a uniform magnetic field is applied.

$$f(x) = \sum_{k<j} w_{kj}\{(1-x_k)x_j + x_k(1-x_j)\} \quad (4)$$

$$= \sum_{k<j} -2w_{kj}x_kx_j + \sum_{k=1}\left(\sum_{j=1} w_{kj}\right)x_i. \quad (5)$$

Consider mapping the max cut problem onto quantum-dot spin glass. We construct a quantum-dot spin glass with fifteen quantum dots and ten electrons, as shown in Fig. 6(b). We define the "up" polarization of the spin to represent the endpoint being in G_1 and "down" to represent the endpoint being in G_2. If we let

$$J_{kj} = -2w_{kj} \quad (6)$$

and

$$J_{kk} = \sum_{j=1} w_{kj} \quad (7)$$

then the expression of the cost function becomes equal to that of Hamiltonian (3). But, the sign of the cost function is opposite to that of Hamiltonian (3). Thus, minimizing the energy function of the spin glass is analogous to maximizing the cost function of the max cut problem. Consequently, an optimal solution can be obtained as long as the spin glass converges to its ground state.

In some combinatorial optimization problems, in addition to a cost function, there is a set of constraint that are imposed on the problems. Figure 7(a) shows such an example — the independent set problem. *Given a graph G of ten endpoints with weights on nineteen branches $w_{kj} = w_{jk} = 1$, the problem is defined as that of finding a maximal independent set G_s of endpoints, i.e. finding a subset G_s in G such that for all endpoints k, j in G_s the weight w_{kj} is 0 (This is a constraint) and such that G_s is maximal.* The space of the solutions is putted under a constraint that w_{kj} must be 0 for endpoints k and j in G_s. (In contrast, there is no such a constraint in the max cut problem, all combination of the variables may be the solutions). To formulate the problem, we use a variable x_k to represent the kth endpoint, and define $x_k = 1$ if the endpoint is in G_s, otherwise $x_k = 0$. Then the cost function to be maximized is defined

$$f(x) = \sum_k x_k \quad (8)$$

subject to the constraint

$$w_{kj}x_kx_j = 0, \quad (9)$$

where w_{kj} is 1 if endpoints k and j are connected by a branch, otherwise $w_{kj} = 0$.

We implement the problem in a quantum-dot spin glass, as shown in Fig. 7(b). The "up" polarization of the spin to represent the endpoint in G_s and "down" to represent the endpoint outside G_s. To satisfy the constraint (9), the spin interaction coefficients that correspond the branches (in Fig.7(a)), are taken to be -1 (antiferromagnetic). Furthermore, to make each spin polarization to trend "up," we apply a uniform magnetic field (along the z axis) to the spin glass. The Zeeman splitting is set to be little smaller than spin interaction coefficient J_{kj}. Thus, minimizing the energy function of the spin glass is analogous to maximizing the cost function of the independent set problem.

3.3 Results

We analyzed the ground states of the quantum-dot spin glasses (Figs. 6(b) and 7(b)) using the Heisenberg Hamiltonian and by simulated annealing [7], [8]. Figure 8 shows the typical development of the system energy for the max-cut-problem spin glass. In the initial arrangement, the parallel electron spins at higher energy in the quantum dot array. Then the system energy decreases with changing eigenstate. Finally the spin glass reaches one of its ground states, as shown in Fig. 8(b). The "up" spin represents the endpoint being in G_1 and "down" represents it being in G_2. The ground state gives one of the optimal solutions to the max cut problem. Furthermore, Fig. 7(b) shows the calculated ground state of the independent-set-problem spin glass. The "up" spins make up the maximal independent set. These results show that quantum-dot spin glass can perform analog computation.

