Modeling Nanowire Transistors in a New Framework for Contribution from Spin

Neema Menon.S [#], Dr. K. A. NarayananKutty [*]

[#] *M.Tech VLSI Design,*
Amrita Vishwa Vidyapeetham University, Coimbatore, India

[*]*Professor, Dept. Of ECE,*
Amrita Vishwa Vidyapeetham University, Coimbatore, India

***Abstract*— This work concentrates on the mathematical modeling of Nanowire Transistors. Nanowire Transistor's density of states characteristics were modelled using differential equation approach utilizing Cauchy's Integral theorem. The spin states were mathematically modelled using multi electron equation and results were closer to practical variation in Voltage-Current characteristics for Silicon nanowires which are presented.**

***Keywords*— VLSI, SNWT, CNT, VLS, MBE, FET, DOS, SCF, CB.**

I. INTRODUCTION

From the VLSI domain point of view, the focus is always on size reduction, area conservation and reducing power dissipation. All these factors accounts for the efficiency of the transistor. this work focuses on modeling Nanowire Transistors. Nanowire transistors have compact size and electron confinement in one dimension. Nanowires have a lateral dimension of about 1nm. Due to their compact size, area efficient designs make use of Nanowire Transistors. Silicon nanowires[1] are focused to be used in next generation MESFETs[5]. Most of the research has been devoted in developing such nanoscale silicon devices. Silicon nanowires have the advantage of compatibility with current Si complementary metal-oxide semiconductor. Due to their compatibility, they can be used in integrated circuit technology. Conductivity of Silicon nanowires can be controlled very well by doping them. Nanowire Transistors have electron confinement in the channel region. Due to the spin polarization effects, Spin states get modified under the control of applied gate voltage. Spin states are modelled in accordance with solution of Cauchy's integral theorem. Their voltage – current characteristics are modelled using the multi-electron equation.

Nanowire[1] is a wire like structure with a diameter or lateral dimension of 1nanometer. Materials used for fabricating nanowires are Ag, Cu (metals), Si, Ge, GaAs, GaN (semiconductors) etc. Applications are in Nanowire transistors, Nanowire memory cell, Nanowire LED etc. If we compare Nanowires with the carbon nanotubes, Nanodevices have high integration density. Due to the device scaling the parameters such as threshold voltage and on/off current are being affected. CNTs and semi conducting nanowires acts as active components. CNT based applications are hindered due to difficulties in fabricating uniform carbon nanotubes. CNTs have several nanometers of length. Nanowires can be fabricated with distinct chemical composition, structure, size and morphology. From the fundamental physics point of view, low dimensional nanowire structure is an ideal platform to probe the properties due to reduced device size and ideal material properties. With the addition of each electron coloumb energy will be greater than thermal energy. Therefore electrical properties are determined by chemical composition. Fabrication of nanowires is by a process called VLS (Vapour Liquid Solid process).

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Fabrication of Silicon nanowires[2] is step by step process which is given below:

Step 1: p-type bulk silicon substrate is used as a starting material.

Step 2: Local Oxidation Of Silicon is done. As a result Si3N4 is deposited by electron beam lithography as a hard mask to protect underlying silicon from source or drain doping and gate etching.

Step 3: Highly doped As source or Drain implantation is done.

Step 4: After SiO2 deposition and electron beam lithography to define gate region oxide over fin is removed but oxide on source or drain region remains the same.
Step 5: Etching is carried out using Si3N4 hard mask to Sifin and high fanout source or drain regions. Si3N4 was formed to protect fin channel from etching at bottom gate region.
Step 6: Substrate implantation and nitride hardmask removal is done.
Step 7: Cylindrical shape channel is formed.
Step 8: etching, metal deposition and metal patterning is done.

II. NANOWIRE TRANSISTOR

Consider the generic structure of a nanowire transistor[3].

