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Method for Determining Weight Coefficients for Quantum Boltzmann Machine Neuron Devices

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A method for designing weight coefficients in the quantum Boltzmann machine (QBM) neuron device is proposed. The exchange interaction coefficient corresponds to the weight coefficient of the QBM neuron. A quantitative clarification of the dependence of the exchange interaction coefficient on two physical factors is given: the interval and the barrier height between the nearest-neighbor dots. It is demonstrated that the weight coefficient of the QBM neuron device can be controlled by specifying the values for these two physical factors during the design phase.

KEYWORDS: quantum dot, Boltzmann machine, neuron device, weight coefficient, single electron

1. Introduction

One of the challenges in the field of nanoelectronics is the development of new functional devices that utilize quantum mechanical effects. A quantum device can produce stochastic operations naturally because electrons in a quantum structure behave like probabilistic waves. We have previously proposed a quantum-Boltzmann-machine (QBM) neuron device that utilizes a probabilistic architecture for information processing.[1)] In this paper we propose a method for specifying the weight coefficients in the QBM neuron device.

The Boltzmann machine[2)] (BM) is a kind of feedback neural network based on a stochastic architecture. Figure 1(a) is a schematic diagram of the BM neural network. It is composed of a number of identical binary-state neurons. The connection between each neuron and its mate is characterized by a particularized weight coefficient. The neuron receives input signals x_i that are weighted with weight coefficients $w_i (i = 1, 2, \ldots n)$, as shown in Fig. 1(b). The neuron produces the weighted sum of the input signals and generates its output state of 1 or 0 with a probability. The probability that the neuron will produce an output of 1 is given by the following sigmoid function,

$$f(s) = \frac{1}{1 + \exp\left(\dfrac{s}{C}\right)} \tag{1}$$

$$S = \sum_{i=1}^{n} x_i w_i + w_0 \tag{2}$$

where S is the weighted sum of the input signals, and C is a control parameter that must be changed during the simulated annealing process. The BM can solve various problems such as combinatorial optimization, association, and pattern recognition. For implementation of the BM neuron network circuit, the weight coefficients must be controllable.

In this paper we propose a method for controlling weight coefficients in the QBM neuron device. First we briefly describe the operation of the QBM neuron device and its characteristics, in §2. Then we propose the method for controlling the weight coefficients, in §3. After that we analyze the weight coefficients and present analytical results, in §4. Finally, we summarize the main results, in §5.

2. QBM Neuron Device

Figure 2 depicts the structure of the proposed QBM neuron device and its operating characteristics. The QBM consists of a two-dimensional (2D) arrangement of coupled quantum dots. Each quantum dot is occupied by a single electron. The arrow represents the polarization of the electron spin. The device has n inputs and one output. It has an operating dot that plays a leading role in the QBM operation. The operating dot is connected to each input by an input line. The exchange interaction coefficient between the operating dot and the input dot for the i-th input line is denoted by $J_i (i = 1, 2, 3, \ldots n)$. The exchange interaction coefficient corresponds to the weight coefficient of the neuron.

We analyzed the entire operation of the QBM neuron device, using the Monte Carlo method.[1)] For simplicity, all the coefficients of the exchange interaction between the operating dot and the input dots were assumed to have the same value for J_s(i.e., $J_1 = J_2 = \ldots = J_s$). Figure 2(b) shows the probability of output 1 for different values of the temperature T as a function of the local field of the spin polarizations at the input dots. The probability shows an approximately sigmoid characteristic that is consistent with eq. (1). The results demonstrated that the device can perform stochastic operation of the BM neuron.

3. Method for Specifying Weight Coefficients

In the QBM neuron device, the exchange interaction coefficient corresponds to the weight coefficient of the QBM neuron. Construction of the QBM neuron network requires control of the weight coefficients. We propose a method for specifying the exchange interaction coefficients. These coefficients depend on physical factors such as the dot diameter and both the interval and the barrier height between the nearest-neighbor dots. Here we will clarify quantitatively the dependence of the exchange interaction coefficient on both the interval and the barrier height between the nearest-neighbor dots, and show a practical method for controlling the physical factors.

