Non-equilibrium charge transport through quantum dot in magnetic field

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***Abstract*—Magnetic field effects the charge transport in quantum dot.The grain(quantum dot) I-V characteristics are subject to change due to magnetic field, extent of variation in the Quantum Dot I-V characteristics is function of magnetic field strength, size and type of the Quantum Dot. We present the study of the I-V characteristics of the grain in non-equilibrium and steady state conditions in a magnetic field. We use non-equilibrium green function based technique for the computations.**

***Index Terms*—GreenFunction,QuantumDot,Landég-factor,Bohrmagnetron,Nanoelectronics,Kondo effect.**

I. Introduction

The Consistent scaling of MOSFET device dimensions in accordance with Moore's law and 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 Nano Ribbon(GNR)[1]. These new devices are different in operation and require modelling and study in the light of quantum mechanics[10]. Many mathematical and physical approaches like Scattering Theory, Non-equilibrium Green's Function(NEGF) theory, Time Driven(Dependent) Density Functional Theory(TDDFT) along with Many Body Perturbation Theory(MBPT) are developed by established researchers which can be used in modelling and understanding of these device characteristics.Device engineering and application needs the latest approaches of quantum device modelling. Engineers must think about charge carriers as quantum entities at the atomistic scale[2]. Extensive theoretical and practical research work is being conducted since from decades to understand the characteristics and working of nano scale devices. The quantum devices will be working in various environmental conditions like High or Low Temperature, intense magnetic fields

In this paper we present V-I characteristic study of Non-equilibrium steady state quantum transport in magnetic field with NEGF technique.Section II contains discussion about hamiltonian of the quantum system under study, in section III a steady state current expression is derived using NEGF approach and section IV discusses the quantum dot energy level computation and in section V we discuss about the results of simulating the V-I characteristics in magnetic field.

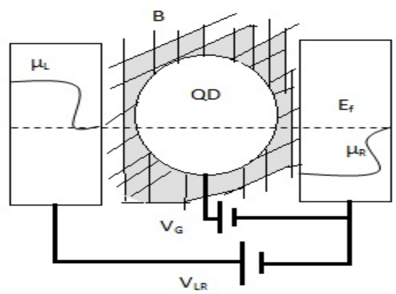

Fig. 1. Schematic representation of the quantum dot in magnetic field

II. Quantum System Hamiltonian Model

System under study consists of a quantum dot made of single impurity connected to two metallic leads represented as right(R or E) and left(L) leads. The two metallic leads are connected to a battery to establish the potential difference such that lead L is at potential level μ_L and lead R is at potential level μ_R, $\mu_L > \mu_R$. A gate probe is used to control the quantum transport through the QD and it is driven with a static potential or voltage V_G, its not considered as a lead. We consider that a magnetic field with energy ε_M is setup in the vicinity of the QD system. Entire setup is shown in figure(1). To analyse the quantum transport characteristics of the quantum dot with NEGF approach a proper hamiltonian description is required. The hamiltonian of the grain(quantum dot) setup under study is described as[7], [13].

$$H_{Total} = \sum H_{Cent} + H_{Tunnel} + H_{\beta} \tag{1}$$

Where H_{Total} on the left side of the equation is the total hamiltonian of the entire setup, H_{Cent} corresponds to hamiltonian of the central region or quantum dot,H_{Tunnel} describes tunneling energy relation between the leads and the grain. Last term H_{β} is for energy description of the quantum leads where β stands for left/right leads.The leads are considered to be metallic, net hamiltonian for the leads that includes contribution from the left and right leads is described as[4], [3], [21].

$$H_{\beta} = \sum_{k,\sigma} \varepsilon^{\sigma}_{k\beta} a^{\sigma\dagger}_{k\beta} a^{\sigma}_{k\beta} + \sum_{k,\sigma} v_o (a^{\sigma\dagger}_{k\beta} a^{\sigma}_{k+1\beta} + h.c.) \tag{2}$$

here ${\varepsilon^{\sigma}}_{k\beta}$ represents the localised energy levels of the electrons in the leads in state k with spin σ and υ_o is the hopping integral; The operator $a^{\sigma\dagger}_{k\beta}(a^{\sigma}_{k\beta})$ creates (annihilates) electron having spin $\sigma(\sigma=\uparrow,\downarrow)$ at lattice point k inside the leads.To keep the analysis simple and to evaluate the magnetic field effect on charge transport through the dot we consider the energy levels inside the quantum dot to be interaction free, with this the hamiltonian describing the central region or quantum dot is[3].

