Unit 5 – Nano Devices and Quantum computing

Introduction - Quantum confinement - Quantum structures: quantum wells, wires and dots - Band gap of nanomaterials. Tunneling - Single electron phenomena: Coulomb blockade - Resonant- tunneling diode - single electron transistor - quantum cellular automata - Quantum system for information processing - quantum states - classical bits - quantum bits or qubits - CNOT gate - multiple qubits - quantum gates - advantage of quantum computing over classical computing (qualitative).

5.1. Introduction

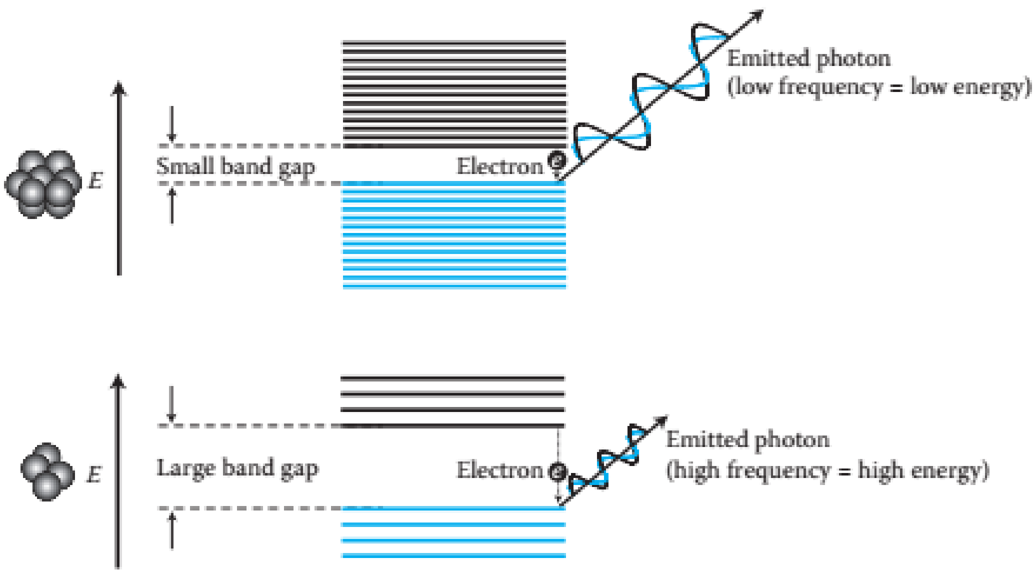
The current growth of technology suggests that reductions are needed in the dimensions of devices and active materials. The Pentium of 1993, used an 800nm technology which consists of 310000 transistors per square inch on ICs. The Pentium 4 "Prescott" of 2004, used a 90 nm technology which consists of 125000000 transistors per square inch on IC. Extensive research is going on to reduce the dimension further.

Nanoelectronics refer to the use of nanotechnology in electronic components. Nanoelectronics are sometimes considered as disruptive technology because present candidates are significantly different from traditional transistors.

5.2. Quantum size effect – Confinement

When the size of a nanocrystal becomes smaller than the deBroglie wavelength, electrons and holes gets spatially confined, electrical dipoles gets generated, the discrete energy levels are formed. As the size of the material decreases, the energy separation between adjacent levels increases. The density of states of nanocrystals is positioned in between discrete (as that of atoms and molecules) and continuous (as in crystals).

Quantum size effect is most significant for semiconductor nanoparticles. In semiconductors, the bandgap energy is of the order of few electron volts and increases with a decrease in particle size.



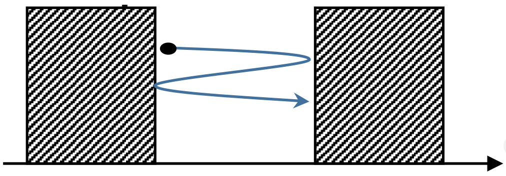
When photons of light fall in a semiconductor, only those photons with energy are absorbed and a sudden rise in absorption is observed when the photon energy is equal to the bandgap.

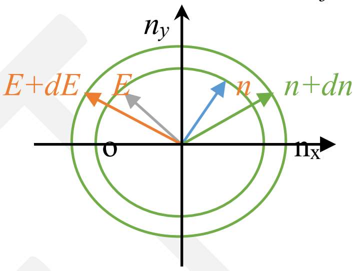
As the size of the particle decreases, absorption shifts towards the shorter wavelength (blue shifts) indicating an increase in the bandgap energy .A change in absorption causes a change in the colour of the semiconductor nanoparticle.

For example, bulk cadmium sulphide is orange in colour and has a bandgap of 2.42eV. It becomes yellow and then ultimately white as its particle size decreases and the bandgap increases.

5.3. Quantum structures: Density of states in quantum well, quantum wire and quantum dots.

The quantum well can be displayed with dimensions of length a, where the electrons of effective mass are confined in the well as shown in fig.





The two dimensional density of states is the number of states per unit area and unit energy. Consider the electron in a two dimensional bounded region of space. We want to find how many quantum states lie within a particular energy, say, between E and E+dE as shown in Figure. The reduced phase space now consists only the x- y plane and n_x and n_y coordinates. In 2D space, $n^2 = n_x^2 + n_y^2$

Derivation

The number of available states within a circle of radius 'n' is given by $\frac{1}{4}\pi n^2$

Here only one quarter of circle will have positive integer values

The number of states within a circle of radius $n+dn$ is given by $\frac{1}{4}\pi(n+dn)^2$

The number of available energy states lying in an energy interval E and $E+dE$

$$Z'(E)dE = \frac{1}{4}\pi\left[(n+dn)^2 - n^2\right]$$

$$= \frac{\pi}{4}\left[n^2 + dn^2 + 2ndn - n^2\right]$$

As dn^2 is very small, we can neglect dn^2. Therefore we get,

$$Z'(E)dE = \frac{\pi}{4}[2ndn] = \frac{\pi}{2}ndn \quad (1)$$

We know that $n^2 = \frac{8m^*E}{h^2}a^2$ (2)

(or) $n = \left[\frac{8m^*E}{h^2}\right]^{1/2} a$ (3)

(or) $dn = \left[\frac{8m^*}{h^2}\right]^{1/2} a \frac{1}{2} E^{-1/2} dE$ (4)

Substitute the value of equation (3) and (4) in equation (1), we get

$$Z'(E)dE = \frac{\pi}{2}\left[\frac{8m^* E}{h^2}\right]^{1/2} a \left[\frac{8m^*}{h^2}\right]^{1/2} a \frac{1}{2} E^{-1/2} dE$$

m* is the effective mass in the quantum well

$$Z'(E)dE = \frac{\pi}{4}\left[\frac{8m^*}{h^2}\right] a^2 dE \qquad (5)$$

Put $a^2 = A$ area of circle.

According to Pauli's exclusion principle each energy level can occupy two electrons of opposite spin

i.e., $Z'(E)dE = 2 \times \frac{\pi}{4}\left[\frac{8m^*}{h^2}\right] AdE$

Number of quantum states per unit area and unit energy is

$$\frac{Z'(E)dE}{AdE} = 2 \times \frac{\pi}{4}\left[\frac{8m^*}{h^2}\right]$$

$Z'(E) = \frac{\pi}{2}\left[\frac{8m^*}{h^2}\right]$ (or) $Z'(E) = \frac{\pi}{2}\left[\frac{8m^*}{(2\pi\hbar}\right]$ [since $h^2 = 4\pi\hbar$] (6)

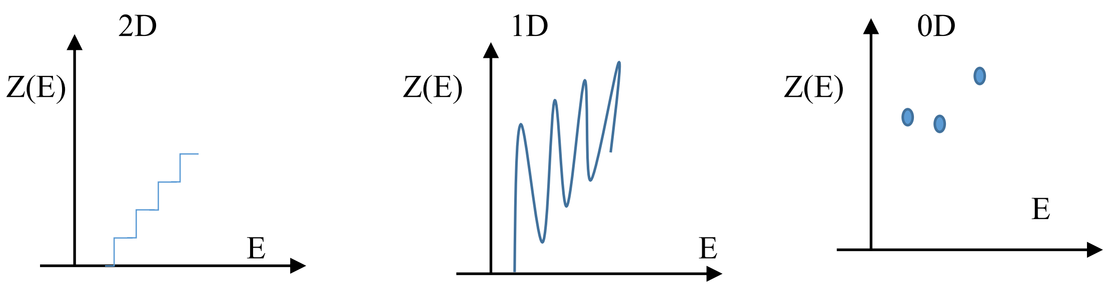
The density of states in two dimensional is given by $Z'(E)^{2D} = \frac{m^*}{\pi\hbar}$ for $E >= E_0$ (7)

Where E_0 is the ground state of quantum well

$$Z'(E)^{2D} = \frac{m^*}{\pi\hbar}\sum \sigma(E - E_n) \qquad (8)$$

Where E_n are the energies of quantized states and $\sigma(E - E_n)$ is step function.

From equation (7), the density of states in two dimension is constant with respect to the energy. i.e., $Z'(E)^{2D} \infty E^0 =$ constant



Density of states in quantum wire

Consider the one dimensional system, the quantum wire in which only one direction of motion is allowed. (eg. Along x – direction).

In one dimension, such as for a quantum wire, the density of states is defined as the number of available states per unit length per unit energy around an energy *E*. The electron inside the wire are confined in a one dimensional infinite potential well with zero potential inside the wire and infinite potential outside the wire.

At $x = 0$; $V(x) = 0$ for an electron inside the wire

At $x = a$; $V(x) = \alpha$ for an electron outside the wire

The reduced phase space now consists only the x plane and n_x coordinates are shown in figure.

In one dimensional space $n^2 = n_x^2$

The number of available energy states lying in an interval of length is

$$Z'(E)dE = n + dn - n = dn \qquad (1)$$

Substitute the value of *dn* from equation (4), we get

$$Z'(E)dE = \left[\frac{8m^*}{h^2}\right]^{1/2} a\frac{1}{2}E^{-1/2}dE \qquad (2)$$

According to Pauli's exclusion principle, two electrons of opposite spin can occupy each energy state.

$$Z'(E)dE = 2\times\left[\frac{8m^*}{h^2}\right]^{1/2} a\frac{1}{2}E^{-1/2}dE$$

Number of quantum states per unit length and unit energy is $\frac{Z'(E)dE}{adE} = \left[\frac{8m^*}{h^2}\right]^{1/2} E^{-1/2}$

$$\text{(or)}\ Z'(E) = \left[\frac{8m^*}{4\pi^2\hbar}\right]^{1/2} E^{-1/2} = Z'(E)^{1D} = \left[\frac{2m^{*1/2}}{\pi\hbar}\right] E^{-1/2} \qquad (3)$$

If the electron has potential energy E_0 we have $Z(E)^{1D} = \frac{1}{\pi\hbar}\sqrt{\frac{2m^*}{(E - E_0)}}\,(E \geq E_0) \qquad (4)$

From equation (4) the density of states in one dimensional system has a functional dependence on energy $Z(E)^{1D} \propto E^{-1/2}$

For more than one quantized state, the one dimensional density of states is given by

$$Z(E)^{1D} = \frac{1}{\pi\hbar}\sum\sqrt{\frac{2m^*}{(E - E_0)}}\,\sigma(E - E_n) \qquad (5)$$

Where E_n are the energies of the quantized states of the wire and $\sigma(E-E_n)$ is the step function. The density of states in quasi-continum (or) quantum wire is shown in figure. The discontinuities in the density of states are known as **Van Hove Singularities**

Density of states in Quantum dot

In a zero dimensional system, the density of states are truly discrete and they don't form a quasi continum.

In zero dimensional system (quantum dot), the electron is confined in all three spatial dimensions and hence to motion of electron is possible. Each quantum state of a zero dimensional system can therefore be occupied by only two electrons. So the density of states for a quantum dot is merely a delta function.

$$Z(E)^{0D} = 2\sqrt{(E-E_0)} \qquad (6)$$

Here, the factor 2 accounts for spin. For more than one quantum state, the density of states is given by $Z(E)^{0D} = \sum_n 2\delta\sqrt{(E-E_0)}$

5.4. The electron density in bulk material and size dependent of Fermi energy

The bulk material is a collection of atoms having properties that are from individual atoms. The nanomaterials gives unique electronic properties.one of the mayor difference in nanomaterials with respect to bulk materials is the number of available energy states. In a bulk material, the states within each energy sublevel are so close that they blend into a band.
The total number of electron states N with energies up to E, can be determined based on the equation $N = \frac{\pi}{3}\left[\frac{8m}{h^2}\right]^{3/2} E^{3/2}.V$ (1)

Here, we represent the volume as *V*, *m* is the mass of an electron an *h* is the Planck's constant.

The number of energy states per unit volume is given by $n = \frac{N}{V} = \frac{\pi}{3}\times\left[\frac{8m}{h^2}\right]^{3/2} E^{3/2}$ (2)

Density of states is defined as number of available electron energy states per unit volume, per unit energy i.e., Z(E) = dn / dE (3)
Hence equation (2) becomes,

$$Z(E) = \frac{\pi}{3}\times\left(\frac{8m}{h^2}\right)^{3/2}\times\frac{3}{2}E^{1/2}$$

(or) $$Z(E) = \frac{\pi}{2}\times\left(\frac{8m}{h^2}\right)^{3/2} E^{1/2} \qquad (4)$$

From equation (4), the density of states for a bulk material is directly proportional to square root of energy

i.e., Z(E) α $\sqrt{E}$ (5)

The relevant application of density of states is that it provides information about nanomaterials.

Here, the Fermi function gives the probability of occupation by the free electrons in a given energy state.

i.e., $f(E)=\frac{1}{1+e^{\frac{E-E_f}{kT}}}$ (6)

Then, the number of free electrons per unit volume is $n_e=\int_0^{\alpha} F(E)Z(E)dE$

Put F(E) = 1 at T = 0K, then $n_e=\frac{\pi}{2}\times\left(\frac{8m}{h^2}\right)^{3/2}\int_0^{\alpha} E^{1/2}dE$

(or) $n_e=\frac{\pi}{3}\times\left(\frac{8m}{h^2}\right)^{3/2} E_f(0)^{3/2}$ (7)

Size dependence of Fermi energy

In terms of the distribution of energy, solid have thick energy bands, whereas atoms have thin, discrete energy states. Hence to make a solid behave electronically more like an atom, we need to make it about the same size as an atom.