We will calculate the exchange interaction coefficient in the following procedure. An array of coupled quantum dots, as shown in Fig. 3, is used as an analytical model. Each dot is occupied by a single electron. $\psi_1(\psi_2)$ is an electron wave function at dot 1 (dot 2). E_0 is the ground state of a single

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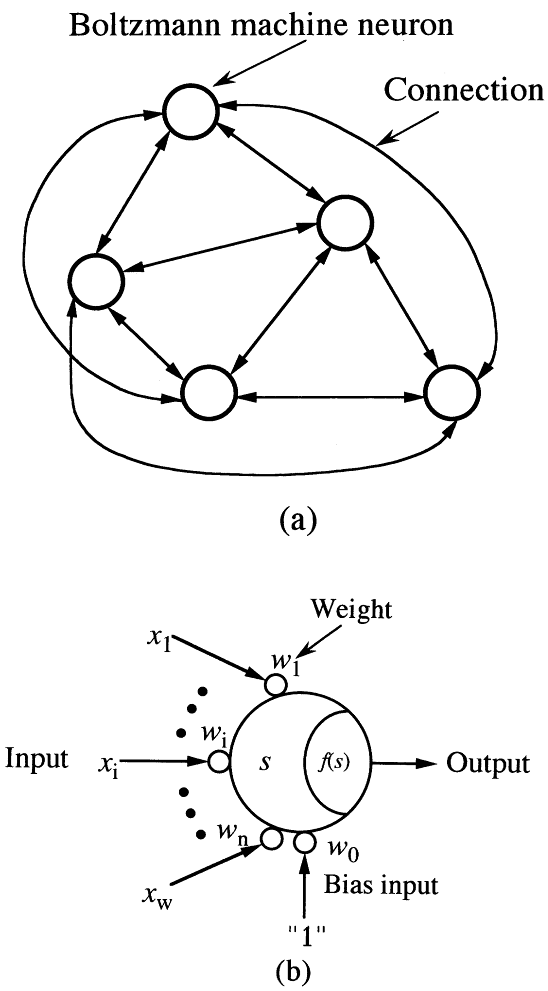

Fig. 1. (a) A schematic diagram of Boltzmann machine neural network; and (b) a model of a Boltzmann machine neuron.

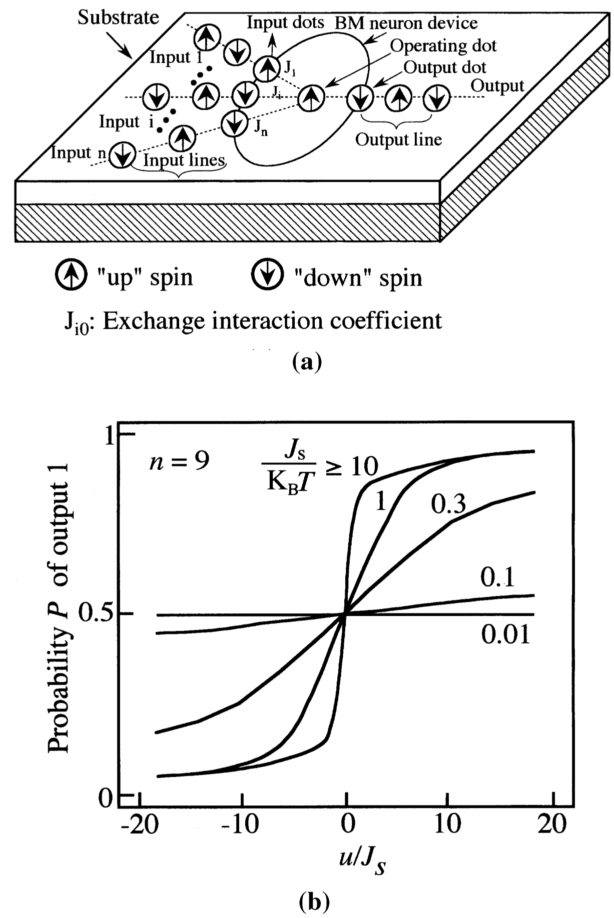

Fig. 2. (a) Quantum-coupled single electrons (quantum dots) in a two-dimensional arrangement constituting a QBM. (b) The probability of output 1 of the nine-input QBM neuron device for different values of temperature T as a function of the weighted sum of the spin polarizations at the input dots. All the strengths of interaction between the operating dot and the input dots are assumed to have the same value:$|J_s| = 10$ meV; the strength of interaction between nearest-neighbor dots in the input lines is set at 50 meV.

electron at a quantum dot. First we calculate the transfer energy t, using the overlay integral,

$$t = \int \psi_1 \{V(x) + E_0\} \psi_2 dx \tag{3}$$

where $V(x)$ is the potential profile of the coupled quantum dots.