$$H_{Cent} = \sum_{\sigma} \varepsilon^{\sigma}_{id} a^{\sigma\dagger}_0 a^{\sigma}_0 \tag{3}$$

where $a^{\dagger}_0$ denotes the electron creation operator , a_0 denotes the electron annihilation operator inside the quantum dot and $\varepsilon^{\sigma}_{id}$ is the interaction free effective quantum dot energy level. The hamiltonian H_{Tunnel} describes tunneling of charge between the quantum dot and the leads with symmetric tunneling conditions and is given as

$$H_{Tunnel} = \sum_{\beta}\sum_{k} \upsilon_c a^{\sigma}_{k\beta} a^{\sigma\dagger}_0 \tag{4}$$

where $a^{\sigma\dagger}_0$ is electron creation operator inside the dot and υ_c is the hopping integral between the leads(considering same type of leads) and the grain (quantum dot).

III. NEGF and Current calculation:

Quantum dot current is established by the flow of charge carriers to and from the leads in non-equilibrium condition which is set under various conditions like thermal agitation at high temperature, potential difference. To compute the current under such scenarios at nano-scale we use NEGF approach where the electron state in the leads and dot are described by the green functions[9]. The current is computed using the Landauer formula[2], [5], [7], [8], [11].

$$I = -\frac{\imath e}{2\pi}\int\{[\Gamma_E(\varepsilon)-\Gamma_L(\varepsilon)]\boldsymbol{G}^{<}(\varepsilon) \\ +[f_E(\varepsilon)\Gamma_E(\varepsilon)-f_L(\varepsilon)\Gamma_L(\varepsilon)][\boldsymbol{G}^R(\varepsilon)-\boldsymbol{G}^A(\varepsilon)]\}d\varepsilon \tag{5}$$

where e is the charge of electron, $\Gamma_E(\varepsilon)(\Gamma_L(\varepsilon))$ represents energy coupling or tunneling barrier width between the E(L) lead and the quantum dot.$f_E(\varepsilon)$ and $f_L(\varepsilon)$ are the energy band distribution (fermi dirac distribution) functions for the leads E and L respectively.$G^{<}(\varepsilon)$,$G^A(\varepsilon)$ and $G^R(\varepsilon)$ are the lesser,advanced and retarded green functions of the quantum dot which are defined as[14], [7], [5], [15].

$$\boldsymbol{G}^{<}(\varepsilon) = \boldsymbol{G}^R(\varepsilon)\Sigma^{<}\boldsymbol{G}^A(\varepsilon) \\ \boldsymbol{G}^{R,A}(\varepsilon) = \frac{1}{\varepsilon^{\sigma}-\varepsilon^{\sigma}_{id}-\Sigma^{R,A}} \tag{6}$$

in the above equations $\Sigma^{R,A}$ corresponds to the advanced or retarded self energy of the leads and $\Sigma^{<}$ describes the lesser self energy of the leads which are defined as [2], [14], [20].

$$\Sigma^{R,A} = \sum_k \frac{\upsilon_k^2}{\varepsilon^{\sigma}-\varepsilon^{\sigma}_{id}\pm\imath\Delta} \\ \Sigma^{R,A} = \Lambda(\varepsilon) \mp \frac{\imath}{2}\Gamma(\varepsilon) \\ \Gamma(\varepsilon) = \Gamma_E(\varepsilon)+\Gamma_L(\varepsilon) \\ \Lambda(\varepsilon) = \Lambda_E(\varepsilon)+\Lambda_L(\varepsilon) \\ \Sigma^{<} = \imath[\Gamma_E(\varepsilon)f_E(\varepsilon)+\Gamma_L(\varepsilon)f_L(\varepsilon)] \tag{7}$$

The substitution of $\Sigma^{R,A}$, $\Sigma^{<}$ and $G^{R,A}(\varepsilon)$ from equation (6)and(7) with the following manipulation for the product $\boldsymbol{G}^R(\varepsilon)\boldsymbol{G}^A(\varepsilon)$ as

$$\boldsymbol{G}^R(\varepsilon)\boldsymbol{G}^A(\varepsilon) = \frac{\boldsymbol{G}^R(\varepsilon)-\boldsymbol{G}^A(\varepsilon)}{\frac{1}{\boldsymbol{G}^R(\varepsilon)}-\frac{1}{\boldsymbol{G}^A(\varepsilon)}} \tag{8}$$

we get an expression for total current I as similar to Meir-Wingreen formula for steady state current[7].

