



Computational study of electronic transport property of a quantum dot
in a single electron transistor

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Science in Applied Physics and Electronics

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DECLARATION

I hereby declare that the thesis titled “Computational study of electronic transport property of a quantum dot in a single electron transistor” is submitted to the Department of Mathematics and Natural Sciences of BRAC University in partial fulfilment of the requirements for the degree of Bachelor of Science in Applied Physics and Electronics. This research is the work of my own and has not been submitted elsewhere. Every work that has been used as reference for this work has been cited properly.

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Abstract

Microscopic object's conductance behaviours are totally different from those of the macroscopic ones and cannot be understood, let alone deciphered using classical approach. Nanoscale systems' electron transport is not diffusive and has different carrier transport mechanism based on the contact type. Quantum dots are artificial atoms with the fascinating possibility of exploring their atomic states by applying current and voltage to them. They can be used to make single electron transistors where the quantum dot is kept separated from the source, drain and gate terminal by tunnel barriers. Quantum tunnelling causes current to flow when specific electrochemical potential requirements are met which can be achieved by varying the gate voltage. During this a phenomenon called Coulomb blockade is observed which is basically the appearance of oscillations in the conductance as a function of gate voltage. This is unique because it can only be observed for quantum dots and not in bulk materials. The conductance of the single electron transistor also varies with the temperature. All these characteristic behaviours can be deduced by carefully constructing and solving the rate equations. The acquired equations were then simulated using Python programs to plot the graphs for current versus voltage, differential conductance versus voltage, differential conductance versus temperature and maximum conductance versus temperature. The achieved graphs clearly depict how the current and the differential conductance are related to different source drain voltage at different gate voltages. The discrete conductance peak indicates different atomic states. Furthermore, it also outlines the fact that differential conductance depends on temperature and its value decreases as the temperature increases.

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Chapter 1

Electron Transport

1.1 Bulk material conductance

Conductance of macroscopic object can be best understood through Ohm's law which ties the dimension of the object to its electrical conductance. It states that the conductance, G of a rectangular conductor is directly proportional to its width, W but inversely proportional to its length, L by some factor σ which is the conductivity of the material, i.e.

$$G = \frac{\sigma W}{L}$$

However as we delve into the smaller dimensions of structures the Ohm's law no longer applies. This is because the conductivity which is dependent on the charge carrier density and the mean free path gets disrupted as the size becomes smaller. When it comes to nanometer scale devices, electron transport can occur through well-resolved quantum states. Transport in semiconductor quantum dots, metal nanoparticles, and molecules can all be understood within a similar framework, in terms of the energies of the states and the rates for transitions between states. [7]

1.2 How electron transport is affected in nanoscale systems

When it comes to nanoscale systems electron transport will no longer be a diffusive process as described by Ohm's law as the mean free path will be greater than the size itself. As this happens the charge carriers will not scatter within the conductor anymore. Another reason for

the drastic change is due to the role played by the contact between the macroscopic electrode and the nanoscale conductor on the total conductance. The type of the contact itself plays an immense role on how the carriers are transported. On top of all these the fact that the nanoscale object has a large charge addition energy and a quantized excitation spectrum cannot be ignored as well as these play vital role when carrier transport takes place at low temperatures. Based on all these it can easily be deduced that the well know conventional macroscopic theories cannot be used to decode the behaviours depicted at smaller scales.

1.3 Quantum dots

Quantum dots, (QD) are artificial atoms. Like natural atoms, they contain a discrete number of electrons and have a discrete spectrum of energy levels. [14] However, they are more commonly known as semiconductor nano-particles with a size of order 100nm [20] which obeys quantum mechanical principle of quantum confinement. It's emission and absorption spectra corresponding to the energy band gap is governed by quantum confinement principles in infinite well potential. The energy band gap increases as the quantum dot decreases in size. This is because the smaller quantum dots have stronger confinement making the energy gap larger. Similarly, a larger size gives a smaller energy gap. [1] A semiconductor quantum dot, is made out of roughly a million atoms with an equivalent number of electrons. Virtually all electrons are tightly bound to the nuclei of the material. However the number of free electrons in the dot can be very small; between one and a few hundred. This tiny fraction of free electrons are the ones which act as the conduction electrons. By attaching a gate to the quantum dot and applying a voltage this small fraction can be varied from a single free electron to a several thousands of free electrons. The deBroglie wavelength of these electrons is comparable to the size of the dot, and the electrons occupy discrete quantum levels and have a discrete excitation

spectrum. A quantum dot has another characteristic usually known as the charging energy which is the energy required to add or remove a single electron from the dot. [12]. The atom-like behaviour of these dots is studied by measuring their transport properties by their ability to carry an electric current.

Quantum dot's applications is quite an impressive array that includes single-electron trap, single-electron turnstile and pump, *single electron transistor*, (*SET*) oscillators, supersensitive electrometry, detection of infrared radiation, voltage state logics, charge state logics, background-charge-insensitive memory, NOVORAM, electrostatic data storage and so on. The list apparently is quite long, impressive and versatile. It is also increasingly expanding because just by subjecting the quantum dot to different permutations and combinations of different types of electrodes or applied voltages all these were achieved. [18]

1.4 Single electron transistor

A single-electron transistor consists of a conducting island which is the quantum dot in this case that is kept separated from the source, drain and gate terminal using insulating barriers. Their effective nuclear charge is controlled by metallic electrodes. Electrons can only transfer between the island and the source and drain terminals by quantum tunnelling through the barriers. For such devices to operate at room temperature, which is essential if they are to be used in realistic circuits, the islands must be smaller than 10 nanometres across. Moreover, the potential energy of the tunnel barriers must be high enough to localize electrons on the island. They exude an unique and spectacular property which is the current through them or the capacitance between their leads can vary by many orders of magnitude when their charge is changed by a single electron. [14]

In single molecule device the electronic spectrum is quantized with the typical energy scale of eV. By applying some voltage between the electrodes the conductance can be measured by

measuring the amount of current flowing through it. In SET, the single-electron charging effect is used to precisely control the charging of individual electrons on a conducting island. Electrons are transferred to the island from source and drain terminals by tunnelling across potential barriers. The charging of the island by a single-electron can be controlled by a gate terminal. The SET has the advantages of very low power consumption, better immunity from statistical charge fluctuation, and very high scalability compared to conventional complementary metal-oxide-semiconductor devices. [22] They are also highly diversified and have wide range of functionality. Their ability to permit self-assembly makes it easier to fabricate them in such small dimensions. Also a metallic quantum dot has a very small energy level separation at the Fermi level, so that the change in Fermi level by the transfer of a single electron from dot to leads may be neglected. The ground state of such a system corresponds to the minimum value of $U(N)$. [23]

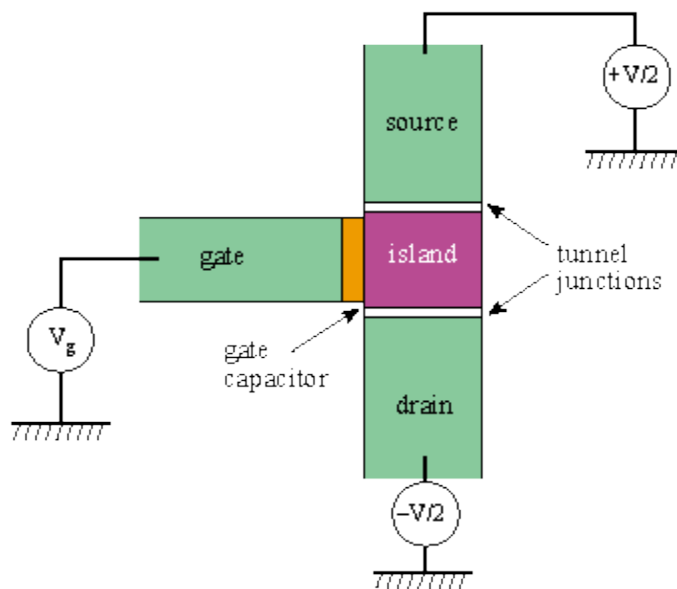


Figure 1.1: Single electron transistor

1.5 Quantum tunnelling

As it has been already stated that quantum dot is loosely connected to the source and the drain electrode through insulating barriers the idea of considering current through it might be frowned upon and found confusing as well. However, despite of the small gap quantum tunnelling allows current to pass through the infinitesimally small gap. In order to understand this phenomenon one has to adopt the quantum mechanical approach.