Hence rearranging equation (7) , we get $E_f(0)=\frac{h^2}{8m}\times\left(\frac{3n_e}{\pi}\right)^{2/3}$ (8)

In the above equation, 'n' is the only variable.

Equation (8) suggests that the fermi energy of a conductor depends on the number of free electrons 'N' per unit volume 'V' $E_F(0)\alpha(n)^{2/3}\alpha\left(\frac{N}{V}\right)^{2/3}$ (9)

Since the electron density is a property of the material, the fermi energy does not vary with material's size. E_F is same for a particle or for a brick of copper. Hence the energy state will have the same range for small volume and large volume of atoms. But for small volume of atoms we get larger spacing between states. This is applicable to semiconductors and insulators.

Let us consider that all states up to $E_F(0)$ are occupied by a total of free electrons (N).

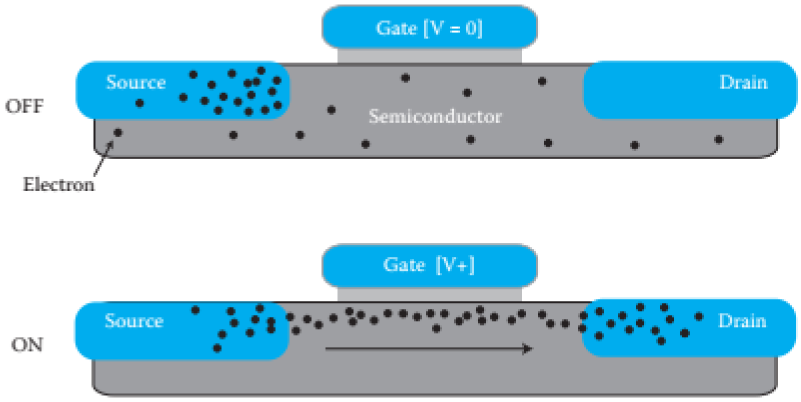
$\Delta E=\frac{E_F(0)}{N}$ (10)

From equation (9) & (10), $\Delta E\alpha\frac{1}{V}$ (11)

Thus, the spacing between energy states is inversely proportional to the volume of the solid. The energy sublevel and the spacing between energy states within it will depend on the number of atoms as shown in figure. At one point, we know that an energy sublevel must be divided as many times as there are atoms in a solid, which eventually results too many splits to differentiate. Hence, we just refer to each sublevel as a solid energy band. On the other hand, a single atom in the sublevel contain only one discrete energy state. If we reduce the volume of s solid, the tiny piece of material behaves electronically like an artificial atom.

5.5. Single electron phenomena

Transistors are what computers used to compute-tiny switches turning on and off, transferring and amplifying signals, making logic decisions. Today, microchips have over a billion transistors, each one turning on and off a billion times every second. These chips require manufacturing processes with roughly 100-nm resolution. And every year this resolution drops, enabling even smaller transistors, so that even more of them can be squeezed into the same amount of space. Rather than moving torrents of electrons through transistors, it may very well be practical and necessary to move electrons *one at a time.* We can use transistors to make sensitive amplifiers, electrometers, switches, oscillators, and other digital electronic circuits all of which operate using single electrons



Rules for single electron phenomena to occur

Tunnelling is the way electrons cross both the physical barriers and the energy barriers separating a quantum dot from the bulk material that surrounds it. If any electron on one side of the barrier could just tunnel across it, there would not be any isolation. The dot would not be a quantum dot because it would still essentially be part of the bulk.

So we need to be able to control the addition and subtraction of electrons. We can do this with voltage biases that force the electrons around. There are two rules for preventing electrons from tunnelling back and forth from a quantum dot.

(i) Coulomb blockade effect

(ii) Overcoming uncertainity

Rule1: Coulomb Blockade effect

A quantum dot has a capacitance, C_{dot}, a measure of how much electric charge it can store

$$C_{dot} = G\,\varepsilon\,d \qquad (1)$$

Here, ε is the permittivity of the material surrounding the dot, *d* is the diameter of the dot, and *G* is a geometrical term (if the quantum dot is a disk, $G = 4$; if it is a spherical particle, $G = 2\pi$). An object isolated in space can store charge on its own and therefore can have a capacitance.

The energy needed to add one negatively charged electron to the dot is known as the charging energy, $E_C = \frac{e^2}{2C_{dot}}$ (2)

We know that the coulomb blockade can prevent unwanted tunnelling. Hence we can keep the quantum dot isolated, the condition for this is given by $E_C \gg$ (3)

Rule2: Overcoming uncertainity

The uncertainty in the energy of a system is inversely proportional to how much time we have to measure it. Specifically, the energy uncertainty, ΔE, adheres to this relationship

$$\Delta E \approx \frac{h}{\Delta t} \quad (4)$$

Here, h is Planck's constant and Δt is the measurement time. Since it is a tiny capacitor, the time we use for Δt is the capacitor's time constant (the characteristic time a capacitor takes to acquire most of its charge). The time constant of a capacitor is RC, where R is the resistance and C is the capacitance. In our case, the resistance is the tunnelling resistance, R_t, and the capacitance is C_{dot}. This gives us $\Delta t = R_t C_{dot}$ (5)

Our goal is to keep electrons from tunnelling freely back and forth to and from the dot. To ensure this, *the uncertainty of the charging energy must be less than the charging energy itself.*

For maintaining electron isolation in quantum dot, we need $\Delta E_c < E_c$ (6)

Substituting equation (2), (4) and (5) in (6), we get $\frac{h}{R_t C_{dot}} < \frac{e^2}{2C_{dot}}$ (7)

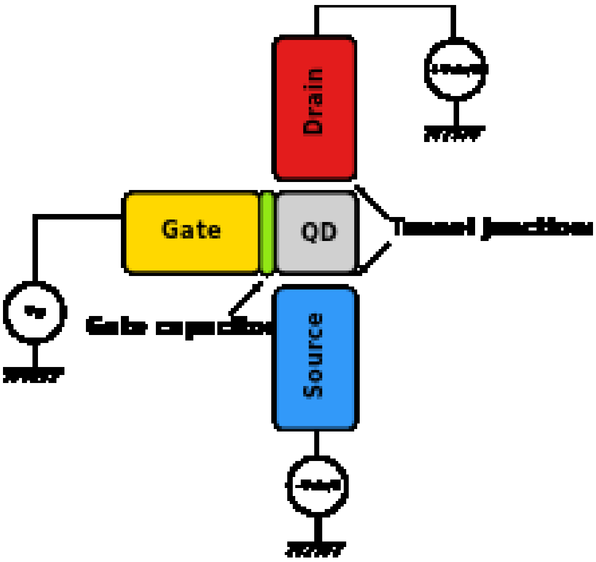
In otherwords, $R_t \gg$ (8)

Meeting this criterion is often as simple as making sure the insulating material surrounding the dot is thick enough. These two rules help in building a single-electron transistor (SET)

5.6. Single electron transistor (SET)

Principle

A transistor with three terminal switching device made from a quantum dot that controls the current from source to rain one electron at a time is called single electron transistor



Construction

The single electron transistor (SET) is built like a conventional Field Emitting Transistor (FET). It has tunnelling junctions in place of *pn* – junctions and quantum dot in place of the channel region of the FET. To control tunnelling, a voltage bias to the gate electrode is applied. A separate voltage bias is applied between source and drain electrodes for the current direction. For current to flow, gate bias voltage must be large enough to overcome the coulomb blockade energy.

Working

1. The purpose of SET is to individually control the tunnelling of electrons into an out of the quantum dot. To do this, we must first stop random tunnelling by choosing the right circuit geometry and materials. If an electron comes or goes from the dot. It will on purpose
2. To control tunnelling, we apply a voltage bias to the gate electrode. There is also a voltage difference between the source and the drain that indicates the direction of current. Here, we can say that current and electron flow in the same direction and we will consider the electrode from which the electrons originate.
3. This is similar to the working of FET, where the gate voltage creates an electric field that alters the conductivity of the semiconducting channel below it, enabling current to flow from source to drain.
4. Applying a voltage to the gate in an SET creates an electric field and change the potential energy of the dot with respect to the source and drain. This gate voltage controlled potential difference can make electrons in the source attracted to the dot and simultaneously electrons in the dot attracted to the drain.
5. For current to flow, this potential difference must be atleast large enough to overcome the energy of the coulomb blockade.

The energy "*E*" needed to move a charge *e* across a potential difference *V* is given by $E=Ve$

So, the voltage that will move an electron onto or off the quantum dot is given by

$$V = \frac{E_c}{e} \quad (or) \quad V = \frac{\frac{e^2}{2C_{dot}}}{e} = \frac{e}{2C_{dot}} \qquad (1)$$

With this voltage applied to quantum dot, an electron can tunnel through coulomb blockade of the quantum dot.

Working for single electron transistor in nutshell

A single electron transistor is shown in figure. As opposed to the semiconductor channel in a field effect transistor, the SET has an electrically isolated quantum dot located between the source and drain.

1. The SET is OFF mode. The corresponding potential energy diagram shows that it is not energetically favourable for electrons in the source to tunnel to the dot as shown in figure.
2. The SET is ON mode. At the lowest setting electrons tunnel one at a time, via the dot, from the source to the drain as shown in figure.
3. This is made possible by first applying the proper gate voltage, $V_{gate} = e/2C_{dot}$, so that the potential energy of the dot is made low enough to encourage an electron to tunnel through the coulomb blockade energy barrier to the quantum dot.
4. Once the electron is on it, the dots potential energy rises as shown in figure
5. The electron then tunnels through the coulomb blockade on the other side to reach the lower potential energy at the drain as shown in figure.
6. With the dot empty and the potential lower again the process repeats as shown in figure.

Advantages

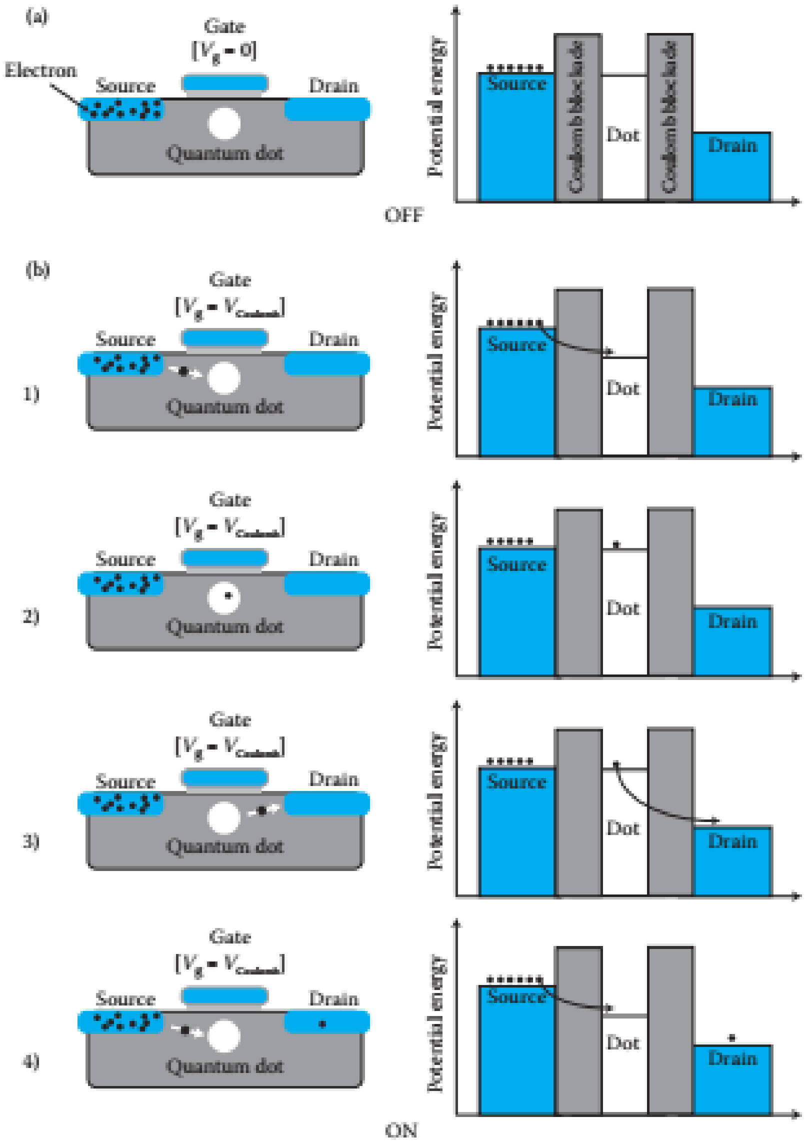
1. The fast information transfer velocity between cells is carried out via electrostatic interactions only.
2. No wire is needed between arrays. The size of each cell can be can be as small as 2.5nm. This made them suitable for high density memory.
3. This can be used for the next generation quantum computer.

Limitations

1. In order to operate SET circuit at room temperature, the size of the quantum dot should be smaller than 10*nm*
2. It is very hard to fabricate by traditional optical lithography and semiconductor processes
3. The method must be developed for connecting the individual structures into logic circuits and these circuits must be arranged into larger 2D patterns.

Applications

1. SET are used in sensor and digital electronic circuits
2. Variety of digital logic functions, including AND or NOR gates, is obtained based on SET operating at room temperature.
3. It is used for mass storage
4. It is used in highly sensitive electrometer.
5. SET can be used as a temperature probe, particularly in the range of very low temperatures.
6. SET is a suitable measurement setup for single electron spectroscopy.
7. It is used for the fabrication of homo-dyn receiver operating at frequencies between 10 and 300 *MHz*



5.7. Quantum Cellular Automata

Introduction

The continuing down scaling of device dimensions in microelectronics technology has led to faster devices and denser circuit with obvious benefits to chip performance. There is much expectation that the availability of very dense device arrays might lead to a new paradigms for information processing based on locally interconnected architectures such as cellular automata (CA)

We focus here on the idea of employing CA architectures which are compatible with nanometer scale quantum devices. Quantum Cellular Automata is a new nanotechnology with potential for applying in building future computers. This technology is a realization of the circuit design at the nano scale.

Quantum Cellular Automata technology is one of the emerging technologies that can be used for replacing CMOS technology. It has attracted significant attention in the recent years due to its extremely low power dissipation, high operation frequently and smaller in size.

Definition

A quantum cellular automata consists of an array of quantum device cells in a locally interconnected architectures.

Concept

According to quantum cellular automata, logical states or values are demonistrated by the position of electrons rather than voltage levels. By applying proper implements of this QCA technology, significant low density of 10^{12} devices/cm^3 and very low power consumption (near to zero) are achievable.

