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QUANTITATIVE EXPERIMENTATION OF CURRENT DENSITY IN NANOSCALE DEVICE FROM COMPLEX RANDOM ENERGY USING GREEN'S FUNCTION FORMALISM

Asif Hassan

Student, Khulna University of Engineering & Technology, Khulna, Bangladesh
Email: hassanstrong_08@hotmail.com

ABSTRACT

A realistic prediction of carrier transport is the noble achievement in nanodevices inflamed by non-equilibrium Green's function method (NEGF). Recursive algorithm is one of the convenient implementation of tracing electron transport through the device of measuring current density .Starting from the charge density the current passed through the infinitesimal device can be calculated from complex random channel energy matrix assuming uniform dimension.

Keywords: Carrier transport, non-equilibrium Green's function method, recursive algorithm, current density, charge density, complex random channel energy.

INTRODUCTION

In semiconductor physics the essential ingredient is extensively signified into the working facts of nanoscale device engineers. Electrons and holes as semi-classical particles with an effective mass were suitable for their quantum behavior measurement. Quantum mechanics which are beginning to play a progressively important role in conventional metal oxide semiconductor devices performance as it contracts below the one hundred nanometer regime [1]. Graphene itself is a 2D nanoscale device one of the tremendous achievement in semiconductor with nanometer size has started entrance into the study of quantum mechanics intensively. Self-consistent solution of a wave equation is used to describe the quantum mechanical transport, Poisson's equation for the statistics of the particle. Landauer-Buttiker formalism is suitable in the absence of electron-electron and electron- phonon interactions [2, 3]. The statistics is embodied into the device by Fermi-Dirac distribution of particles produce from the (source, drain and gate) contacts and the wave equation is in Schrodinger's equation form seen in this formalism [4,5]. Due to scattering mechanism the wave function of an electron loses phase coherence that has an internal degree of freedom named as phonons. An irreversible loss of phase information to phonon degrees of freedom has occurred for phase-incoherent scattering. Loss of phase information is significant when device dimensions become comparable with the scattering lengths because of phonons and phase-breaking mechanisms. One approach provides a good description for nanoscale

devices for accurate modeling named as NEGF. The Boltzmann equation accounts for the energy and momentum relaxation due to scattering mechanisms, in quantum mechanical device modeling under the semi classical device, in otherwise NEGF approach is necessary to account for energy, momentum, and quantum mechanical phase relaxation. Dyson's equation is a very useful quantum mechanical method that relates the Green's function of the full system [6].Calculation of Green's functions of electron and hole respectively (G^n and G^p) solved by an algorithm that is valid for the block tridiagonal form of matrix at first is discussed [7].Using MATLAB simulation electron and hole correlation functions outcome, charge density, current density, current density upon uniform dimensional volume of the cascaded frame in nanoscale device is calculated.

METHODOLOGY

The NEGF method is among the most widely employed methods to describe carrier dynamics in open quantum systems [8, 9]. The numerical solution is extremely demanding as basic NEGF equations are complex, mathematically unwieldy. Judgment of NEGF's adequacy for other problems is difficult because a wide range of different approximations for particular devices and situations have been established and employed. In NEGF calculations most common approximation is to make zero all scattering processes [10]. The main equation which dominates over a device is given by [11]:

$$G^R=(E-H_0-\sum^R)^{-1} \quad \text{Eq.(A.1)}$$

$$G^< = G^R \sum^< G^R \quad \text{Eq.(A.2)}$$

$$\sum^< = G^< D^< \quad \text{Eq.(A.3)}$$

$$\sum^R = G^R D^R + G^R D^< + G^< D^R \quad \text{Eq.(A.4)}$$

Where G^R=Retarded Green's functions.

$G^<$=Lesser Green's functions.

$\sum^<$=Lesser self-energies.

D=Sum of all environmental Green's functions.