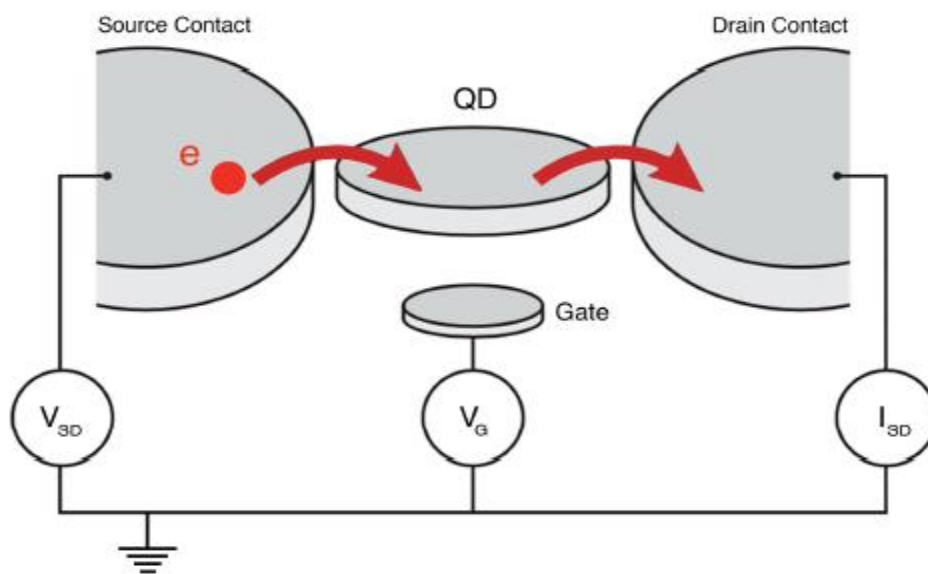


Figure 1.2: Quantum dot coupled to a source and gate via tunnel barriers

Considering the gap between the electron and the electrodes as potential barriers with height $V(r)$ and the quantum dot as an infinite spherical potential well [11]. According to classical physics, a particle of energy E , less than the height $V(r)$ of the barrier, cannot escape making the region inside the barrier classically forbidden. However due to the wave-particle duality, the particle's associated wave function has to be continuous at the barrier as well as at the other side of the barrier thereby giving rise to a considerable probability of the particle tunnelling through the classically forbidden region with an unchanged before and after amount of energy due to the energy conservation principle, i.e.

$$V(r) = \begin{cases} 0 & \text{when } r \leq R \\ \infty & \text{when } r > R \end{cases}$$

Radial equation for inside the well:

$$\frac{d^2u}{dr^2} = \left[\frac{l(l+1)}{r^2} - k^2 \right] u$$

$$\frac{-\hbar^2}{2m} \frac{d^2u}{dr^2} = Eu$$

$$U(r) = A \sin kr + B \cos kr$$

When angular momentum, $l = 0$

$$\frac{d^2u}{dr^2} = -k^2 u \quad \text{where } k = \frac{\sqrt{2mE}}{\hbar}$$

$$U(0) = U(R)$$

$$U(R) = A \sin kR$$

$$kR = n\pi$$

$$k = \frac{n\pi}{R}$$

$$E_N = \frac{n^2 \pi^2 \hbar^2}{2mR^2}$$

Therefore the characteristic energy scale is

$$\frac{\pi^2 \hbar^2}{mR^2} = \Delta E$$

Now shifting the focus on the Fermi level of electrode connected to the quantum dot, i.e. their electrochemical potentials. Assuming the electrochemical potential of the source is μ_S and the electrochemical potential of the drain as μ_D . By definition the energy should be equal to charge multiplied by voltage, i.e. $\mu_S - \mu_D = eV_{SD}$ where V_{SD} is the applied voltage and $e =$ charge of electron $= -1.602 \times 10^{-19}$ C. Considering that the available energy states lying beneath the μ_S and μ_D are filled with an electron and the above energy states are empty. Current is conducted only when electron can tunnel onto the quantum dot from the source electrode and from there to the drain electrode. As soon as an energy state in the range of μ_S and μ_D becomes available electron is tunneled by changing the number of electrons on the quantum dot between N and $N+1$. If no tunnelling occurs the number remains unchanged, i.e. N . [2]

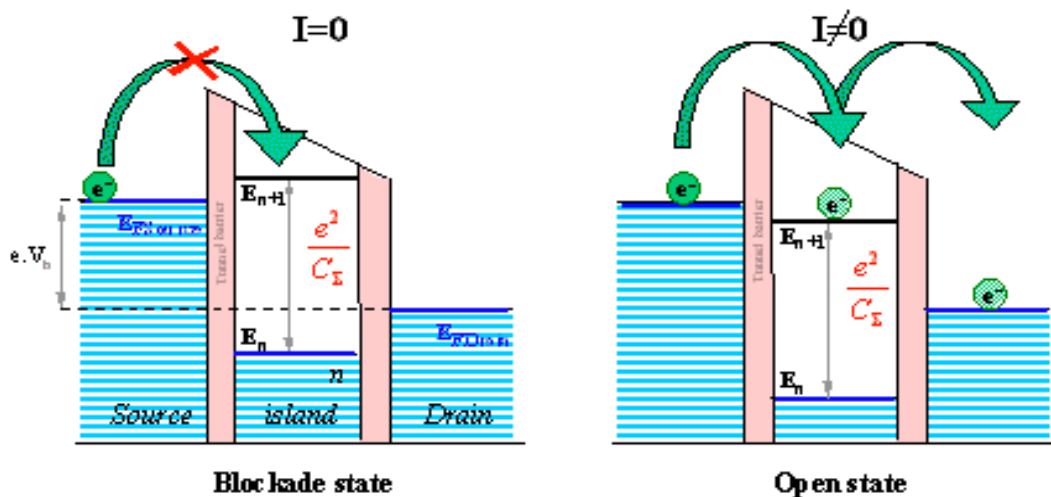


Figure 1.3: Energy states during blocked state and open state

1.6 Conditions for quantum tunnelling to take place

If tunnelling is allowed to the source and drain electrodes, then the number of electrons N adjusts itself until the energy of the whole circuit is minimized. When tunnelling occurs, the charge on the island suddenly changes by the quantized amount e . The associated change in the Coulomb energy is conveniently expressed in terms of the capacitance C of the island. An extra charge e changes the electrostatic potential by the charging energy, $E_C = \frac{e^2}{C}$. This charging energy becomes important when it exceeds the thermal energy, $k_B T$. A second requirement is that the barriers are sufficiently opaque such that the electrons are located either in the source, in the drain, or on the island. This means that quantum fluctuations in the number N due to tunnelling through the barriers is much less than one over the time scale of the measurement which is roughly the electron charge divided by the current. This requirement translates to a lower bound for the tunnel resistances, R_t of the barriers. Considering the typical time to charge or discharge the island $\Delta t = R_t C$. The Heisenberg uncertainty relation: $\Delta E \Delta t = \frac{e^2}{C} \times R_t C > h$ implies that R_t should be much larger than the resistance quantum $\frac{h}{e^2} = 25.813 \text{ k}\Omega$ in order for the energy uncertainty to be much smaller than the charging energy. So the two conditions for observing effects due to the discrete nature of charge are:

$$R_t \gg \frac{h}{e^2}$$

$$\frac{e^2}{C} \gg k_B T$$

The first criterion can be met by weakly coupling the dot to the source and drain leads. The second criterion can be met by making the dot small. Since the capacitance of an object scales with its radius R , for a sphere, $C = 4\pi\epsilon_1\epsilon_0 R$ and for a flat disc, $C = 8\pi\epsilon_1\epsilon_0 R$ where ϵ_r is the dielectric constant of the material surrounding the object. While the tunnelling of a single

charge changes the electrostatic energy of the island by a discrete value, a voltage V_G applied to the gate with capacitance of C_G can change the island's electrostatic energy in a continuous manner. In terms of charge, tunnelling changes the island's charge by an integer while the gate voltage induces an effective continuous charge $q = C_G \times V_G$ that represents the charge that the dot would like to have. This charge is continuous even on the scale of the elementary charge e . If we sweep V_G the buildup of the induced charge will be compensated in periodic intervals by tunnelling of discrete charges onto the dot. This competition between continuously induced charge and discrete compensation leads coulomb oscillations in a measurement of the current as a function of gate voltage at a fixed source-drain voltage. Another important criteria in order to be able to resolve quantized energy levels, the energy level spacing has to be $\Delta E \gg k_B T$ because unless this the whole system falls under the regime of classical dot causing all the previous approaches to be inapplicable. [16]

Chapter 2

Coulomb Blockade Theory

A manifestation of the Coulomb blockade is the appearance of oscillations in the conductance as a function of gate voltage, at temperatures above those expected for resonant tunnelling of non-interacting electrons. Coulomb-blockade oscillations in semiconductors were originally observed and identified in disordered quantum wires, where they result from a break-up of the narrow channel into a few segments separated by tunnel barriers. [21] After the discovery of conductance oscillations periodic in the gate voltage in a disordered quantum wire, and the identification of this phenomenon as Coulomb-blockade oscillations, it has become clear that in certain regimes single electron tunnelling is the dominant transport mechanism in semiconductor nanostructures. This is crucial because of the possibility to study the interplay between size and charge quantization effects, which is not feasible in metallic grains because of the small Fermi wavelength in a metal. [23]

2.1 Basic concepts of a single electron transistor

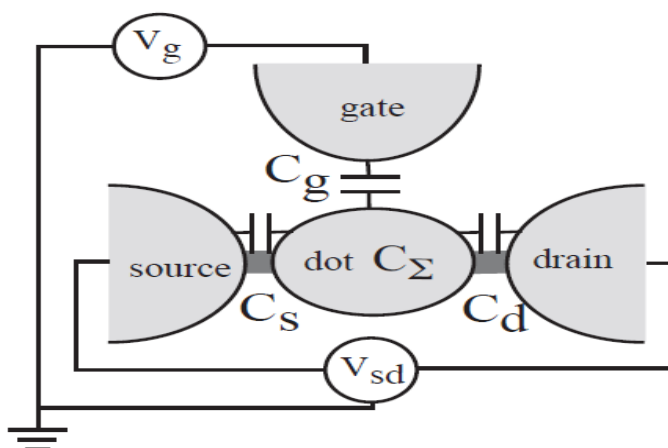


Figure 2.1: Schematic drawing of a typical electrode arrangement for a single electron transistor.

