International Journal of Electrical and Electronics Research ISSN 2348-6988 (online)
Vol. 3, Issue 2, pp: (631-638), Month: April - June 2015, Available at: www.researchpublish.com

Non-Equilibrium Charge Transport in Quantum Dots: NEGF and Single Electron Approaches

[1]Mahesh Koti, [2]Dr.Vinaydatt V Kohir

[1,2] Dept of Electronics and Communication Engineering, PES College of Engineering, Mandya, 574101, India

Abstract: **In this paper we present a quantum transport study of quantum dot in steady state in presence of static gate potential. We consider a quantum dot coupled to the two metallic leads. The quantum dot under study is modelled through Anderson Impurity Model (AIM) and the hopping parameter modulated through voltage drop between leads and the dot central region. Based on the Landauers formula derived from Non Equilibrium Greens Function and Single electron theory, the essential ingredients of transport properties are revealed. We show that the results out of two approaches closely agree with each other.**

Keyword: **GreenFunction, QuantumDot, Single Electron Method, Nanoelectronics.**

I. INTRODUCTION

Consistent scaling of MOSFET device dimensions as per Moore's law as predicted and analysed by ITRS is enforcing introduction of new technology and devices such as Quantum Dots(QD),Carbon Nano Tubes(CNT) and Graphene Nao Ribbon(GNR). These new devices are different in operation and require modelling and study in the light of quantum mechanics. Many mathematical and physical approaches like Time Dependent Density Functional Theory (TDDFT), Many Body Perturbation Theory (MBPT), Scattering Theory and Non-equilibrium Green Function (NEGF) theory are developed by established researchers which can be used in modelling and understanding of these device characteristics. [2, 23, 20, 7, 10, 14, 17, 6, 4, 9, 1, 25, 22, 12, 15, 19, 24, 18, 5, 11, 3, 13, 8, 16, 31]. Application of these devices requires characteristic and performance study under different environmental conditions.In this paper we present the our study of Non-equilibrium steady state V-I characteristics of Quantum dot with static gate potential subjected to magnetic field interaction. Green, Julian Schwinger, Landauer, Kadanoff and Bayem can be considered to be the pioneers of the quantum transport field. Todya many research groups around the world are making their effort and contributions towards this transport study which has lead to many approaches for the study of quantum transport, every approach reveals different characteristics of the transport. The quantum transport cannot be governed by the conventional classical electron transport as it has the flavours of quantum phenomena, one has to consider these quantum phenomena like coulomb blockade and kondo effect to describe the quatnum transport completely.

Landauer derived the expression for quantum current through the application of scattering theory but it is applicable only under equilibrium conditions but for the non equilibrium quantum transport one has to adopt either many-body approach or non equilibrium green function approach with time dependent density functional theory or multiple probe battery method. Every method has its own complexities and intricacies in analysis and implementation, to this list we have one recent method added by schmuel better known with the name of single electron approach. In this paper we adopt this recently proposed single electron method to study the quantum transport through a quantum dot under non equilibrium conditions for steady state case[24].

The system for TD quantum transport study can be prepared through two different approaches leading to two schemes.In one scheme the electrodes are put in equilibrium with the anode and cathode terminals of the battery, but without plugging

any mesoscopic device in between.Current starts to flow when a mesoscopic device is plugged in. In other scheme electrodes are connected to the mesoscopic device and the system i.e mesoscopic device along with electrodes are in equilibrium, current starts to flow when this system is connected to the battery terminals. The former scheme is more suited for landauer transport and the later is best for the DFT. It has been proved that the two schemes closely agree with respect to their results in the non interacting case.

As stated earlier in this work we adopt the recently developed TD quantum transport called single electron approach, to study the fermion transport through the strongly correlated quantum dot. We consider the first scheme of system preparation where both the electrodes will be in equilibrium with battery terminals, the potential difference is established through electrochemical potentials of the set of reservoirs[6].

