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# Controlled NOT GATE using Quantum Dots

Amar Prakash Sinha

Department of ECE, BIT Sindri, Jharkhand, India

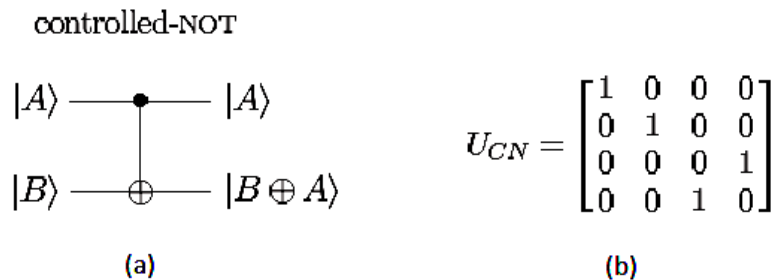
**ABSTRACT:** The single QD with the confined electrons can be treated as an artificial atom. Artificial molecules can be constructed by turning on tunnelling between quantum dots. Double-quantum dots are the simplest coupled QD systems where dots are placed either vertically (Pi, et al., 2001; Imamura, et al., 1999) or laterally. In a vertical double-quantum dot, each dot contains approximate rotational symmetry so that the angular quantum numbers are well defined (Imamura, et al., 1999; Bayer, et al., 2001) while in lateral double quantum dot, this symmetry is absent due to coupling between the two dots (Cha, et al., 2002). Coupled quantum dot systems with a few electrons have been extensively investigated in regard to many body effects such as Coulomb blockade (Stafford, et al., 1994; Weis, et al., 1993; Vaart, et al., 1995; Pfannkuche, et al., 1995; Crouch, et al., 1997; Waugh, et al., 1995). From the experiments by Van Der Vaart (Vaart, et al., 1995), it can be seen that the electron transfer between dots occurs when the discrete energy-level of one of the dot matches with the other dot of the coupled dots. Coupling between two or more quantum dots can be used for CNOT gate and QCA structures which are extensively used in quantum computation.

## I. INTRODUCTION

CNOT gate present a link between classical gates and the quantum gates, because the operation of quantum dot CNOT gate has quantum mechanical premises solely, though it resembles with classical XOR gate. We can realize digital operations using Quantum dot CNOT gate in a similar way as in classical logical gates. In addition to this, the control bit remains unchanged in QD CNOT gate which make logical operation reversible. This reversibility makes it the building block with which the Shor’s algorithm is realized.

There are two major approaches for realizing CNOT gate operation, one exploiting spin state and the other exploiting orbital state. While using spin state particularly natural implementation is provided by a spin -1/2 atomic nucleus, such as <sup>1</sup>H, and this is the approach used in majority of nuclear magnetic resonance (NMR) implementations. A two-qubit quantum computer can be built from two spin ±1/2 nuclei. There must be some sort of spin–spin interaction, so that two-qubit logic gates can be constructed. This is easily achieved by using two inequivalent nuclei in a molecule. NMR technique provides a nice coherent time. However, on increasing the number of correlated spins might eventually lead to nonseparable states(Jones, 2012; Braunstein, et al., 1998). The orbital state can also be exploited for making a CNOT capacitively coupled qubit pair. We achieve a strong electrostatic dipole coupling between two charge qubits. The large coupling energy enables us to completely and coherently turn on/off of one qubit by pulse-driving the charge on the other qubit. A CNOT operation is demonstrated based on this effect and is addressed and simulated as a part of this paper.

The QD CNOT gate is presented in Fig. 1(a), in which line |A> is called the control line because a logical state of this line decides about the state of the output of line|B>, known as the target line. In the control line, the output state is always the same as the input state. The CNOT gate works like a NOT gate for target qubit if the control line is in logical state 1. In the opposite case, line |B> copies the input state to the output. All the logical states of the CNOT gate are scheduled in the truth table shown in Fig. 1(b). The matrix representation of the controlled-NOT,  $U_{CN}$ , is written with respect to the amplitudes for |00>, |01>, |10>, and |11> in that order.



