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ABSTRACT

Here we present the novel idea of Quantum-dot Controlled-NOT (QCNOT) gate. We have simulated the Controlled-NOT (CNOT) gate using orbital state of electron wavefunction. Asymmetric coupled QDs structure made by InAs dots on GaAs substrate have been simulated. The simulation results were very encouraging realization of CNOT gate. Quantum tunnelling is the responsible prime parameter for the realization of CNOT gate. Consequently, the interdot separation is the major factor to be controlled. The effect of QD separation for optimum coupling had been utilized. We also studied controlled-notrolled-NOT (CCN) gate (also known as Toffloi gate) which, is an extension of CNOT gate, have two control and one target qubit. Universal gate analogous to classical CMOS/TTL is realized by CCN which at certain condition provide the truth table equivalent to NAND gate.

Keywords: NAND, QDOT, TTL, Wavelength, Structure.

I. INTRODUCTION

Quantum logic gates provide fundamental examples of conditional quantum dynamics. They could form the building blocks of general quantum information processing systems which have recently been shown to have many interesting non-classical properties. Although coherence is difficult to maintain through entire calculation process, CNOT gate has immerged as a formidable candidate to replace the classical logic gates. However, it will be more efficient to combine the quantum computational circuit and the conventional VLSI circuit on the same chip . Thus Kane proposed the Silicon based quantum dot computer using NMR of dopants (phosphorous). In similar fashion Tanamoto's work is also based on Silicon substrate using orbital states for logic operation. Mechanism of a controlled switching on and off of the exchange interaction between spin qubits has been advocated by numerous authors to be most promising candidate for quantum logic operation . Parallel research on orbital states based CNOT or charge qubits using coupled asymmetric QDs have been reported and advocated as the best possible candidate for quantum logic operations .

In this paper we have presented quantum mechanical model of controlled-NOT gate (CNOT Gate) using QDs. The model is composed of two set of asymmetric QDs with single electron. In the present piece of work, we extend the model to a two-dimensional nanostructure and take into account all the two-electron states with discrete energy levels. The structure of this paper is as follows. In section 2 we have discussed about the basic idea of CNOT gate, and computational method has been described in section 3. We have presented the results of simulations for CNOT structure with variation in parameters in 4. Conclusions are presented at last.

Preliminaries

To understand the concept of quantum logic gates led us to understand its primitive 'quantum bit' or 'qubit'. We treat qubit as abstract mathematical object. Two possible states of qubits are states $|0\rangle$ and $|1\rangle$. But unlike classical bits

qubits can present linear combination of $|0\rangle$ and $|1\rangle$ states, often called superposition.

$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$$
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where α and β are complex numbers. When we measure a qubit, we get result '0' with probability $|\alpha^2|$ and result '1' with probability $|\beta^2|$. So,

$$\mathbf{x}|\boldsymbol{\alpha}^2| + |\boldsymbol{\beta}^2| = \mathbf{1}$$

Thus we can say in general a qubit's state is a unit vector in a two dimensional complex vector space (Bloch sphere). When measured a qubit gives either '0' or '1' probabilistically. For example a qubit in $\frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|0\rangle$ state gives the result '0' fifty percent of the result '1' fifty percent of the time. In similar manner if we take two qubits than

result '0' fifty percent of time and the result '1' fifty percent of the time. In similar manner if we take two qubits than 67



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$$|\psi\rangle = \alpha_{00}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|10\rangle + \alpha_{11}|11\rangle \qquad 3$$

With, $\sum_{x \in \{0,1\}^2} |\alpha_x|^2 = 1$ or,

$$|\alpha_{00}|^2 + |\alpha_{01}|^2 + |\alpha_{10}|^2 + |\alpha_{11}|^2 = 1$$

Moreover, the measurement outcomes are strangely correlated according to EPR paradox [12]. According to John Bell the measurement correlations in quantum systems are stronger than could ever exist between classical systems [13].

As infinitely many superposition of $|0\rangle$ and $|1\rangle$ states can be obtained, infinitely many one qubit operation can be performed theoretically. For example X (NOT), Z and H (Hadamard). Matrix representation may be given by:

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$H = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

$$5$$

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Figure 3.1 represents the function of these unitary gates.



Fig. 1: Qubit logic gates.

