Simulation of Controlled Physical Quantum Gates by using Mathematica

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Summary
Physical realization of single and two qubit quantum gates are studied. Hamiltonians of physical system is solved. We discussed constraint of physical parameters of the Hamiltonian to construct controlled quantum gates. We presented a Mathematica program to demonstrate input-output relations of quantum gates. Finally, we will simulate a basic single-qubit quantum computer which contain each input, operation and output and the physical realization of CNOT gate by using Ising interaction of two qubit quantum system.

Key words:
Quantum Computation, Qubit, Hamiltonian.

1. Introduction

Nowadays, the recent manufacturing, technology, medicine, researches and ...etc, depending on the computational machines. The first mechanical computers were built from rather than 2000 years beforehand, and generation of the modern electronic computers started in the last century. [1] From the first electrical computer, that was constructed in 1943 in England to decoding the German's messages during the world war II, till now, the technology of computers has passed the fifth generation. Each revolution in the efficiency and cost of computers, born a new generation in the scope, whereby, makes deeply effects on the human's life.

We are at the critical point of traditional computers, because, according to Moor's law, the squeezing of computer chips, duplicated every 18 months, [2] and in the dimension of atoms, the quantum effects appear, so we need to handle a new logic to construct the next generation of computers.

There are many researchers who work in the scope, to realize physical systems, whether by empirical results, or by simulating theoretical computations. Current centers of research in quantum computing include D-Wave, DARPA (Defense Advanced Research Projects Agency) with the U.S. military [11], Clarendon Laboratory at Oxford or the Centre for Quantum Computing in Cambridge, both in the UK, MIT [12], IBM [13], Oxford University[14], and the Los Alamos National Laboratory. [3]

The computers, in general contain three main parts:

1. The input of information as encoded qubits.
2. A quantum process unit consisting of quantum gates to accomplish unitary transformations on input data.[5]
3. The last part (which is the important part, because it is referring to the time of operation) is a measurement of the output state and break down the superposition of states to the computational basis of the individual qubits. The block diagram of a general form of a quantum computer is as follows:

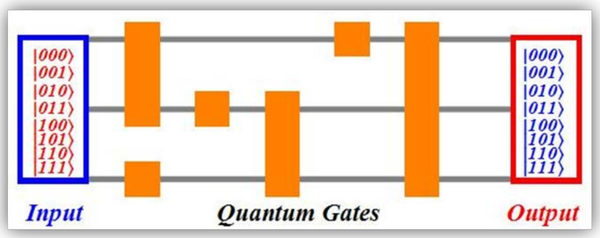

Fig. 1 A block diagram of a quantum computer, which consisting of three parts: input information, quantum unit processor (QUP) and the last part is a measurable states of quantum information.

In this paper we want to simulate some physical quantum systems, in general, that by controlling their parameters, we can freeze the state of qubit to demonstrate the quantum memory, or evaluate them from initial states to any arbitrary final states, to show the quantum operations in the quantum circuits. Furthermore, we have used the computer algebra system Wolfram Mathematica, as a program to solve the Schrödinger equation and plot some graphs a demonstrate the results in term of Bar Chart in three dimensions.

2. Quantum computation

The quantum computation (or nano computation) and quantum information based on some postulates of quantum mechanics. [6,7] but nowadays, they are not just a branch of physics but many mathematicians, chemist and computer scientists attempt whether experimentally or in

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theory. This area, trying to study for developing computer technology and based on quantum' s principles. [8]

The goal of quantum computing is to find a new definition for defining instruments (transistors, bit, get...etc.) by using new techniques for harnessing quantum effects in the nano scale material. To get this aim one has to know about quantum mechanics and information science.