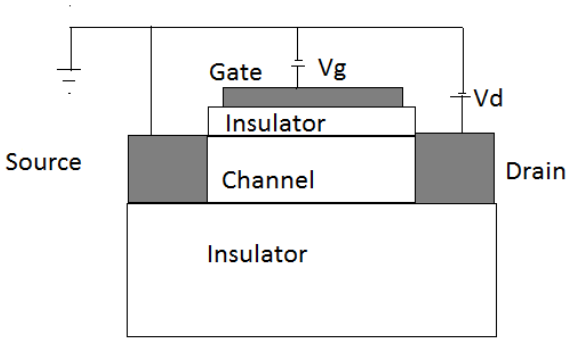

Fig.1 Device structure of Nanowire Transistors

It consists of a semi-conducting channel, separated by an insulating layer made of silicon dioxide isolating the channel from the metallic gate. Insulator thickness should be thick enough to ensure that no current flows to the gate terminal and thin enough to ensure that gate voltage can control the electron density in the channel. Regions marked Source and Drain are the two contact pads which are highly conducting. Resistance of the channel determines the current that flows from source to drain when a drain voltage is applied. The gate voltage is used to control the electrons in the channel. Thus its resistance can be controlled, as a voltage controlled resistor. Difference lies in the channel length which is reduced from micrometre range to one nanometre. So from the VLSI point of view they are more compact and therefore area efficient. To model the flow of current, we have to plot the equilibrium energy level diagram and locate the Fermi level. Current flows when an external battery is connected between the terminals of the device. Thus the contacts will maintain two different Fermi levels. The channel will be driven in to a non equilibrium state. Current can be calculated further. In equilibrium state, average number of electrons in any energy level is typically not an integer but a probability which is given by the Fermi function:

$$f_0(E-\mu) = 1/\{1+\exp\left[\frac{E-\mu}{K_BT}\right]\} \quad (1)$$

where E is the energy level, μ is the Fermi energy and T is the absolute temperature.

Energy levels within a few K_BT of μ are occasionally empty and occasionally full. So the average number of electrons lies between 0 and 1. They cannot exceed 1 because Pauli's Exclusion principle forbids more than 1 electron per level. Conduction depends on the availability of states around E= μ. Battery lowers energy levels μ_1 and μ_2 in the drain contact with respect to source contact and maintains them at distinct levels separated by qV_D.

$$\mu_1 - \mu_2 = qV_D \quad (2)$$

The different electro-chemical potentials give rise to two different Fermi levels. This is because source keeps pumping electrons into it to maintain equilibrium. But equilibrium is not established as drain keeps pulling electrons to establish equilibrium.

Say the Source contact would like to see $f_1(\epsilon)$ electrons. Similarly drain contact $f_2(\epsilon)$ electrons. f_1 and f_2 are Source and drain Fermi functions respectively. N is the average number of electrons at steady state. Net flux across the source contact is proportional to (f_1-N) and net flux across drain contact is proportional to (f_2-N).

Currents across the two terminals are given by

$$I_1 = q\gamma_1/\hbar(f_1 - N) \quad (3)$$

$$I_2 = q\gamma_2/\hbar(f_2 - N) \quad (4)$$

$\gamma_1/\hbar$ and $\gamma_2/\hbar$ are the escape rates at which electrons are initially placed in the level ϵ. It will escape into source and drain contacts respectively. γ_1 and γ_2 have the dimensions of energy. At steady state, there is no flux into or out of the channel. Therefore,

$$I_1 + I_2 = 0 \quad (5)$$

$$N = (\gamma_1 f_1 + \gamma_2 f_2)/(\gamma_1 + \gamma_2) \quad (6)$$

$$I_1 = I = -I_2 = q/\hbar\left[\frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}\right][f_1(\epsilon) - f_2(\epsilon)] \quad (7)$$

Three cases are to be considered:

Case 1: No current flows if $f_1(\epsilon) = f_2(\epsilon)$=1. Fermi Level is below both μ_1 and μ_2.

Case 2: No current flows if $f_1(\epsilon) = f_2(\epsilon)$=0. Fermi Level is above both μ_1 and μ_2.

Case 3: Current flows only when level lies within few $K_B T$ μ_1 and μ_2. Here current flows.

Consider a small voltage applied across the device. Assume $\mu_1 > \varepsilon > \mu_2$.

$$f_1(\varepsilon) = f_0(\varepsilon - \mu) = 1$$

$$f_2(\varepsilon) = f_0(\varepsilon - \mu) = 0$$

$$I = \frac{q}{\hbar}\left[\frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2}\right] = q\gamma_1/2\hbar \quad (8)$$

Since $\gamma_1 = \gamma_2$.