4. Discussion

Fabrication of the spin glass requires control of the in-

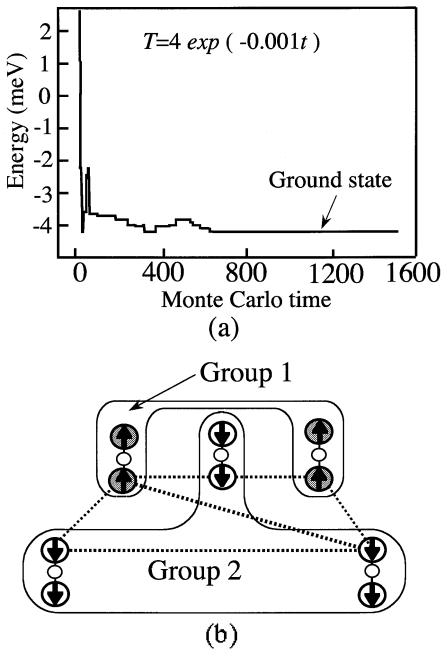

Fig. 8 (a) Typical development of the energy of the max-cut-problem spin glass, the initial temperature T_0 is set to 4 K and temperature T is decreased exponentially, and (b) one optimal solution (group 1 and group 2) to the max cut problem.

terval and barrier height between near neighbor quantum dots. Optimum design of these two physical factors can be achieved through appropriate arrangement of the quantum dots and selection of the barrier materials. Several methods can produce a 2D array of quantum dots [3], [9]. We have considered a selective-area-nanodeposition method [3] for the fabrication of our 2D array of quantum dots. In this method nucleation sites are first created on the substrate by means of a scanning tunneling microscope (STM) tip, and then nano-sized particles are deposited on it. The particles tend to occupy the nucleation sites first. The accuracy of the interaction coefficient depends on the fabrication accuracy of the distance between the dots in the quantum-dot spin glass. A simple estimate for a GaAs/AlGaAs quantum-dot spin glass, as shown Fig. 6(b), indicates that the interaction coefficient is approximately in proportion to the distance between the quantum dots. If the distance between the quantum dots can be controlled in an atomic scale (about 0.3 nm), an accuracy of the interaction coefficient, that is smaller than 0.1 meV, is readily achievable.

Furthermore, the desired value for exchange interaction coefficient J can also be obtained by changing the materials serving as barriers between the near neighbor dots. For example, to nullify the spin interaction between quantum dots, we only remove the film between the input lines by electron beam lithography and etching, and form an air gap to prevent spin interaction between the quantum dots. Figure 6(c) shows a possible layout of the quantum-dot spin glass corresponding to the max cut problem in Fig. 6(b). The diameter of the central dots is designed to be smaller than the other quantum dots so that the ground state level of the single electron in the central dot is higher than that in the other quantum dots. Therefore, the sign and magnitude of the interaction coefficient J_{kj} between the spins of two electrons can be controlled by the position of the central dot and the distance (or barrier material) between the quantum dots.

It is also important to detect the spin polarization of the electrons at the quantum dots. It is probable that a magnetic STM/AFM (atomic force microscope) tip can be used to measure the spin polarization of the dot [3], [7]. In an STM/AFM, the tunneling current depends on the relative spin polarization of the tip and the quantum dot. If the spin of the tip is known, the spin polarization of the quantum dot can be determined by measuring the tunneling current. Details of the writing (reading) mechanism are not mentioned here.

In analog computation, the ground state of the coupled-quantum-dot spin glass is mapped to an optimal solution of the problem. The dynamics of spin glass is considered to be the computational process. To quantify the computation speed, it will be necessary to model the dynamics of spin glass. The actual dynamical evolution of spin glass is extremely complicated because the system is in contact with the environment. The dynamics strongly depends on the energy-dissipation processes, such as the phonon and photon emission process. In future research the dynamics will be investigated systematically.

5. Conclusion

We proposed a novel analog-computation system using quantum-dot spin glass. We constructed a 2D array of quantum dots by mixing two-dot (antiferromagnetic interaction) and three-dot (ferromagnetic interaction) systems. Simulation results indicate that the quantum-dot array shows spin-glass-like behavior. We then mapped two combinatorial optimization problems onto quantum-dot spin glass and found their optimal solutions. The results demonstrate that quantum-dot spin glass can perform analog computation.

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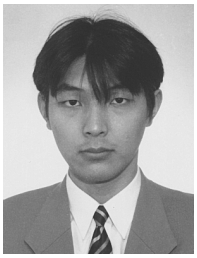

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