Now a method is used to simplify the above term is Dyson's equation for G.For this at first subdividing the device layers into two regions Z and Z' .So the Green's function equation for the device is written as from Dyson's equation

AG=I Eq.(A.5)

In matrix form it can be written as

$$\begin{pmatrix} A_{Z,Z} & A_{Z,Z'} \\ A_{Z',Z} & A_{Z',Z'} \end{pmatrix}\begin{pmatrix} G_{Z,Z} & G_{Z,Z'} \\ G_{Z',Z} & G_{Z',Z'} \end{pmatrix} = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} \quad \text{Eq.(A.6)}$$

Where G=$\begin{pmatrix} G_{Z,Z} & G_{Z,Z'} \\ G_{Z',Z} & G_{Z',Z'} \end{pmatrix}$

Recursive algorithm is one of the solution procedure of Green's function.At first retarded Green's function is calculated by[6]:

$P=A_{z/,z/} - A_{z/,z} * gLz_{z,z} * A_{z,z/}$ Eq.(A.7)

$gLZ^{/}_{(z/,z/)}=1/P$ Eq.(A.8)

Then full Green's function is calculated by[6]:

$G_{z,z}=gLZ_{z,z}+ gLZ_{z,z} *(A_{z,z/} * G_{z/,z/} * A_{z/,z}) * gLZ_{z,z}$ Eq.(A.9)

Again upto n layer of our device's G^n is calculated by the recursive algorithm of Green's function is

$gnLZ^{/}_{(z/,z/)}=\left(gLZ^{/}_{(z/,z/)} {}^{in}_{z/}\right)*\left[\sum^{in}_{z/,z/} + {}^{in}_{z/}\right]$conjugate$(gLZ^{/}_{(z/,z/)})$ Eq.(A.10)

Where $\sum^{in}_{z/,z/}$=In-scattering self-energy of diagonal element.

${}^{in}_{z/}=A_{z/,z} * gnLz_{z,z}$ *conjugate$(A_{z,z/})$

At last full electron correlation function in terms of left- connected Green's f unction is calculated [6]:

$G^n_{z,z} = gnLZ_{(z,z)} - [\, gnLZ_{(z,z)} *$ conjugate$(A_{z,z/})$*conjugate$(G_{z/,z})\,]$-$gLz_{z,z}$

$* A_{z,z/} * G^n_{z/,z}$ Eq.(A.11)

Where $G^n_{z/,z} = - G_{z/,z/} * A_{z/,z} * gnLZ_{(z,z)} - [G^n_{z/,z/} *$conjugate$(A_{z/,z}) *$ conjugate$(gLz_{z,z})]$

Now lower diagonal Green's function $G^n_{z/,z}$ and main Green's function is calculated by substituting $G^n_{z/,z}$ into above equation .From this the charge (n_q(E)) and current density ($J^{n_{q\to q+1}(E)}$) can be measured by [6]:

$n_q(E) = 2\frac{G^n_{q,q}(E)}{2\pi}$ Eq.(A.12)

Here $G^n_{q,q}$ (E) = $G^n_{z,z}$.

$J_{q\to q+1}(E) = \frac{ie\,\hbar}{2m\alpha} 2\,\frac{1}{2\pi}\left[G^n_{q,q+1}(E) - G^n_{q+1,q}(E)\right]$ Eq.(A.13)

where q=Z and q+1=$Z^{/}$

$Z, Z^{/}$ = Upper diagonal elements.

$Z^{/}, Z$ =Lower diagonal elements.

$Z^{/}, Z^{/}$ = Diagonal elements.

e=Electron's charge=$1.6*10^{-19}$ coloumb.

ħ = Reduced Plank's constant =$1.054*10^{-34}$(J s.)

m=Electron's mass=$9.11*10^{-31}$ kg.

a=Grid spacing=5 (uniform).

$G^n_{q,q+1}$ (E) = $G^n_{z,z/}$ = Upper diagonal electron Green's function.

$G^n_{q+1,q}$ (E)= $G^n_{z/,z}$ = Lower diagonal electron Green's function.

i=Indicates complex value.

The charge and current density per unit volume is measured. Then current passing through the device is found if the volume is known. For uniform dimension in a 3D device (if its dimension is equal to L/2 in all three direction) the volume can be written as

V= $(L/2)^3$ Eq.(A.14)

And current can be calculated through channel which is molded from number of numerous frames

I=$\sum_i^f J_n(i) * V$ Eq.(A.15)

Where f=number of nanoscale frame is used in the device.

The row matrix of the current which pass through the device is

I (k) =J_n (k)*V k=1, 2, 3----length of (Jn) Eq.(A.16)

The current density can be calculated in exponential and logarithm form

J_{ne} (k) =exp(J_n ((k)) Eq.(A.17)

And

J_{ni}(k)=log(J_n(k)) Eq.(A.18)

RESULTS

At first by using recursive algorithm retarded Green's function is designed from random complex value of lower, upper and diagonal matrix co-efficient channel energy ($A_{z/,z}$, $A_{z,z/}$, $A_{z/,z/}$) at meV scale. The diagonal elements should be more than the lower and upper elements. The input are $\sum^{in}_{z/,z/}$, $\sum^{out}_{z/,z/}$ (Out-scattering self-energy of diagonal element), above noted matrix co-efficient elements and size of matrix (N_p=7) otherwise output are electron Green's function parameters. In this stage we have observed electron Green's function response for given random diagonal matrix co-efficient of channel energy.