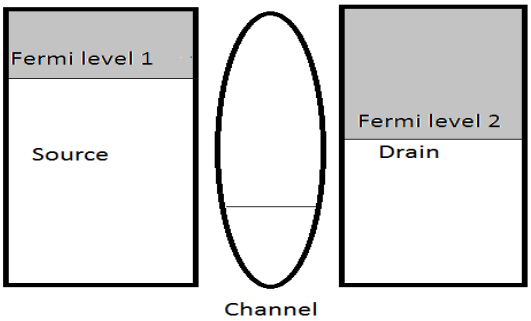

Fig.2 Fermi energy levels in a nanowire transistor after an external applied voltage

III. SPIN MODELING USING DENSITY OF STATES FUNCTION

Density of states equation[4] is given by

$$D_s(E) = \left(\frac{\gamma}{2\pi}\right)/[(E-\varepsilon)^2 + (\gamma/2)^2] \quad (9)$$

For showing the 2 spins which are degenerate (this means having same energy), we need to update the equation as below:

$$D_s(E) = \left(\frac{\gamma}{2\pi}\right)/[(E-0.25)^2 + (\gamma/2)^2] \quad (10)$$

$$D_s(E) = D_s(E) + \left(\frac{\gamma}{2\pi}\right)/[(E+0.25)^2 + (\gamma/2)^2] \quad (11)$$

The same density of states function can be compared to Cauchy's solution for wave equation. Cauchy's solution for wave equation is given below:

$$u(x,t) = \left(\frac{1}{2}\right)[e^{-(x-ct)2} + e^{-(x+ct)2} \quad (12)$$

Density of states function can be related to the equation above as

$$u(x,t) = u(E,\varepsilon) \quad (13)$$

IV. CAUCHY'S PROBLEM FOR WAVE EQUATION

$$U_{tt} = C^2 U_{xx} \quad (14)$$

Where c is a constant, x is the position of the wave and t is the time instant with the arbitrary but fixed initial data.

$$U(x,0) = f(x) \quad (15)$$

$$U_t(x,0) = g(x) \quad (16)$$

Applying Fourier Transform

$$F\{u(x,t)\} = U(k,t) \quad (17)$$

To the system gives

$$\frac{d^2U}{dt^2} + C^2K^2U = 0 \quad (18)$$

$$U(k,0) = F(k) \quad (19)$$

$$\frac{du}{dt} = G(k) \quad (20)$$

The solution of the transformed system is

$$U(k,t) = Ae^{ickt} + Be^{-ickt} \quad (21)$$

Where A and B are constants which are to be determined from the transformed data so that

$$A + B = F(k) \quad (22)$$

$$A - B = \left(\frac{1}{ikc}\right)G(k) \quad (23)$$

Solving for A and B we obtain,

$$U(k,t) = 1/2[F(k)\left(e^{ickt} + e^{-ickt}\right) + \left(\frac{G(k)}{2ick}\right)\left(e^{ickt} - e^{-ickt}\right) \quad (24)$$

Thus the inverse Fourier transform yields the solution

$$u(x,t) = \left[\frac{1}{2}\right)\left[\left(\frac{1}{\sqrt{2\pi}}\right)\int_{-\infty}^{\infty} F(k)\left(e^{ik(x+ct)} + e^{ik(x-ct)}\right)\right]dk + \left(\frac{1}{2c}\right)\left[\left(\frac{1}{\sqrt{2\pi}}\right)\int_{-\infty}^{\infty} F(k)\left(e^{ik(x+ct)} + e^{ik(x-ct)}\right)\right]dk$$

We use the following results:

$$f(x) = \left(\frac{1}{\sqrt{2\pi}}\right)\int_{-\infty}^{\infty} e^{ik(x)} F(k)\,dk \quad (25)$$

$$g(x) = \left(\frac{1}{\sqrt{2\pi}}\right)\int_{-\infty}^{\infty} e^{ik(x)} G(k)\,dk \quad (26)$$

Solution in the final form is given by:

$$u(x,t) = \left(\frac{1}{2}\right)[e^{-(x-ct)2} + e^{-(x+ct)2}] \quad (27)$$

Initial wave is found to split into two similar waves propagating in the opposite direction with unit velocity.