By investigating the TD evolution of the current through the quantum dot, we find an agreement with Ref NEGF current results. We observe the drop of current through the quantum dot as source to drain voltage increases beyond the critical bias voltage leading to NDR effect[1]. We show the variation in charcteristics NDC curve as a function of the control potential or gate potential. In particular we show that the current equation modelled through NEGF approach takes large value and diverges when a gate potential is applied, whereas the single electron approach leads to converging result.

This is indeed very interesting to see that the current equation modelled through single electron approach shows the NDR under the absence of interactions due to the finite bandwidth of electrodes as put forth by baldea and koppel and as uphold through MPB method study of anna.

Our paper is organised as follows. In the next section we introduce the hamiltonian model of quantum system for our study. In the first part of the section III the I-V characteristics of the non-interacting quantum dot obtained with single electron approach is discussed and results are validated against the NEGF results. Section IV is about the NDC effect with single electron approach in comparision to NEGF results[5].

II. HAMILTONIAN OF THE QUANTUM SYSTEM

We consider the simplest possible model of the quantum dot interacting with the left and the right electrodes with the chemical potentials μ_l and μ_r respectively which is illustrated tgrough schematic representation in Figure(1). The total hamiltonian H $_{Total}$ of the system is split up into three parts as Central hamiltonian H $_{Cent}$, Contact hamiltonian H $_{Contact}$ and Tunneling hamiltonia H $_{T}$ corresponding to the Quantum dot, electrodes and the coupling respectively.We discuss about each of these terms in the following paragraphs.

$$H_{Total} = H_{Cent} + H_{Tunnel} + H_{Contact} \quad (1)$$

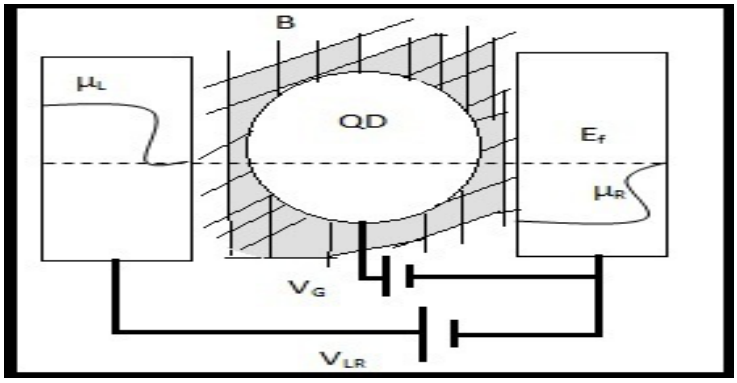

Figure 1: Schematic representation of the quantum dot connected to two metallic leads

A. Central Region Hamiltonian:H $_{Cent}$

We consider the central region to be noninteracting with time dependent energy level which is nothing but the local gate energy that depends on the external gate voltage applied.To keep our analysis simple we are considering the static gate voltage case and making the central region energy independent of Kohn-Sham dynamics and electron phonon interactions.

$$H_{Cent} = V_G(t)c_0^{\dagger}c_0 \quad (2)$$

Here $c_0^{\dagger}$ denotes the electron creation operator , c $_0$ denotes the electron annihilation operator inside the quantum dot and

V $_G$(t) is the gate potential that describes the quantum dot energy level.

B. Contact Hamiltonian:$H_{Contact}$

The left and the right leads are modelled as infinite non-interacting fermionic baths,37â€“39 and are initially assumed to be in equilibrium with chemical potentials μ_l and μ_r respectively, where the difference μ_l-μ_r = ΔV_{lr} is the applied voltage bias. The contacts/leads Hamiltonian is given by

$$H_{Contact} = \sum_{k,l} \varepsilon_{k,l}(t) c_{kl}^{\dagger} c_{kl} + \sum_{k,r} \varepsilon_{k,r}(t) c_{kr}^{\dagger} c_{kr} + \sum_{k,l} \upsilon_0 c_{kl}^{\dagger} c_0 + \sum_{k,l} \upsilon_0 c_{kr}^{\dagger} c_0 \qquad (3)$$

In above equation $\varepsilon_{k,l}$(t) and $\varepsilon_{k,r}$(t) represents energy level of the left and right leads respectively where k corresponds to the k th energy state and the terms c $^{\dagger}_{kl}$, c $_{kl}$ and c $^{\dagger}_{kr}$, c $_{kr}$ stands for the k th state energy level electron creation and annihilation operators inside the left and right leads respectively.υ_0 is the hopping parameter.