**Fig.** Ошибка! Текст указанного стиля в документе отсутствует. **1:** (a) scheme of the CNOT gate A being control and B being target qubit and (b) Truth table of CNOT gate (Moskal, et al., 2004).



Quantum logic gates provide fundamental examples of conditional quantum dynamics. They 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 emerged as a plausible 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 (Tanamoto, 2000). Thus Kane (Kane, 1998) proposed the silicon based quantum dot computer using NMR of dopants (phosphorous). In similar fashion Tanamoto's (Tanamoto, 2000) 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 (Moskal, et al., 2007; Loss, et al., 1998; Levy, 2001; Leuenberger, et al., 2001; Feng, 2003). 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 (Balandin, et al., 1998; Szafran, 2008; Li, et al., 2014; Barenco, et al., 1995).

In this chapter we have presented quantum mechanical model of controlled-NOT gate (CNOT Gate) using orbital state based qubits. 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 chapter is as follows. In section 3.2, we have discussed about the basic idea of CNOT gate, formulation of problem is presented in section 3.3 and computational method has been described in section 3.4. We have presented the results of simulations for CNOT structure with variation in parameters in 3.5 and conclusions are presented in section 3.6.

## II. CONCEPT OF QUANTUM LOGIC GATES

The concept of quantum logic gates are based on the 'quantum bit' or 'qubit'. We treat qubit as abstract mathematical object. But unlike classical bits qubits can be presented as linear combinations of  $|0\rangle$  and  $|1\rangle$  states, often called superposition.

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \quad 1$$

where  $\alpha$  and  $\beta$  are complex numbers. When we measure a qubit, we get result '0' with probability  $|\alpha|^2$  and result '1' with probability  $|\beta|^2$  such that

$$|\alpha|^2 + |\beta|^2 = 1. \quad 2$$

Thus we can say in general that 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  $\frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$  state gives the result '0' fifty percent of time and the result '1' fifty percent of the time. In similar manner if we take two qubits then

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

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

$$|\alpha_{00}|^2 + |\alpha_{01}|^2 + |\alpha_{10}|^2 + |\alpha_{11}|^2 = 1. \quad 4$$

Moreover, the measurement outcomes are strangely correlated according to EPR paradox (Einstein, et al., 1935). According to John Bell the measurement correlations in quantum systems are stronger than could ever exist between classical systems (Bell, 1964).

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:



$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \tag{5}$$

$$Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \tag{6}$$

$$H = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}. \tag{7}$$

Fig. 2. represents the function of these unitary gates.

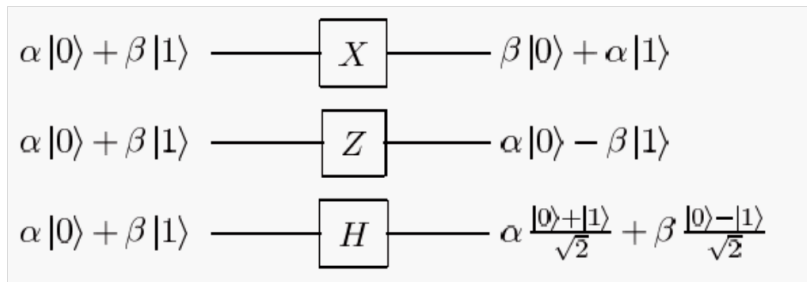


Fig. 2: Qubit logic gates.

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) (Tanamoto, 2000; Barenco, et al., 1995) where  $\epsilon_1$  shows a *control qubit* and  $\epsilon_2$  shows a *target qubit*. The value of  $\epsilon_1$  remains unchanged, whereas that of  $\epsilon_2$  is changed only if  $\epsilon_1 = 1$ . (Fig.1 gives the pictorial presentation and transfer matrix). In addition to this a quantum controlled-NOT gate has a variety of properties and applications like (Barenco, et al., 1995):

- 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 (Bennett, et al., 2000). In this chapter we show the quantum gates of the semiconductor coupled quantum dots, emphasizing their controlled-NOT operation.