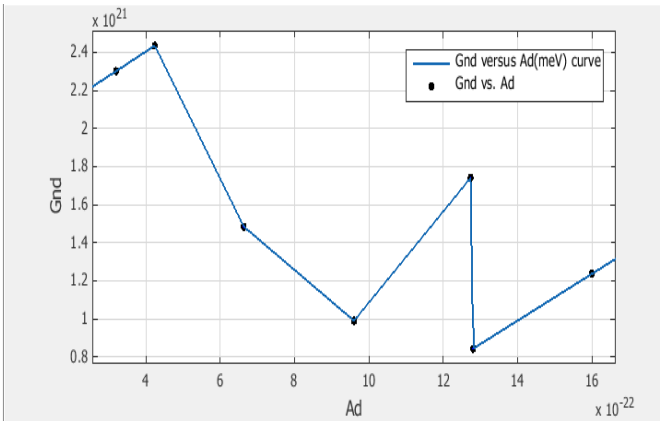

Fig. A.1: Electron Green's function response versus diagonal matrix co-efficient of channel energy (meV).

The Green's function response become worsening as the channel energy of diagonal element increasing. At 7.96+5.12i meV the Green's function response is $1.7407*10^{21}$.Then we have observed the charge density for lower diagonal elements

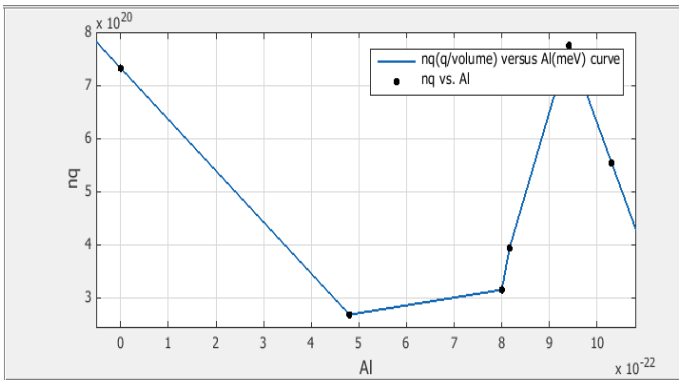

Fig. A.2: Charge density (q/volume) for electron versus lower diagonal matrix co-efficient of channel energy (meV).

The maximum charge transferred through the channel is $5.5409*10^{20}$ coulomb /volume at 6.43+2.6i meV channel energy. Here $2.6853*10^{20}$ coulomb /volume is the minimum charge transfer through our designed device. We have also experimented for upper diagonal matrix co-efficient of channel energy which shows sinusoidal behavior over the device.

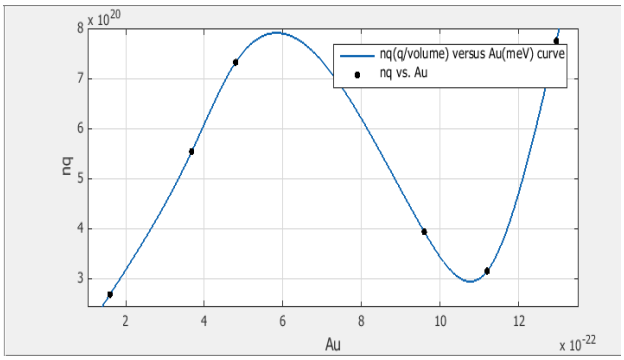

Fig.A.3: Charge density (q/volume) for electron versus upper diagonal matrix co-efficient of channel energy (meV).

By using previous value, on electron Green's function response we have calculated the current density per unit volume for corresponding lower diagonal matrix co-efficient of channel energy.

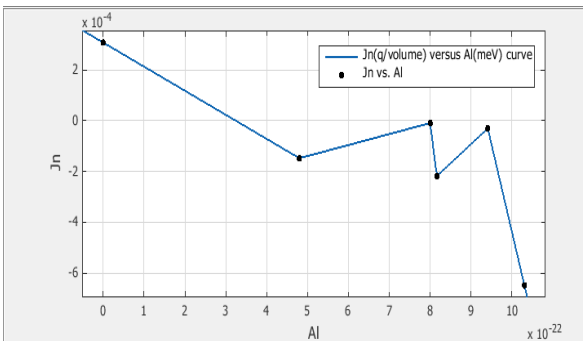

Fig.A.4: Current density (A/volume) for electron versus upper diagonal matrix co-efficient of channel energy (meV).