C. Coupling Hamiltonian:H_{Tunnel}

The rate at which electrons tunnel from the leads into the central region i.e, the quantum dot depends on the terminal potential applied at the leads in general we can refer the lead with more positive potential as source and the other as drain. the hamiltonian describing this impact is written as[9]:

$$H_{Tunnel} = \sum_{k,l} \upsilon_{k,l}(t) c_{kl}^{\dagger} c_0 + \sum_{k,r} \upsilon_{k,r}(t) c_{kr}^{\dagger} c_0 \qquad (4)$$

The time dependence of the tunneling through the lead potential can be considered very subtle and can be replaced with a constant factor as described through the following equation:

$$H_{Tunnel} = \sum_{k,l} \upsilon_{k,l} c_{kl}^{\dagger} c_0 + \sum_{k,r} \upsilon_{k,r} c_{kr}^{\dagger} c_0 (5)$$

Considering symmetric conditions of tunneling from both sides of the leads and static potential case the above equation reduces to [8].

$$H_{Tunnel} = \sum_{k} \upsilon_c (c_{kl}^{\dagger} c_0 + c_{kr}^{\dagger} c_0 + h.c.) \ (6)$$

III. NON EQUILIBRIUM GREENS FUNCTION (NEGF) APPROACH

The current is established through the quantum dot with biasing of the quantum dot through the left and right leads. the current comprises of two parts the left and the right part due to tunneling of electrons from leads into the quantum dot and from quantum dot into the leads. The current is controlled perimetrically by the tunneling factor, biasing potential and the effective gate field/potential. The quantum mechanism establishing current through the dot under non equilibrium conditions can be described in detail with the green functions. We denote the current entering the quantum dot with $I_E(t)$ and current leaving the quantum dot with $I_L(t)$. Total current $I(t)$ through the quantum dot considering the system to be in linear boundary conditions excluding the external temperature and field impact is average of the two components. Here we are considering the steady state conditions hence

$$I_E(t) = I_E \qquad (7)$$

$$I_L(t) = I_L \qquad (8)$$

$$I(t) = I \qquad (9)$$

The total current through the quantum dot is:

$$I = \frac{I_E + I_L}{2} \qquad (10)$$

Considering the symmetrical coupling on left and right sides of the quantum dot and both leads to be made of same type material, ignoring the direction of charge movement one can establish the following condition.

$$I_E = I_L = \dot{Q} \qquad (11)$$

In the above equation $\dot{Q}$ denotes the rate of charge movement through the quantum dot that is nothing but the current. To compute the total charge flowing through the quantum dot, we need to analyse the elcetron density which is controlled by the field established in the left and right leads connected to the quantum dot and also one must consider the impact of gate potential on the net charge inside the quantum dot. Following set of equations are to arrive at the mathematical description

of this physical phenomena[7]. Net charge inside the quantum dot can be computed as

$$Q = e\langle \aleph \rangle \qquad (12)$$

In the above equation the notation $\langle \aleph \rangle$ denotes the electron/fermion density in the central region or quantum dot and notation e denotes electron charge which is constant, from equations (8) and (9) we can see

$$I_E = I_L = \frac{\partial}{\partial t}\{e\langle \aleph \rangle\}$$

$$I_E = I_L = e\frac{\partial}{\partial t}\langle \aleph \rangle \qquad (13)$$

To compute electron density we use the quantum statistics equation derived from solution of one particle Schrö dinger equation [12].