Electrostatic energy of the dot: [16]

$$E_{es} = \frac{(-eN + Q_0)^2}{2C}$$

The integer part of the excess charge in the dot is $eN = e(N - N_0)$, where N is the number of electrons in the dot, and the elementary charge e is taken positive. N_0 is the number of electrons at zero gate voltage and zero bias voltage (so $N_0 > N$), which compensates the positive background charge originating from the donors. Q_0 represents the continuous part of the excess charge.

$$Q_0 = C_S V_S + C_D V_D + C_G V_G$$

Since V_{SD} is very small $Q_0 \approx C_G V_G$

$$C_{total} = C_S + C_D + C_G$$

Assumptions made for calculating $U(N)$:

- 1) Quantum levels can be calculated independently of the number of electrons on the dot.
- 2) Parameterizing coulomb interactions amongst and between the electrons on the dot and environment electrons by capacitance.
- 3) Capacitance is independent of dot electrons.

$$U(N) = \sum_{i=1}^N E_p + \frac{(-eN + C_G V_G)^2}{2C_{total}}$$

Electrochemical potential of the dot with N electrons:

$\mu_{(N)}$ = minimum energy for adding the Nth electron to the dot

$\mu_{(N)} = U(N) - U(N-1)$ where $U(N)$ = total ground state energy for N electrons

$$\mu_{(N)} = E_N + \frac{(-eN + C_G V_G)^2}{2C_{total}} - \frac{(N-1)^2 e^2}{2C_{total}}$$

Or

$$\mu_{(N)} = E_N + \frac{(C_G V_G)^2}{2C_{total}} - \frac{(2Ne C_G V_G)^2}{2C_{total}} + \frac{(Ne)^2}{2C_{total}} - \left[\frac{(Ne)^2}{2C_{total}} - \frac{2Ne^2}{2C_{total}} + \frac{e^2}{2C_{total}} \right]$$

Ignoring $(C_G V_G)^2$ since V_G is very small:

$$\mu_{(N)} = E_N + \frac{(N-1/2)e^2}{C_{total}} - \frac{eC_G V_G}{C_{total}}$$

Here E_N is the electrochemical potential and the rest is electrostatic potential.

As long as $\mu_{(N)}$ is in between μ_S and μ_D the Nth electron can be added to the dot.

$$\mu_{(N)} = E_N + \frac{(N-1/2)e^2}{C_{total}} + eV_{dot} \text{ where } V_{dot} = \frac{1}{C_{total}} \sum_{i=S,D,G} C_i V_i$$

Taking $V_D = 0$

$$V_{dot} = \frac{c_S}{c_{total}} V + \frac{c_G}{c_{total}} V_G$$

Since V_{dot} does not depend on electrons available on the dot, the charge addition energy $E_c + \Delta E$ does not change in this case but the position of $\mu_{(N)}$ relative to the electrodes' Fermi levels is affected by V and V_G . So by changing these two voltages the electrodes' electrochemical potentials can be changed as well. To summarize the effect:

Taking $\Delta\mu_{(N)} \approx e\Delta V_{dot}$

$$\frac{\Delta\mu_{(N)}}{e} \approx \frac{c_S}{c_{total}} \Delta V + \frac{c_G}{c_{total}} \Delta V_G$$

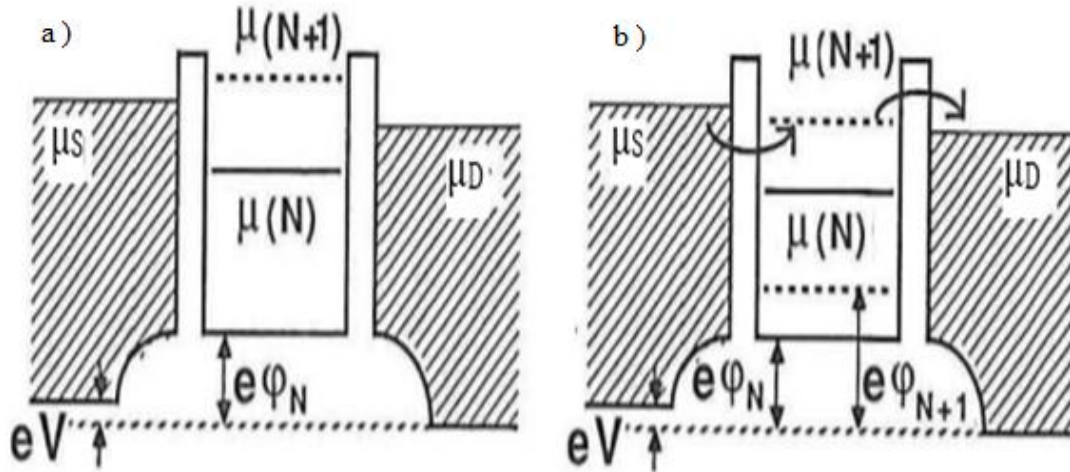


Figure 2.2: Two situations for different gate voltages

a) Coulomb blockade of electron tunneling when $\mu_{(N)} < \mu_D < \mu_S < \mu_{(N+1)}$

b) One by one electron tunneling at the N to $N + 1$ transition when $eV \ll \mu_{(N+1)} - \mu_{(N)}$ and $\mu_D < \mu_{(N+1)} < \mu_S$

When the number of electrons is changed by one change in electrochemical potential will be: [16]

$$\mu_{(N+1)} - \mu_{(N)} = E_{(N+1)} - E_N + \frac{e^2}{C} \quad \text{where } C = C_{total}$$

Or

$$\mu_{(N+1)} - \mu_{(N)} = \Delta E + \frac{e^2}{C}$$

The addition energy $\mu_{(N+1)} - \mu_{(N)}$ is large for a small capacitance and a large energy splitting ΔE between 0D-states. It is important to note that the charging energy, $\frac{e^2}{C}$ to the energy gap exists only at the Fermi energy. Below $\mu_{(N)}$ the energy states are only separated by the single-particle energy differences ΔE . These energy differences ΔE are the excitation energies of a dot with constant number N . A non-zero addition energy can lead to a blockade for tunnelling of electrons on and off the dot, where N electrons are localized on the dot. The $(N+1)^{\text{th}}$ electron cannot tunnel on the dot, because the resulting electrochemical potential $\mu_{(N+1)}$ is higher than the potentials of the reservoirs. So, for $\mu_{(N)} < \mu_S, \mu_D < \mu_{(N+1)}$ the electron transport is blocked, which is known as the Coulomb blockade. Another reason is because the charge addition energy is quite large in this case. The Coulomb blockade can be removed by changing the gate voltage, to align $\mu_{(N+1)}$ between μ_S and μ_D . When this happens an electron can tunnel from the left reservoir on the dot. The electrostatic increase is $\frac{e^2}{C}$ due to the change in the conduction band bottom. Since $\mu_{(N+1)} > \mu_D$, one electron can tunnel off the dot to the right reservoir, causing the electrochemical potential to drop back to $\mu_{(N)}$. A new electron can now tunnel on the dot and repeat the cycle of N to $N+1$ and back to N again.

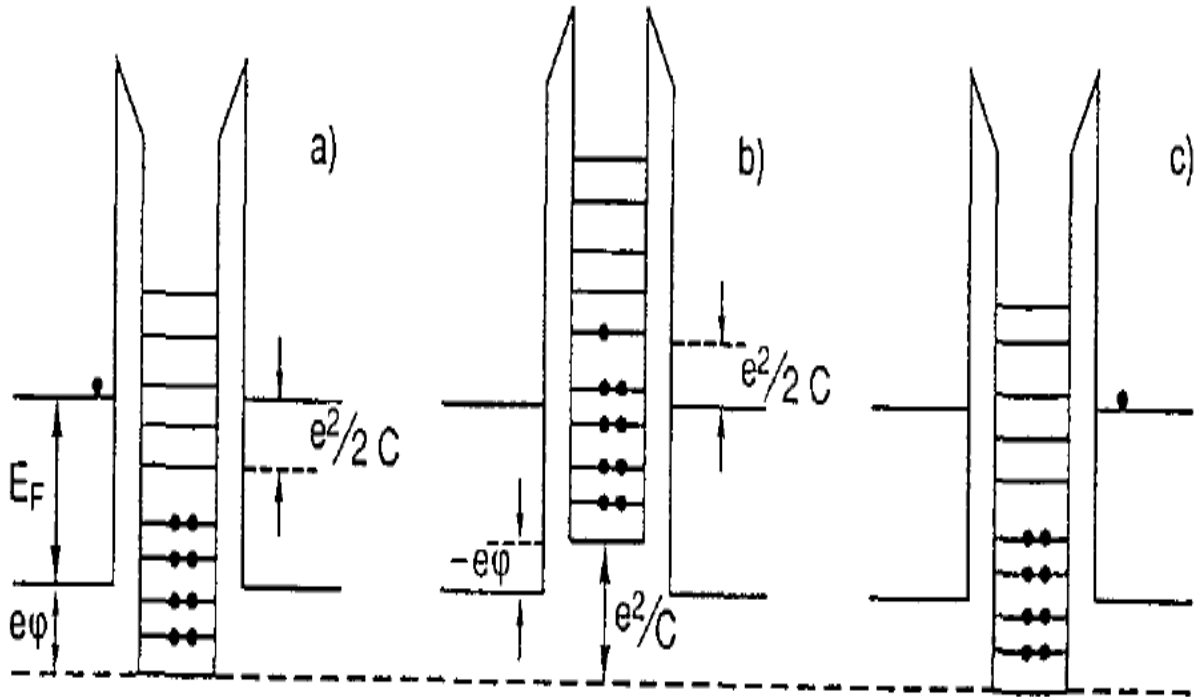


Figure 2.1: Single-electron tunneling through a quantum dot, under the conditions of $E_N +$