V. SELF CONSISTENT FIELD EQUATION

Current equation for different Fermi levels[6][4] for source and drain is given by:

$$I_1 = I = -I_2 = q/\hbar[\frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}][f_1(\epsilon) - f_2(\epsilon)]$$

(28)

Integrating to obtain a distribution of states:

$$I = q/\hbar \int_{-\infty}^{\infty} dE\, D_s(E)[\frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}][f_1(\epsilon) - f_2(\epsilon)]$$

(29)

If the bias applied is very small, then density of states function is a constant.

$$I = q/\hbar[\frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}] \int_{-\infty}^{\infty} dE\, D_s(E)$$

(30)

The above equation is valid when

$$f_1(\epsilon) - f_1(\epsilon) = 1 \text{ for } \mu_1 \geq E \geq \mu_2, 0 \text{ otherwise}$$

If the bias is small enough and the density of states is assumed to be a constant over $\mu_1 \geq E \geq \mu_2$.

Maximum current and conductance is when

$$\mu_1 - \mu_2 = qV_D$$

(31)

Therefore the conductance is given by

$$G = \frac{q^2}{h}[\frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}]$$

(32)

If $\gamma_1 = \gamma_2$, then the conductance becomes

$$G = q^2/2h$$

(33)

Similarly the number of electrons at steady state is given by

$$N = (\gamma_1 f_1(\epsilon) + \gamma_2 f_2(\epsilon))/(\gamma_1 + \gamma_2)$$

(34)

Number of electrons at steady state for broadened energy levels is given by

$$N = \int_{-\infty}^{\infty} dE\, D_s(E)(\gamma_1 f_1(\epsilon) + \gamma_2 f_2(\epsilon))/(\gamma_1 + \gamma_2)$$

(35)

Here U_L is the Laplace potential. C_E is the total capacitance. E accounts for electrostatic which means forces that the electric charges exert on each other. Total potential energy in the channel = electrostatic potential x charge of an electron.

$$U_L = \left(\frac{C_G}{C_E}\right)(-qV_G) + \left(\frac{C_D}{C_E}\right)(-qV_D)$$

(36)

$$U = U_L + \left(\frac{q^2}{C_E}\right)\Delta N$$

(37)

Here ΔN is the change in number of electrons.

$$q^2/C_E = U_0$$

(38)

Here U_0 is the single electron charging energy. If we include the effect of potential U then we get,

$$N = \int_{-\infty}^{\infty} dE\, D_s(E - U)(\gamma_1 f_1(\epsilon) + \gamma_2 f_2(\epsilon))/(\gamma_1 + \gamma_2)$$

(39)

Similarly the current also gets modified to

$$I = q/\hbar \int_{-\infty}^{\infty} dE\, D_s(E - U)[\frac{\gamma_1\gamma_2}{\gamma_1+\gamma_2}][f_1(\epsilon) - f_2(\epsilon)]$$

(40)