$$\langle \aleph \rangle = \langle \Psi(t)|^2 \qquad (14)$$

From equation (14) one can observe that to compute the electron density one should compute the system wave function i.e, $\langle \Psi|$. The above equation holds good for both the left and the right electrodes hence the suffix is not taken into account. The wave function can be computed from the Schrödinger equation

$$i\,\partial_t \langle \Psi(t)| = H(t)\langle \Psi(t)| \qquad (15)$$

Substituting equation (14) in (13) and simplifying:

$$I_{E(L)} = e\frac{\partial}{\partial t}\{\langle \Psi|^2\}$$

$$I_{E(L)} = 2e\frac{\partial}{\partial t}\{\langle \Psi|\} \quad (16)$$

from equation(16)

$$I_{E(L)} = -2ie\{H\langle \Psi|\}$$

$$I_{E(L)} = -2ie\{H_{Cent} + H_{Tunnel} + H_{Contact}\}\{\langle \Psi|\} \qquad (17)$$

H $_{Cent}$ and H $_{Contact}$ commutes with the dot wave function [30], considering this into account the above equation is simplified as

$$I_{E(L)} = -2ie\{H_{Tunnel}\langle \Psi| - \langle \Psi|H_{Tunnel}\} \quad (18)$$

In the above equation H $_{Tunnel}$ corresponds to the tunneling hamiltonian for the left and right coupling and the terms $\langle \Psi|$ and $-\langle \Psi|$ corresponds to the non-equilibrium state of the quantum dot due to the potential difference between the dot and the leads, which results in inflow and outflow of electrons through the quantum dots i.e. nothing but the creation and annihilation operation which can be symbolically represented by the fermion annihilation and creation operators of the quantum dot with this one can re write the above equation in terms of tunneling hamiltonian and fermion operators as[13, 30]:.

$$I_{E(L)} = -2ie\{\textstyle\sum_k \upsilon_k\langle c_k^\dagger c_0\rangle - \upsilon_k^*\langle c_0^\dagger c_k\rangle\} \quad (19)$$

To solve the above equation to analyse the relation between current through the quantum dot ,bias potentials and tunneling parameters in quantized fields we use the propagation functions or green functions a technique primarily investigated by Schwinger and further applied explicitly by many in their theoretical work of non equilibrium quantum transport study [2, 7, 27, 8, 8, 28].

Here we introduce two green functions considering potential or energy variation into account as:

$$G^<_{(k,0)}(\varepsilon) = i\langle c_k^\dagger c_0\rangle$$

$$G^<_{(0,k)}(\varepsilon) = i\langle c_0^\dagger c_k\rangle \qquad (20)$$

Green function complex conjugation property states that

$$G^<_{(k,0)}(\varepsilon) = -[G^<_{(0,k)}(\varepsilon)]^* \qquad (21)$$

with above property of green function and using equation (22) current through the quantum dot (21) can be expressed as

$$I_{E(L)} = -2ie\{\sum_k \upsilon_k G^{<}_{(k,0)}(\varepsilon)\} \qquad (22)$$

to compute the contribution of left and right leads to the central quantum dot current we need to evaluate the lesser green function $G^{<}_{(k,0)}(\varepsilon)$ which can be accomplished using contour tracing but it is complex. The complexity of contour tracing can be simplified by converting contour into real time integrals and this procedure is known by the name of analytic continuation. We follow here Langreth formulation [26] as discussed earlier we consider the energy or potential dependence of the current hence we take the Langreth formulation for energy ignoring temporal dependency as we are interested in steady state rather than the dynamic response and also we ignore the energy state and write a general form of the lesser green function as.

$$G^{<}(\varepsilon) = \int_{-\infty}^{\infty} \upsilon^{*}[G^{R}(\varepsilon)\mathrm{g}^{<}(\varepsilon) + G^{<}(\varepsilon)\mathrm{g}^{A}(\varepsilon)]\, d\varepsilon \qquad (23)$$

where $G^{R}(\varepsilon)$, $G^{<}(\varepsilon)$ are the retarded and lesser green function's respectively of the quantum dot and $\mathrm{g}^{<}(\varepsilon)$, $\mathrm{g}^{A}(\varepsilon)$ are the lesser and advanced green functions respectively for the leads.