The basic controlled-NOT operation is given by $|\epsilon_1\rangle|\epsilon_2\rangle \rightarrow |\epsilon_1\rangle|\epsilon_1 \oplus \epsilon_2\rangle$ (modulo 2) [11,1] where ϵ_1 shows a *control qubit* and ϵ_2 shows a *target qubit*. The value of ϵ_1 remains unchanged, whereas that of ϵ_2 is changed only if $\epsilon_1 = 1$. (Fig. 3 gives the pictorial presentation and transfer matrix). Moreover in addition to this a quantum controlled-NOT gate has a variety of properties and applications like [11]:

- Transforms superposition into entanglement: $(\alpha|0\rangle + \beta|1\rangle)|0\rangle \rightarrow \alpha|0\rangle|0\rangle + \beta|1\rangle|1\rangle$
- This transformation of superposition into entanglements can be reversed by applying the same controlled– NOT operation again.
- Quantum state swapping can be achieved by cascading three quantum controlled–NOT gates.

The entanglement plays an important role in quantum cryptography gates [14]. In this paper we show the quantum gates of the semiconductor coupled quantum dots, emphasizing their controlled-NOT operation.

1. **Computational method**

Crouch *et al.* [15] and Waugh *et al.* [16] showed that, if the tunnelling barrier is low and the coupling of the two dots is strong, the coupled dots behave as a large single dot in a Coulomb blockade phenomenon. This means that, if the tunnelling barrier between the dots is sufficiently small, it is possible that only one electron exists in the coupled dots. We can consider the electronic state of the two coupled dots in the range of the free-electron approximation at the first step of investigation. When two dots of different size are coupled and one excess electron is inserted, the system can

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be treated as a two-state system where the energy levels of the total coupled-dot system show the localized state of the wave function reflecting the different energy levels of the independent isolated dots. When gate bias voltage is applied and the potential slope is changed, there appears a gate bias voltage at which the two energy levels of the original single dots coincide, and the electron transfers to another dot. If we regard the perfect localization of the charge in one of the coupled dots as the $|0\rangle$ state and that in the other dot as the $|1\rangle$ state, we can constitute a *qubit* by the coupled quantum dots. Here we have considered that if electronic state is localized at bigger dot than the qubit is in $|0\rangle$ state and if the electronic state (wave function) is localized in smaller dot than the qubit is in $|1\rangle$ state.



Fig.2: Confinement potential of two asymmetric QD pair, control qubit 'a' and target qubit 'b'.

For simulation we have taken two coupled asymmetric QDs as given in fig.2. Where the asymmetric coupled dots 'a' are taken as control qubit and dots 'b' are taken as target qubit. The schematic diagram for CNOT is given in Fig. 3.

The diameter for QD a1 and b1 is taken to be 6nm and that of a2 and b2 is 4nm. InAs dots upon GaAs substrate are assumed which has the band difference of 570meV at conduction band. The confinement potential of QDs is considered to have Gaussian shape. The distance between centres of coupled asymmetric QDs is 6nm (let's call it m) and the distance between the centres of qubits is taken to be 10nm (let's call it n). All dimensions are taken in AU for simulation.



Fig.3: Schematic diagram of CNOT gate using coupled asymmetric QDs solid lines show path of electron tunnelling. Dotted lines show electric fields generated between dots or channel.

The wave function of control qubit is first determined, solving the Hamiltonian

$$\frac{\hbar}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\psi + V(x, y)\psi = E\psi \qquad 8$$

With V(x,y) for the control qubit is taken as



$$V(x, y) = V_0 exp\left(\frac{\left(\left(x - \frac{m}{2}\right)^2 + \left(y + \frac{n}{2}\right)^2\right)}{2\sigma_1^2}\right) + V_0 exp\left(\frac{\left(\left(x + \frac{m}{2}\right)^2 + \left(y + \frac{n}{2}\right)^2\right)}{2\sigma_2^2}\right) + x * \xi_1$$

Where ξ_1 is the electric field applied through the gate 1 as given in Fig. 3. $\sigma_1 \& \sigma_2$ gives the width of dot. Now the wave function obtained by this process provides the probability density of electron found in the control qubit. Now the Hamiltonian 3.8 is solved for the target qubit, in which the coulombic interaction due to the wave function is added in the potential term V(x,y):

$$V(x, y) = V_0 exp\left(\frac{\left(\left(x - \frac{m}{2}\right)^2 + \left(y - \frac{n}{2}\right)^2\right)}{2\sigma_1^2}\right) + V_0 exp\left(\frac{\left(\left(x + \frac{m}{2}\right)^2 + \left(y - \frac{n}{2}\right)^2\right)}{2\sigma_2^2}\right) + q^2 |\psi| / 4\pi\varepsilon_0 \varepsilon_{sc} ((x - x_1)^2 + (y - y_1)^2)^{\frac{1}{2}} + x * \xi_2$$
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Here \mathcal{E}_{sc} is the relative permittivity of the semiconductor QD, ξ_2 is the potential applied through gate 2, x_1 and y_1 are the coordinates of wave function of control qubit and x and y are the coordinates of target qubit (this has to be added in recursion for every coordinates of wavefunction of control qubit and coordinates of target qubit).