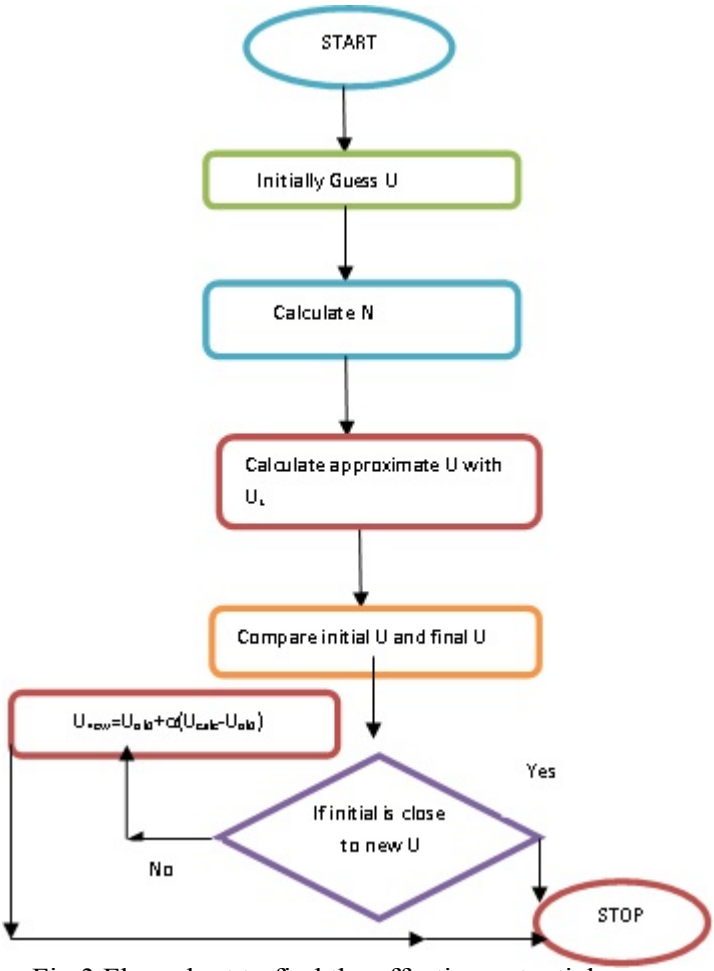

Fig.3 Flow chart to find the effective potential.

VI. MULTI ELECTRON PICTURE

If there are N numbers of spins, there will be 2^N levels introduced. If we consider a single spin, it will be either empty or full[7][8]. So for N spins 2^N levels will be there. Here we are considering 2 spins. So the number of levels will be $2^N = 2^2 = 4$. The 4 levels can be written as 00, 01, 10 and 11. In neutral state, system will be in either 01 or 10 state. So the total energy is given by

$$E_0 = E_{10} = E_{01} \quad (41)$$

One electron energy level =energy levels with nuclear potential + Self-Consistent potential.

$$E_{11} = E_0 + \varepsilon + \frac{U_0}{2} \quad (42)$$

Similarly

$$E_{00} = E_0 - \varepsilon + \frac{U_0}{2} \quad (43)$$

Pauli's exclusion principle forbids the existence of one electron per energy level. Therefore the total probability of electron existence in 00, 01, 10 and 11 states will be equal to 1.

$$\Sigma P_\alpha = 1 \quad (44)$$

$$\Sigma P_\alpha = 1 = P_{00} + P_{01} + P_{10} + P_{11} \quad (45)$$

Addition of an electron in a transition can be defined as affinity and removal of an electron in a transition is called as ionisation. So the rate at which electron enters any level depends on its electron availability. The Exit rate from any level depends on availability of empty states. Here the transitions from 00 state to 01 or 10 states are shown. If it gains an elecron and moves in to 01 or 10 state, then the escape rates of electrons from 00 to 01 or 10 state is given by

$$R(00 \to 01 \text{ or } 10)\frac{\gamma_1}{\hbar}f_1^1 + \frac{\gamma_2}{\hbar}f_2^1 \quad (46)$$

Transitions from 01 or 10 to 00 has a different escape rate given by

$$R(10 \text{ or } 01 \to 00) = \frac{\gamma_1}{\hbar}(1 - f_1^1) + \frac{\gamma_2}{\hbar}(1 - f_2^1) \quad (47)$$

Here

$$f_1^1 = f_0(\varepsilon_1 - \mu_1) \quad (48)$$

$$f_2^1 = f_0(\varepsilon_1 - \mu_2) \quad (49)$$

Here the transitions from 01 or 10 states to 00 state are shown. If it gains an elecron and moves in to 11 state, then the escape rates of electrons from 01 or 10 state to 11 is given by

$$R(01 \text{ or } 10 \to 11) = \frac{\gamma_1}{\hbar}f_1^{11} + \frac{\gamma_2}{\hbar}f_2^{11} \quad (50)$$

Transitions from 11 to 10 or 01 has a different escape rate given by

$$R(10 \text{ or } 01 \to 11)\frac{\gamma_1}{\hbar}(1 - f_1^{11}) + \frac{\gamma_2}{\hbar}(1 - f_2^{11}) \quad (51)$$

Here $f_1^{11} = f_0(\varepsilon_2 - \mu_1)$ (52)

$$f_2^{11} = f_0(\varepsilon_2 - \mu_2) \quad (53)$$

$$\varepsilon_2 = \varepsilon + \frac{U_0}{2} \quad (54)$$

$\varepsilon_2 > \varepsilon_1$ since it requires more energy to add an electron when an electron is present already due to interaction energy. Using the rate constants we can find the probabilities of transistions from one level to other level.