$$I = \frac{e}{2\pi}\int\frac{\Gamma_E(\varepsilon)\Gamma_L(\varepsilon)}{[(\varepsilon^{\sigma}-\varepsilon^{\sigma}_{id}-\Lambda(\varepsilon))^2+\frac{\Gamma^2(\varepsilon)}{4}]}d\varepsilon \tag{9}$$

where $\Lambda(\varepsilon)$ denotes the vertex function which serves the purpose of weighing the scattering events of fermions [14].The energy functions $\Lambda(\varepsilon)$ and $\Gamma(\varepsilon)$ depends on type of the leads (super conducting leads, ferromagnetic leads or metallic leads) and type of the contacts(Single Channel or Multi channel). In this paper we are conisder the metallic leads for which the the two parameters are taken as[4], [16], [20]:

$$\Lambda_{E(L)}(\varepsilon) = \frac{\upsilon_c^2}{2\upsilon_o^2}\varepsilon_{E(L)} \tag{10}$$

$$\Gamma_{E(L)}(\varepsilon) = \frac{\upsilon_c^2}{\upsilon_o^2}\Theta(2\upsilon_o-|\varepsilon_{E(L)}|)\sqrt{4\upsilon_0^2-\varepsilon^2_{E(L)}} \tag{11}$$

where $\Theta(2\upsilon_o-|\varepsilon_{E(L)}|)$ is the heaviside step function of energy of the lead $\varepsilon_{E(L)}$ and hopping integral υ_o.

IV. Quantum dot or impurity energy level:ε_{id}

Numerical analysis of the quantum dot current requires the lead potential,tunneling width,vertex function and the quantum dot or impurity energy level to be defined[19], [22].Our interest is in the analysis of magnetic field impact on the non-equilibrium current under steady state conditions we consider the partial analysis and computation of the dot energy level considering the empirical values for the rest of three parameters. To simplify the task of vigorous physical and mathematical inspection of the situation under study, we consider the magnetic field interaction impact to be associated with the dot energy level only i.e magnetic energy interaction with the lead energy level is very low in comparison to the dot energy interaction with the magnetic field and we also assume our analysis to be Kondo effect[18] and electron-electron interaction free,i.e.temperature $T << \Gamma(\varepsilon)$ (otherwise kondo effect will be appreciable) and $U=0$(electron-electron interaction energy inside the quantum dot).We use the Kohn-Sham hamiltonian model with local density approximation to compute $\varepsilon_{id}^{\sigma}$[4], [12], [3].

$$\varepsilon_{id}^{\sigma} = V_G + U + \varepsilon_{xc}^{\sigma} + \varepsilon_{m}^{\sigma} \quad (12)$$

the first term is the localised QD energy, which is taken through gate potential[4],second term is the Hartree potential calculated from the electron density, the third term is XC(Exchange Correlation potential) containing the effects of exchange and correlation between electrons,the last or fourth term represents external magnetic field interaction induced energy or potential.As discussed above $U = 0$ and $\varepsilon_{xc}^{\sigma} = 0$ with this the effective potential of the QD is

$$\varepsilon_{id}^{\sigma} = V_G + \varepsilon_{m}^{\sigma} \quad (13)$$

in the above equation V_G is the static gate potential which is established to a fix value and ε_{m}^{σ} is the magnetic field induced delta energy change that depends on the type of the quantum dot(ferromagnetic,semiconductor,graphene,metallic),dimension and geometry of the quantum dot.The parametric dependency of the delta energy change can be modelled as a linear parameter as the experiments shows the linear shift in the quantum dot energy levels when the setup consisting quantum dot is subjected to the magnetic field[6].