Thus quantum cellular automata (QCA) is an abstract model of quantum computation devised in analogy to conventional models of cellular automata.

Advantages

1. Low power dissipation
2. High operating frequency
3. Smaller in size
4. It replaces CMOS technology.

Applications

1. It can used for designing general purpose computational circuits
2. It is used in memory circuits and other computational and sequential circuit designs.

5.8. QUANTUM SYSTEM FOR INFORMATION PROCESSING

The Quantum phenomena can be applied to Quantum Computing Quantum information science and Quantum metrology. The Progresses of all these technologies are mutually dependent on each other. They share the same laws of physics, Common hardware and related works.

Quantum information science deals with the methods of the information in a quantum system. It includes statistics of Quantum mechanics along with their limitations, it provides a core for all other applications such as quantum Computing, networking, sensing and metrology

Quantum Communication and Networking explains the exchange of information by encoding it in to a quantum Cryptography. It is the subset of quantum Communication in which Quantum Properties help to design the secure communication System.

Quantum Sensing and metrology: is the Quantum systems which are used to measure important physical Properties (e.g. electric and magnetic fields, temperature, etc.,) . The system has more accuracy than classical systems. Quantum Sensors are based on Qubits. They are carried out using the experimental quantum systems.

Quantum Computing deals with the Quantum mechanical properties of Super position, entanglement and interference to enact Computation In Common, a Quantum Computer Consists of a collection of quantum bits (Qubits). The Qubits are isolated from the environment for their Quantum state to perform the Computation

These Qubits are organized and manipulated to set an algorithms and to get a result. The high Probability from the measurement of final state produces the result.

Several ways such as nuclear magnetic resonance, optical and solid state techniques and ion traps are used to build Quantum Computers. The fundamental Concept that has been need to handle the Quantum Computers using the above ways are given below.

(a) Harmonic oscillation Quantum Computer

In this system, discrete eigen states are represented as n x, where n = 0, 1, 2,.... α; these represent qubits . The lifetime of Qubits depend on the Quality factor of the cavity.

A Single quantum harmonic oscillator will have a 2^n energy states in Hilbert Space. But, a classical harmonic oscillator has n energy states in the same Hilbert Space

(b) Optical Phonon Quantum Computer

In these Computers, Photon can represent a quantum bit. Photons can be made to interact with eachother using non-linear optical media. Mirrors, Phase shifters and beam splitters are the accessible devices for manipulating the photon states

The required Single photons can be created using attenuated laser. These photons are defected with photo detectors. Thus a quantum Computer can be made using these optical components.

(c) Optical Cavity quantum electrodynamic Computer

In this, Coupling of Single atom to a few optical modes takes place. It is done by placing single atom in optical cavities of very high Q.

The cavity electrodynamic system consists of Fabry Perot cavity containing a few atoms to which the optical field is coupled. The photons in the cavity have an opportunity to interact many times with the atoms before escaping.

The single photon can be good carrier of quantum information. They are created by attenuated lasers and they are measured at the output wing photo multiplier.

(d) Ion trap quantum Computer

In electromagnetic traps, a number of charged atoms are isolated and trapped. Then the atoms are cooled so that their kinetic energy is much less than their spin energy. After this, the incident monochromatic light can selectively cause transitions between energy states of lowest level vibrational modes of ions. These transitions can be made to perform quantum computation. The main components of the ion trap quantum computers are the electromagnetic trap with lasers, photo detectors of ions.

(e) Nuclear magnetic resonance computer

These computers are based on the spins of atomic nucleus. This will be nearly ideal for quantum computation if only spin - spin coupling be large and controllable. Magnetic field pulses are applied to spins in a strong magnetic field.
The coupling between spins of atoms can be provided by chemical between the neighbouring atoms. The processing magnetic moment induces the output. These proposals shows that the quantum are more suitable for information processing.

5.9. Quantum states

The quantum state of a system is described by a complex function ψ, which depends on the coordinate x and on time

i.e., Quantum state = ψ (x,t)

The wave function encodes all the information about the system. We know $|\psi(x,t)|^2\, dx$ is the probability of finding the position of the particles and yields a result in the interval $x \rightarrow x + dx$

The total probability of finding the particles somewhere along the real axis must be unity, thus we can write $|\psi|^2 = \int \psi^* \psi\, dx = \int |\psi(x,t)|^2 dx = 1$

In quantum mechanics, a different notation is called Dirac notation is used to represent quantum states. The inner product of two vectors u and v is denoted by <u | v>

The left part $\langle u|$ is called bra and the right part $|v\rangle$ is called as ket. Thus in the direct notation, also known as the bra-ket notation, an inner product is denoted by < > bracket.

5.10. Classical bit

A Classical bit can be either 0 or 1

Information in digital representation uses a sequence of bits. Each bit is basically the charge of an electron. If the electron is charge, the bit is assumed to carry a value 1; alternatively if the electron is not charged the bit carries a value 0.

Definition

Thus a bit also known as a classical bit can be in state 0 or state 1, and measuring a bit at any time results in one of two possible outcomes.

5.11. Single Quantum bit

Definition

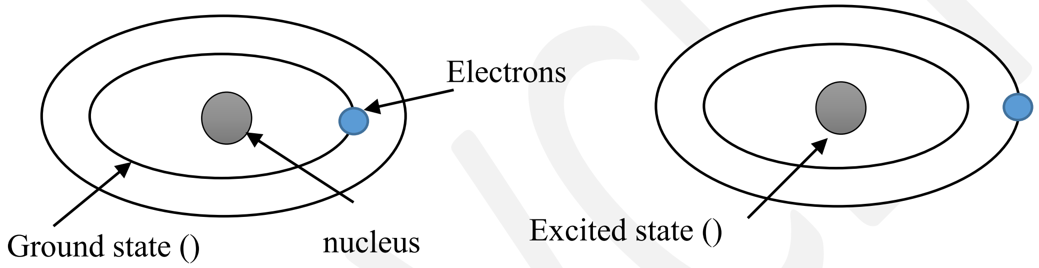
A qubit (quantum bit) is the basic unit of information in quantum computing. A qubit uses the quantum mechanical phenomena of superposition to achieve a linear combination of two states.

Explanation

A classical binary bit can only represent a single binary value such as either 0 or 1, i.e., it can only be in one of two possible states.

A qubit, however, can be represented as 0, 1 or any portion of 0 and 1 in superposition of both states, with a certain probability of being 0 and a certain probability of being 1.

Let us consider an electron in a hydrogen atom which will be in its ground state as shown in figure or in an excited state as shown in figure.



In classical system, it is assumed that excited state represent and the ground state represent.

But in qunatum system, the electron will exist in a linear superposution of the ground and excited state . i.e., it will exist in the ground state with probability amplitude α and in excited state with probability amplitude β.

This type of two state quantum system is referred to as single qubit, and its actual state ψ can also be any linear combination (or superposition) of these states.

i.e., $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ (1)

Where $|\psi\rangle$ is the state of the qubit and $|0\rangle$ and $|1\rangle$ are the computational basis states. The coefficeints α and β are complex numbers and are called as probability amplitudes.

If α is the probability amplitude of 0 state, then the probability of qubit being in 0 state is $\alpha\alpha^* = |\alpha|^2$ where α^* is the complex conjugate of α

However, $|\alpha|^2 + |\beta|^2 = 1$ (2)

The qunatum state ψ in equation (1) can be written as unit column vector in a two dimensional complex plane (Hilbert space) spanned by the two basis vectors.

Here, a qubit with state $|0\rangle$ is represented by column vector $\begin{pmatrix}1\\0\end{pmatrix}$ (3)

A qubit with state $|1\rangle$ is represented by column vector $\begin{pmatrix}0\\1\end{pmatrix}$ (4)

Substitting (3) and (4) in (1), we get

$$|\psi\rangle = \alpha\begin{pmatrix}1\\0\end{pmatrix} + \beta\begin{pmatrix}0\\1\end{pmatrix}$$

(or) $|\psi\rangle = \begin{pmatrix}\alpha\\0\end{pmatrix} + \begin{pmatrix}0\\\beta\end{pmatrix}$

(or) $|\psi\rangle = \begin{pmatrix}\alpha\\\beta\end{pmatrix}$ (5)

Equation (5) is the vector representing an arbitary qubit state

Interference

(1) As discussed, classical bit can only be in a single state, whereas, a qubit cannot only be in one of the two discrete states, it can also exist simultaneously in a blend of some of these states.

(2) The proportions of $|0\rangle$ and $|1\rangle$ in the blended states need not be equal and can be arbitary.

(3) Thus an infinite number of possible combinations of $|0\rangle$ and $|1\rangle$ is possible in a qubit, provided the constraint $|\alpha|^2 + |\beta|^2 = 1$ is satisified

5.12. Multiple Qubits

Consider a system of two qubits in a four dimensional vector space. In this Hilbert space, four computational basis states represented as $|00\rangle$, $|01\rangle$, $|10\rangle$ and $|11\rangle$

The superposition of these states gives a state vector $|\psi\rangle$ given as linear combination of the basis vectors $|\psi\rangle = \alpha_{00}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|10\rangle + \alpha_{11}|11\rangle$ (1)

Where α_{00}, α_{01}, α_{10}, α_{11} are complex coefficeints, the probabilities of the four states are $|\alpha_{00}|^2$, $|\alpha_{01}|^2$, $|\alpha_{10}|^2$ and $|\alpha_{11}|^2$.

The normaziliation of equation (1) is the sum of the square of the probailities of the coefficeint in the state is 1

i.e., $|\alpha_{00}|^2 + |\alpha_{01}|^2 + |\alpha_{10}|^2 + |\alpha_{11}|^2 .= 1$ (2)

Before the measurement, the state of the two qubits is uncertain. After the measurement, the state is certain i.e., $|00\rangle$, $|01\rangle$, $|10\rangle$ and $|11\rangle$. If only the first bit is observed,

The probability for the first qubit is 0

$$P_0^{'} = |\alpha_{00}|^2 + |\alpha_{01}|^2 \tag{3}$$

Similarly, probaility for 1 is

$$P_1^{'} = |\alpha_{10}|^2 + |\alpha_{11}|^2 \tag{4}$$

Sum of the two probabilities is unity

Therefore, $P_0^{'} + P_1^{'} = 1$ (5)

Let $|\psi_0^{'}\rangle$ and $|\psi_1^{'}\rangle$ be the states after the measurement when the first qubits are 0 and 1 respectively. These states are given by

$$|\psi_0^{'}\rangle = \frac{\alpha_{00}|00\rangle + \alpha_{01}|01\rangle}{\sqrt{|\alpha_{00}|^2 + |\alpha_{01}|^2}} \quad \text{and} \tag{6}$$

$$|\psi_1^{'}\rangle = \frac{\alpha_{10}|10\rangle + \alpha_{11}|11\rangle}{\sqrt{|\alpha_{10}|^2 + |\alpha_{11}|^2}} \tag{7}$$

Similarly, for the measurement for second qubit

The probability for second qubit to 0 and 1.

$$P_0^{"} = |\alpha_{00}|^2 + |\alpha_{10}|^2 \tag{8}$$

$$P_1^{"} = |\alpha_{01}|^2 + |\alpha_{11}|^2 \tag{9}$$

and the sum of the second probavility is unity (1)

Therefore $P_0^{"} + P_1^{"} = 1$ (10)

The corresponding states after measurements are

$$|\psi_0^{"}\rangle = \frac{\alpha_{00}|00\rangle + \alpha_{10}|10\rangle}{\sqrt{|\alpha_{00}|^2 + |\alpha_{10}|^2}} \quad \text{and} \tag{11}$$

$$|\psi_1^{"}\rangle = \frac{\alpha_{01}|01\rangle + \alpha_{11}|11\rangle}{\sqrt{|\alpha_{01}|^2 + |\alpha_{11}|^2}} \tag{12}$$

Now, let us consider special state of two qubits system with $\alpha_{00} = \alpha_{11} = \frac{1}{\sqrt{2}}$ and $\alpha_{01} = \alpha_{10} = 0$ .This state is called **Bell state** and this pair of qubit is called EPR (Einstein, Podoisky and Rosen) pair

When the two qubit system is in the Bell state, the probability of first qubt as 0 is $\frac{1}{2}$ and that of 1 is $\frac{1}{2}$.

Therefore, after measurements, states are

$$|\psi_0^{'}\rangle = |00\rangle$$

$$|\psi_0^{'}\rangle = \frac{\alpha_{00}|00\rangle + \alpha_{10}|10\rangle}{\sqrt{|\alpha_{00}|^2 + |\alpha_{10}|^2}}$$

$$\alpha_{00} = \frac{1}{\sqrt{2}} \text{ and } \alpha_{10} = 0$$

Therefore, $|\psi_0^{'}\rangle = \dfrac{\frac{1}{\sqrt{2}}|00\rangle + 0|10\rangle}{\sqrt{\left(\frac{1}{\sqrt{2}}\right)^2 + 0^2}} = \dfrac{\frac{1}{\sqrt{2}}|00\rangle}{\frac{1}{\sqrt{2}}}$

Therefore, $|\psi_0^{'}\rangle = |00\rangle$ (13)

Similarly, $|\psi_1^{'}\rangle = |11\rangle$ (14)

Likewise, for second qubit

$$|\psi_0^{"}\rangle = |00\rangle$$

$$|\psi_0^{"}\rangle = \frac{\alpha_{00}|00\rangle + \alpha_{10}|10\rangle}{\sqrt{|\alpha_{00}|^2 + |\alpha_{10}|^2}}$$

$$\alpha_{00} = \frac{1}{\sqrt{2}} \text{ and } \alpha_{10} = 0$$

Therefore, $|\psi_0^{"}\rangle = \dfrac{\frac{1}{\sqrt{2}}|00\rangle + 0|10\rangle}{\sqrt{\left(\frac{1}{\sqrt{2}}\right)^2 + 0^2}} = \dfrac{\frac{1}{\sqrt{2}}|00\rangle}{\frac{1}{\sqrt{2}}}$

Therefore, $|\psi_0^{"}\rangle = |00\rangle$ (15)

Similarly, $|\psi_1''\rangle = |11\rangle$ (16)

These are four special states called Bell states and form an orthonormal basis as

$$|\beta_{00}\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$$

$$|\beta_{01}\rangle = \frac{|01\rangle + |10\rangle}{\sqrt{2}}$$

$$|\beta_{10}\rangle = \frac{|00\rangle - |11\rangle}{\sqrt{2}}$$

$$|\beta_{11}\rangle = \frac{|01\rangle - |10\rangle}{\sqrt{2}}$$

Where the first one $|\beta_{00}\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$ is involved in many quantum computation and quantum information. The quantum state of n qubit system is specified by 2^n amplitudes. So far seven qubit quantum computer has been buid.