$\left(N - \frac{1}{2}\right) \frac{e^2}{C} = E_F + e\phi$ for the case that the charging energy is comparable to the level

spacing. In panel (a) $N - 1$ electrons occupy the dot. The N^{th} level in the dot is empty. In

panel (b) an electron has tunneled into this level. The potential difference ϕ between dot and

leads has decreased by $\frac{e}{C}$ (becoming negative), because of the added electron. Finally, in

panel (c) the added electron tunnels out of the dot, resetting the potentials to the initial state

of panel (a). [23]

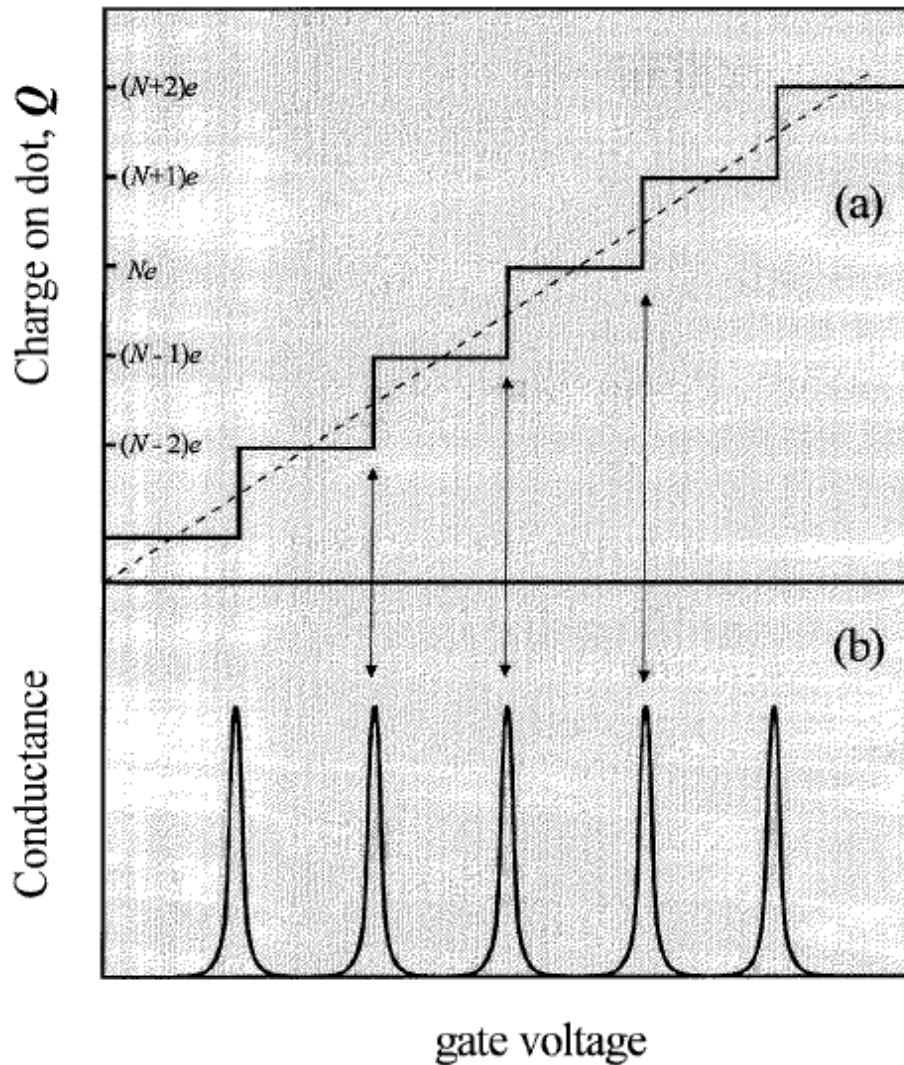


Figure 2.4: Single-electron charging and the origin of periodic conductance peaks. The quantity of charge that represents the minimum electrostatic energy plotted as the broken line in (a). In a quantum dot where the discreteness of charge must be taken into account, the actual charge in the QD is the integer multiple of e closest to the continuous quantity Q , shown by the full line in (a). The schematic plot of conductance peaks in (b) illustrates that periodic conductance peaks correspond to gate voltages associated with charge-degeneracy points, where the charge in a QD is free to fluctuate by e . [19]

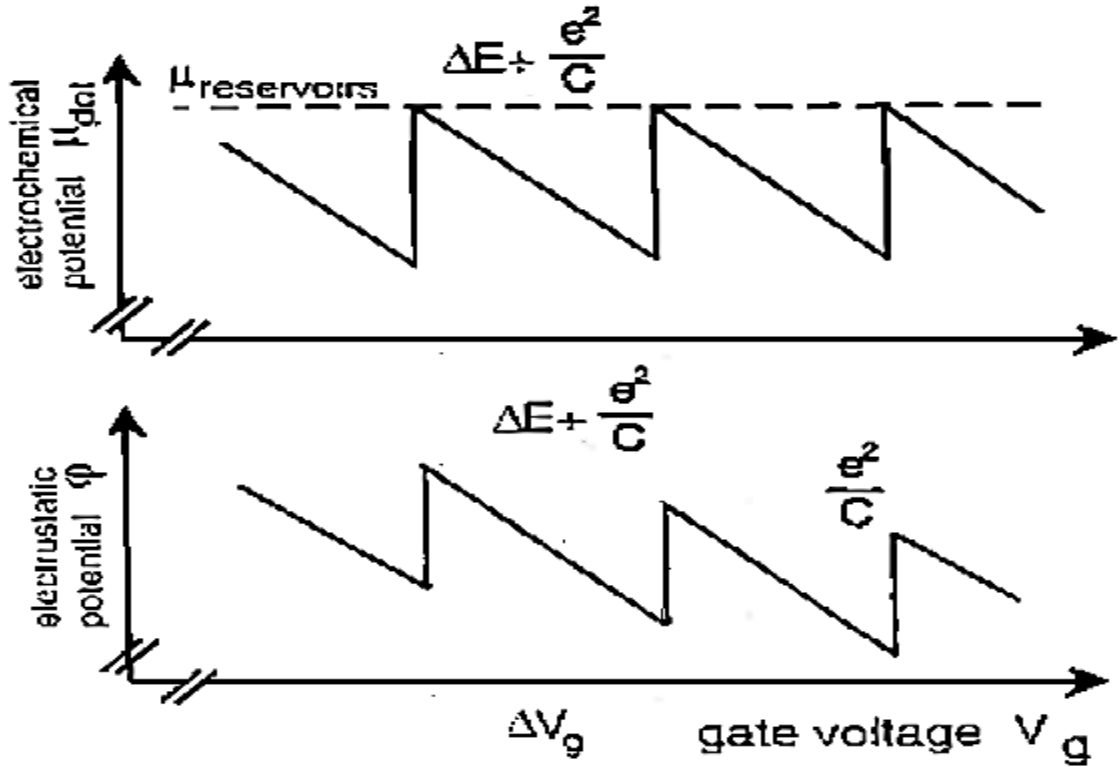


Figure 2.5: Schematic comparison, as a function of gate voltage, between the electrochemical potential in the dot $\mu_{(N+i)}$, and the electrostatic potential.

2.2 Single level quantum dots

For single level quantum dots only two charge states are taken into account due to their availability, i.e. N and $N+1$ in their ground states. Additional assumptions are made for simplification and convenience purpose, i.e. $\mu_D = 0$ and voltage $V = V_G = 0$ thereby modifying the previously established equations slightly.

$$\mu_{(N+1)} = E_0 + eV_{dot} \text{ where } E_0 = \text{ground state energy}$$

Assuming the crossing potential as V_c , $e = -|e|$, $E_0 > 0$ and $V = 0$. When $V_G = 0$, i.e. $V_G < V_c$ the dot will be in its N state as $\mu_{(N+1)}$ greater than μ_S and μ_D which will both be equal to zero. So no current will flow.

When V_G is not equal to zero and is greater than V_c the $N + 1$ state will always be occupied.

This is because

$$\mu_{(N+1)} = E_0 - |e| V_{dot}$$

$$E_0 < |e| V_{dot}$$

$$E_0 < |e| \frac{C_G V_G}{C_{total}}$$

Therefore,

$$|e| V_G > E_0 \frac{C_{total}}{C_G}$$

Current will only flow when $V_G \approx V_C$ because this will cause the $\mu_{(N+1)}$ to be in the range of μ_s and μ_D .

$$\text{By putting } V_G = V_C \text{ we get } |e| V_C > E_0 \frac{C_{total}}{C_G}$$

Therefore V_C can be defined as

$$V_C = \frac{E_0 C_{total}}{|e| C_G}$$

This means the conductance versus V_G graph will show only one peak where the value of V_G will be equal to that of V_C . This happens due to Coulomb oscillation because at $V_G = V_C$ the N and $N+1$ charge states will have equal energy thereby allowing the electron to move to and fro the dot.