We can represent every quantum gates by using either Dirac notations or Hubbard operators X^{rc}, (where X is represented a unit matrix element and each r and c are the rows and column number respectively).
Hubbard operators obey the following rule:

$$X^{rc}X^{mn} = X^{rn}\delta_{cm} \quad (1)$$

where $\delta_{cm} = \begin{cases} 0 \ if \ c \neq m \\ 1 \ if \ c = m \end{cases}$

On the other side, Dirac notations can be used. The notation, bra⟨ | is represented row vector and ket or (state vector) was symbolized in the form | ⟩ is the column vector. Also by taking conjugated of ket we get bra. [6] ⟨|⟩ each half is so-called bra and ket respectively .[9]
A vector in space C^n and vector in complex space C^{n*} are denoted respectively by[10]:

$$|x\rangle = \begin{pmatrix} x_1 \\ x_2 \\ \cdot \\ \cdot \\ x_n \end{pmatrix}, \ \langle y| = \{y_1, y_2 \dots, y_n\} \quad (2)$$

$$where \ x_n, y_n \in \mathbb{C}$$

Dirac notations similarly can be used to construct quantum gates from basic unit matrices:

$$X^{rc} = |r-1\rangle\langle c-1| \quad (3)$$

The above equation is an outer product (kronecker product) [16-20]. Also the inner product of a two orthogonal vector, is satisfied:

$$\langle n|m\rangle = \delta_{nm}, \quad (4)$$

$$where \quad \delta_{nm} = \begin{cases} 1 \ when \ n = m \\ 0 \ when \ n \neq m \end{cases}$$

Definition :
Direct product, kronecker product and sometimes outer product [21-23]), is one of linear algebra's rules for matrices, to increase their dimensions. Suppose A_{pq} and B_{ij} are two complex vectors so their tensor product be:

$$C_{pi} = A_{pq} \otimes B_{ij} \quad (5)$$

And in bra-ket form notation we have:

$$|A\rangle \otimes |B\rangle or |A\rangle|B\rangle \quad (6)$$

3. Single-Qubit Quantum system

First of all, we can imagine a single-qubit at an arbitrary time:

$$|\Psi(t)\rangle = \alpha(t)|0\rangle + \beta(t)|1\rangle \quad (7)$$

And by acting a physical operator, we can manipulate this qubit. To evolve the state we can use time-dependent Schrödinger equation:

$$i\hbar \frac{\partial \Psi(t)}{\partial t} = H \, \boldsymbol{\Psi(t)} \quad (8)$$

Here, ™ is equal to $\sqrt{-1}$, □□is Planck's constant (1.6×10^{-31}J.s) per 2π and *H* is a quantum observable quantity, is so called Hamiltonian that has the form:

$$H = \Delta\sigma_x + k\sigma_y + \varepsilon\,\sigma_z = \begin{pmatrix} \varepsilon & \Delta - i\,k \\ \Delta + i\,k & -\varepsilon \end{pmatrix} \quad (9)$$

Here Δ, k and □are some parameters which are depending on the systems we can supposed in the real physical experiment, and finally σ_x, σ_y and σ_z are Pauli's matrices [4]. By solving the Schrödinger equation we can get:

$$\Psi(t) = e^{\frac{i H t}{\hbar}} \Psi(0) = U \, \Psi(0) \quad (10)$$

Here, U is a unitary transformation, that can transform the state $\boldsymbol{\Psi}$, from an initial time (t = 0) to any arbitrary time (t):

$$U = e^{\frac{i H t}{\hbar}}$$

$$\Psi(0) = \alpha(0) + \beta(0) = \begin{pmatrix} \alpha(0) \\ \beta(0) \end{pmatrix} = \begin{pmatrix} a + i\,b \\ c + i\,d \end{pmatrix} \quad (12)$$

By now, we can use "Wolfram Mathematica" as a powerful program to simulate the single qubit system, and investigate it as a general. By taking the Hamiltonian in the Schrödinger equation, we can get a solution in the matrix form:

$$\begin{pmatrix} \text{Cos}[t\omega] - \frac{i\varepsilon\,\text{Sin}[t\omega]}{\omega\hbar} & -\frac{(k+i\Delta)\text{Sin}[t\omega]}{\omega\hbar} \\ \frac{(k-i\Delta)\text{Sin}[t\omega]}{\omega\hbar} & \text{Cos}[t\omega] + \frac{i\varepsilon\,\text{Sin}[t\omega]}{\omega\hbar} \end{pmatrix}$$