From the above figure it can be observed that the maximum positive current (because Green's function amplitude response is complex) through the device is 0.3072mA.We have also found negative current for taking Jn as a complex value. Later we have taken also current density for upper diagonal element.

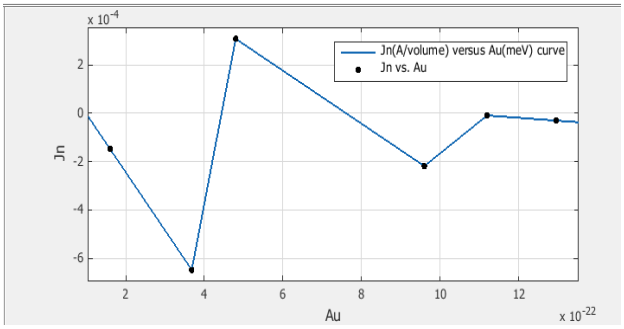

Fig.A.5: Current density (A/volume) for electron versus upper diagonal matrix co-efficient of channel energy (meV).

At last we have observed the current passing through our device (cascade of many small frames) for their corresponding frame number. We have also measured the total current 0.0117A through cascaded form of many small frames. As the number of frame is used the current is increased.

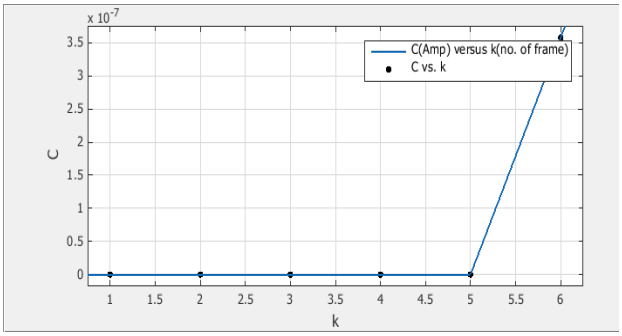

Fig.A.6: Current (A) for electron pass versus number of small frame (k) used in our device.

CONCLUSION

In this paper we have mainly amplified the application of Green's function formalism in nanoscale device.It is used to characterize the device operating condition efficiently than semi-classical techniques. There is some problem in our simulation such like negligible and negative current because of random and complex value of channel energy but which more than in practical in our laboratory is. We have also taken exponential and logarithm value of current density which gives constant value. Upon this the quantum capacitance can be well designed and really movement of electron can be explored.

REFERENCES

1. D.Frank,R.Dennard,E.Nowak,P.Soloman,Y.Taur,and H.-S.Wong, "Device scaling limits of Si MOSFETs and their application dependencies"Proc.of the IEEE,vol.89,pp.259-288,2001.
2. M. Buttiker , Phys.Rev. B 46 , 12485-12507 (1992) .
3. S. Datta ,"Electronic Transport in Mesoscopic Systems",Cambridge University Press, Cambridge,UK , (1997) .
4. R .Lake, G .Klimeck, R .C.Bowen and D .Jovanovic, J. Appl. Phys. 81, 7845 (1997) .
5. G . Klimeck, D . Blanks and R . Lake, "Nanoelectronic Modeling Tool (NEMO) , User 's Manual and Reference Guide", Raytheon, 1998 .
6. M. P. Anantram , Mark S. Lundstrom, Fellow IEEE ,and Dmitri E. Nikonov, "Modeling of Nanoscale Device", 0018- 9219, Vol. 96, No. 9, September 2008 .
7. A.Svizhenko, M . P.Anantram,T. R.Govinda n, B. Biegel, and R.Venugopal, "Two dimensional quantum mechanical modeling of nano transistors", J. Appl. Phys. vol .91 , p. 2343, 2002 .
8. L.P.Kadanoff and G.Baym,"Quantum Statistical Mechanics",(Benjamin, Menlo Park, CA, 1962).

9. L. V. Keldysh, Sov. Phys. JETP 20, 1018 (1965) .
10. T. Kubis, P. Vogl, "Assessment of approximations in n onequilibrium Green's function theory", PhysRevB.83.195304, 2011.
11. H. Haug and A.-P. Jauho, "Quantum Kinetics in Transport and Optics of Semiconductors" (Springer, Berlin, 1996).