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Quantum Transport in Magnetic Field

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***Abstract*—**Charge transport through nanodevices is af- fected by the device geometry and dimensions along with environmental conditions like temperature of operation, ex- ternal electric and magnetic fields.V-I characteristics of the quantum dot are subject to change under the influence of the magnetic field,extent of variation in V-I characteristics of the Quantum Dot are function of magnetic field strength, size and type of the Quantum Dot. We present the model of V-I characteristic equation with study of V-I characteristics of the quantum dot in non-equilibrium and steady state condi- tions in time varying magnetic field. We use non-equilibrium green function based approach for the computations.The time varying magnetic field induces sinusoidal response in the current. The sinusoidal response current is a function of magnetic field strength, type of quantum dot(geometry and material), dimensions of the quantum dot, frequency of the field oscillations and applied lead potential difference.

I. Introduction

Recently theoretical and experimental research commu- nities have shown a good interest in transport properties of one dimensional quantum systems. With consistent scaling and optimization the semiconductor microelectron- ics devices are approaching atomic or molecular scale. Electronics at atomic scale needs to be addressed with new devices that can work with few or single electrons and these new devices cannot be modelled and governed with classical electronics as they reveal many quantum characteristics like coloumb blockade, kondo effect. The study and modelling of these atomic or molecular devices require understanding and application quantum physics.

Charge transport through these devices has been most fascinating part so far where different theoretical tech- niques have been developed like Time Dependent Den- sity Functional Theory(TDDFT), Non-Equilibrium Green Function(NEGF), Generalised Motion of Equation Method (GME), Master Rate Equation method (MRE). Using these methods one can model and study the charge transport through the atomic scale or molecular devices under various environmental conditions like potential non- equilibrium, temperature variation, nuclear spin interaction and external magnetic field. In this paper we present the study and analysis of current voltage (I-V) characteristics of the Quantum Dot(QD) one of the nanodevice or molec- ular scale device, in presence of the sinusoidal magnetic field using NEGF approach.

In section II we present quantum dot system along with its Hamiltonian representation, section III we present model of NEGF current equation, section IV discusses about simulation results and section V is the conclusion.

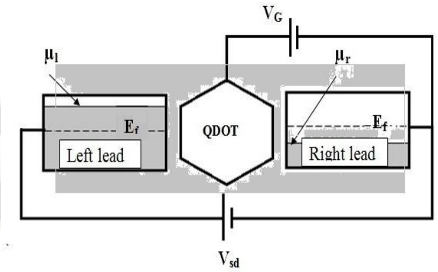


Fig. 1. Quantum dot (nanodevice) in magnetic field, gray colour shade represents magnetic environment

II. Quantum Dot System and Hamiltonian:

We consider the quantum dot coupled to the two metallic leads via tunneling barriers and the QD is also capacitively coupled to the gate.We use anderson impurity model for the quantum dot, whose Hamiltonian can be written as:

$$H_{Total} = \sum_{\sigma} \epsilon^{\sigma}_{id} a^{\sigma\dagger}_{0} a^{\sigma}_{0} + \sum \epsilon^{\sigma}_{k\beta} a^{\sigma\dagger}_{k\beta} a^{\sigma}_{k\beta} + \sum_{k,\sigma} \upsilon_o (a^{\sigma\dagger}_{k\beta} a^{\sigma}_{k+1\beta} + h.c.) + \sum_{\beta} \sum_{k}^{\sigma} \upsilon_{k\beta} a_{k\beta} a^{\dagger}_{0} \quad (1)$$

where the first term represents quantum dot interaction free energy level, second term represents the contact hamiltonian, third term represents tunneling hamiltonian the last term represents energy interaction between the dot and contacts.$\epsilon^{\sigma}{}_{k\beta}$ are the on-site energies of the electrons in the leads in state k with spin σ and υ_o is the hopping integral; $a^{\sigma\dagger}_{k\beta}$ ($a^{\sigma}_{k\beta}$) is the creation (annihilation) operator for an electron with spin $\sigma(\sigma =\uparrow, \downarrow)$ at lattice point k in the leads. $a^{\dagger}_{0}$ denotes the electron creation operator , a_0 denotes the electron annihilation operator inside the quantum dot and ϵ^{σ}_{id} is the interaction free effective quantum dot energy level.To keep the analysis simple and to evaluate the magnetic field effect on charge transport through quantum dot we consider the energy levels inside the quantum dot to be interaction free.