2.3 Fermi functions for single level quantum dots

The single level quantum dot has single-electron energy levels at E_p ($p = 1, 2, \dots$), labeled in ascending order and measured relative to the bottom of the potential well. Each level contains either one or zero electrons. Spin degeneracy can be included by counting each level twice, and other degeneracies can be included similarly. Each reservoir is taken to be in thermal equilibrium at Temperature, T and chemical potential E_F . A continuum of states is assumed in the reservoirs, occupied according to the Fermi-Dirac distribution [3]

$$f(E - E_f) = \left[1 + \exp\left(\frac{E - E_f}{k_B T}\right) \right]^{-1}$$

Therefore for Source

$$f_s = \left[1 + \exp\left(\frac{\mu_{(N+1)} - \mu_s}{k_B T}\right) \right]^{-1}$$

Simplifying $\mu_{(N+1)}$ by putting the value of E_0 and V_{dot}

$$\mu_{(N+1)} = |e| \left(\frac{C_G V_C}{C_{\text{total}}} \right) - |e| \left(\frac{C_G V_G + C_S V}{C_{\text{total}}} \right)$$

Therefore,

$$\mu_{(N+1)} = -|e| \left[\frac{C_G (V_G - V_C) + C_S V}{C_{\text{total}}} \right]$$

Putting $V_{SD} = V = V_{dot}$ and $e = -|e|$

$$\frac{\mu_S - \mu_D}{-|e|} = V_{SD}$$

Therefore,

$$-|e|V = \mu_S \text{ since } \mu_D = 0$$

Finally f_s becomes

$$f_s = \left[1 + \exp \left(\frac{\mu_{(N+1)} + |e|V}{k_B T} \right) \right]^{-1}$$

For Drain

$$f_D = \left[1 + \exp \left(\frac{\mu_{(N+1)} - \mu_D}{k_B T} \right) \right]^{-1}$$

But since $\mu_D = 0$ and $V_D = 0$ Fermi-Dirac distribution for drain is

$$f_D = \left[1 + \exp \left(\frac{\mu_{(N+1)}}{k_B T} \right) \right]^{-1}$$

2.4 Rate equations for single level quantum dots

Since the fluctuation between the two available states is completely random statistical approach has to be adopted to figure out the probability of the dot being in a certain state. Assuming P_0 as the probability of the dot being in the N state and P_1 as the probability of the dot being in the $N+1$ state the rate of change of P_0 and P_1 can be depicted by referring

to the non-equilibrium probability distribution P as a stationary solution of the kinetic equation [3] which is:

$$\begin{aligned}
\frac{\delta}{\delta t} P(\{n_i\}) &= 0 \\
&= - \sum_p P(\{n_i\}) \delta_{n_p,0} [\Gamma_p^l f(E^{vl}(N) - E_F) + \Gamma_p^r f(E^{vr}(N) - E_F)] \\
&\quad - \sum_p P(\{n_i\}) \delta_{n_p,1} [\Gamma_p^l [1 - f(E^{f,l}(N) - E_F) + \Gamma_p^r [1 \\
&\quad - f(E^{f,r}(N) - E_F)]] \\
&\quad + \sum_p P(n_1, \dots, n_{p-1}, n_{p+1} \dots) \delta_{n_p,0} \\
&\quad \times [\Gamma_p^l [1 - f(E^{f,l}(N+1) - E_F) + \Gamma_p^r [1 - f(E^{f,r}(N+1) - E_F)]] \\
&\quad + \sum_p P(n_1, \dots, n_{p-1}, n_{p+1} \dots) \delta_{n_p,1} \\
&\quad \times [\Gamma_p^l [f(E^{i,l}(N-1) - E_F) + \Gamma_p^r [1 - f(E^{i,r}(N-1) - E_F)]]
\end{aligned}$$

So,

$$\begin{aligned}
\frac{\delta P_0}{\delta t} &= -P_0[\Gamma_S f_S + \Gamma_D f_D] - P_0[\Gamma_S(1 - f_S) + \Gamma_D(1 - f_D)] + P_0[\Gamma_S(1 - f_S) + \Gamma_D(1 \\
&\quad - f_D)] + P_1[\Gamma_S(1 - f_S) + \Gamma_D(1 - f_D)]
\end{aligned}$$

Therefore,

$$\frac{\delta P_0}{\delta t} = -P_0[\Gamma_S f_S + \Gamma_D f_D] + P_1[\Gamma_S(1 - f_S) + \Gamma_D(1 - f_D)]$$

Similarly,

$$\begin{aligned}\frac{\delta P_1}{\delta t} = & -P_1[\Gamma_S f_S + \Gamma_D f_D] - P_1[\Gamma_S(1-f_S) + \Gamma_D(1-f_D)] + P_0[\Gamma_S f_S + \Gamma_D f_D] \\ & + P_1[\Gamma_S f_S + \Gamma_D f_D]\end{aligned}$$

Therefore,

$$\frac{\delta P_1}{\delta t} = P_0[\Gamma_S f_S + \Gamma_D f_D] - P_1[\Gamma_S(1-f_S) + \Gamma_D(1-f_D)]$$

Here $\frac{\delta P_0}{\delta t}$ and $\frac{\delta P_1}{\delta t}$ are the rate equations. By solving these two we can find in turn find the probability P_0 and P_1 .

Taking $\frac{\delta P_0}{\delta t} = 0$ and assuming total probability, i.e $P_0 + P_1 = 1$

$$-P_0[\Gamma_S f_S + \Gamma_D f_D] + (1-P_0)[\Gamma_S(1-f_S) + \Gamma_D(1-f_D)] = 0$$

Or

$$[\Gamma_S + \Gamma_D] - P_0[\Gamma_S + \Gamma_D] - \Gamma_S f_S - \Gamma_D f_D = 0$$

Therefore,

$$P_0 = \frac{\Gamma_S(1-f_S) + \Gamma_D(1-f_D)}{\Gamma_S + \Gamma_D}$$

2.5 Current equation for single level quantum dots

Assuming that the stationary current [3] through the left barrier equals that through the right barrier which is given by

$$I = -e \sum_{p=1}^{\infty} \sum_{\{n_i\}} \Gamma_p^l P(\{n_i\}) \times \{ \delta_{n_p,0} f(E^{l,l}(N) - E_F) - \delta_{n_p,1} [1 - f(E^{F,l}(N) - E_F)] \}$$

By putting the previously acquired value and solving the above equation we get the current for the single level quantum dot.

$$\frac{I}{|e|} = -P_0 \Gamma_S f_S + P_1 \Gamma_S (1 - f_S)$$

Or

$$\frac{I}{|e|} = -P_0 \Gamma_S f_S + (1 - P_0) (\Gamma_S - \Gamma_S f_S)$$

Or

$$\frac{I}{|e|} = \Gamma_S (1 - P_0 - f_S)$$

Or

$$\frac{I}{|e|} = \frac{\Gamma_S \Gamma_D (f_D - f_S)}{\Gamma_S + \Gamma_D}$$

Taking $\Gamma = \frac{\Gamma_S \Gamma_D}{\Gamma_S + \Gamma_D}$ we finally get:

$$I = |e| \Gamma (f_D - f_S)$$

In the equation given above the current amplitude is dependent on Γ , i.e. higher the value of Γ higher will be the current amplitude and $(f_D - f_S)$ determines whether current will

actually flow or not. This is because when $f_D = f_S$ current will become zero. Since f_D and f_S are both connected to $\mu_{(N+1)}$ which in turn is dependent on the value of μ_S and μ_D current will also not be conducted unless $\mu_{(N+1)}$ lies in between the μ_S and μ_D .

2.6 Conductance equation for single level quantum dots

Since conductance, G is related to current and voltage in the manner $G = \frac{I}{V}$ by differentiating the acquired current equation with respect to voltage, V we can find the differential conductance for the single level dot.

$$\frac{dI}{dV} = |e|\Gamma \left[\frac{\delta(f_D - f_S)}{\delta\mu_{(N+1)}} \frac{\delta\mu_{(N+1)}}{\delta V} - \frac{\delta f_S}{\delta V} \right]$$

$$\frac{\delta f_D}{\delta\mu_{(N+1)}} = \frac{-\exp\left(\frac{\mu_{(N+1)}}{k_B T}\right)}{k_B T \left[1 + \exp\left(\frac{\mu_{(N+1)}}{k_B T}\right)\right]^2}$$

$$\frac{\delta f_S}{\delta\mu_{(N+1)}} = \frac{-\exp\left(\frac{\mu_{(N+1)} + |e|V}{k_B T}\right)}{k_B T \left[1 + \exp\left(\frac{\mu_{(N+1)} + |e|V}{k_B T}\right)\right]^2}$$

$$\frac{\delta f_D}{\delta\mu_{(N+1)}} - \frac{\delta f_S}{\delta\mu_{(N+1)}} = \frac{\exp\left(\frac{\mu_{(N+1)} + |e|V}{k_B T}\right)}{k_B T \left[1 + \exp\left(\frac{\mu_{(N+1)} + |e|V}{k_B T}\right)\right]^2} - \frac{-\exp\left(\frac{\mu_{(N+1)}}{k_B T}\right)}{k_B T \left[1 + \exp\left(\frac{\mu_{(N+1)}}{k_B T}\right)\right]^2}$$

$$\frac{\delta\mu_{(N+1)}}{\delta V} = -|e| \left[\frac{C_S}{C_{total}} \right]$$

$$\frac{\delta f_S}{\delta V} = -|e| \frac{\exp\left(\frac{\mu_{(N+1)} + |e|V}{k_B T}\right)}{k_B T \left[1 + \exp\left(\frac{\mu_{(N+1)} + |e|V}{k_B T}\right)\right]^2}$$