$$\mathrm{g}^{<}(t,t') = i\langle c_k^{\dagger}(t')c_k(t)\rangle = if_{(E)L}(\varepsilon)e^{-i\int_{t'}^{t}E(\tau)\,d\tau}\mathrm{g}^{r,a}(t,t') = \mp i\Theta(\pm t \mp t')\langle\{c_k(t), c_k^{\dagger}(t')\}\rangle$$

$$= \mp i\Theta(\pm t \mp t')e^{-i\int_{t'}^{t}\varepsilon(\tau)\,d\tau} \qquad (24)$$

where $f_{(E)L}(\varepsilon)$ is the fermi dirac distribution function of energy given as

$$f_{(E)L}(\varepsilon) = \frac{1}{1+e^{\frac{\varepsilon-\mu}{k_B T}}} \qquad (25)$$

where μ is the chemical potential for the lead, k_B is the Boltzmann's constant and T is temperature of the lead.Substituting for lead green function's and quantum dot system lesser green function from equation (23) and (24) into equation (22).

$$I_{E(L)} = -2eImag\{\sum_k \upsilon_k \int \varepsilon(\tau 1)\, d\tau 1 \times e^{\int \varepsilon(\tau)\,d\tau}\upsilon_k^{*} \times [G^{R}(\varepsilon)f_{(E)L}(\varepsilon) + G^{<}(\varepsilon)]\} \qquad (26)$$

Time limits are not taken into account as we are interested in the steady state current with fixed bias. The discrete sum over the k energy levels can be replaced with integral form of density of states in the leads considering infinitesimal leads. Here we introduce tunneling width function which depends on density function $\rho_{E(L)}$ as

$$\Gamma_{E(L)}(\varepsilon) = 2\pi \sum \rho_{E(L)}(\varepsilon)\upsilon_k\upsilon_k^{*} \times e^{i\int \varepsilon(\tau)\,d\tau} \qquad (27)$$

The general expression for the current due to tunneling of fermions from left or right leads under steady state fixed bias condition is

$$I_{E(L)} = -\frac{ie}{\pi}\int \Gamma_{E(L)}(\varepsilon)(G^{<}(\varepsilon) + f_{E(L)}(\varepsilon)[G^{R}(\varepsilon) - G^{A}(\varepsilon)])d\varepsilon \qquad (28)$$

considering symmetrical conditions on either side of coupling under steady state the total current flowing through the quantum dot as taken from equation(2) is

$$I = \frac{I(E)-I(L)}{2} \qquad (29)$$

the minus sign indicates the current due to leaving of fermions. With the substitution of the current contributions from equation (28) we get the total current expression:

$$I = -\frac{ie}{2\pi}\int \{[\Gamma_E(\varepsilon) - \Gamma_L(\varepsilon)]G^{<}(\varepsilon) + [f_E(\varepsilon)\Gamma_E(\varepsilon) - f_L(\varepsilon)\Gamma_L(\varepsilon)][G^{R}(\varepsilon) - G^{A}(\varepsilon)]\}d\varepsilon \qquad (30)$$

$G^{<}(\varepsilon)$,$G^{R}(\varepsilon)$ and $G^{A}(\varepsilon)$ are defined as[28, 30].

$$G^{<}(\varepsilon) = G^{R}(\varepsilon)\Sigma^{<}G^{A}(\varepsilon)$$

$$G^{R,A}(\varepsilon) = \frac{1}{\varepsilon - V_G - \Sigma^{R,A}}$$

in the above equations $\Sigma^{R,A}$ corresponds to the retarded or advanced self energy of the leads and $\Sigma^{<}$ describes the lesser self energy of the leads which are defined as [28, 13].

$$\Sigma^{R,A} = \sum_k \frac{v_k^2}{\varepsilon - V_G \pm i\Delta}$$

$$\Sigma^{R,A} = \Lambda(\varepsilon) \mp \frac{i}{2}\Gamma(\varepsilon)$$

$$\Gamma(\varepsilon) = \Gamma_E(\varepsilon) + \Gamma_L(\varepsilon)$$

$$\Lambda(\varepsilon) = \Lambda_E(\varepsilon) + \Lambda_L(\varepsilon)$$

$$\Sigma^{<} = \sum_{k,(E)L} v_k^2 g^{<}_{k(E)L}(\varepsilon)$$

$$\Sigma^{<} = i[\Gamma_E(\varepsilon) f_E(\varepsilon) + \Gamma_L(\varepsilon) f_L(\varepsilon)] \qquad (31)$$