### III. FORMULATION OF THE PROBLEM

Crouch *et al.* (Crouch, et al., 1997) and Waugh *et al.* (Waugh, et al., 1995) 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 be treated as a two-state system where the energy levels of the total coupled-dot system shows 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 (wavefunction) is localized at bigger dot then the qubit is in  $|0\rangle$  state and if the electronic state is localized in smaller dot then the qubit is in  $|1\rangle$  state. Two sets of such asymmetric dots must be considered, representing controlled and target qubit, and similar consideration has to be taken for modelling  $|0\rangle$  and  $|1\rangle$  states for both qubits.

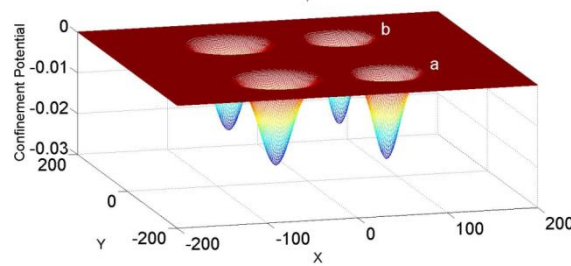


Fig. Ошибка! Текст указанного стиля в документе отсутствует.3: Confinement potential of two asymmetric QD pair, control qubit ‘a’ and target qubit ‘b’.

IV. COMPUTATIONAL METHOD

For simulation we have taken two coupled asymmetric QDs as shown in Fig.4, where the asymmetric coupled dots ‘a’ are taken as control qubit and dots ‘b’ are taken as target qubit. The schematic diagram for CNOT gate is shown in Fig. 4.

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 570 meV 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.

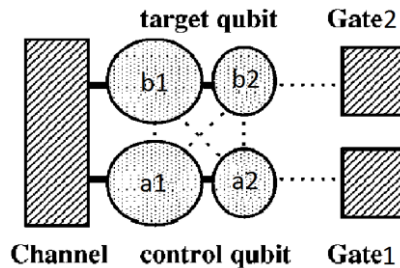


Fig. 4: Schematic diagram of CNOT gate using coupled asymmetric QDs solid lines show path of electron tunnelling. Dotted lines show electric fields generated between dots or channel.

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

$$\hat{H}\psi = -\frac{\hbar^2}{2m^*} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \psi + V(x,y)\psi = E\psi \tag{8}$$

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

$$V(x,y) = -V_0 \left[ \exp \left\{ -\left( \frac{\left( (x-\frac{m}{2})^2 + (y+\frac{n}{2})^2 \right)}{2\sigma_1^2} \right) \right\} + \exp \left\{ -\left( \frac{\left( (x+\frac{m}{2})^2 + (y-\frac{n}{2})^2 \right)}{2\sigma_1^2} \right) \right\} \right] + x\xi_0 \tag{9}$$

where  $\xi_1$  is the electric field applied through the gate 1 as shown in Fig. 4.  $\sigma_1$  &  $\sigma_2$  provides the width of dots. The wave function obtained by this process provides the probability density of electron found in the control qubit. 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  $V(x,y)$ :

$$V(x,y) = -V_0 \left[ \exp \left\{ -\left( \frac{\left( (x-\frac{m}{2})^2 + (y-\frac{n}{2})^2 \right)}{2\sigma_1^2} \right) \right\} + \exp \left\{ -\left( \frac{\left( (x+\frac{m}{2})^2 + (y-\frac{n}{2})^2 \right)}{2\sigma_1^2} \right) \right\} \right] + q^2 |\psi|^2 / 4\pi\epsilon_0\epsilon_{sc} ((x-x_1)^2 + (y-y_1)^2)^{\frac{1}{2}} + x * \xi_2 \tag{10}$$



here  $\epsilon_{sc}$  is the relative permittivity of the semiconductor QD,  $\xi_2$  is the potential applied through gate 2,  $x_1$  and  $y_1$  are the coordinates of wavefunction of control qubit,  $x$  and  $y$  are the coordinates of target qubit (this has to be added in recursion for coordinate 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 as described in section 1.8 and used in second chapter.