The exchange interaction coefficient equals half of the energy difference between the antiferromagnetic and ferromagnetic states of the electron spins. We estimate the value of exchange interaction coefficient J using the extended Hubbard model,[3)]

$$H = \sum_{k,j,\sigma} t_{kj} c^{+}_{k,\sigma} c_{j,\sigma} + \frac{1}{2} \sum_{k,\sigma} U n_{k,\sigma} n_{k,-\sigma} \tag{4}$$

where $c_{k\sigma^+}$ ($c_{k\sigma}$) is the creation (annihilation) operator for an electron at the quantum dot k with spin σ, $n_{k,\sigma}$ is the number operator of the electron for the quantum dot k and spin σ, t_{kj} is the overlap integral that represents the interdot coupling between two quantum dots k and j; and U is the on-site Coulomb repulsion energy when two electrons are in the same dot, as

$$U = \frac{3q^2}{4\pi\varepsilon_r d} \tag{5}$$

where d is the diameter of the quantum dot and ε_r is the di-

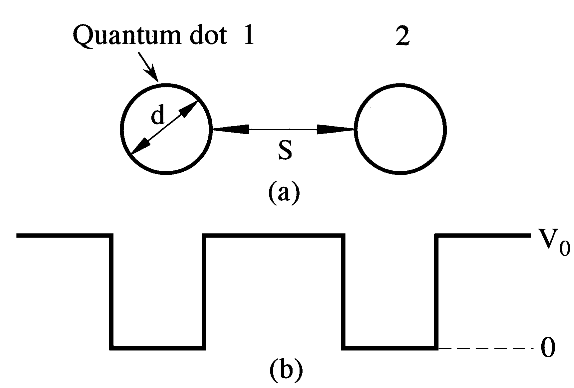

Fig. 3. (a) The coupled quantum dots; and (b) the potential profile seen by two electrons in the coupled quantum dots.

electric constant.

4. Results

Figure 4 shows the calculated transfer energy t values. The barrier height between the coupled quantum dots was assumed to have two different values of 240 and 500 meV. The electron effective mass m^* value was taken to be 0.067 m_0.

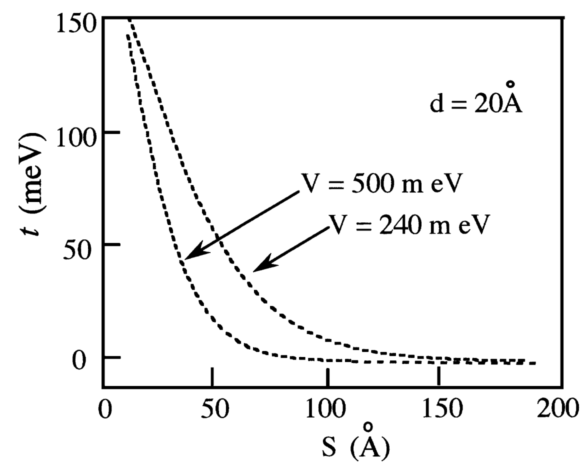

Fig. 4. Dependence of the transfer energy t on the interval between the coupled dots for two barrier height values of 240 and 500 meV.

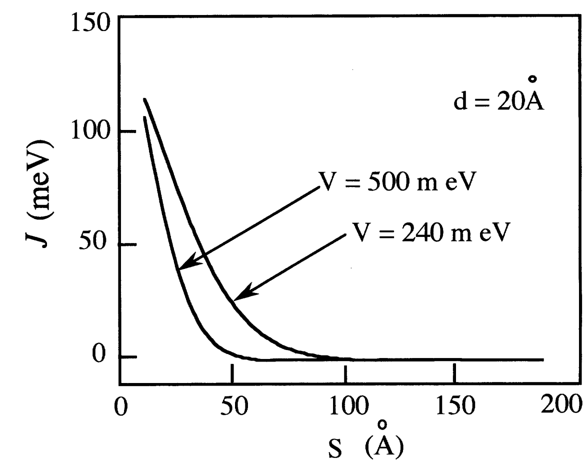

Fig. 6. Dependence of the exchange interaction coefficient t on the interval between the coupled dots for two barrier height values of 240 and 500 meV.