5.13. Quantum Gates

We know that classical logic gates are the building blocks of digital circuits. Similarly, a quantum gate is a basic quantum circuit operating with a small number of qubits and are the building blocks of qunatum gates.

1. Quantum gates are the unitary operator which are constructed with the help of basis vector.
2. Here the basis vector of single qubit is $|0\rangle$ and $|1\rangle$. Similarly for two qubits are $|00\rangle$, $|01\rangle$, $|10\rangle$ and $|11\rangle$.
3. one qubit qunatum state of $|0\rangle$ is represented by column matrixby column vector $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|1\rangle$ by $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$
4. Identity matrix is $I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
5. Qunatum gate is unitary operator with $U^\dagger U = I$ where $U^\dagger = U^{-1}$ and Det $|U| = 1$
6. The qunatum states satisify othronormal condition (self product is allowed)
7. Any single qubit qunatum state is represented by

$$U = e^{i\alpha}\left[I\cos\left(\frac{\theta}{2}\right) - i(\vec{c} \text{ [illegible] } \left(\frac{\cdot}{2}\right)\right)\right]$$

In this equation the square bracket term represents the rotational operator about the arbitary direction and $e^{i\alpha}$ is its phase.

Now, put $\alpha = \left(\frac{\pi}{2}\right); \theta = \pi$

$$U = e^{i\frac{\pi}{2}}\left[I\cos\left(\frac{\pi}{2}\right) - i(\vec{c}\ldots,\ldots\left(\frac{\cdot}{2}\right)\right] \qquad \text{(or) } U = (\vec{c}\ldots,$$

Where σ_n is the polarization state of a qubit along any axis . Here there is only a single bit of information (0 or 1)

5.13.1 SINGLE BIT QUANTUM STATES

Single bit qunatum gate can be constructed by condiering the unitary operator

$U = (\vec{c}\ldots,$ (or) $U = \vec{c}_{x\cdot\cdot x} \cdot \vec{\ }_{y\cdot\cdot y} \cdot \vec{\ }_{z\cdot\cdot z}$ and

if $n_x = (100); n_y = (010); n_z = (001)$ and σ_n is $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

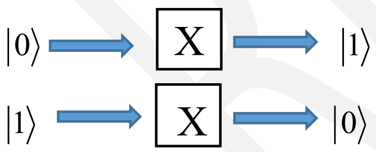
(1) Pauli's X – gate

X	$\|0\rangle$	$\|1\rangle$
$\langle 0\|$	0	1
$\langle 1\|$	1	0

Then $X = |1\rangle\langle 0| + |0\rangle\langle 1|$

Output

(i) $Y|0\rangle = |0\rangle\{|1\rangle\langle 0| + |0\rangle\langle 1|\} = |1\rangle$ (ii) $Y|1\rangle = |1\rangle\{|1\rangle\langle 0| + |0\rangle\langle 1|\} = |0\rangle$



Hence, X gate is also a NOT gate which transpose the components of qubit.

(ii) Pauli's Y - gate

Y	$\|0\rangle$	$\|1\rangle$
$\langle 0\|$	0	$-i$
$\langle 1\|$	i	0

Then $Y = -i|1\rangle\langle 0| + i|0\rangle\langle 1|$

Output

(i) $Y|0\rangle = -i|0\rangle\{|1\rangle\langle 0| + i|0\rangle\langle 1|\} = -i|1\rangle$ (ii) $Y|1\rangle = i|1\rangle\{|1\rangle\langle 0| + i|0\rangle\langle 1|\} = i|0\rangle$

$|0\rangle \longrightarrow$ [Y] $\longrightarrow -i|1\rangle$

$|1\rangle \longrightarrow$ [Y] $\longrightarrow i|0\rangle$

Hence, Y gate multiplies the input qubit by *i* and flip the two components of qubits.

(iii) Pauli's Z – gate

Z	$\|0\rangle$	$\|1\rangle$
$\langle 0\|$	1	0
$\langle 1\|$	0	-1

Then $Z = |0\rangle\langle 0| - |1\rangle\langle 1|$

Output

(i) $Z|0\rangle = |0\rangle\{|0\rangle\langle 0| - |1\rangle\langle 1|\} = |0\rangle$ (ii) $Z|1\rangle = |1\rangle\{|0\rangle\langle 0| - |1\rangle\langle 1|\} = -|1\rangle$

$|0\rangle \longrightarrow$ [Z] $\longrightarrow |0\rangle$

$|1\rangle \longrightarrow$ [Z] $\longrightarrow -|1\rangle$

Z-gate changes the phase (flips the sign) of a qubit

(iv) Hadamard – gate

Here $H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$

H	$\|0\rangle$	$\|1\rangle$
$\langle 0\|$	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$
$\langle 1\|$	$\frac{1}{\sqrt{2}}$	$-\frac{1}{\sqrt{2}}$

Then $H = \frac{1}{\sqrt{2}}\left[|0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| - |1\rangle\langle 1|\right]$

Output

(i) $H|0\rangle = |0\rangle \frac{1}{\sqrt{2}}\{|0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| - |1\rangle\langle 1|\} = \frac{1}{\sqrt{2}}\{|0\rangle + |1\rangle\} = |0\rangle$

(ii) $H|0\rangle = |1\rangle \frac{1}{\sqrt{2}}\{|0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| - |1\rangle\langle 1|\} = \frac{1}{\sqrt{2}}\{|0\rangle - |1\rangle\}$

$$|0\rangle \longrightarrow \boxed{H} \longrightarrow \frac{1}{\sqrt{2}}\{|0\rangle + |1\rangle\}$$

$$|1\rangle \longrightarrow \boxed{H} \longrightarrow \frac{1}{\sqrt{2}}\{|0\rangle - |1\rangle\}$$

H-gate creates superposition state from pure input states.

(v) S – gate (Phase gate)

Here, $S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$

S	$\|0\rangle$	$\|1\rangle$
$\langle 0\|$	1	0
$\langle 1\|$	0	i

Then $S = |0\rangle\langle 0| - i|1\rangle\langle 1|$

Output

(i) $S|0\rangle = |0\rangle\{|0\rangle\langle 0| - i|1\rangle\langle 1|\} = |0\rangle$ (ii) $Z|1\rangle = |1\rangle\{|0\rangle\langle 0| - i|1\rangle\langle 1|\} = i|1\rangle$

$$|0\rangle \longrightarrow \boxed{S} \longrightarrow |0\rangle$$

$$|1\rangle \longrightarrow \boxed{S} \longrightarrow i|1\rangle$$

The S gate is also known as the phase gate, because it represents a 90-degree rotation around the z-axis.

(vi) T – gate (Phase gate)

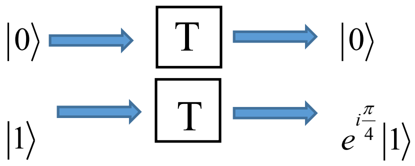
Here, $T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{pmatrix}$

S	$\|0\rangle$	$\|1\rangle$
$\langle 0\|$	1	0
$\langle 1\|$	0	$e^{i\frac{\pi}{4}}$

Then $T = |0\rangle\langle 0| + e^{i\frac{\pi}{4}}|1\rangle\langle 1|$

Output

(i) $T|0\rangle = |0\rangle\left\{|0\rangle\langle 0| + e^{i\frac{\pi}{4}}|1\rangle\langle 1|\right\} = |0\rangle$ (ii) $T|1\rangle = |1\rangle\left\{|0\rangle\langle 0| + e^{i\frac{\pi}{4}}|1\rangle\langle 1|\right\} = i|1\rangle$



The S gate and T gate are connnected by S = T^2.

5.13.2 TWO BITS QUANTUM STATES

Two bit qunatum states are represented by controlled unitary operator

$$CU = \begin{pmatrix} I & O \\ O & U \end{pmatrix}$$

Where I and O are identity and zero matrix and hence the unitary operator U can be resolved as

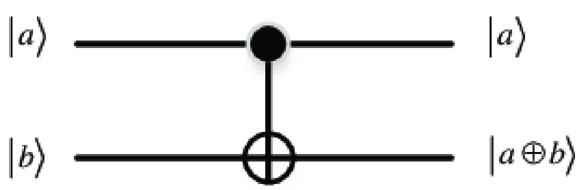
$$U = X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; U = Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}; U = S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$$

Here extension of Pauli's X gate lead to CNOT gate, similarly Z and S gates lead to to CZ and SWAP gates respectively

Here the identity matrix is obtained by the combination of basis states such as $|00\rangle$, $|01\rangle, |10\rangle \, and \, |11\rangle$ as $\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$

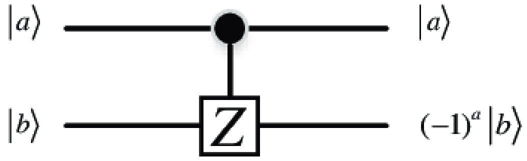
Also, CNOT gate, is used to swap the $|10\rangle \leftarrow$ between third and fouth row in identity matrix. The output after truth table is implemented is given by

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

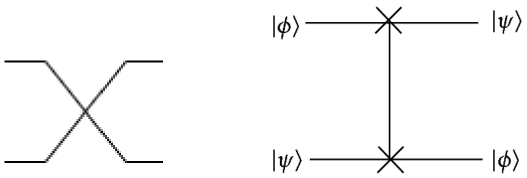


Similarly, CZ gate is obtained, when two qubit quantum states involves in a phase change in $|11\rangle$. As a result the four row has a phase change.The output of the truth table and representation is given by

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



Further, SWAP gate is obtained by interchanging $|01\rangle \rightleftarrows |10\rangle$ in the identitiy matrix to get this swap gate. The output and the symbolic representation are given by



$$\text{SWAP} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

5.14. CNOT gate

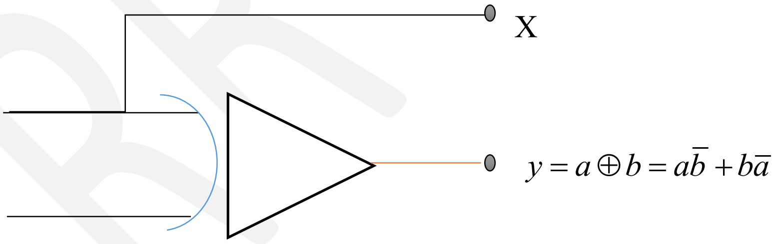
Principle

CNOT gate means controlled NOT gate. It is a quantum logic gate which plays a vital role in the designing of quantum computers.

The CNOT gate will have two qubit operation, wherein the first qubit is referred as the control qubit and the second qubit is referred as the target qubit.

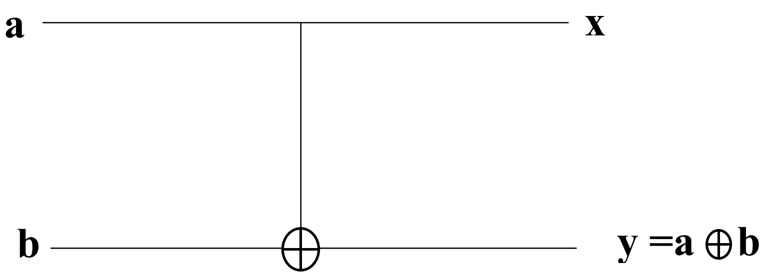
Symbolic Representation

The Symbolic representation of CNOT gate is as shown in figure



Concept

A CNOT gate basically implements a reversible Ex-OR. It can be used to generate entanglement. The CNOT gate can be logically represented as shown in figure.



From figure, we can see that the control (x) and the target (y) are shown as two horizontal lines. Here, we can also notice that the count 'y' depends on the input source 'a' and is shown by an interconnecting vertical line from 'a' to 'y' and to one of the inputs of the EX-OR gate i.e., the target input 'b' as shown in figure.

Logical operation

Inputs

The input a is typically called the source, and input 'b' is known as the target input. Here the x depends on the input a. i.e.,

(i) If source a = 0, then control x = 0; similarly if x = 1, then control x = 1.

Thus *the source is called the control input and controls the application of the NOT operation on the target input*

Outputs

The output of CNOT gate is $y = a \oplus b = a\bar{b} + b\bar{a}$

Here y depends on the source a and target b. i.e.,

(ii) If source a =0, Then the output $y = b$ (i.e., 0)

(iii) When the source a = 1, then the output y will have inverse value of b

Truth table

INPUT		OUTPUT	
Source/Control input	Target qubit	Control qubit	Target output
a	b	x	$y = a \oplus b = a\bar{b} + b\bar{a}$
0	0	0	0
0	1	0	1
1	0	1	1
1	1	1	0

Case (i) When a = 0 and b = 0 or 1, then $y = b$

Case (ii) When a = 1 and b = 0 or 1, then y will be inverse of b

i.e., the inverted value y is controlled by the source a and hence the gate is named as Controlled NOT gate (or) CNOT gate. Hence the inputs can be uniquely determined from outputs by verifying the reversibility of the gate.

Matrix representation of CNOT gate:

$$\mathrm{CNOT} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}.$$

5.15. Quantum Entanglement

From the truth table, we can see that, the target qubit is $|0\rangle$ and the control qubit is either $|0\rangle$ or $|1\rangle$, then the output target y takes the value of control qubit, i.e., it becomes the copy of the control qubit, but control qubit itself does not change.

However, a superposition in the control qubit results in the entaglement of control and target qubits.

Thus, when two or more particles link up in a certain way, no matter how far apart they are in space, their state remains linked. That means they share a common, united quantum state.

So observations of one of the particles can automatically provide information about the other entangled particles, regardless of the distance between them. Any action to one of these particles will invariably impact the other in the entangled system. This united state is known as qunatum entanglement.