The results are described in the next section.

#### IV. RESULTS AND DISCUSSION

We have considered coupled asymmetric confinement potential as shown in Fig. 3 and Fig. 4 to simulate and verify the CNOT gate. The 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 shown in Fig. 5, 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 taken to be in  $|0\rangle$  state.

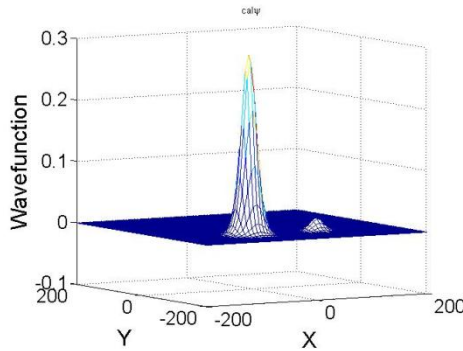


Fig. 5: Wavefunction of control qubit, at ground state representing  $|0\rangle$  state.

The modified potential profile for the target qubit accounting for the coulombic repulsion due to the electron probability density function is shown in Fig. 6.

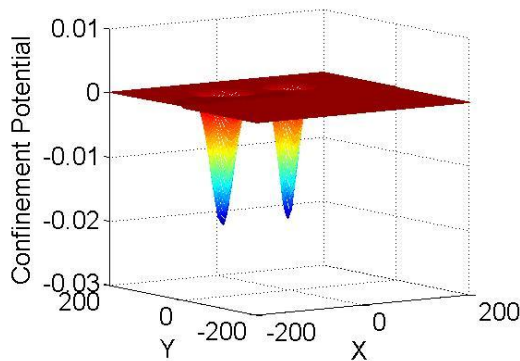
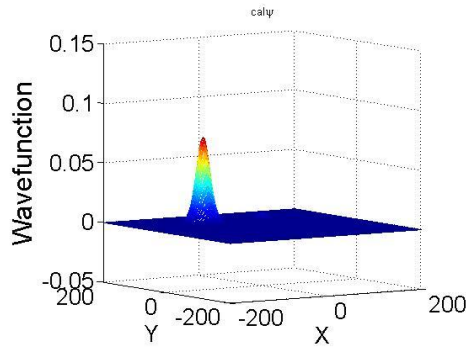
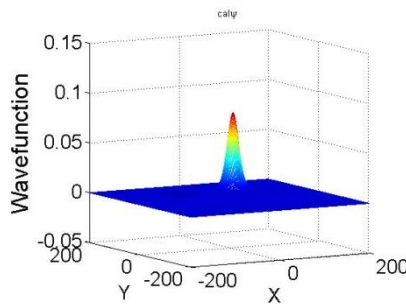


Fig.6: Confinement potential of target qubit constituting the repulsive effect of the probability density of electron in control qubit.

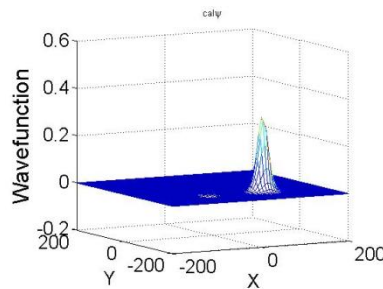


**Fig. 7:** Ground state wavefunction of target dots, concentrated at bigger dot corresponding to  $|0\rangle$  State.

Fig. 7 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 shown in Fig. 8. Here the wavefunction is concentrated in smaller dot which corresponds to  $|1\rangle$  state. The energy eigenvalues of the two target qubit states are  $-0.0128\text{AU}$  and  $-0.0113\text{AU}$ . Hence this simulation shows that the target qubit is not at all affected when the control qubit has  $|0\rangle$  state.

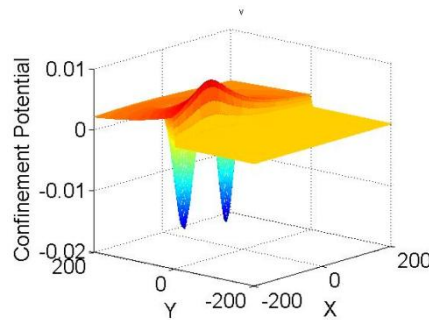


**Fig. 8:** First Excited state of Target dots, wavefunction is concentrated at smaller dot corresponding to  $|1\rangle$  state.