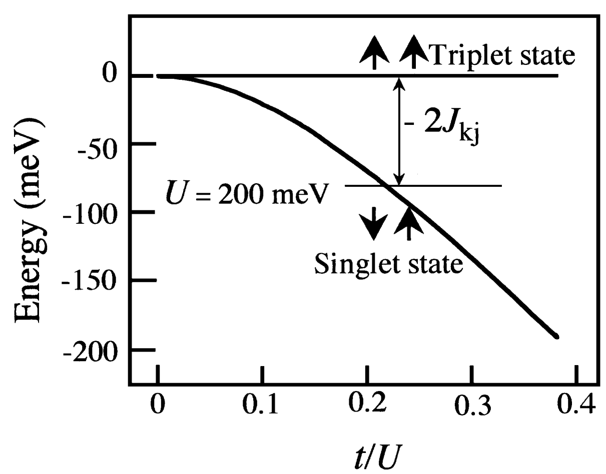

Fig. 5. The levels of the low-energy singlet and triplet states as a function of the transfer energy.

The transfer energy t depends on the interval and the barrier height between the coupled quantum dots. Its values decrease from 150 to 0 meV with the increase of the interval. When the interval is constant, the t value for the barrier height of 240 meV is larger than 500 meV.

As is well known, the two electrons in the coupled quantum dots can be described by singlet and triplet orbital states. Figure 5 shows the calculated dependence of the low-energy singlet and triplet orbital levels on the amplitude of the transfer energy t. The Coulomb repulsion energy U is assumed to be 200 meV and the dielectric coefficient to be 10. The ground state of the two-electron system corresponds to the singlet state, in which the spins of the two electrons are antiparallel (antiferromagnetic). The exciting state is the triplet state, in which the spins are parallel. Thus we find that the exchange interaction coefficient J is equal to half of the energy difference between the singlet and triplet states and that it has a negative value. The value of $|J|$ increases as the overlap integral increases.

Figure 6 shows the values calculated for the exchange interaction coefficient J. The exchange interaction coefficient J depends strongly on the barrier height and the interval between the coupled quantum dots. Its value changes over a wide range, from 110 to 0 meV. These results demonstrated that the weight coefficient of the QBM neuron device can be controlled in the design phase, by selecting the values for two physical factors: the interval and the barrier height between the nearest-neighbor dots.

5. Discussion

Physical implementation of the QBM requires the control of the interval and the barrier height between nearest-neighbor quantum dots. Optimum design of these two physical factors can be achieved through arrangement of the quantum dots and the selection of the barrier materials. Several methods can produce a 2D array of quantum dots. We considered a selective-area-nanodeposition method[4] for the fabrication of our 2D array of quantum dots. In the method nucleation sites are first created on the substrate by means of a STM (scanning tunneling microscope) tip, and then nanosized particles are deposited on it. The particles tend to occupy the nucleation sites first. This method can be used to fabricate the desired arrangement of the dots with angstrom-level resolution.

Furthermore, the desired value for exchange interaction coefficient J can also be obtained by changing the materials serving as barriers between the nearest-neighbor dots. For example, to nullify the spin interaction strength between different input lines (linear arrays), we deposited a barrier-material film over the 2D array of quantum dots formed on an insulating substrate, and then removed the film between the input lines by electron beam lithography and etching.[5] As a result, the quantum dots of one input line were coupled by a finite exchange interaction coefficient, but spin interaction between nearest-neighbor input lines was prevented due to the presence of an air gap.

6. Conclusions

We have proposed a method for determining weight coefficients in the QBM neuron device design. The construction of the QBM neuron network requires the control of the weight coefficients. The exchange interaction coefficient corresponds to the weight coefficient of the QBM neuron. We analyzed quantitatively the dependence of the exchange interaction coefficient on two physical factors: the interval and the barrier height between the nearest-neighbor dots. We found that the exchange interaction coefficient decreases with increase in the interval and increase in the barrier height. These results demonstrated that the weight coefficient of the QBM neuron device can be controlled in the design phase, by means of the specification of the interval and the selection of the barrier materials.

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