The change in the energy level depends on the direction of the magnetic field applied i.e. parallel or perpendicular to the quantum dot. The direction dependency is modelled through the spin, dimensional and geometrical dependency is modelled through the geometrical Landé g-factor, which we denote with g_g. For low dimensional systems the Landé factor strongly depends on the physical dimensions and the magnetic field strength [23]. The dimensional and geometrical dependency of the shift in energy level under magnetic field is noticeable for considerable length and radius of the quantum dots otherwise it is negligible. The variation in energy level of the quantum dot definitely affects the current flow through the quantum dot and its conductance[17]. We model the delta variation in the dot energy level as

$$\varepsilon_{m}^{\sigma} = \sigma g_g \mu_B \quad (14)$$

where σ is the spin factor, g_g geometrical Landé g factor the suffix g is to indicate dimensional and geometrical dependency and μ_B is the Bohr's magnetron. The geometrical Landé g factor is modelled as

$$g_g = g_f g \quad (15)$$

where g is the Landé factor and g_f is the constant to account for the geometry and dimensions of the quantum dot, which we modelled based on the experimental results[23] as.

$$g_f = -1 + e^{(1-\frac{L}{R})} \quad (16)$$

where L denotes the length and R denotes the radius (width) of the quantum dot depending of the quantum dot geometry i.e cylindrical or rectangular dot.If one considers low dimensional quantum dots or quantum dots with few atoms where L and R are approximately close to zero, then $g_f = 1$

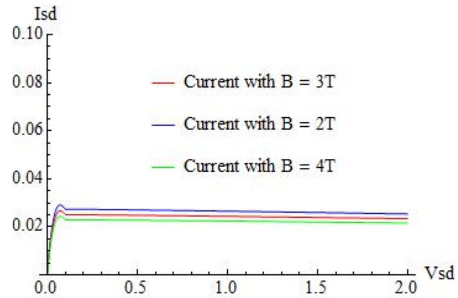

Fig. 2. Quantum Dot I-V plot, for gate voltage (Vg=0), calculated with gf = 2 under variable magnetic field strength with $\sigma = +\frac{1}{2}$

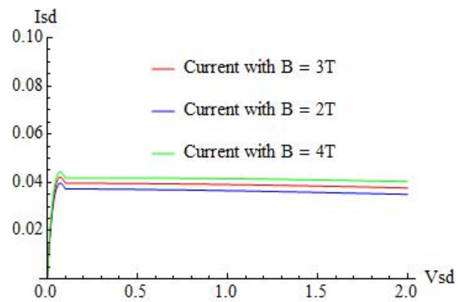

Fig. 3. Quantum Dot I-V plot, for gate voltage (Vg=0), calculated with gf = 2 under variable magnetic field strength with $\sigma = -\frac{1}{2}$

V. RESULTS AND DISCUSSION

In this section we discuss about magnetic field effect on quantum dot I-V characteristics, by applying the current formula derived in section III. To understand the magnetic field impact on I-V characteristics we consider the quantum dot system illustrated in figure (1) with external bias applied i.e under non-equilibrium condition in steady state with zero gate bias. All the results discussed in this section are evaluated for room temperature and for variable magnetic field strength with variable quantum dot dimensions, results are listed in figure(2),(3),(4) and (5) respectively.Other parameters in the expression for current are fixed as $\upsilon_c = -0.1ev, \upsilon_o = -1ev$.

From the graph of Isd versus Vsd in figure and (2),(3),(4) and (5) one can observe that with fixed geometrical dimensions

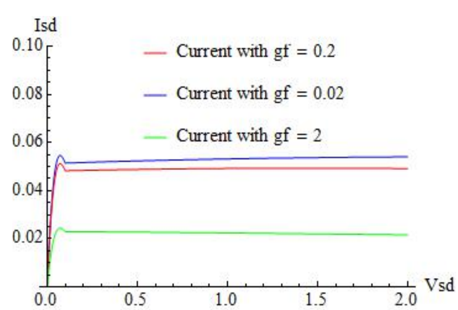

Fig. 4. Quantum Dot I-V plot, for gate voltage (Vg=0), calculated with B = 4T under variable gf with $\sigma = +\frac{1}{2}$

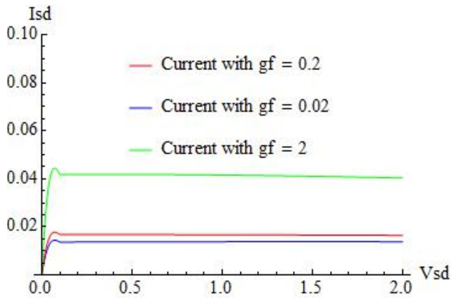

Fig. 5. Quantum Dot I-V plot, for gate voltage (Vg=0), calculated with B = 4T under variable gf with $\sigma = -\frac{1}{2}$

of the quantum dot and variable magnetic field strength with $\sigma = +\frac{1}{2}$ current saturates earlier at higher value (strength) of magnetic field when compared to the lower value(strength), whereas for $\sigma = -\frac{1}{2}$ current saturates earlier at lower magnetic field strength when compared to the higher magnetic field strength.