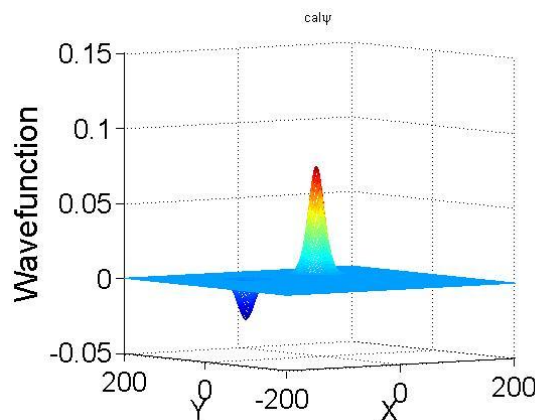
**Fig. 9:** Wavefunction of control qubit, at first excited state representing  $|1\rangle$  state.

Now the operation of CNOT gate is more prominent when we have  $|1\rangle$  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. The wavefunction is concentrated in smaller dot of control qubit, as shown in Fig. 9. The coulombic interaction is added with the confinement potential of the target qubit and the resultant potential distribution is shown in Fig. 10 where the effect of coulombic repulsion due to the probability density of control qubit is more prominent in comparison to the Fig. 6.



**Fig.10:** 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. 11 and 12. The energy eigenvalues of the two target qubit states are  $-0.0093\text{AU}$  and  $-0.0089\text{AU}$ . Thus, we see that if the control bit is  $|0\rangle$  the target bit is unchanged, while if the control bit is  $|1\rangle$  the target bit’s state is flipped from  $|0\rangle$  to  $|1\rangle$  and vice-versa. Hence configuration works as a CNOT gate.



**Fig. 11:** Ground state wavefunction of target dots, concentrated at smaller dot corresponding to  $|1\rangle$  State.

CNOT gate, similar to classical XOR gate, cannot serve as a universal gate. For any combinations of CNOT gate the parity is unchanged. For creating a universal gate we use a gate based on three qubit called Controlled Controlled NOT (CCN) Gate or Toffoli Gate. In this Quantum gate if and only if both of the control lines are at  $|1\rangle$  state, the target bit is inverted. The schematic of QD CCN gate is presented in Fig. 13(a), in which line  $|C1\rangle$  is control line 1 and line  $|C2\rangle$  is control line 2. Combinations of control lines will decide the output of target line  $|T\rangle$ . In the control lines, the output state is always the same as the input state. When any or both of the control lines have  $|0\rangle$  state, the target line  $|T\rangle$  copies the input state to the output. Truth table of QD CCN gate is shown in Fig. 13(b). From the truth table of the CCN gate it is clear that if we apply state  $|1\rangle$  at the target qubit and consider C1 and C2 as inputs and T as output then it replicates the NAND gate. We can use this design for a universal gate.