Substituting all the above equations in $\frac{dI}{dV}$:

$$\frac{dI}{dV} = \frac{|e|^2 \Gamma}{k_B T} \left\{ \frac{C_S}{C_{total}} \left[\frac{\exp\left(\frac{\mu_{(N+1)}}{k_B T}\right)}{\left[1 + \exp\left(\frac{\mu_{(N+1)}}{k_B T}\right)\right]^2} - \frac{\exp\left(\frac{\mu_{(N+1)} + |e|V}{k_B T}\right)}{\left[1 + \exp\left(\frac{\mu_{(N+1)} + |e|V}{k_B T}\right)\right]^2} \right] + \frac{\exp\left(\frac{\mu_{(N+1)} + |e|V}{k_B T}\right)}{\left[1 + \exp\left(\frac{\mu_{(N+1)} + |e|V}{k_B T}\right)\right]^2} \right\}$$

$$f_D - f_D^2 = \frac{\exp\left(\frac{\mu_{(N+1)}}{k_B T}\right)}{\left[1 + \exp\left(\frac{\mu_{(N+1)}}{k_B T}\right)\right]^2}$$

$$f_S - f_S^2 = \frac{\exp\left(\frac{\mu_{(N+1)} + |e|V}{k_B T}\right)}{\left[1 + \exp\left(\frac{\mu_{(N+1)} + |e|V}{k_B T}\right)\right]^2}$$

Or

$$\frac{dI}{dV} = \frac{e^2 \Gamma}{k_B T} \left[(1 - f_D) f_D \frac{C_S}{C_{total}} + (1 - f_S) f_S \left(\frac{C_{total} - C_S}{C_{total}} \right) \right]$$

Finally,

$$\frac{dI}{dV} = \frac{e^2 \Gamma}{k_B T} \left[(1 - f_D) f_D \frac{C_S}{C_{total}} + (1 - f_S) f_S \left(\frac{C_D - C_G}{C_{total}} \right) \right]$$

In the above equation first term will be non-zero when $0 < f_D < 1$ because $\mu_{(N+1)}$ will align with μ_D . The second term will be non-zero when $0 < f_S < 1$ because $\mu_{(N+1)}$ will align with μ_S . So by varying the voltage V and V_G we can easily measure $\frac{dI}{dV}$ and in turn find $\mu_{(N+1)}$.

2.7 How the voltage V changes when μ_{N+1} aligns either μ_S or μ_D

When $\mu_{(N+1)} = \mu_S$

$$e \left[\frac{C_G(V_G - V_C) + C_S V}{C_{total}} \right] = eV$$

Or

$$V = \frac{C_S V}{C_{total}} + \frac{C_G(V_G - V_C)}{C_{total}}$$

Or

$$V = \frac{(V_G - V_C)}{C_{total}} \times \frac{C_{total}}{C_{total} - C_S}$$

Therefore,

$$V = \frac{C_G(V_G - V_C)}{C_D + C_G}$$

When $\mu_{(N+1)} = \mu_D = 0$

$$C_S V + C_G(V_G - V_C) = 0$$

Therefore,

$$V = - \frac{C_G(V_G - V_C)}{C_S}$$

2.8 Temperature dependence of single level coulomb oscillation

In order to figure out how the change in temperature affects coulomb oscillation the differential conductance, $\frac{dI}{dV}$ has to be a bit more simplified. Assuming $V=0$, f_s will become equal to f_D . This in turn further simplifies the $\frac{dI}{dV}$, i.e.

$$\frac{dI}{dV} = \frac{e^2\Gamma \exp\left(\frac{\mu(N+1)}{k_B T}\right) \div 4\exp\left(\frac{\mu(N+1)}{k_B T}\right)}{\left[\frac{1 + \exp\left(\frac{2\mu(N+1)}{k_B T}\right)}{2 \exp\left(\frac{\mu(N+1)}{k_B T}\right)}\right]^2}$$

Or

$$\frac{dI}{dV} = \frac{e^2\Gamma}{k_B T} \frac{1/4}{\left[\cosh\left(\frac{\mu(N+1)}{2k_B T}\right)\right]^2}$$

Or

$$\frac{dI}{dV} = \frac{e^2\Gamma}{4k_B T} \left[\cosh\left(\frac{\mu(N+1)}{2k_B T}\right)\right]^{-2}$$

Putting $\alpha = \frac{C_G}{C_{total}}$ in $\mu_{(N+1)}$ we get

$$\frac{dI}{dV} = \frac{e^2\Gamma}{4k_B T} \left[\cosh\left(\frac{|\alpha(V_G - V_C)|}{2k_B T}\right)\right]^{-2}$$

This shows

$$\text{Peak height} = \frac{e^2\Gamma}{4k_B T} \text{ when } V_G = V_C \text{ and } \cosh\left(\frac{|\alpha(V_G - V_C)|}{2k_B T}\right) = 1$$

This means the maximum conductance value, G_{\max} will be $\frac{e^2\Gamma}{4k_B T}$ at that particular temperature.

Chapter 3

Simulation

In order to resolve and ensure the outcomes of the previously acquired equations simulation can be an effective approach. Since due to the unavailability of fully equipped lab fabrication followed by experiment based deductions was somewhat infeasible simulation is the next best solution to come up with characteristics graph through an artificially computed model.

3.1 Python

When the question to write the code for the equations came up Python seemed like the best option to opt for. The reasons behind it are endless. For starter Python looks more readable thereby providing the ability to program at a faster rate. Python container objects (e.g. lists and dictionaries) that can hold objects of any type, including numbers and lists. For python no casting is required. Python programs are typically much shorter than equivalent programs. This difference can be attributed to Python's built-in high-level data types and its dynamic typing. This means it is much easier to debug which is key when one has a time crunch.

Python provides an interpreted programming language that can be viewed as an extension of the simple command languages already used by scientific programs. Also Python is easily integrated with software written in other languages. As a result, it can serve as both a control language for driving existing programs as well as a glue language for combining different systems together.

Python already has libraries that fit scientific computing like NumPy, Numeric, Numarray, SAGE, etc. It has bindings with R (the statistics language), integrated Matplotlib graphing and can manage computational clusters. The numeric Python extension adds fast array and matrix manipulation. The Scipy library of Python has well known constants available. NumPy provides a multidimensional array object, various derived objects and an assortment of routines for fast operations on arrays, including mathematical, logical, shape manipulation, sorting, selecting, I/O, discrete Fourier transforms, basic linear algebra, basic statistical operations, random simulation and much more.