The above matrix is a 2x2 unitary matrix, that by giving different values to the parameters, one can get, any known single-qubit quantum gates. For instance the matrix U act on a single - qubit in a superposition of two states that has the form:

$$\Upsilon|0\rangle + \xi|1\rangle$$

Here γ and ξ are the probability amplitude for each $|0\rangle$ and $|1\rangle$ and respectively. Since, after evaluation by will have the form:

$$\alpha|0\rangle + \beta|1\rangle$$

That each value α and β are the probability amplitude for new evaluated state.

$$\begin{aligned} \alpha &= -\frac{(k+i\Delta)\xi\text{Sin}[t\omega]}{\omega\hbar} + \gamma\left(\text{Cos}[t\omega] - \frac{i\epsilon\text{Sin}[t\omega]}{\omega\hbar}\right); \\ \beta &= \frac{\gamma(k-i\Delta)\text{Sin}[t\omega]}{\omega\hbar} + \xi\left(\text{Cos}[t\omega] + \frac{i\epsilon\text{Sin}[t\omega]}{\omega\hbar}\right); \end{aligned} \quad (13)$$

By having the probability amplitudes (α and β) we can leave the initial qubit without change during processing, and the operator, operate as a identity matrix; Also we can construct an arbitrary 2x2 unitary matrices that can change the state of qubit during the evaluation.

First of all, we make a 2x2 matrix (or PauliMatrix[0] in Mathematica) to simulate single-qubit memory (storage part of quantum computer) by following considerations:

$$\varepsilon \gg k, \Delta$$

$$\varepsilon = 25 * 10^6; \quad k = 0; \; \Delta = 0; \quad t = 10^{-9}\text{sec};$$

$$\hbar = \frac{1}{2\pi}; \qquad \omega = 2\text{Pi}\sqrt{\Delta^2 + k^2 + \epsilon^2};$$

The real value of Planck's constant is (6.626068×10^{-34} m^2 kg / s) [15], but we take the value 1 to make our computation easy; Also the units of the quantities omitted.

Since, the probability amplitude γ after evaluation transform to α and ξ to β. So, the initial probability amplitudes in principle must not change and remain constant. When the value of γ and ξ is chosen 0 and 1 and vice versa, so the value of α and β must be 0 and 1 respectively, ($\gamma = \alpha$ and $\xi = \beta$) as we can see in the following:

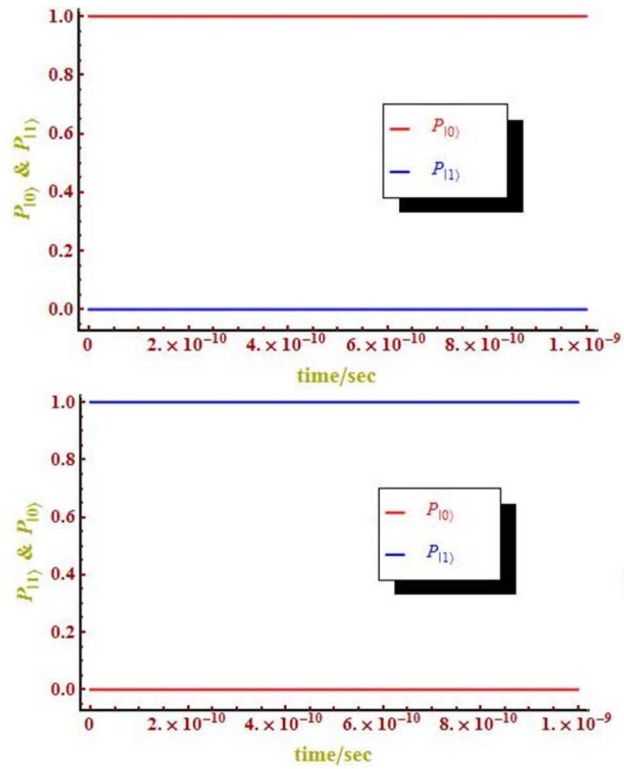


Fig 2 The physical system in the static form (the probability amplitude of each state does not change during the time)

By now, to give a dynamical rule to the quantum system to become a Processor , the NOT gate as an example, (σ_x or its Wolfram Mathematica code is PauliMatrix[1]). We can give new values to the parameters in the probability equation as:

$$(\varepsilon \ll k, \Delta)$$

Now, by taking a new value to the parameter, and after then to finding a value for Δ we can write:

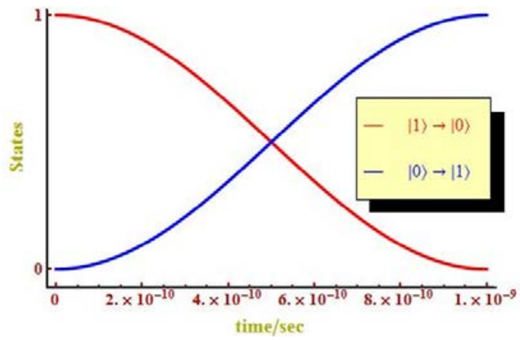
$$\hbar = \frac{1}{2\pi}; \omega = 2\text{Pi}\sqrt{\Delta^2 + k^2 + \epsilon^2};$$

$$\varepsilon = 0; k = 0; t = 10^{-9}\text{sec};$$

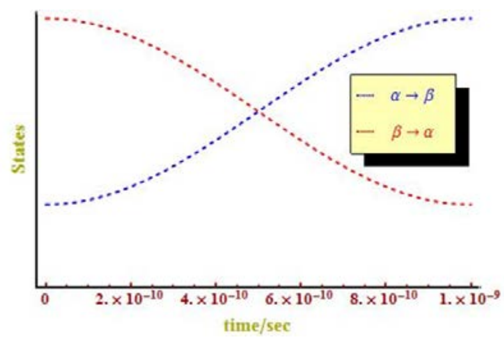
In the above results we can choose any value of them. Our choosing value is:

$(\Delta = 2.5 \times 10^{8} \;\; or \;\; \Delta = -2.5 \times 10^{8})$

The following figures are the results of the single-qubit simulation by using the Mathematica program, in each freezing state of the qubit and dynamical form in term of bases states and superposition of bases states.



(a)



(b)

Fig. 3 The physical system in the dynamical form a) flipping of bases states; b) superposition of states with a different probability amplitudes.

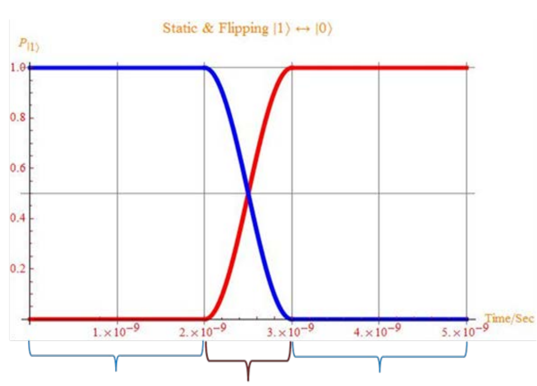


Fig. 4 The overall single quantum system, which is simulated quantum computer, the first, third and second parts demonstrate input, output (that is time-independent without change of the state) and operation (flipping the state from |0⟩ to |1⟩ and vice versa.

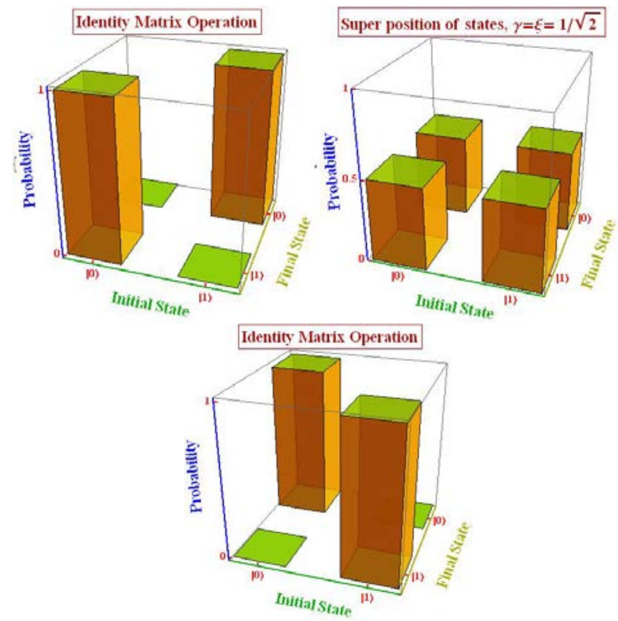


Fig. 5 The physical system in the dynamical, a) flipping of bases states, b) superposition of states, c) statical (the gate does not change states and work as an Identity matrix) form. (Bar Chart representation).