The substitution of $\Sigma^{R,A}$, $\Sigma^{<}$ and $G^{R,A}(\varepsilon)$ from equation (31)and(32) with the following manipulation for the product $G^R(\varepsilon)G^{\mathrm{A}}(\varepsilon)$ as

$$G^R(\varepsilon)G^A(\varepsilon) = \frac{G^R(\varepsilon) - G^A(\varepsilon)}{\frac{1}{G^R(\varepsilon)} - \frac{1}{G^A(\varepsilon)}} \qquad (32)$$

we get an expression for total current I as similar to Meir-Wingreen formula for steady state current[30].

$$I = \frac{e}{2\pi}\int \frac{\Gamma_E(\varepsilon)\Gamma_L(\varepsilon)}{[(\varepsilon - V_G - \Lambda(\varepsilon))^2 + \frac{\Gamma^2(\varepsilon)}{4}]} d\varepsilon \qquad (33)$$

where $\Lambda(\varepsilon)$ denotes the vertex function which serves the purpose of weighing the scattering events of fermions [28] and $\Gamma\varepsilon$ denotes coupling of the leads to the quantum dot, there are different types of models for these two parameters which needs to be selected depending on type of the leads (super conducting leads, ferromagnetic leads or metallic leads) and type of the contacts(Single Channel or Multi channel). Here in this paper we are interested in quantum dot coupled with the metallic leads for which the the two parameters are taken as[4, 11, 3]:

$$\Lambda_{E(L)}(\varepsilon) = \frac{v_c^2}{2v_o^2}\varepsilon_{E(L)} \qquad (34)$$

$$\Gamma_{E(L)}(\varepsilon) = \frac{v_c^2}{v_o^2}\Theta(2v_o - |\varepsilon_{E(L)}|)\sqrt{4v_0^2 - \varepsilon_{E(L)}^2} \qquad (35)$$

where $\varepsilon_{E(L)} = \varepsilon - \mu_{E(L)}$, $\mu_{E(L)}$ is the on site potential of the leads E or L.

IV. SINGLE ELECTRON METHOD

Here we present a brief account of the single electron approach for the derivation of non equilibrium steady state current through the quantum dot presented by Shmuel Gurvitz[6]. Total current consists of two components due to the entering and leaving of electrons from the two leads ignoring the displacement current.

$$I = I_E + I_L \qquad (36)$$

where

$$I_E = \Gamma_E Q_o^L - \Gamma_L Q_o^R \qquad (37)$$

$$I_L = \Gamma_L Q_o^E - \Gamma_E Q_o^L \qquad (38)$$

$$Q_o^\beta = \int \rho_\beta(\varepsilon) f_\beta(\varepsilon) d\varepsilon \qquad (39)$$

Γ_E and Γ_L are the tunneling parameters which are similar to the imaginary part of the self energies for the left or right leads, ρ_β is the electron density parameter where β stands for either left(E) or right(L) leads and ε,$f_\beta(\varepsilon)$ represents energy and fermi-dirac distribution respectively. Q_o^β is the charge contributed by the right or left left lead which is computed from the system wave function $|\Psi(t)\rangle$, that is expressed in terms of the single-electron wave functions i.e, slater product as[13, 6]:

$$|\Psi(t)\rangle = \Pi_k \hat{\Phi}^{(k)}(t)|0\rangle \qquad (40)$$

$\hat{\Phi}^{(k)}(t)|0\rangle$ is the k'th state single electron wave function.Considering the slater product applying the schrödinger equation along with quantum commutation rule and simplifying for the amplitude parameters one obtains intermediate equations

for the quantum charge contributed as listed in equation (37).The hamiltonian used in solving the schrödinger equation is the same as used in NEGF i.e, described in section II.Further with the substitution of equations (38),(39) and(40) into equation(37) considering left and the right leads we obtain.