3.2 Flowchart

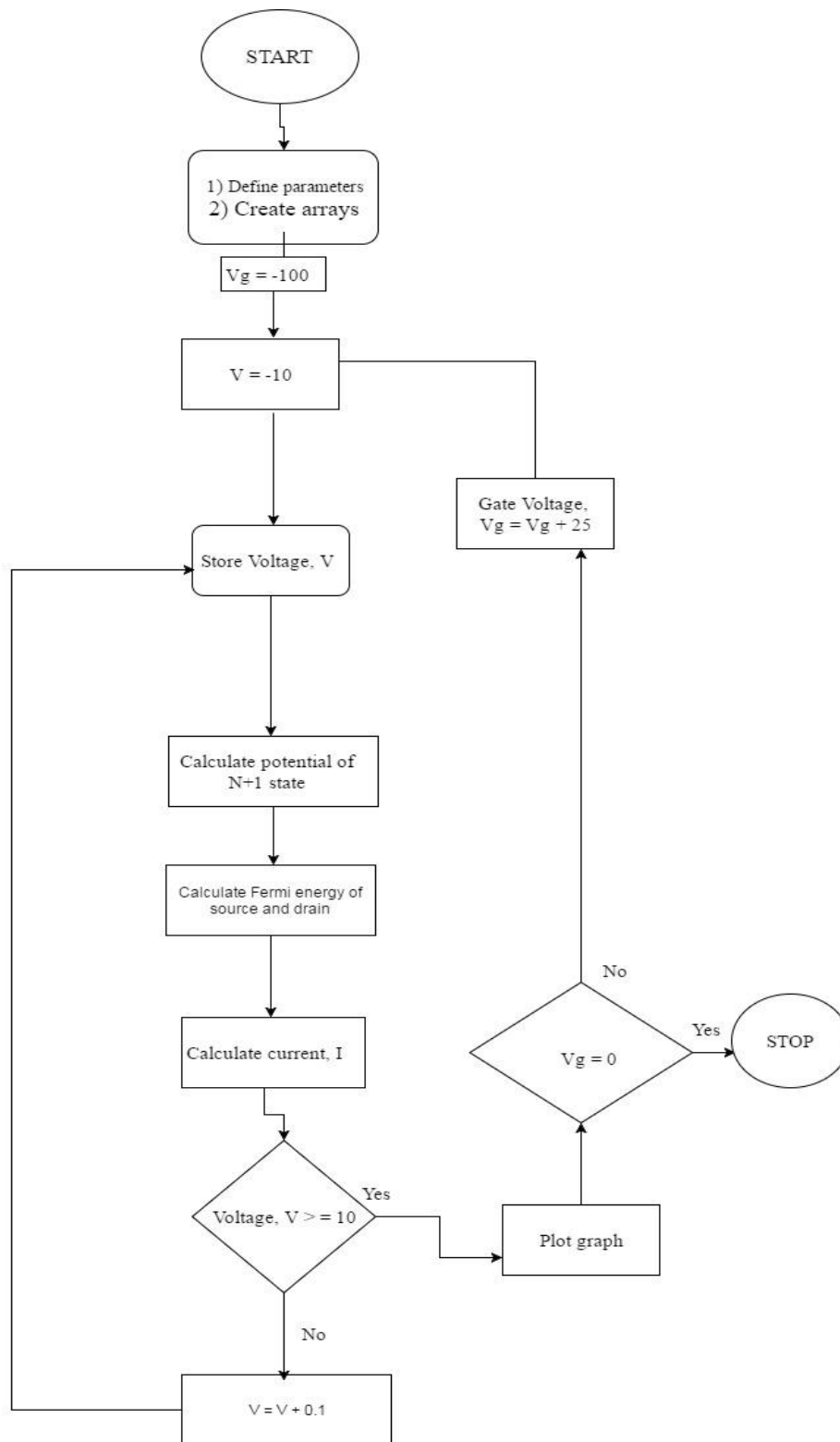


Figure 3.1: Flowchart for calculating and plotting I vs V

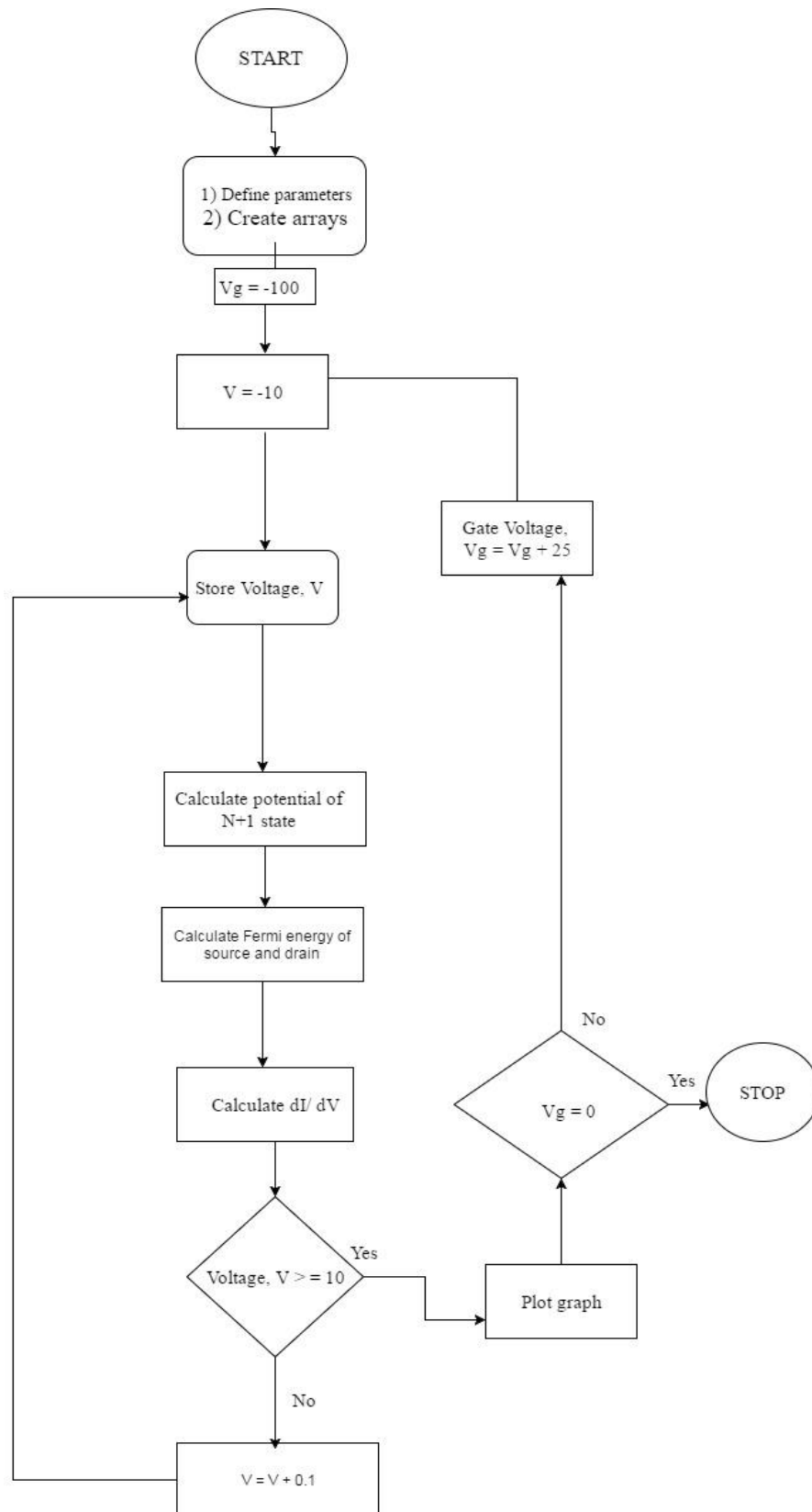


Figure 3.2: Flowchart for calculating and plotting $\frac{dI}{dV}$

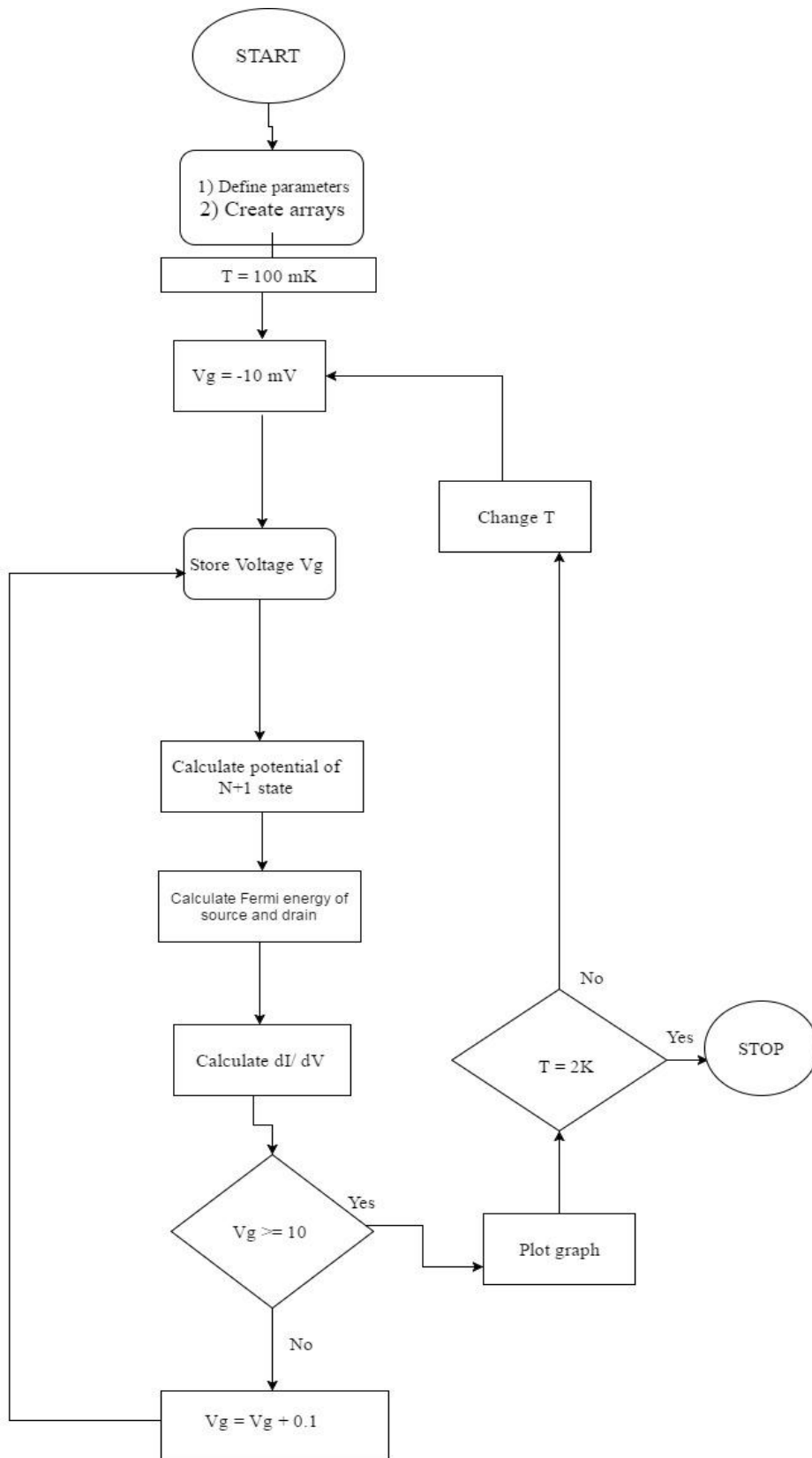


Figure 3.3: Flowchart for plotting $\frac{dI}{dV}$ vs V_G at different temperatures