We have adopted the method based on imaginary time propagation technique to solve the Hamiltonian proposed by Kosloff [17]. The results are described in next section.

II. RESULTS & DISCUSSION

We have considered coupled asymmetric confinement potential as given in Fig. 2 and Fig. 3 to simulate and verify the CNOT gate. First observations have been made with no potential applied on gate 1 and 2. Here we have observed two cases. First when control qubit is in $|0\rangle$ state.

The wavefunction obtained for this condition is given in Fig. 4, where the wavefunction is concentrated in the bigger dot of control qubit which indicates that the electron is present in the bigger dot and hence the qubit is in $|0\rangle$ state.



Fig. 4: wavefunction of qubit, at ground state representing $|0\rangle$ state.



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The modified potential profile for the target qubit accounting for the coulombic repulsion due to the electron probability function will become as given in Fig. 5. The contour is visible in the confinement potential profile.



Fig. 5: Confinement potential of target qubit constituting the repulsive effect of the probability density of electron in control qubit.

Fig. 6 presents the wavefunction at ground state. We can see that wavefunction is concentrated in bigger QD which corresponds to $|0\rangle$ state of target qubit. The first excited state wavefunction is given in Fig. 7. Here the wavefunction is concentrated in smaller dot which corresponds to $|1\rangle$ state. Hence this simulation shows that the target qubit is not at all affected when the control qubit has $|0\rangle$ state.



Fig. 6: Ground state wavefunction of target dots, concentrated at bigger dot corresponding to $|0\rangle$ State.





Fig. 7: First Excited state of Target dots, wavefunction is concentrated at smaller dot corresponding to $|1\rangle$ state.

Now the operation of CNOT gate is more prominent when we apply $|1\rangle$ state at control qubit and simulate the result at target qubit. This is the first excited state of control qubit when no electric field is applied at any gate and the wavefunction is concentrated in smaller dot of control qubit, as given in Fig. 8. The coulombic interaction is added with the confinement potential of the target qubit and the resultant potential distribution is given in Fig. 9 where the contour is more prominent in comparision to the Fig. 5.



Fig.8: wavefunction of control qubit, at first excited state representing $|1\rangle$ state.





Fig.9: Confinement potential of target qubit constituting the coulombic interaction of the probability density of electron in control qubit.

This repulsive coulombic potential due to the wavefunction of control qubit changes the target qubit's ground state to $|1\rangle$ state and first excited state to $|0\rangle$ state as shown in Fig. 10 and 3.11.



Fig.10: Ground state wavefunction of target dots, concentrated at smaller dot corresponding to $|1\rangle$ State.





Fig. 11: First Excited state of Target dots, wavefunction is concentrated at bigger dot corresponding to $|0\rangle$ state.

Can CNOT gate serve as a universal gate? It is similar to classical XOR gate. But XOR gate can never serve as universal gate. Because any combinations of CNOT gate the parity is unchanged. For creating a universal gate we a gate based on three qubit called Controlled Controlled NOT (CCN) Gate or Toffoli Gate. In this Quantum gate if and only if the bits on both of the control lines is 1, than the target bit is inverted. The QD CCN gate is presented in Fig. 12(a), in which line $|C1\rangle$ is control line 1 and line $|C2\rangle$ is control line 2 combinations of which will decide the output of Target line $|T\rangle$. In the control lines, the output state is always the same as the input state. CCN gate works like a CNOT gate only if both control lines are in logical state 1. In the opposite case, line $|T\rangle$ copies the input state to the output. Truth table QD CCN gate is shown in Fig. 12(b). From the truth table of the CCN gate it is clear that if we apply state $|1\rangle$ at the target qubit then it replicates the NAND gate output for the combinations of control qubits C1 and C2. Now we can use it as universal gate.



Fig.12: (a) scheme of the CCN gate C1 & C2 being control and T being target qubit and (b) Truth table of CCN gate



Fig.13: Confinement potential of QD CCN gate used for simulation.

III. CONCLUSION

The novel idea of controlled-NOT gate using QDs is presented. We have exploited orbital state of the electron wavefunction to simulate the CNOT gate. We have also proved that an extension of CNOT gate i.e. CCN gate can present the necessary condition with which any logical operation can be performed.

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