$$\frac{P_{10}}{P_{00}} = (\gamma_1 f_1^1 + \gamma_2 f_2^1)/(\gamma_1(1 - f_1^1) + \gamma_2(1 - f_2^1)) \quad (55)$$

$$\frac{P_{11}}{P_{10}} = (\gamma_1 f_1^{11} + \gamma_2 f_2^{11})/(\gamma_1(1 - f_1^{11}) + \gamma_2(1 - f_2^{11})) \quad (56)$$

$$P_{00} = P_{11} = 1$$

$$P_{01} = P_{10} = 0$$

Fermi functions get modified as shown below:

$$f_0(E - \mu) = 1/\{1 + (\frac{1}{\vartheta})\exp\left[\frac{E - \mu}{K_B T}\right]\} \quad (57)$$

Here ϑ is the degeneracy factor. ϑ =2 means it has 2 spin degeneracy levels[9][10].

We can see that if U_0 is very much greater, the current voltage characteristics in SCF region and CB region differ. More distortions are found in CB region. If U_0 is smaller, current voltage characteristics does not differ a lot. It has least amount of distortions or noise. These distortions can be explained with the Cauchy's solution for wave problem.

$$u(x,t) = \left(\frac{1}{2}\right)[e^{-(x-ct)u} + e^{-(x+ct)u} \quad (58)$$

'C' accounts for all distortions in the wave. We assume C=1 for distortionless wave. In the CB regions distortions are accounted by the equation below:

$$U = U_L + \left(\frac{q^2}{C_\Sigma}\right)\Delta N \quad (59)$$

Here ΔN represent the change in number of electrons due to surrounding effects, ie due noise from the surroundings.