5.16 Difference between classicial and qunatum cmputing

Comparison key	Classical computer	Quantum computer
Basis	Large scale integrated multipurpose computer based classical physics	High speed parallel computer based on quantum mechanics
Information storage	Bit based information storage using voltage/ charge or magnetism	Qubit based information storage using electron spin
Bit values	Having either 0 or 1 with a single value at any instant	Qubits have value of 0, 1 , sometime negative and can have both values at the same time
Possible states	Two states, either 0 or 1	It is infinite, it holds combinations of 0 and 1 along with some complex information
Output	Deterministic (repetition on the same input give the same output)	Probabilistic (repetition of computation on superposition states gives probabilistic answers)
Gates used for processing	It is sequential. Example, AND,, OR, NOT, etc.,	Qubit gates process the information parallel.
Scope	Define and limited answer due to algorithm design	Probabilistic and multiple answers are considered due to superposition and entanglement properties.

5.17. Advantages of quantum computing over classical computing

Sl.No	Quantum computing	Classical computing
1.	It is done using qubits	It is done using bits
2.	Here states 0's and 1's can be represented simultaneously	Here, we can represent either 0 or 1. Both cannot be represent simultaneously.
3.	Here, the power increases exponentially in proportion to the number of qubits	The power increases in a 1:1 relationship to the number of transistors.
4.	It is incredibly fast and effective	It is slow and ineffective
5.	They solve complex problems	They do not solve complex problems
6.	It is used to run complex simulation	It is not used for such complex simulation

5.18. Applications

1. It is used in Artificial Intelligence and Machine learning
2. It plays a vital role in drug design and development.
3. They are applied in cyber security and cryptography
4. It is used in weather forecasting.
5. They are used in logistics optimisation, financial modelling, etc.,
6. In research and development, quantum computing are used in computational science research.

Part – A Questions

1. **Define Nano materials.**

Nano phase materials are newly developed materials with grain size at the nanometre range (10^{-9}) in the order of 1 – 100 nm.

2. **What is quantum confinement?**

The effect is achieved by reducing the volume of a solid so that the energy levels within it becomes discrete is called quantum confinement.

3. **What is quantum structure?**

When the bulk material is reduced in its size, atleast one of its dimension, in order of few nanometers, then the structure is known as quantum structure.

4. **What is quantum size effect?**

When the size of nanomaterial becomes smaller than the deBroglie wavelength, electrons and holes gets spatially confined, electrical dipoles gets generated, the discrete energy levels are formed. As the size of the material decreases, the energy separation between adjacent level increases. The density of states of nanocrystals is positioned in between discrete and continuous for atoms/molecules and crystals. This effect is significant for semiconductor nanoparticles.

5. **What is single electron phenomena?**

The phenomena of keeping single electron or quantum dot in isolation without tunnelling.

6. Define Coulomb-Blockade effect.

The charging effect which blocks the injection or rejection of a single charge into or from a quantum dot is called Coulomb blockade effect.

7. What is single electron tunnelling?

The quantization of charge can dominate and tunnelling of single electron across leaky capacitors carriers the current. This is called single electron tunnelling.

8. What is single electron transistor?

A transistor made from a quantum dot that controls the current from source to drain one electron at a time is called single electron transistor.

9. Explain the rules which used for the single electron phenomena?

(i) The energy needed to add one electron to the dot, or charging energy E_C must be significantly higher than the thermal energy of an electron $E_c = \frac{e^2}{2C_{dot}} >> K_B T$

(ii) The uncertainity of the charging energy must be less than the charging energy itself.

$$R_t >> \frac{h}{e^2}$$

10. What are the limitations of single electron transistor?

In order to operate SET at room temperature, the size of quantum dot should be less than 10nm.

It is very hard to fabricate optical lithography and semiconducting process by traditional way.

The methods must be developed for connecting individual structures into logic circuits and these circuits must be arranged in larger 2D particles.

11. What are the applications of single electron transistor?

A variety of digital logic functions are obtained based on SET operating at room temperature.

Used for mass data storage

Used in high sensitive electrometer.

SET is used as temperature probe for very low temperature ranges.

SET is used for single electron spectroscopy.

SET is used in homo-dyan receiver operating between 10 and 300 MHz

12. What is Quantum cellular automata?

it is an emerging nanotechnology. CMOS technology has a lot of limitations while scaling into a nano-level. In order to improve the performance of a system, new nano technology approach should be taken into account. QCA is a optable replacement of CMOS.

13. What are the advantages of QCA?

It is edge driven meaning an input is brought to an edge of a QCA block. This also means that no power line need to routed internally.

The QCA system should be very low power system because there is no current flowing. Only enough energy needs to add to lift the electrons from their ground states to higher states.

The QCA cells are very small.

14. Define Hilbert space.

Hilbert space is defined as an infinite dimensional vector space with an inner product and its associated norm

$$|\psi_0\rangle = \alpha_0|0\rangle + \alpha_1|1\rangle + ... + \alpha_{n-1}|n-1\rangle$$

15. Define classical bits.

A Classical bit can be either 0 or 1

Information in digital representation uses a sequence of bits. Each bit is basically the charge of an electron. If the electron is charge, the bit is assumed to carry a value 1; alternatively if the electron is not charged the bit carries a value 0.

16. What is qubit?

A qubit is a mathematical model of microscopic physical system such as the spin of electron or the polarization of a photon. It also exists in the continuum of intermediate states or superposition states.

17. What are the difference between bits and qubits?

Sl.No	Bits	Qubits
1.	The device computes by manipulating those bits using logic gates	The device computes by manipulating those bits using quantum logic gates
2.	A classical computer has a memory made up of bits where each bit hold either a one or zero	A qubits can hold a one, a zero or crucially a superposition of these
3.	Bits are used in classical computers	Qubits are use in quantum computer
4.	Information is stored in bits which take the discrete values 0 and 1	Information is stored in quantum bits. A qubit can be in state $\|0\rangle$ and $\|1\rangle$, but it can

		also be in a superposition of these states as $\|\psi\rangle = \alpha\|0\rangle + \beta\|1\rangle$. If we think a qubit as a vector, then superposition of state is just vector addition.
5.	Processing of bits are slow	Processing of qubits are faster
6.	Circuit is based on classical physics.	Circuit is based on quantum mechanics

18. Define one qubit quantum state.

A one qubit gate transforms an input qubit $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ in to an output qubit

Mathematically a gate is represented by 2 x 2 unitary operator matrix with basis qunatum states such as $|0\rangle \, and \, |1\rangle$

19. What are advantages of quantum computer over classical computer?

Sl.No	Quantum computing	Classical computing
1.	It is done using qubits	It is done using bits
2.	Here states 0's and 1's can be represented simultaneously	Here, we can represent either 0 or 1. Both cannot be represent simultaneously.
3.	Here, the power increases exponentially in proportion to the number of qubits	The power increases in a 1:1 relationship to the number of transistors.
4.	It is incredibly fast and effective	It is slow and ineffective
5.	They solve complex problems	They do not solve complex problems
6.	It is used to run complex simulation	It is not used for such complex simulation

20. What are the differences between classical and quantum computers?

Comparison key	Classical computer	Quantum computer
Basis	Large scale integrated multipurpose computer based classical physics	High speed parallel computer based on quantum mechanics
Information storage	Bit based information storage using voltage/ charge or magnetism	Qubit based information storage using electron spin
Bit values	Having either 0 or 1 with a single value at any instant	Qubits have value of 0, 1 , sometime negative and can have both values at the same time
Possible states	Two states, either 0 or 1	It is infinite, it holds combinations of 0 and 1

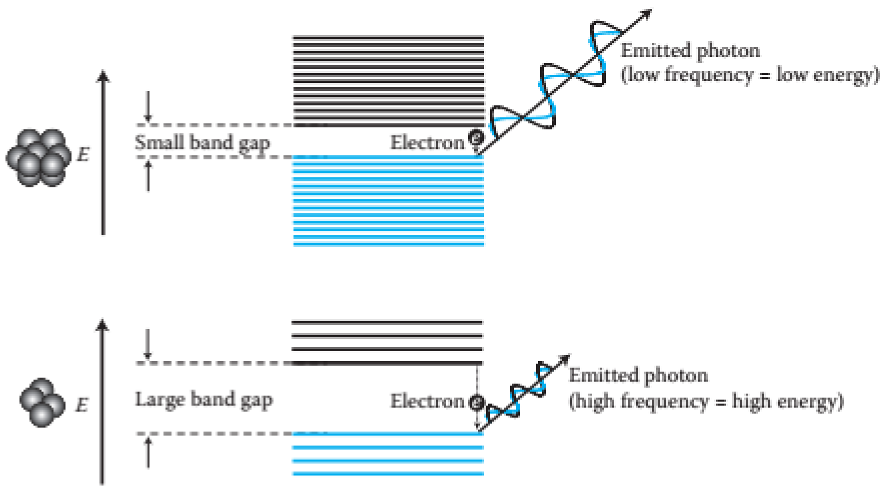
		along with some complex information
Output	Deterministic (repetition on the same input give the same output)	Probabilistic (repetition of computation on superposition states gives probabilistic answers)
Gates used for processing	It is sequential. Example, AND,, OR, NOT, etc.,	Qubit gates process the information parallel.
Scope	Define and limited answer due to algorithm design	Probabilistic and multiple answers are considered due to superposition and entanglement properties.

Part – B questions

1. **Define quantum confinement and quantum structures in nanomaterial.**

When the size of a nanocrystal becomes smaller than the deBroglie wavelength, electrons and holes gets spatially confined, electrical dipoles gets generated, the discrete energy levels are formed. As the size of the material decreases, the energy separation between adjacent levels increases. The density of states of nanocrystals is positioned in between discrete (as that of atoms and molecules) and continuous (as in crystals).

Quantum size effect is most significant for semiconductor nanoparticles. In semiconductors, the bandgap energy is of the order of few electron volts and increases with a decrease in particle size.



When photons of light fall in a semiconductor, only those photons with energy are absorbed and a sudden rise in absorption is observed when the photon energy is equal to the bandgap.

As the size of the particle decreases, absorption shifts towards the shorter wavelength (blue shifts) indicating an increase in the bandgap energy .A change in absorption causes a change in the colour of the semiconductor nanoparticle.

For example, bulk cadmium sulphide is orange in colour and has a bandgap of 2.42eV. It becomes yellow and then ultimately white as its particle size decreases and the bandgap increases.

2. Discuss the electron density in bulk material and size dependent of Fermi energy.

The bulk material is a collection of atoms having properties that are from individual atoms. The nanomaterials gives unique electronic properties.one of the mayor difference in nanomaterials with respect to bulk materials is the number of available energy states. In a bulk material, the states within each energy sublevel are so close that they blend into a band.

The total number of electron states N with energies up to E, can be determined based on the equation $N = \frac{\pi}{3}\left[\frac{8m}{h^2}\right]^{3/2} E^{3/2}.V$ (1)

Here, we represent the volume as V, m is the mass of an electron an h is the Planck's constant.

The number of energy states per unit volume is given by $n = \frac{N}{V} = \frac{\pi}{3}\times\left[\frac{8m}{h^2}\right]^{3/2} E^{3/2}$ (2)

Density of states is defined as number of available electron energy states per unit volume, per unit energy i.e., Z(E) = dn / dE (3)

Hence equation (2) becomes,

$$Z(E) = \frac{\pi}{3}\times\left(\frac{8m}{h^2}\right)^{3/2} \times \frac{3}{2} E^{1/2}$$

(or) $Z(E) = \frac{\pi}{2}\times\left(\frac{8m}{h^2}\right)^{3/2} E^{1/2}$ (4)

From equation (4), the density of states for a bulk material is directly proportional to square root of energy

i.e., Z(E) α √E (5)

The relevant application of density of states is that it provides information about nanomaterials.

Here, the Fermi function gives the probability of occupation by the free electrons in a given energy state.

i.e., $f(E) = \frac{1}{1+e^{\frac{E-E_f}{kT}}}$ (6)

Then, the number of free electrons per unit volume is $n_e = \int_0^{\alpha} F(E)Z(E)dE$

Put F(E) = 1 at T = 0K, then $n_e = \frac{\pi}{2}\times\left(\frac{8m}{h^2}\right)^{3/2} \int_0^{\alpha} E^{1/2}dE$

(or) $n_e = \frac{\pi}{3}\times\left(\frac{8m}{h^2}\right)^{3/2} E_f(0)^{3/2}$ (7)

Size dependence of Fermi energy

In terms of the distribution of energy, solid have thick energy bands, whereas atoms have thin, discrete energy states. Hence to make a solid behave electronically more like an atom, we need to make it about the same size as an atom.

Hence rearranging equation (7) , we get $E_f(0) = \frac{h^2}{8m} \times \left(\frac{3n_e}{\pi}\right)^{2/3}$ (8)

In the above equation, ‘n’ is the only variable.

Equation (8) suggests that the fermi energy of a conductor depends on the number of free electrons ‘N’ per unit volume ‘V’ $E_F(0) \alpha (n)^{2/3} \alpha \left(\frac{N}{V}\right)^{2/3}$ (9)

Since the electron density is a property of the material, the fermi energy does not vary with material’s size. E_F is same for a particle or for a brick of copper. Hence the energy state will have the same range for small volume and large volume of atoms. But for small volume of atoms we get larger spacing between states. This is applicable to semiconductors and insulators.

Let us consider that all states up to $E_F(0)$ are occupied by a total of free electrons (N).

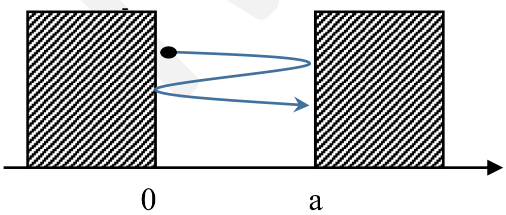
$$\Delta E = \frac{E_F(0)}{N} \quad (10)$$

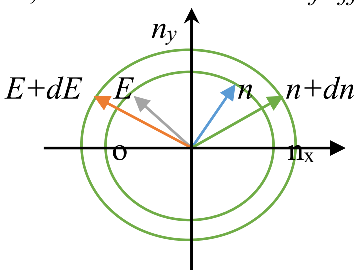
From equation (9) & (10), $\Delta E \alpha \frac{1}{V}$ (11)

Thus, the spacing between energy states is inversely proportional to the volume of the solid. The energy sublevel and the spacing between energy states within it will depend on the number of atoms as shown in figure. At one point, we know that an energy sublevel must be divided as many times as there are atoms in a solid, which eventually results too many splits to differentiate. Hence, we just refer to each sublevel as a solid energy band. On the other hand, a single atom in the sublevel contain only one discrete energy state. If we reduce the volume of s solid, the tiny piece of material behaves electronically like an artificial atom.

3. Discuss density of states in quantum well, quantum wire and quantum dot structure.

The quantum well can be displayed with dimensions of length a, where the electrons of effective mass are confined in the well as shown in fig.