4. Two-Qubits Quantum system

The state of two-qubit quantum gate controlled by solution time evaluation Schrodinger equation:

$$|\emptyset(t)\rangle = e^{\frac{-i\,H\,t}{\hbar}}\,|\emptyset(0)\rangle = U\,|\emptyset(0)\rangle \qquad (14)$$

Each of the states of $|\emptyset(t)\rangle$ and $|\emptyset(0)\rangle$ are represented by a 4x1 matrices which are called column matrices because they have four rows and one column. Therefore, the operator ($U = e^{\frac{-i\,H\,t}{\hbar}}$) is a square 4x4 matrix.

In general for a system that has an anisotropic interaction the Hamiltonian is represented by:

$$H = H_a + H_b + H_i \qquad (15)$$

In the above equation H_a , H_b and H_i are the Hamiltonian for first qubit, second qubit and energy interaction between them respectively. And each of them in general can represented as follows:

$$\begin{aligned} H_a &= \Delta_a \sigma_{xa} + k_a \sigma_{ya} + \varepsilon_a\, \sigma_{za} \\ H_b &= \Delta_b \sigma_{xb} + k_a \sigma_{yb} + \varepsilon_b\, \sigma_{zb} \\ H_i &= J_x \sigma_{xa}\sigma_{xb} + J_y \sigma_{ya}\sigma_{yb} + J_z \sigma_{za}\sigma_{zb} \end{aligned} \qquad (16)$$

In the above equations Δ_a, Δ_b, k_a, k_b, □ and □ are the parameters of both qubits (a and b), also J_x , J_y and J_z are coupling constants. So the Hamiltonian of the system become:

$$H = \Delta_a\sigma_{xa} + k_a\sigma_{ya} + \varepsilon_a\,\sigma_{za} + \Delta_b\sigma_{xb} + k_a\sigma_{yb} + \varepsilon_b\,\sigma_{zb} + J_x\sigma_{xa}\sigma_{xb} + J_y\sigma_{ya}\sigma_{yb} + J_z\sigma_{za}\sigma_{zb} \quad (17)$$

There are, σ_{xa}, σ_{ya} and σ_{za} the tensor products of Pauli matrices with 2x2 Identity matrix and σ_{xb}, σ_{yb} and σ_{zb} are the tensor product of 2x2 Identity matrix with each x, y and z, Pauli matrices, respectively. By taking the result of each of the above outer products in Hamiltonian equation, we can get:

$$H = \begin{pmatrix} \varepsilon_a+\varepsilon_b+J_z & \Delta_b-ik_b & \Delta_a-ik_a & J_x-J_y \\ \Delta_b+ik_b & \varepsilon_a-\varepsilon_b-J_z & J_x+J_y & \Delta_a-ik_a \\ \Delta_a+ik_a & J_x+J_y & -\varepsilon_a+\varepsilon_b-J_z & \Delta_b-ik_b \\ J_x-J_y & \Delta_a+ik_a & \Delta_b+ik_b & -\varepsilon_a-\varepsilon_b+J_z \end{pmatrix} \quad (18)$$

There are several actions and reaction between two qubits [24,25], which is demonstrated in the table 1:

Table 1: The Interaction between two quantum bits

Relations	Interaction Name	Comment
$J_x = J_y = J_z$	Heisenberg interaction	The general form of most two qubit systems, (spin coupled quantum dot) is one of them
$J_x = J_y = 0$	Ising Interaction	To simulate the interaction between superconducting Josephson junction
$J_z = 0$	XY Interaction	-
$J_x = J_y$	XXZ Interaction	-

In our purpose, we chose Ising Interaction. Also we give the zero value to each (k_a and Δ_a),whereby the Hamiltonian get the following form:

$$H = \begin{pmatrix} J_z+\varepsilon_a+\varepsilon_b & -ik_b+\Delta_b & 0 & 0 \\ ik_b+\Delta_b & -J_z+\varepsilon_a-\varepsilon_b & 0 & 0 \\ 0 & 0 & -J_z-\varepsilon_a+\varepsilon_b & -ik_b+\Delta_b \\ 0 & 0 & ik_b+\Delta_b & J_z-\varepsilon_a-\varepsilon_b \end{pmatrix} \quad (19)$$