VII. RESULTS AND DISCUSSION

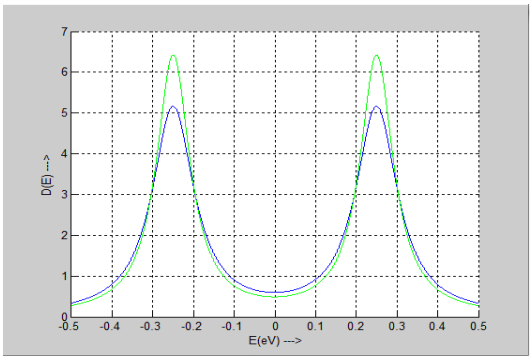

Fig. 4 Density of states characteristics for γ =0.5 and α=2

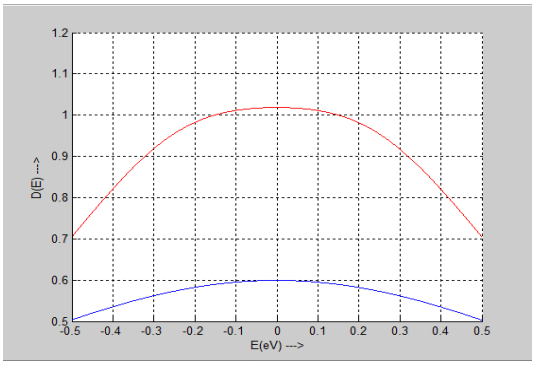

Fig. 5 Density of states characteristics for γ =1 and α=1

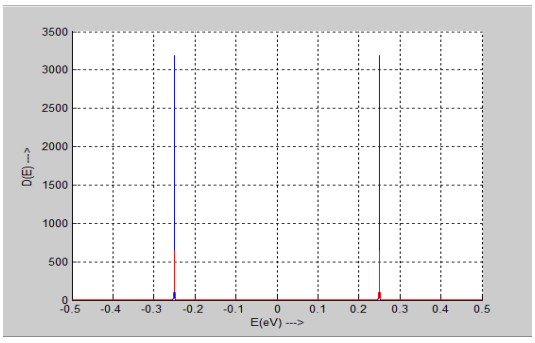

Fig. 6 Density of states characteristics for γ =0.01 and α=100

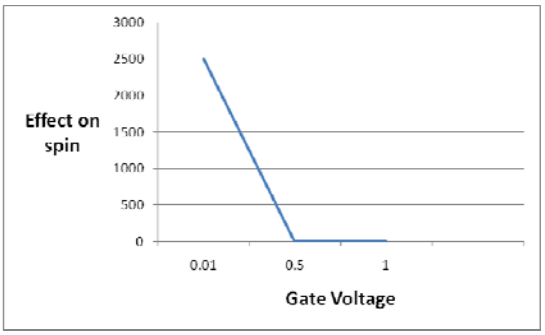

Fig.7 Effect on Spin versus Gate voltage plot

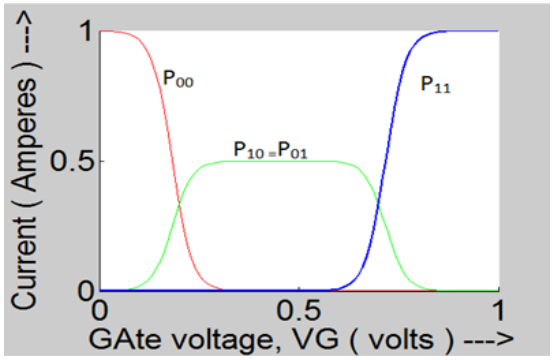

Fig. 8 Current-gate voltage characteristics

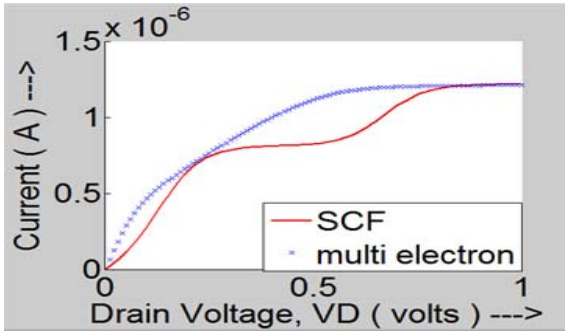

Fig. 9 Current-voltage characteristics for greater values of U_0

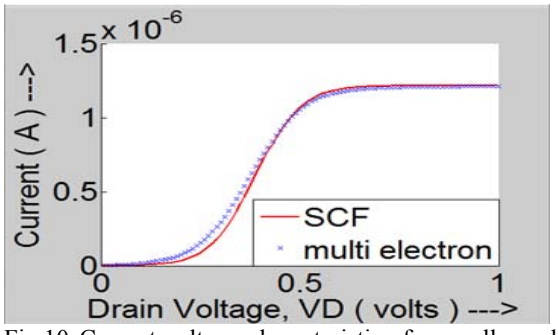

Fig.10 Current-voltage characteristics for smaller values of U_0

As the value of γ decreases, the value of c increases and noise will become more and more prominent. Here we can see the difference in density of states function amplitude. This is due to the value of c. c includes the effect of noises in the propagating waves. As the value of γ decreases, the value of c increases.

'C' accounts for all distortions in the wave. We assume C=1 for distortionless wave. In the CB regions distortions are accounted by the equation below:

$$U = U_L + \left(\frac{q^2}{C_\Sigma}\right)\Delta N$$

Here ΔN represent the change in number of electrons due to surrounding effects, ie due noise from the surroundings.

VIII. CONCLUSION AND FUTURE WORK

We can see that probability of finding an electron at the 2 spin states is high and at middle level the probability of finding an electron is very low. We can see that if U_0 is very much greater, the current voltage characteristics in SCF region and CB region differ. More distortions are found in CB region. It has least amount of distortions or noise. These distortions can be explained with the Cauchy's solution for wave problem. If U_0 is smaller, current voltage characteristics does not differ a lot. They tend to be more or less similar. Nanowire transistors were modelled mathematically using mathematical equations. Nanowire Transistors were modelled using differential equation approach utilizing C Cauchy's Integral theorem. The spin states were mathematically modelled using multi-electron equation and results were closer to practical variation in Voltage-Current characteristics. Analysis of the Voltage-Current characteristics in the Coulomb Blockade region and Self Consistent Field region were done. For lower energy both the regions had similar Voltage-Current characteristics whereas for higher energy the Self Consistent Field region has distortion in characteristics compared to Coulomb Blockade region which is close to practical variation.

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