With fixed magnetic field strength for $\sigma = +\frac{1}{2}$, current saturates earlier at higher geometrical factor g_f strength when compared to the lower geometrical factor g_f, whereas for $\sigma = -\frac{1}{2}$ current saturates earlier at lower geometrical factor g_f when compared to the geometrical factor g_f.

VI. Conclusion

In this paper a modified expression for the quantum dot current has been reported which accounts for the impact of static magnetic field on the dot current. The expression is derived with NEGF approach. The expression is analysed with the simulation under various device dimensions and field strengths. The reported expression can be applied to quantum dot device applications which works in or in the vicinity of the magnetic field.

References

[1] G. I. Bourianoff, J. A. Hutchby, V. V. Zhirnov, and J. E. Brewer,*"Extending the road beyond CMOS"*,IEEE Circuits Devices Mag., vol. 18,pp. 2841, Feb. 2002.

[2] Mark Lundstrom,Anantram, D E.Nikonov,*"On Modeling of nanoscale devices "*,IEEE Proceedings,vol. 96,issue 9,pp. 1511-1550.

[3] Matveev K.A. and Glazman L.I. and ,*"Coulomb correlations in the tunneling through resonance centers"*,JETP Lett, Vol.48,no.7,pp.445-448,1988.

[4] Stamenova, Pertsova and Sanvito, *"Time-dependent electron transport through a strongly correlated quantum dot:multiple-probe open boundary conditions approach"*,Journal of Physics: Condensed Matter, vol. 25,no. 10, p.105501, 2013.

[5] S Datta, *"Quantum devices"*,Journal of Superlattices and Microstructures,vol.6, issue 1, pp 83-93, 1989.

[6] Sebastian Schmitt and Frithjof B. Anders, *"Nonequilibrium Zeeman-splitting in quantum transport through nanoscale junctions"*,Phys. Rev. Lett, vol. 107,2011.

[7] A Pekka Jauho, N S Wingreen and Y Meir,*"Time-dependent transport in resonant-tunneling systems"*,Phys. Rev. B, vol. 50, issue 8,pp.5528-5544, Aug. 1994.

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

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

[10] V Lindberg and B Hellsing,*"Metallic Quantum Dots"*,J. Phys.: Condens. Matter,vol.17,pp. s1075-ss1094,2005.

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

[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] Chen L.Y. and C S.Ting,*"Dynamic prop's of db resonant-tunneling structures"*,Phys. Rev. B, vol.43,issue 3, Jan.1991.

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

[15] Langreth,*"Linear and Non-linear Electron Transport in Solids"*,NATO ASI Series,vol.17,series B,pp. 3-18,1976.

[16] Haobin Wang and Michael Thoss,*"Numerically exact, TD study of correlated electron transport in molecular junctions"*,Journal of Chem.Phys,vol.135,issue.24,pp.244506,Non.2011.

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

[18] D Mahalu,D Goldhaber,Hadas Shtrikman, David Abusch-Magder, U.Meirav and Kastner,*"Kondo effect in a SET"*,NATURE,vol.391,pp.156-159,Jan.1998.

[19] Mohammad K. ELSAID,*"The Energy Spectrum of Two-Electron Semiconductor Quantum Dots"*,Turk J Phys,vol.32,pp.79-84,2008.

[20] Nitzan, V Mujica, Mao, W Davis, M Kemp, A Roitberg and Ratner ,*"Electron transfer in molecules and molecular wires"*,ACP ,vol.107,pp.403-429,199.

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

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

[23] N. Porras and J. R. Meja-Salazar,*"Lande g-Factor and Cyclotron Effective Mass in a Cylindrical GaAs Pillbox Under the Influence Of Magnetic Field"*,R Colomb de Fsica,Vol. 40, No.1, Abril 2008.