$$I = \int [\rho_E(\varepsilon)\Gamma_L(\varepsilon)f_E(\varepsilon) - \rho_L(\varepsilon)\Gamma_E(\varepsilon)f_L(\varepsilon)]d\varepsilon \qquad (41)$$

The density of electrons contributed by the leads can be computed from the equation

$$\rho_\beta(\varepsilon,t) = \frac{1-2\cos(\varepsilon-\varepsilon_o)te^{-\frac{\Gamma(\varepsilon,t)t}{2}}+e^{-\Gamma(\varepsilon,t)t}}{(\varepsilon-\varepsilon_o)^2+\frac{\Gamma^2(\varepsilon,t)}{4}}\frac{\Gamma_\beta(\varepsilon,t)}{2\pi} \qquad (42)$$

for steady state fixed bias conditions $t \to \infty$ density becomes independent of time and we obtain

$$\rho_\beta(\varepsilon) = \frac{\Gamma_\beta(\varepsilon)}{2\pi[(\varepsilon-\varepsilon_o)^2+\frac{\Gamma^2(\varepsilon)}{4}]} \qquad (43)$$

replacing ε_o with V_G gate potential which is responsible for the dot energy and substituting for $\rho_\beta(\varepsilon)$ into equation (40) one obtains steady state current expression which coincides with Landauer formula.

$$I = \frac{e}{2\pi}\int \frac{\Gamma_E(\varepsilon)\Gamma_L(\varepsilon)}{[(\varepsilon-V_G)^2+\frac{\Gamma^2(\varepsilon)}{4}]}d\varepsilon \qquad (44)$$

in the above equation we have taken charge of electron into consideration as the density of electrons should be weighed to compute current. The numerical computation of the current in equation (45) requires value of $\Gamma(\varepsilon)$ which can be taken from the equation (36).

V. CONCLUSION

One can compare the two steady state current expressions (34) and (45) to find that the only difference between the two is vertex function which represents the real part of the lead's retarded or advanced self energy that accounts for the weighing of the scattering events of the fermions.

REFERENCES

[1] Anti Pekka Jauho, Ned S Wingreen and Yogal Meir,"Time-dependent transport in interacting and noninteracting resonant-tunneling systems ",Phys Rev B., vol. 50,pp. 5528â€“5544, Aug. 1994.

[2] M P.Anantram, Mark S.Lundstrom, Dmitri E.Nikonov,"Modelling of inelastic effects in molecular electronics",Journal of Physics:Conf Series.,vol. 35,pp. 313-323, 2006.

[3] A. Pertsova, M. Stamenova and S. Sanvito,"Coulomb correlations in the tunneling through resonance centersTime-dependent electron transport through a strongly correlated quantum dot: multiple-probe open boundary conditions approach",Journal of Physics: Condensed Matter, Vol.48,2013.

[4] Ioan BÃ¢ldea and Horst KÃ¶ppel, "Sources of negative differential resistance in electric nanotransport",Phys Rev B, vol. 81,pp.193401, 2013.

[5] Yigal Meir and Ned S Wingreen, "Landauer Formula for the Current through an Interacting Electron Region",Phys Rev Letters,vol.68, pp 2512-2515, 1989.

[6] Shmuel Gurvitz, "Single-electron approach for time-dependent electron transport",arXiv,2014.

[7] L Y.Chen and C S.Ting,"Dynamic properties of double-barrier resonant-tunneling structures",Phys. Rev. B, vol.43,issue 3,Jan.1991.

[8] T. V. Ramakrishnan and Patrick A. Lee,"Disordered electronic systems",Reviews of Modern Physics,Vol. 57, No. 2,pp. 287-337,April 1985.

[9] Ned S.Wingreen, Karsten W.Jacobsen and John W.Wilkins,"Inelastic scattering in resonant tunneling",Phys. Rev. B., Vol. 40, pp. 11834, December 1989.

[10] Daniel S.Fischer and P A.Lee,"A Relation Between Conductivity and Transmission Matrix", Phys. Rev. B., Vol 23, PP. 6853, 1981.