The two dimensional density of states is the number of states per unit area and unit energy.

Consider the electron in a two dimensional bounded region of space. We want to find how many quantum states lie within a particular energy, say, between E and E+dE as shown in Figure.

The reduced phase space now consists only the x- y plane and n_x and n_y coordinates.

In 2D space, $n^2 = n_x^2 + n_y^2$

Derivation

The number of available states within a circle of radius 'n' is given by $\frac{1}{4}\pi n^2$

Here only one quarter of circle will have positive integer values

The number of states within a circle of radius $n+dn$ is given by $\frac{1}{4}\pi(n+dn)^2$

The number of available energy states lying in an energy interval E and $E+dE$

$$Z'(E)dE = \frac{1}{4}\pi\left[(n+dn)^2 - n^2\right]$$

$$= \frac{\pi}{4}\left[n^2 + dn^2 + 2ndn - n^2\right]$$

As dn^2 is very small, we can neglect dn^2. Therefore we get,

$$Z'(E)dE = \frac{\pi}{4}[2ndn] = \frac{\pi}{2}ndn \qquad (1)$$

We know that $n^2 = \frac{8m^*E}{h^2}a^2$ (2)

$$\text{(or)}\quad n = \left[\frac{8m^*E}{h^2}\right]^{1/2} a \qquad (3)$$

$$\text{(or)}\quad dn = \left[\frac{8m^*}{h^2}\right]^{1/2} a\frac{1}{2}E^{-1/2}dE \qquad (4)$$

Substitute the value of equation (3) and (4) in equation (1), we get

$$Z'(E)dE = \frac{\pi}{2}\left[\frac{8m^*E}{h^2}\right]^{1/2} a\left[\frac{8m^*}{h^2}\right]^{1/2} a\frac{1}{2}E^{-1/2}dE$$

m* is the effective mass in the quantum well

$$Z'(E)dE = \frac{\pi}{4}\left[\frac{8m^*}{h^2}\right]a^2dE \qquad (5)$$

Put $a^2 = A$ area of circle

According to Pauli's exclusion principle each energy level can occupy two electrons of opposite spin

i.e., $Z'(E)dE = 2\times\frac{\pi}{4}\left[\frac{8m^*}{h^2}\right]AdE$

Number of quantum states per unit area and unit energy is

$$\frac{Z'(E)dE}{AdE} = 2\times\frac{\pi}{4}\left[\frac{8m^*}{h^2}\right]$$

$$Z'(E) = \frac{\pi}{2}\left[\frac{8m^*}{h^2}\right] \text{ (or) } Z'(E) = \frac{\pi}{2}\left[\frac{8m^*}{(2\pi\hbar}\right] \qquad [\text{ since } h^2 = 4\pi\hbar \;] \qquad (6)$$

The density of states in two dimensional is given by $Z'(E)^{2D} = \frac{m^*}{\pi\hbar}$ for E >= E_0 (7)

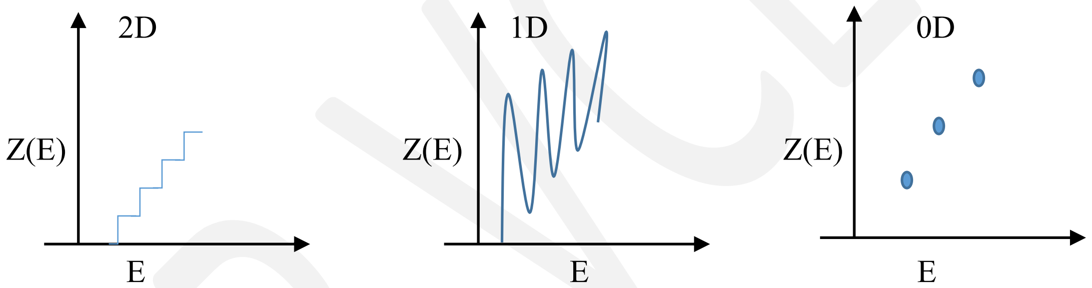
Where E_0 is the ground state of quantum well

$$Z'(E)^{2D} = \frac{m^*}{\pi\hbar}\sum\sigma(E - E_n) \qquad (8)$$

Where E_n are the energies of quantized states and $\sigma(E - E_n)$ is step function.

From equation (7), the density of states in two dimension is constant with respect to the energy.

i.e., $Z'(E)^{2D} \infty E^0$ = constant



Density of states in quantum wire

Consider the one dimensional system, the quantum wire in which only one direction of motion is allowed. (eg. Along x – direction).

In one dimension, such as for a quantum wire, the density of states is defined as the number of available states per unit length per unit energy around an energy *E*. The electron inside the wire are confined in a one dimensional infinite potential well with zero potential inside the wire and infinite potential outside the wire.

At $x = 0$; V(x) = 0 for an electron inside the wire

At $x = a$; V(x) = α for an electron outside the wire

The reduced phase space now consists only the x plane and n_x coordinates are shown in figure.

In one dimensional space $n^2 = n_x^2$

The number of available energy states lying in an interval of length is

$Z'(E)dE = n + dn - n = dn$ (1)

Substitute the value of *dn* from equation (4), we get

$$Z'(E)dE = \left[\frac{8m^*}{h^2}\right]^{1/2} a\frac{1}{2}E^{-1/2}dE \qquad (2)$$

According to Pauli's exclusion principle, two electrons of opposite spin can occupy each energy state.

$$Z'(E)dE = 2\times\left[\frac{8m^*}{h^2}\right]^{1/2} a\frac{1}{2}E^{-1/2}dE$$

Number of quantum states per unit length and unit energy is $\frac{Z'(E)dE}{adE} = \left[\frac{8m^*}{h^2}\right]^{1/2} E^{-1/2}$

$$\text{(or)}\;\; Z'(E) = \left[\frac{8m^*}{4\pi^2\hbar}\right]^{1/2} E^{-1/2}s \;=\; Z'(E)^{1D} = \left[\frac{2m^{*1/2}}{\pi\hbar}\right]E^{-1/2} \qquad (3)$$

If the electron has potential energy E_0 we have $Z(E)^{1D} = \frac{1}{\pi\hbar}\sqrt{\frac{2m^*}{(E-E_0)}}\,(E \geq E_0)$ (4)

From equation (4) the density of states in one dimensional system has a functional dependence on energy $Z(E)^{1D}$ α $E^{-1/2}$

For more than one quantized state, the one dimensional density of states is given by

$$Z(E)^{1D} = \frac{1}{\pi\hbar}\sum\sqrt{\frac{2m^*}{(E-E_0)}}\,\sigma(E-E_n) \qquad (5)$$

Where E_n are the energies of the quantized states of the wire and $\sigma(E-E_n)$ is the step function. The density of states in quasi-continum (or) quantum wire is shown in figure. The discontinuities in the density of states are known as **Van Hove Singularities**

Density of states in Quantum dot

In a zero dimensional system, the density of states are truly discrete and they don't form a quasi continum.

In zero dimensional system (quantum dot), the electron is confined in all three spatial dimensions and hence to motion of electron is possible. Each quantum state of a zero dimensional system can therefore be occupied by only two electrons. So the density of states for a quantum dot is merely a delta function.

$$Z(E)^{0D} = 2\sqrt{(E-E_0)} \qquad (6)$$

Here, the factor 2 accounts for spin. For more than one quantum state, the density of states is given by $Z(E)^{0D} = \sum_n 2\delta\sqrt{(E-E_0)}$

4. Describe the construction and working of single electron transistor.

Principle

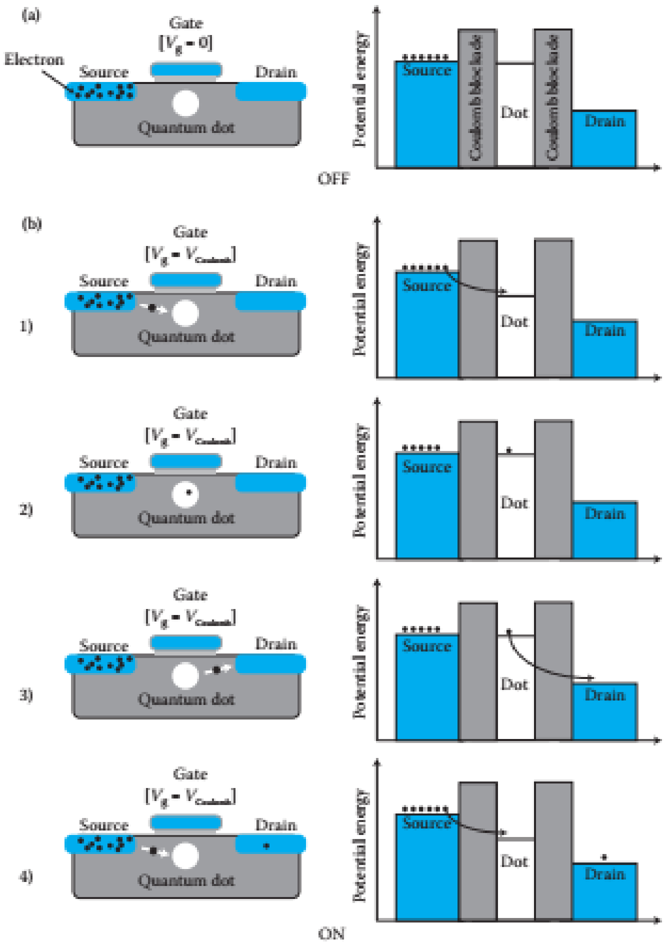
A transistor with three terminal switching device made from a quantum dot that controls the current from source to rain one electron at a time is called single electron transistor

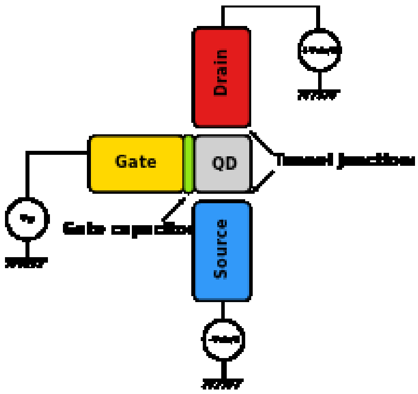
Construction

The single electron transistor (SET) is built like a conventional Field Emitting Transistor (FET). It has tunnelling junctions in place of *pn* – junctions and quantum dot in place of the channel region of the FET. To control tunnelling, a voltage bias to the gate electrode is applied. A separate voltage bias is applied between source and drain electrodes for the current direction. For current to flow, gate bias voltage must be large enough to overcome the coulomb blockade energy.

Working

1. The purpose of SET is to individually control the tunnelling of electrons into an out of the quantum dot. To do this, we must first stop random tunnelling by choosing the right circuit geometry and materials. If an electron comes or goes from the dot. It will on purpose.





2. To control tunnelling, we apply a voltage bias to the gate electrode. There is also a voltage difference between the source and the drain that indicates the direction of current. Here, we can say that current and electron flow in the same direction and we will consider the electrode from which the electrons originate.

3. This is similar to the working of FET, where the gate voltage creates an electric field that alters the conductivity of the semiconducting channel below it, enabling current to flow from source to drain.
4. Applying a voltage to the gate in an SET creates an electric field and change the potential energy of the dot with respect to the source and drain. This gate voltage controlled potential difference can make electrons in the source attracted to the dot and simultaneously electrons in the dot attracted to the drain.
5. For current to flow, this potential difference must be atleast large enough to overcome the energy of the coulomb blockade.

The energy "*E*" needed to move a charge *e* across a potential difference *V* is given by $E=Ve$

So, the voltage that will move an electron onto or off the quantum dot is given by

$$V=\frac{E_c}{e} \quad (or) \quad V=\frac{\frac{e^2}{2C_{dot}}}{e}=\frac{e}{2C_{dot}} \qquad (1)$$

With this voltage applied to quantum dot, an electron can tunnel through coulomb blockade of the quantum dot.

Working for single electron transistor in nutshell

A single electron transistor is shown in figure. As opposed to the semiconductor channel in a field effect transistor, the SET has an electrically isolated quantum dot located between the source and drain.

1. The SET is OFF mode. The corresponding potential energy diagram shows that it is not energetically favourable for electrons in the source to tunnel to the dot as shown in figure.
2. The SET is ON mode. At the lowest setting electrons tunnel one at a time, via the dot, from the source to the drain as shown in figure.
3. This is made possible by first applying the proper gate voltage, $V_{gate} = e/2C_{dot}$, so that the potential energy of the dot is made low enough to encourage an electron to tunnel through the coulomb blockade energy barrier to the quantum dot.
4. Once the electron is on it, the dots potential energy rises as shown in figure
5. The electron then tunnels through the coulomb blockade on the other side to reach the lower potential energy at the drain as shown in figure.
6. With the dot empty and the potential lower again the process repeats as shown in figure.

Advantages

1. The fast information transfer velocity between cells is carried out via electrostatic interactions only.
2. No wire is needed between arrays. The size of each cell can be can be as small as 2.5nm. This made them suitable for high density memory.
3. This can be used for the next generation quantum computer.

Limitations

1. In order to operate SET circuit at room temperature, the size of the quantum dot should be smaller than 10*nm*
2. It is very hard to fabricate by traditional optical lithography and semiconductor processes
3. The method must be developed for connecting the individual structures into logic circuits and these circuits must be arranged into larger 2D patterns.

Applications

1. SET are used in sensor and digital electronic circuits
2. Variety of digital logic functions, including AND or NOR gates, is obtained based on SET operating at room temperature.
3. It is used for mass storage
4. It is used in highly sensitive electrometer.
5. SET can be used as a temperature probe, particularly in the range of very low temperatures.
6. SET is a suitable measurement setup for single electron spectroscopy.
7. It is used for the fabrication of homo-dyn receiver operating at frequencies between 10 and 300 *MHz*

5. Explain quantum cellular automata.

Introduction

The continuing down scaling of device dimensions in microelectronics technology has led to faster devices and denser circuit with obvious benefits to chip performance. There is much expectation that the availability of very dense device arrays might lead to a new paradigms for information processing based on locally interconnected architectures such as cellular automata (CA)

We focus here on the idea of employing CA architectures which are compatible with nanometer scale quantum devices. Quantum Cellular Automata is a new nanotechnology with potential for applying in building future computers. This technology is a realization of the circuit design at the nano scale.