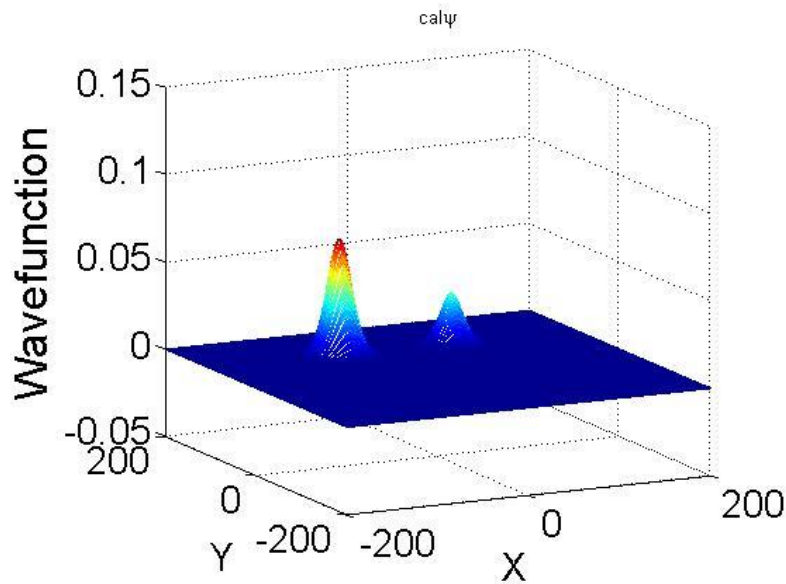


Fig. 12: First Excited state of Target dots, wavefunction is concentrated at bigger dot corresponding to  $|0\rangle$  state.

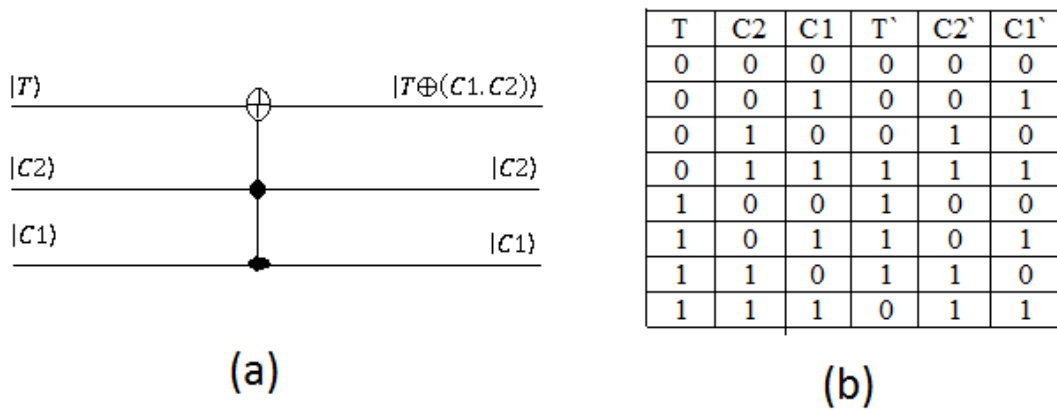


Fig. 13: (a) Scheme of the CCN gate C1 & C2 being control and T being target qubit and (b) Truth table of CCN gate

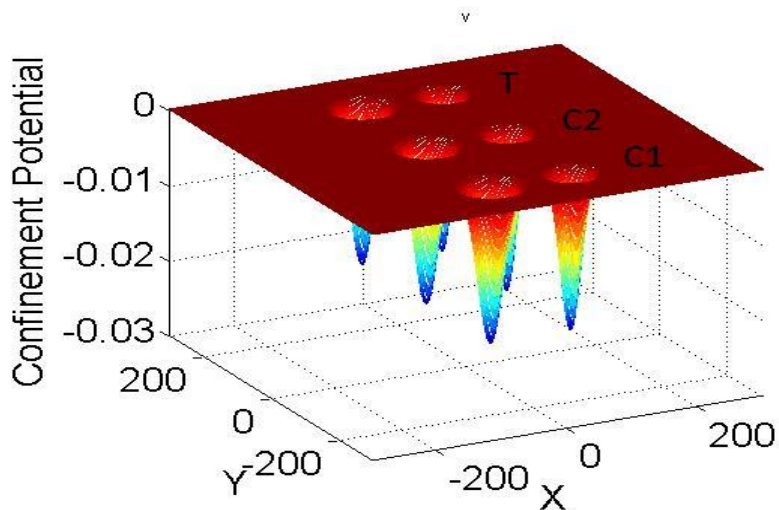


Fig. 14: Confinement potential of QD CCN gate used for simulation.