[11] Abraham Nitzan,"Electron transmission through molecules and molecular interfaces",arXiv reprint cond-mat, pp. 0102300, 2001.

[12] W. Kohn and L. J.Sham, "Self-consistent Equations Including Exchange and Correlation Effects",Phys. Rev.,vol.140,issue 4A,pp. 1133-1138,1965.

[13] Richard E.Prange,"Tunneling from a many particle point of view",UM Technical Report,pp.1- 14,1992.

[14] L I Glazman and K Matveev,"Coulomb correlations in the tunneling through resonancecenters",JETP Lett, Vol. 48, pp. 445, 1988.

[15] Leo P. Kouwenhoven,Charles M. Marcus, "Electron Transport In Quantum Dots",Proc of Advanced Study Institute on Mesoscopic Electron Transport,pp. 1-110, 1997.

[16] S. H. Son, B. H. Choi, K. H. Cho and S. W. Hwang,"Single-Electron Tunneling Through a Heavily Doped GaAs Quantum Dot", Journal of the Korean Physical Society, Vol. 41, pp. 953-955, December 2002.

[17] R.W.Godby, M.Schlüter and L.J.Sham,"Self-energy operators and exchange-correlation potentials in semiconductors", Phys. Rev. B, Vol. 37, pp. 159-175, June 1988.

[18] A. Levy Yeyati, J. C. Cuevas, A. Lopez-Davalos, and A. Martin-Rodero,"Resonant tunneling through a small quantum dot coupled to superconducting leads", Phys. Rev. B, Vol. 55, pp. 6137-6140, March 1997.

[19] S. Kurth and G. Stefanucci,"Time-dependent bond-current functional theory for lattice hamiltonians:Fundamental theorem and application to electron transport", Journal of Chem Phys, Vol. 391, pp. 164-172, 2011.

[20] Carsten A.Ullrich and Zeng-hui Yang,"A brief compendium of time-dependent density-functional theory",Brazilian Journal of Physics, Vol. 44, pp. 154-188, 2014.

[21] G Stefanucci, S Kurth, A Rubio and EKU Gross,"Time-dependent approach to electron pumping in open quantum systems", Phys. Rev. B, Vol. 77, pp. 075339, 2008.

[22] San-Huang Ke, Rui Liu,Weitao Yang and Harold U. Baranger,"Time dependent transport through molecular junctions", Journal of Chem Phys, Vol. 132, pp. 234105-1, 2010.

[23] A. Aviram and M. A. Ratner,"Molecular Rectifiers", Chemical Physics Lett, Vol. 29, pp. 277-283, 1974.

[24] R. Landauer,"Spatial variation of currents and fields due to localized scatterers in metallic conduction",IBM J. RES. DEVELOP, vol.32, issue 3,pp.306-316,May. 1988.

[25] Julian Schwinger, "On Gauge Invariance and Vaccum Polarization",Phy.Rev, vol.82, issue 5,pp.664-679, June. 1951.

[26] D.C.Langreth,"Linear and Non-linear Electron Transport in Solids",NATO Advanced Study Institute Series,vol.17,series B,pp. 3-18,1976.

[27] S. Datta, "Electronic Conduction in Mesoscopic Systems", Cambridge, U.K.: Cambridge Univ.Press, 1996

[28] G D.Mahan,"Many-Particle Physics",Kluver Academic,3rd edition.

[29] D.Goldhaber-Gordon,Hadas Shtrikman, D Mahalu, David Abusch-Magder, U.Meirav and M.A.Kastner,"Kondo effect in a single-electron transistor",NATURE,vol.391,pp.156-159,Jan.1998.

[30] V Mujica, A Nitzan, Ya Mao, W Davis, M Kemp, A Roitberg and MA Ratner ,"Electron transfer in molecules and molecular wires: geometry dependence, coherent transfer, and control ",Advances in chemical physics ,vol.107,pp.403- 429,199.

[31] Shmuel A.Gurvitz,"Quantum interference in resonant tunneling and spin measurements", IEEE Trans.Nanotechnology, vol. 4,no. 1,Jan.2005.