III. NEGF current equation in Magnetic field:

With the application of potential difference between the leads charge transport is initiated for time $t > 0$.The current or charge transport through the dot is a function of various environmental conditions, as we are intended to study the impact of time varying or sinusoidal magnetic field on the charge transport we consider only the magnetic field induced variations in the magnetic field while assuming the other environmental effects to be subtle.NEGF current equation for the quantum dot with a potential difference in a magnetic field can be modelled as:

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

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

$$\Lambda_{E(L)}(\varepsilon) = -\frac{\upsilon_c^2}{2\upsilon_o^2}\varepsilon_{E(L)} \qquad (3)$$

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

Current through the QD is a function of various parameters one of them is dot energy level which depends on the applied potential difference, interactions and external field impact.We perform the partial analysis i.e. we compute the dot energy level considering the empirical values for the rest of three parameters. To simplify the complex mathematical inspection of the situation , we consider the magnetic field interaction only with the dot energy level excluding magnetic energy interaction with the lead energy level. We use the Kohn-Sham hamiltonian with local density approximation to compute ε^σ_{id} [4], [12], [3].

$$\varepsilon^\sigma_{id} = V_G + U + \varepsilon^\sigma_{xc} + \varepsilon^\sigma_m \qquad (5)$$

where first term is the QD on site energy, which acts as gate voltage[4],second term is the Hartree potential , 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.

$$\varepsilon^\sigma_{id} = \varepsilon^\sigma_m \qquad (6)$$

$$\varepsilon^\sigma_m = \sigma g_g \mu_B B \qquad (7)$$

where σ is the spin factor, g_g geometrical Lande´ g factor the suffix g is to indicate dimensional and geometrical dependency,μ_B is the Bohr's magnetron and B is the magnetic field strength. The geometrical Lande´ g factor is modelled as

$$g_g = g_f g \qquad (8)$$ fac

where g is the Lande´
account for the geometry and dimensions of the quantum dot.

$$g_f = -1 + e^{(1-\frac{L}{R})} \qquad (9)$$

where L is the length of the quantum dot and R is the rad ... quantum dot depending on the geometry i.e cylindrical or rectangular ... uantum dots or

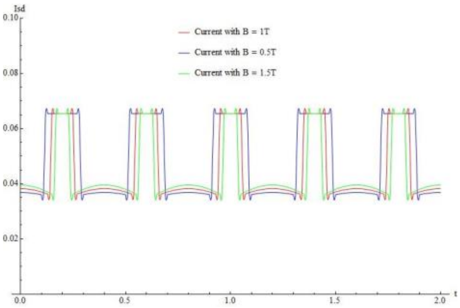


Fig. 2. Quantum Dot I-V plot at gate voltage (Vg=0), calculated with g = 1 under variable magnetic field strength with $\sigma = +\frac{1}{2}$

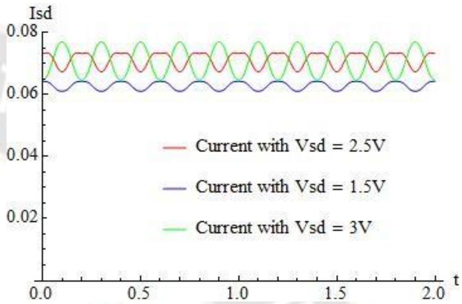


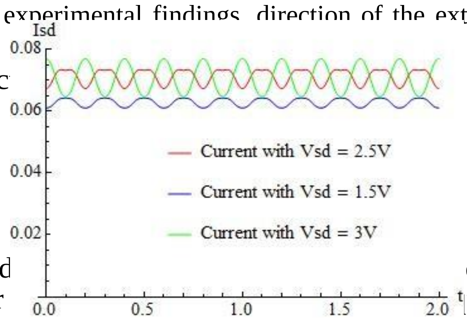
Fig. 3. Quantum Dot I-V plot at gate voltage (Vg=0), calculated with g = 1 under variable potential Vsd and $\sigma = -\frac{1}{2}$

IV. Results and Discussion

In this section we discuss about the effect of time varying magnetic field on V-I characteristics, by applying the current formula of section III. To understand the impact of magnetic field on V-I 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 constant gate bias. All the results discussed in this section are evaluated for different static field values,time varying magnetic field and different quantum dot dimensions and material, results are listed in figure(2),(3),(4),(5),(6),(7) and (8) respectively.Other parameters in the expression for current are fixed as $\upsilon_c = -0.1ev, \upsilon_o = -1ev$.