As we can see, the final Hamiltonian 4x4 matrix, consists of 8 elements, that by giving desire values to the parameters we can solve Schrödinger equation to get CNOT gate which is the important universal quantum gate. So the value of the remains entries being as follows:

$H_{11} = 1\,, H_{12} = 0\,, H_{21} = 0\,, H_{22} = 1\,,$

$H_{33} = 0\,, H_{34} = 1\,, H_{43} = 1\,, H_{44} = 0$

Therefore, we give the numerical values to each parameter as follows:

$$k = 0;\ \Delta = 25 \times 10^6;\ \varepsilon_b = 48.4 \times 10^6;\ \varepsilon_a = 0;$$
$$\xi = 48.5 \times 10^6;\ t = 10 \times 10^{-9}\text{sec};\ \hbar = \frac{1}{2\pi};$$

By now, we can represent the final states of two-qubit bases states in the figure 6.

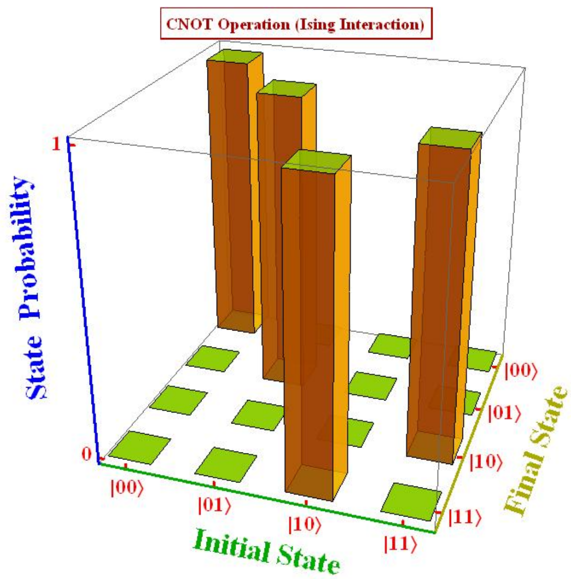


Fig. 6 The Bar Chart in three dimensions, that shows the physical realization of CNOT gate, by using Ising interaction.

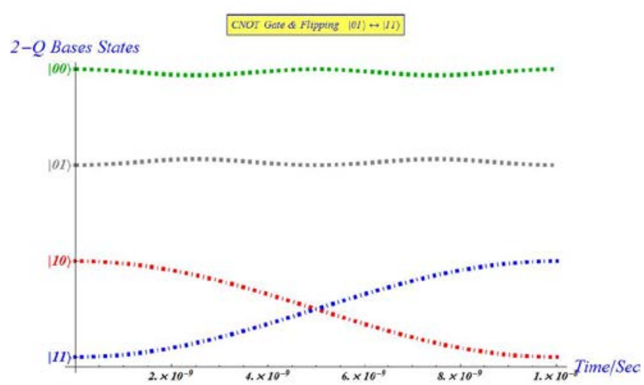


Fig. 7 The physical realization of CNOT gate, by using Ising interaction.

5. Conclusions

The physical realization for single qubit and two qubit have demonstrated and the results have shown as the Bar Chart in three dimensions by using a package of "Wolfram Mathematica" program. We could successfully simulate a quantum computer for a single qubit in three time intervals, from (0 to 2) nano seconds the state of qubit remains constant as an input, from (2-3) nano seconds the qubit under operation, flips its state as a not gate in the classical gate which the 0 flips to 1 and vice versa; finally the evaluated state from (3-5) nano seconds, get a constant value.

We can see that the parameter (ε) works as a switch. When its value is so greater than the values (Δ and k), the state of qubit does not change and the operator acts as a 2x2 Identity matrix. Otherwise, when the parameters (Δ and k), have a huge value with respect to ε, the operator acts as NOT gate in the single qubit.

In the second-qubit quantum system, by handling Ising interaction and some arbitrary values for the other parameters, we have realized the CNOT gate which is a universal quantum gate like NAND gate in the classical logic gates.

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