Quantum Cellular Automata technology is one of the emerging technologies that can be used for replacing CMOS technology. It has attracted significant attention in the recent years due to its extremely low power dissipation, high operation frequently and smaller in size.

Definition

A quantum cellular automata consists of an array of quantum device cells in a locally interconnected architectures.

Concept

According to quantum cellular automata, logical states or values are demonistrated by the position of electrons rather than voltage levels. By applying proper implements of this QCA technology, significant low density of 10^{12} devices/cm^{3} and very low power consumption (near to zero) are achievable.

Thus quantum cellular automata (QCA) is an abstract model of quantum computation devised in analogy to conventional models of cellular automata.

Advantages

1. Low power dissipation
2. High operating frequency
3. Smaller in size
4. It replaces CMOS technology.

Applications

1. It can used for designing general purpose computational circuits
2. It is used in memory circuits and other computational and sequential circuit designs.

6. Explain quantum computing for information processing.

The Quantum phenomena can be applied to Quantum Computing Quantum information science and Quantum metrology. The Progresses of all these technologies are mutually dependent on each other. They share the same laws of physics, Common hardware and related works.

Quantum information science deals with the methods of the information in a quantum system. It includes statistics of Quantum mechanics along with their limitations, it provides a core for all other applications such as quantum Computing, networking, sensing and metrology

Quantum Communication and Networking explains the exchange of information by encoding it in to a quantum Cryptography. It is the subset of quantum Communication in which Quantum Properties help to design the secure communication System.

Quantum Sensing and metrology: is the Quantum systems which are used to measure important physical Properties (e.g. electric and magnetic fields, temperature, etc.,) . The system has more accuracy than classical systems. Quantum Sensors are based on Qubits. They are carried out using the experimental quantum systems.

Quantum Computing deals with the Quantum mechanical properties of Super position, entanglement and interference to enact Computation In Common, a Quantum Computer Consists of a collection of quantum bits (Qubits). The Qubits are isolated from the environment for their Quantum state to perform the Computation

These Qubits are organized and manipulated to set an algorithms and to get a result. The high Probability from the measurement of final state produces the result.

Several ways such as nuclear magnetic resonance, optical and solid state techniques and ion traps are used to build Quantum Computers. The fundamental Concept that has been need to handle the Quantum Computers using the above ways are given below.

(a) Harmonic oscillation Quantum Computer

In this system, discrete eigen states are represented as n x, where n = 0, 1, 2,.... α; these represent qubits . The lifetime of Qubits depend on the Quality factor of the cavity.

A Single quantum harmonic oscillator will have a 2^{n} energy states in Hilbert Space. But, a classical harmonic oscillator has n energy states in the same Hilbert Space

(b) Optical Phonon Quantum Computer

In these Computers, Photon can represent a quantum bit. Photons can be made to interact with eachother using non-linear optical media. Mirrors, Phase shifters and beam splitters are the accessible devices for manipulating the photon states

The required Single photons can be created using attenuated laser. These photons are defected with photo detectors. Thus a quantum Computer can be made using these optical components.

(c) Optical Cavity quantum electrodynamic Computer

In this, Coupling of Single atom to a few optical modes takes place. It is done by placing single atom in optical cavities of very high Q.

The cavity electrodynamic system consists of Fabry Perot cavity containing a few atoms to which the optical field is coupled. The photons in the cavity have an opportunity to interact many times with the atoms before escaping.

The single photon can be good carrier of quantum information. They are created by attenuated lasers and they are measured at the output wing photo multiplier.

(d) Ion trap quantum Computer

In electromagnetic traps, a number of charged atoms are isolated and trapped. Then the atoms are cooled so that their kinetic energy is much less than their spin energy. After this, the incident monochromatic light can selectively cause transitions between energy states of lowest level vibrational modes of ions. These transitions can be made to perform quantum computation. The main components of the ion trap quantum computers are the electromagnetic trap with lasers, photo detectors of ions.

(e) Nuclear magnetic resonance computer

These computers are based on the spins of atomic nucleus. This will be nearly ideal for quantum computation if only spin - spin coupling be large and controllable. Magnetic field pulses are applied to spins in a strong magnetic field.

The coupling between spins of atoms can be provided by chemical between the neighbouring atoms. The processing magnetic moment induces the output. These proposals shows that the quantum are more suitable for information processing.

7. Explain single qubit and two qubit quantum gates.

We know that classical logic gates are the building blocks of digital circuits. Similarly, a quantum gate is a basic quantum circuit operating with a small number of qubits and are the building blocks of qunatum gates.

1. Quantum gates are the unitary operator which are constructed with the help of basis vector.
2. Here the basis vector of single qubit is $|0\rangle$ and $|1\rangle$. Similarly for two qubits are $|00\rangle$, $|01\rangle$, $|10\rangle$ and $|11\rangle$. This is obtained in 4x1 matrix by the tensor product of $|0\rangle$ and $|1\rangle$

3. one qubit qunatum state of $|0\rangle$ is represented by column matrixby column vector $\begin{pmatrix}1\\0\end{pmatrix}$ and $|1\rangle$ by $\begin{pmatrix}0\\1\end{pmatrix}$. Similarly for two qubits of $|00\rangle, |01\rangle, |10\rangle \; and \; |11\rangle$ states as

$$\begin{pmatrix}1\\0\\0\\0\end{pmatrix}\begin{pmatrix}0\\1\\0\\0\end{pmatrix}\begin{pmatrix}0\\0\\1\\0\end{pmatrix}\begin{pmatrix}0\\0\\0\\1\end{pmatrix}$$

4. Identity matrix is $I = \begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}$
5. Qunatum gate is unitary operator with $U^{\dagger}U = I$ where $U^{\dagger} = U^{-1}$ and Det $|U| = 1$
6. The qunatum states satisify othronormal condition (self product is allowed)
7. Any single qubit qunatum state is represented by

$$U = e^{i\alpha}\left[I\cos\left(\frac{\theta}{2}\right) - i(\vec{c}\ldots,\ldots\left(\frac{\cdot}{2}\right)\right]$$

In this equation the square bracket term represents the rotational operator about the arbitary direction and $e^{i\alpha}$ is its phase.

Now, put $\alpha = \left(\frac{\pi}{2}\right); \theta = \pi$

$$U = e^{i\frac{\pi}{2}}\left[I\cos\left(\frac{\pi}{2}\right) - i(\vec{c}\ldots,\ldots\left(\frac{\cdot}{2}\right)\right] \quad \text{(or)} \; U = (\vec{c}\ldots,$$

Where σ_n is the polarization state of a qubit along any axis . Here there is only a single bit of information (0 or 1)

SINGLE BIT QUANTUM STATES

Single bit qunatum gate can be constructed by condiering the unitary operator

$U = (\vec{c}\ldots,$ (or) $U = \vec{c}_{x\cdot\cdot x} \cdot \vec{\;}_{y\cdot\cdot y} \cdot \vec{\;}_{z\cdot\cdot z}$ and

if $n_x = (100); n_y = (010); n_z = (001)$ and σ_n is $\sigma_x = \begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}; \sigma_y = \begin{pmatrix}0 & -i\\i & 0\end{pmatrix}; \sigma_z = \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix}$

(1) Pauli's X – gate

X	$\lvert 0\rangle$	$\lvert 1\rangle$
$\langle 0\rvert$	0	1
$\langle 1\rvert$	1	0

Then $X = |1\rangle\langle 0| + |0\rangle\langle 1|$

Output

(i) $Y|0\rangle = |0\rangle\{|1\rangle\langle 0| + |0\rangle\langle 1|\} = |1\rangle$ (ii) $Y|1\rangle = |1\rangle\{|1\rangle\langle 0| + |0\rangle\langle 1|\} = |0\rangle$

$|0\rangle \longrightarrow \boxed{X} \longrightarrow |1\rangle$

$|1\rangle \longrightarrow \boxed{X} \longrightarrow |0\rangle$

Hence, X gate is also a NOT gate which transpose the components of qubit.

(ii) Pauli's Y - gate

Y	$\|0\rangle$	$\|1\rangle$
$\langle 0\|$	0	$-i$
$\langle 1\|$	i	0

Then $Y = -i|1\rangle\langle 0| + i|0\rangle\langle 1|$

Output

(i) $Y|0\rangle = -i|0\rangle\{|1\rangle\langle 0| + i|0\rangle\langle 1|\} = -i|1\rangle$ (ii) $Y|1\rangle = i|1\rangle\{|1\rangle\langle 0| + i|0\rangle\langle 1|\} = i|0\rangle$

$|0\rangle \longrightarrow \boxed{Y} \longrightarrow -i|1\rangle$

$|1\rangle \longrightarrow \boxed{Y} \longrightarrow i|0\rangle$

Hence, Y gate multiplies the input qubit by *i* and flip the two components of qubits.

(iii) Pauli's Z – gate

Z	$\|0\rangle$	$\|1\rangle$
$\langle 0\|$	1	0
$\langle 1\|$	0	-1

Then $Z = |0\rangle\langle 0| - |1\rangle\langle 1|$

Output

(i) $Z|0\rangle = |0\rangle\{|0\rangle\langle 0| - |1\rangle\langle 1|\} = |0\rangle$ (ii) $Z|1\rangle = |1\rangle\{|0\rangle\langle 0| - |1\rangle\langle 1|\} = -|1\rangle$

$|0\rangle \longrightarrow \boxed{Z} \longrightarrow |0\rangle$

$|1\rangle \longrightarrow \boxed{Z} \longrightarrow -|1\rangle$

Z-gate changes the phase (flips the sign) of a qubit

(iv) Hadamard – gate

Here $H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$

H	$\|0\rangle$	$\|1\rangle$
$\langle 0\|$	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$
$\langle 1\|$	$\frac{1}{\sqrt{2}}$	$-\frac{1}{\sqrt{2}}$

Then $H = \frac{1}{\sqrt{2}}\left[|0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| - |1\rangle\langle 1|\right]$

Output

(i) $H|0\rangle = |0\rangle \frac{1}{\sqrt{2}}\left\{|0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| - |1\rangle\langle 1|\right\} = \frac{1}{\sqrt{2}}\left\{|0\rangle + |1\rangle\right\} = |0\rangle$

(ii) $H|0\rangle = |1\rangle \frac{1}{\sqrt{2}}\left\{|0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| - |1\rangle\langle 1|\right\} = \frac{1}{\sqrt{2}}\left\{|0\rangle - |1\rangle\right\}$

$$|0\rangle \longrightarrow \boxed{H} \longrightarrow \frac{1}{\sqrt{2}}\left\{|0\rangle + |1\rangle\right\}$$

$$|1\rangle \longrightarrow \boxed{H} \longrightarrow \frac{1}{\sqrt{2}}\left\{|0\rangle - |1\rangle\right\}$$

H-gate creates superposition state from pure input states.

(v) S – gate (Phase gate)

Here, $S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$

S	$\|0\rangle$	$\|1\rangle$
$\langle 0\|$	1	0
$\langle 1\|$	0	i

Then $S = |0\rangle\langle 0| - i|1\rangle\langle 1|$

Output

(i) $S|0\rangle = |0\rangle\left\{|0\rangle\langle 0| - i|1\rangle\langle 1|\right\} = |0\rangle$ (ii) $Z|1\rangle = |1\rangle\left\{|0\rangle\langle 0| - i|1\rangle\langle 1|\right\} = i|1\rangle$

$$|0\rangle \longrightarrow \boxed{S} \longrightarrow |0\rangle$$

$$|1\rangle \longrightarrow \boxed{S} \longrightarrow i|1\rangle$$

The S gate is also known as the phase gate, because it represents a 90-degree rotation around the z-axis.

(vi) T – gate (Phase gate)

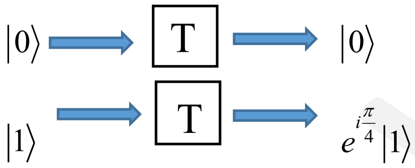
Here, $T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{pmatrix}$

S	$\vert 0\rangle$	$\vert 1\rangle$
$\langle 0\vert$	1	0
$\langle 1\vert$	0	$e^{i\frac{\pi}{4}}$

Then $T = |0\rangle\langle 0| + e^{i\frac{\pi}{4}}|1\rangle\langle 1|$

Output

(i) $T|0\rangle = |0\rangle\left\{|0\rangle\langle 0| + e^{i\frac{\pi}{4}}|1\rangle\langle 1|\right\} = |0\rangle$ (ii) $T|1\rangle = |1\rangle\left\{|0\rangle\langle 0| + e^{i\frac{\pi}{4}}|1\rangle\langle 1|\right\} = i|1\rangle$



The S gate and T gate are connnected by S = T^2.

TWO BITS QUANTUM STATES

Two bit qunatum states are represented by controlled unitary operator

$$CU = \begin{pmatrix} I & O \\ O & U \end{pmatrix}$$

Where I and O are identity and orthogonal matrix and hence the unitary operator U can be resolved as

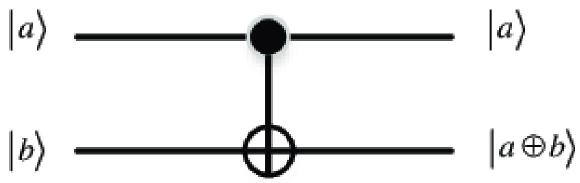
$$U = X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; U = Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}; U = S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$$

Here extension of Pauli's X gate lead to CNOT gate, similarly Z and S gates lead to to CZ and SWAP gates respectively

Here the identity matrix is obtained by the linear combination of basis states $|00\rangle$, $|01\rangle, |10\rangle \; and \; |11\rangle$ as $\begin{pmatrix}1\\0\\0\\0\end{pmatrix}\begin{pmatrix}0\\1\\0\\0\end{pmatrix}\begin{pmatrix}0\\0\\1\\0\end{pmatrix}\begin{pmatrix}0\\0\\0\\1\end{pmatrix} = \begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix}$

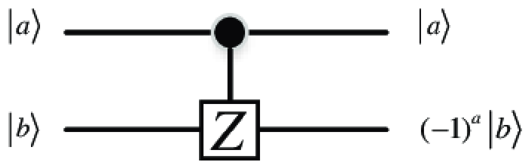
Also, CNOT gate, is used to swap the $|10\rangle \longleftarrow$ between third and fouth row in identity matrix. The output after truth table is implemented is given by

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

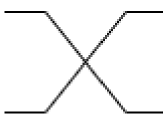


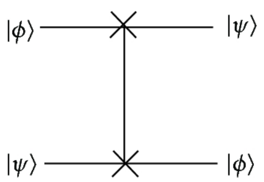
Similarly, CZ gate is obtained, when two qubit quantum states involves in a phase change in $|11\rangle$. As a result the four row has a phase change.The output of the truth table and representation is given by

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



Further, SWAP gate is obtained by interchanging $|01\rangle \longleftarrow$ in the identitiy matrix to get this swap gate. The output and the symbolic representation are given by





$$\text{SWAP} = \begin{bmatrix}1&0&0&0\\0&0&1&0\\0&1&0&0\\0&0&0&1\end{bmatrix}$$

8. Write a short note on single qubit and multiple qubits.

Single Qubit

Definition

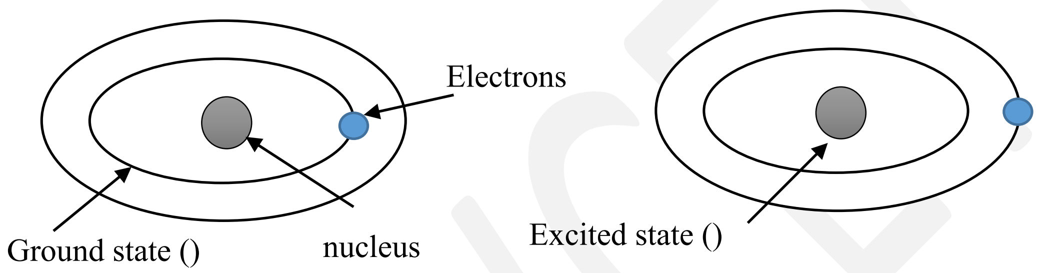
A qubit (quantum bit) is the basic unit of information in quantum computing. A qubit uses the quantum mechanical phenomena of superposition to achieve a linear combination of two states.