V. Conclusion

We deduced an expression to relate the I-V characteristic of quantum dot with the geometrical dimensions and the magnetic field. Simulation results are inline with experimental findings, direction of the external magnetic



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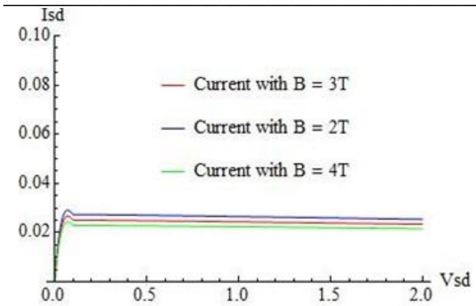

Fig. 4. Quantum Dot I-V plot at gate voltage (Vg=0), calculated with g = 1 under variable potential Vsd and $\sigma = -\frac{1}{2}$

quantum dots with few atoms where L and R are approximately close to zero, then $g_f = 1$

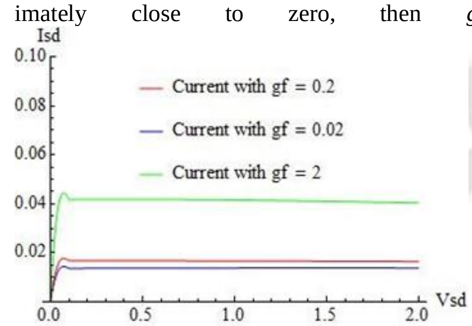

Fig. 5. Quantum Dot I-V plot at gate voltage (Vg=0), calculated with B = 4T under variable g factor and $\sigma = -\frac{1}{2}$

field has impact on the phase of time evolving I-V curves for sinusoidal magnetic field. The expression deduced here is applicable for nano scale devices and can be used in designing and implementation of nano electronic applications.

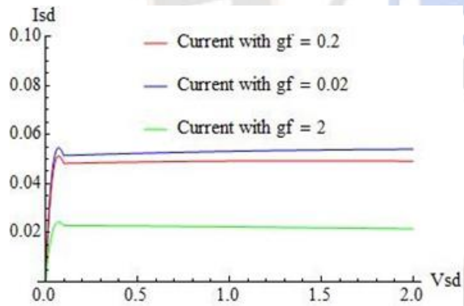

Fig. 6. Quantum Dot I-V plot at gate voltage (Vg=0), calculated with B = 4T under variable g factor and $\sigma = +\frac{1}{2}$

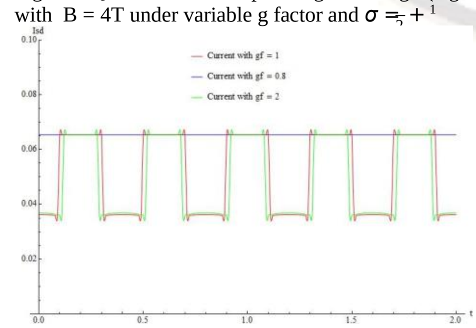

Fig. 7. Quantum Dot I-V plot at gate voltage (Vg=0), calculated under sinusoidal magnetic field with variable g factor and $\sigma = +\frac{1}{2}$

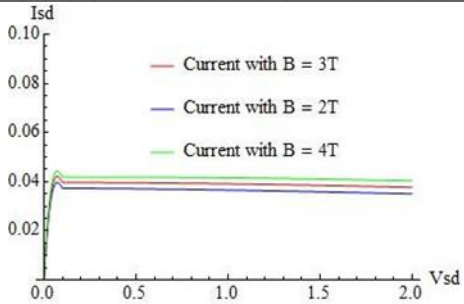

Fig. 8. Quantum Dot I-V plot at gate voltage (Vg=0), calculated with g = 2 under variable magnetic field strength and $\sigma = -\frac{1}{2}$

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