## V. CONCLUSION

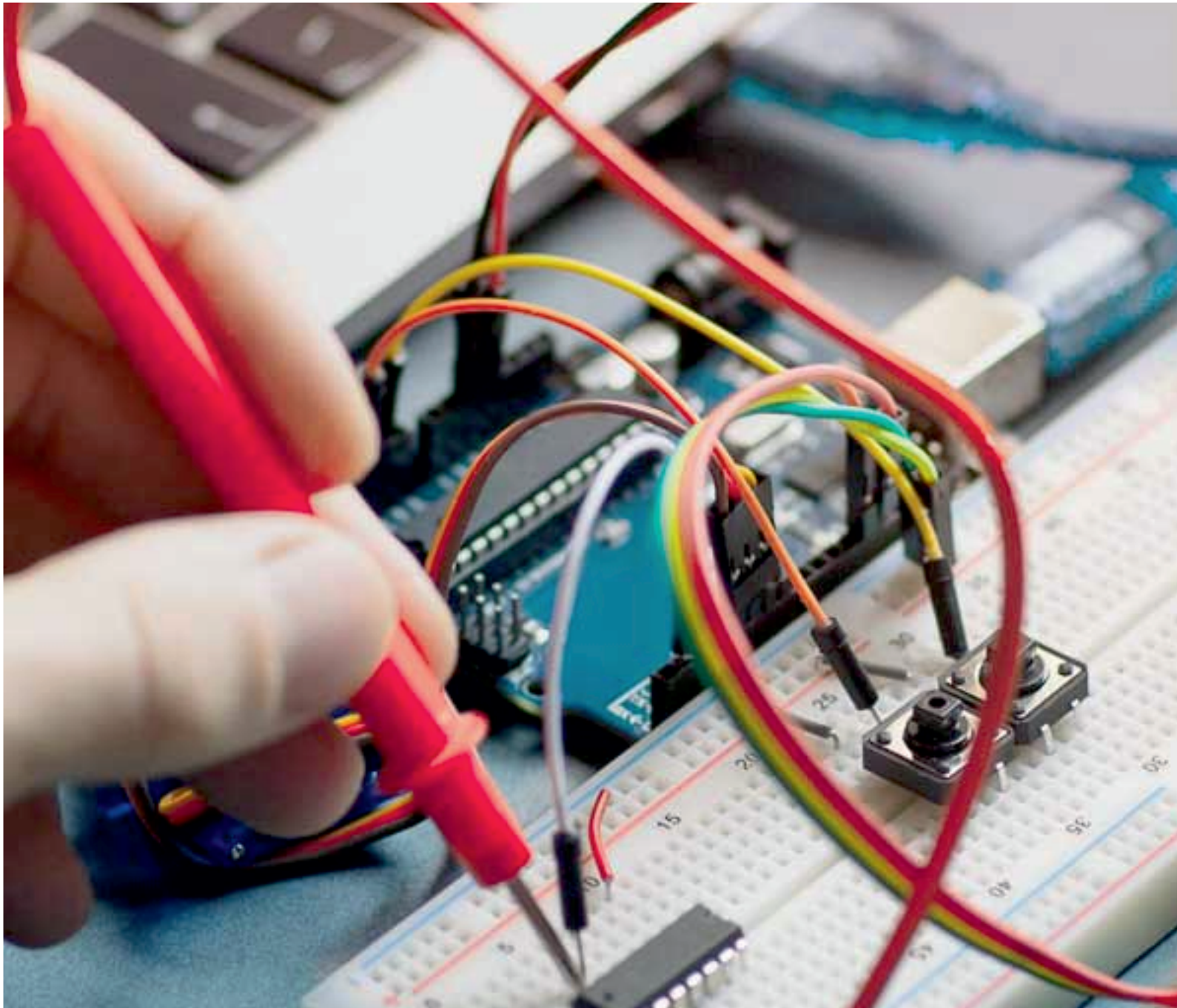
The model of controlled-NOT gate using QDs is presented. We have exploited orbital state of the electron wavefunction to model and simulate the CNOT gate. An extension of CNOT gate i.e. CCN gate can present the necessary condition with which any logical operation can be performed. The CNOT gate is a very important device to perform quantum computation, but another domain also attracted us very much and that is quantum-dot cellular automata (QCA), which we contemplate to be equally promising.

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