Explanation

A classical binary bit can only represent a single binary value such as either 0 or 1, i.e., it can only be in one of two possible states.

A qubit, however, can be represented as 0, 1 or any portion of 0 and 1 in superposition of both states, with a certain probability of being 0 and a certain probability of being 1.

Let us consider an electron in a hydrogen atom which will be in its ground state as shown in figure or in an excited state as shown in figure.



In classical system, it is assumed that excited state represent and the ground state represent.

But in quantum system, the electron will exist in a linear superposition of the ground and excited state. i.e., it will exist in the ground state with probability amplitude α and in excited state with probability amplitude β.

This type of two state quantum system is referred to as single qubit, and its actual state ψ can also be any linear combination (or superposition) of these states.

i.e., $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ (1)

Where $|\psi\rangle$ is the state of the qubit. Here, $|0\rangle$ and $|1\rangle$ are the computational basis states. The coefficients α and β are complex numbers and are called as probability amplitudes.

If α is the probability amplitude of 0 state, then the probability of qubit being in 0 state is $\alpha\alpha^* = |\alpha|^2$ where α^* is the complex conjugate of α

However, $|\alpha|^2 + |\beta|^2 = 1$ (2)

The quantum state ψ in equation (1) can be written as unit column vector in a two dimensional complex plane (Hilbert space) spanned by the two basis vectors.

Here, a qubit with state $|0\rangle$ is represented by column vector $\begin{pmatrix}1\\0\end{pmatrix}$ (3)

A qubit with state $|1\rangle$ is represented by column vector $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ (4)

Substituting (3) and (4) in (1), we get

$$|\psi\rangle = \alpha\begin{pmatrix} 1 \\ 0 \end{pmatrix} + \beta\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

(or) $|\psi\rangle = \begin{pmatrix} \alpha \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ \beta \end{pmatrix}$

(or) $|\psi\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$ (5)

Equation (5) is the vector representing an arbitrary qubit state

Multiple Qubits

Consider a system of two qubits in a four dimensional vector space. In this Hilbert space, four computational basis states represented as $|00\rangle$,$|01\rangle$,$|10\rangle$ and $|11\rangle$

The superposition of these states gives a state vector $|\psi\rangle$ given as linear combination of the basis vectors $|\psi\rangle = \alpha_{00}|00\rangle + \alpha_{01}|01\rangle + \alpha_{10}|10\rangle + \alpha_{11}|11\rangle$ (1)

Where α_{00}, α_{01}, α_{10}, α_{11} are complex coefficients, the probabilities of the four states are $|\alpha_{00}|^2$, $|\alpha_{01}|^2$, $|\alpha_{10}|^2$ and $|\alpha_{11}|^2$.

The normalization of equation (1) is the sum of the square of the probabilities of the coefficient in the state is 1

i.e., $|\alpha_{00}|^2 + |\alpha_{01}|^2 + |\alpha_{10}|^2 + |\alpha_{11}|^2 .= 1$ (2)

Before the measurement, the state of the two qubits is uncertain. After the measurement, the state is certain i.e., $|00\rangle$, $|01\rangle$,$|10\rangle$ and $|11\rangle$. If only the first bit is observed,

The probability for the first qubit is 0

$$P_0' = |\alpha_{00}|^2 + |\alpha_{01}|^2 \quad (3)$$

Similarly, probability for 1 is

$$P_1' = |\alpha_{10}|^2 + |\alpha_{11}|^2 \quad (4)$$

Sum of the two probabilities is unity

Therefore, $P_0' + P_1' = 1$ (5)

Let $|\psi_0'\rangle$ and $|\psi_1'\rangle$ be the states after the measurement when the first qubits are 0 and 1 respectively. These states are given by

$$|\psi_0'\rangle = \frac{\alpha_{00}|00\rangle + \alpha_{01}|01\rangle}{\sqrt{|\alpha_{00}|^2 + |\alpha_{01}|^2}} \quad \text{and} \qquad (6)$$

$$|\psi_1'\rangle = \frac{\alpha_{10}|10\rangle + \alpha_{11}|11\rangle}{\sqrt{|\alpha_{10}|^2 + |\alpha_{11}|^2}} \qquad (7)$$

Similarly, for the measurement for second qubit

The probability for second qubit to 0 and 1.

$$P_0'' = |\alpha_{00}|^2 + |\alpha_{10}|^2 \qquad (8)$$

$$P_1'' = |\alpha_{01}|^2 + |\alpha_{11}|^2 \qquad (9)$$

and the sum of the second probability is unity (1)

Therefore $P_0'' + P_1'' = 1$ (10)

The corresponding states after measurements are

$$|\psi_0''\rangle = \frac{\alpha_{00}|00\rangle + \alpha_{10}|10\rangle}{\sqrt{|\alpha_{00}|^2 + |\alpha_{10}|^2}} \quad \text{and} \qquad (11)$$

$$|\psi_1''\rangle = \frac{\alpha_{01}|01\rangle + \alpha_{11}|11\rangle}{\sqrt{|\alpha_{01}|^2 + |\alpha_{11}|^2}} \qquad (12)$$

Now, let us consider special state of two qubits system with $\alpha_{00} = \alpha_{11} = \frac{1}{\sqrt{2}}$ and $\alpha_{01} = \alpha_{10} = 0$ .This state is called **Bell state** and this pair of qubit is called EPR (Einstein, Podolsk and Rosen) pair

When the two qubit system is in the Bell state, the probability of first qubit as 0 is $\frac{1}{2}$ and that of 1 is $\frac{1}{2}$. Therefore, after measurements, states are $|\psi_0'\rangle = |00\rangle$

$$|\psi_0'\rangle = \frac{\alpha_{00}|00\rangle + \alpha_{10}|10\rangle}{\sqrt{|\alpha_{00}|^2 + |\alpha_{10}|^2}}$$

$\alpha_{00} = \frac{1}{\sqrt{2}}$ and $\alpha_{10} = 0$

Therefore, $\left|\psi_0^{'}\right\rangle = \dfrac{\frac{1}{\sqrt{2}}|00\rangle + 0|10\rangle}{\sqrt{\left(\frac{1}{\sqrt{2}}\right)^2 + 0^2}} = \dfrac{\frac{1}{\sqrt{2}}|00\rangle}{\frac{1}{\sqrt{2}}}$

Therefore, $\left|\psi_0^{'}\right\rangle = |00\rangle$ (13)

Similarly, $\left|\psi_1^{'}\right\rangle = |11\rangle$ (14)

Likewise, for second qubit

$\left|\psi_0^{''}\right\rangle = |00\rangle$

$$\left|\psi_0^{''}\right\rangle = \frac{\alpha_{00}|00\rangle + \alpha_{10}|10\rangle}{\sqrt{|\alpha_{00}|^2 + |\alpha_{10}|^2}}$$

$\alpha_{00} = \dfrac{1}{\sqrt{2}}$ and $\alpha_{10} = 0$

Therefore, $\left|\psi_0^{''}\right\rangle = \dfrac{\frac{1}{\sqrt{2}}|00\rangle + 0|10\rangle}{\sqrt{\left(\frac{1}{\sqrt{2}}\right)^2 + 0^2}} = \dfrac{\frac{1}{\sqrt{2}}|00\rangle}{\frac{1}{\sqrt{2}}}$

Therefore, $\left|\psi_0^{''}\right\rangle = |00\rangle$ (15)

Similarly, $\left|\psi_1^{''}\right\rangle = |11\rangle$ (16)

These are four special states called Bell states and form an orthonormal basis as

$$|\beta_{00}\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$$

$$|\beta_{01}\rangle = \frac{|01\rangle + |10\rangle}{\sqrt{2}}$$

$$|\beta_{10}\rangle = \frac{|00\rangle - |11\rangle}{\sqrt{2}}$$

$$|\beta_{11}\rangle = \frac{|01\rangle - |10\rangle}{\sqrt{2}}$$

Where the first one $|\beta_{00}\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$ is involved in many quantum computation and quantum information. The quantum state of n qubit system is specified by 2^n amplitudes. So far seven qubit quantum computer has been build.

9. Explain the difference between classical bits and qubits. Explain the process behind the CNOT gate.

Sl.No	Bits	Qubits
1.	The device computes by manipulating those bits using logic gates	The device computes by manipulating those bits using quantum logic gates
2.	A classical computer has a memory made up of bits where each bit hold either a one or zero	A qubits can hold a one, a zero or crucially a superposition of these
3.	Bits are used in classical computers	Qubits are use in quantum computer
4.	Information is stored in bits which take the discrete values 0 and 1	Information is stored in quantum bits. A qubit can be in state $|0\rangle$ and $|1\rangle$, but it can also be in a superposition of these states as $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$. If we think a qubit as a vector, then superposition of state is just vector addition.
5.	Processing of bits are slow	Processing of qubits are faster
6.	Circuit is based on classical physics.	Circuit is based on quantum mechanics

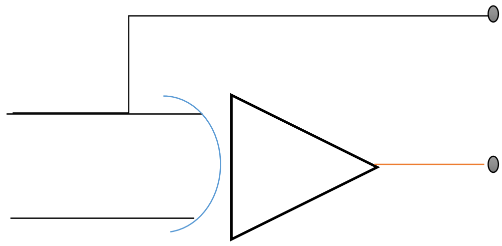
CNOT gate

Principle

CNOT gate means controlled NOT gate. It is a quantum logic gate which plays a vital role in the designing of quantum computers. The CNOT gate will have two qubit operation, wherein the first qubit is referred as the control qubit and the second qubit is referred as the target qubit.

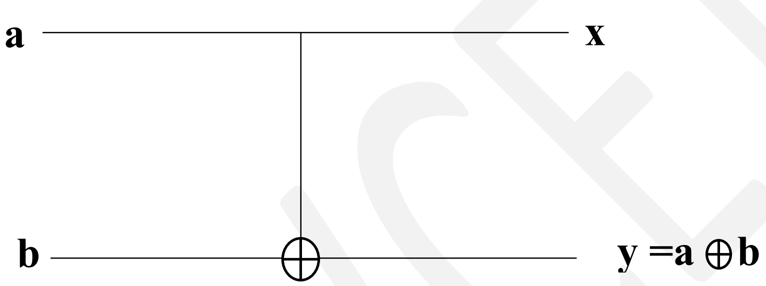
Symbolic Representation

The Symbolic representation of CNOT gate is as shown in figure



Concept

A CNOT gate basically implements a reversible Ex-OR. It can be used to generate entanglement. The CNOT gate can be logically represented as shown in figure.



From figure, we can see that the control (x) and the target (y) are shown as two horizontal lines. Here, we can also notice that the count ‘y’ depends on the input source ‘a’ and is shown by an interconnecting vertical line from ‘a’ to ‘y’ and to one of the inputs of the EX-OR gate i.e., the target input ‘b’ as shown in figure.

Logical operation

Inputs

The input a is typically called the source, and input ‘b’ is known as the target input. Here the x depends on the input a. i.e.,

(i) If source $a = 0$, then control $x = 0$; similarly if $x = 1$, then control $x = 1$.

Thus *the source is called the control input and controls the application of the NOT operation on the target input*

Outputs

The output of CNOT gate is $y = a \oplus b = a\bar{b} + b\bar{a}$

Here y depends on the source a and target b. i.e.,

(ii) If source a =0, Then the output $y = b$ (i.e., 0)

(iii) When the source $a = 1$, then the output y will have inverse value of b

Truth table

INPUT		OUTPUT	
Source/Control input	**Target qubit**	**Control qubit**	**Target output**
a	**b**	**x**	$y = a \oplus b = a\bar{b} + b\bar{a}$
0	0	0	0
0	1	0	1
1	0	1	1
1	1	1	0

Case (i) When $a = 0$ and $b = 0$ or 1, then $y = b$

Case (ii) When $a = 1$ and $b = 0$ or 1, then y will be inverse of b

i.e., the inverted value y is controlled by the source a and hence the gate is named as Controlled NOT gate (or) CNOT gate. Hence the inputs can be uniquely determined from outputs by verifying the reversibility of the gate.

Matrix representation of CNOT gate:

$$\mathrm{CNOT} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}.$$

Quantum Entanglement

From the truth table, we can see that, the target qubit is $|0\rangle$ and the control qubit is either $|0\rangle$ or $|1\rangle$, then the output target y takes the value of control qubit, i.e., it becomes the copy of the control qubit, but control qubit itself does not change.

However, a superposition in the control qubit results in the entanglement of control and target qubits.

Thus, when two or more particles link up in a certain way, no matter how far apart they are in space, their state remains linked. That means they share a common, united quantum state.

So observations of one of the particles can automatically provide information about the other entangled particles, regardless of the distance between them. Any action to one of these particles will invariably impact the other in the entangled system. This united state is known as quantum entanglement.