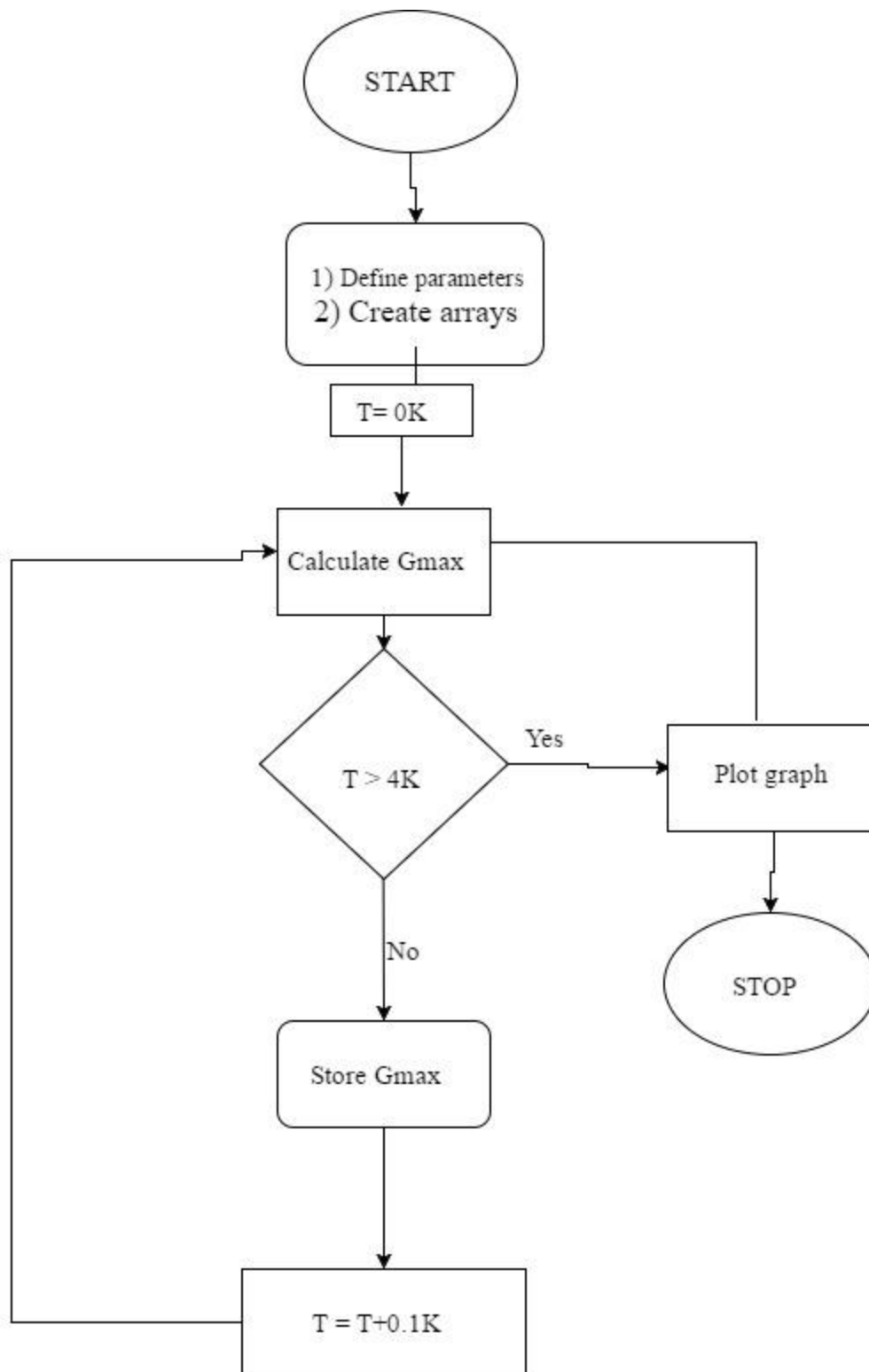


Figure 3.4: Flowchart for plotting peak height vs temperatures

3.3 Sample codes

For current versus source drain voltage graph for different gate voltages:

```
import math

import numpy as np

from math import exp, expm1

from decimal import Decimal

import matplotlib.pyplot as plt

#the constants are assigned with specific values

gamma = 5 * math.pow(10, 9)

kb = 1.3807 * math.pow(10, -23)

t = 1.5

ctotal = 100

cd = 38

cs = 57

cg = 5

e = 1.602 * math.pow(10, -19)

#This array stores current

current1 = []

current2 = []

current3 = []

current4 = []

current5 = []
```

```

#this sets the voltages and the gate voltages

VG = np.arange(-100*math.pow(10,-3),25*math.pow(10,-3),25*math.pow(10,-3))

voltage = np.arange(-10*math.pow(10,-3), 11*math.pow(10,-3), 0.1*math.pow(10,-3))

#this acts as the voltage loop for a particular gate voltage

for vol in voltage:

    meu = -(e/ctotal)* ((cg*VG[0])+(cs*vol))

    fd = math.pow((1+(np.exp(meu/(kb*t))))), -1)

    fs = math.pow((1 + (np.exp(((meu+(e*vol))/(kb*t))))), -1)

    I = e * gamma *(fd-fs)

    current1.append(I)

    .....

    .....

#for plotting the multiple graphs

plt.gca().set_color_cycle(['red', 'green', 'blue', 'yellow', 'black'])

plt.plot(voltage, current1)

plt.plot(voltage, current2)

plt.plot(voltage, current3)

plt.plot(voltage, current4)

plt.plot(voltage, current5)

plt.xlabel('Voltage(V)')

plt.ylabel('Current(nA)')

plt.show()

```


For $\frac{dI}{dV}$ versus source drain voltage graph for different gate voltages:

```
import math

import numpy as np

from math import exp, expm1

from decimal import Decimal

import matplotlib.pyplot as plt

#the constants are assigned with specific values

gamma = 5 * math.pow(10, 9)

kb = 1.3807 * math.pow(10, -23)

t = 1.5

ctotal = 100

cd = 38

cs = 57

cg = 5

e = 1.602 * math.pow(10, -19)

#this sets the voltages and the gate voltages

VG = np.arange(-100*math.pow(10,-3),25*math.pow(10,-3),25*math.pow(10,-3))

voltage = np.arange(-10*math.pow(10,-3),11*math.pow(10,-3),0.1*math.pow(10,-3))

#this acts as the array for  $\frac{dI}{dV}$ 

dibydvarray1 = []

dibydvarray2 = []
```

```

dibyvarray3 = []
dibyvarray4 = []
dibyvarray5 = []

#this acts as the voltage loop for a particular gate voltage
for vol in voltage:

    meu = -(e/ctotal)* ((cg*VG[0])+(cs*vol))

    fd = math.pow((1+(np.exp(meu/(kb*t)))), -1)

    fs = math.pow((1 + (np.exp(((meu+(e*vol))/(kb*t))))), -1)

    dibydv = ((math.pow(e,2)* gamma)/(kb*t)) * (((1-fd)*fd)*(cs/ctotal)) + (((1-
fs)*fs)*((cd+cg)/ctotal))

    dibyvarray1.append(dibydv)

#for plotting the multiple graphs
plt.gca().set_color_cycle(['red', 'green', 'blue', 'yellow', 'black'])

plt.plot(voltage, dibyvarray1)
plt.plot(voltage, dibyvarray2)
plt.plot(voltage, dibyvarray3)
plt.plot(voltage, dibyvarray4)
plt.plot(voltage, dibyvarray5)

plt.xlabel('Voltage(V)')
plt.ylabel('dI/dV')

plt.show()

```

For $\frac{dI}{dV}$ versus voltage graph for different temperature:

```
import math

import numpy as np

from math import exp, expm1

from decimal import Decimal

import matplotlib.pyplot as plt

#the constants are assigned with specific values

gamma = 5 * math.pow(10, 9)

kb = 1.3807 * math.pow(10, -23)

t = 1.5

ctotal = 100

cd = 38

cs = 57

cg = 5

e = 1.602 * math.pow(10, -19)

alpha = cg/ctotal

#this sets the voltages and the temperatures

T = [100*math.pow(10,-3),160*math.pow(10,-3),300*math.pow(10,-3), 1, 2]

voltage = np.arange(-10*math.pow(10,-3),11*math.pow(10,-3),0.1*math.pow(10,-3))

dibydvarray1 = []
```

```

#this acts as the voltage loop for a particular temperature
for vol in voltage:

    coshvalue = np.cosh((e*alpha*vol)/(2*kb*T[0]))

    dibydv = (((math.pow(e,2)*gamma)/(4*kb*T[0]))*math.pow(coshvalue, -2))

    dibydvarray1.append(dibydv)

#for plotting the multiple graphs
plt.gca().set_color_cycle(['red', 'green', 'blue', 'yellow', 'black'])

plt.plot(voltage, dibydvarray1)
plt.plot(voltage, dibydvarray2)
plt.plot(voltage, dibydvarray3)
plt.plot(voltage, dibydvarray4)
plt.plot(voltage, dibydvarray5)

plt.xlabel('Voltage(V)')
plt.ylabel('dI/dV (S)')

plt.show()

```

For G_{max} versus temperature:

```

import math

import numpy as np

from math import exp, expm1

from decimal import Decimal

import matplotlib.pyplot as plt

```

```

#constants are assigned specific values

gamma = 5 * math.pow(10, 9)

kb = 1.3807 * math.pow(10, -23)

ctotal = 100

cd = 38

cs = 57

cg = 5

e = 1.602 * math.pow(10, -19)

# sets the temperature

T = np.arange(0,4.2,.2)

#array for  $G_{max}$ 

gmaxvaluearray = []

#loop for  $G_{max}$  at a particular temperature

for t in T:

    gmax = ((math.pow(e,2)* gamma)/(4*kb*t))

    gmaxvaluearray.append(gmax)

#for plotting the graph
plt.plot(T, gmaxvaluearray)
plt.xlabel('T(K)')
plt.ylabel('peak height (S)')
plt.show()

```

Chapter 4

Results

Each obtained equation for current versus voltage, V , corresponding differential conductance versus voltage, V , differential conductance with $V = 0$ and finally maximum conductance versus temperature were simulated using Python. The common values used for the variables are listed below:

$$\Gamma = 5 \text{ GHz}$$

$$e = |e| = 1.602 \times 10^{-19} \text{ C}$$

$$C_D = 38 \text{ } \mu\text{F}$$

$$C_S = 57 \text{ } \mu\text{F}$$

$$C_G = 5 \text{ } \mu\text{F}$$

$$C_{total} = 100 \text{ } \mu\text{F}$$

$$E_0 = 0$$

$$V_C = 0$$

$$k_B T = 1.3806 \times 10^{-23} \text{ J}$$

4.1 Current versus source drain voltage graph for different gate voltages

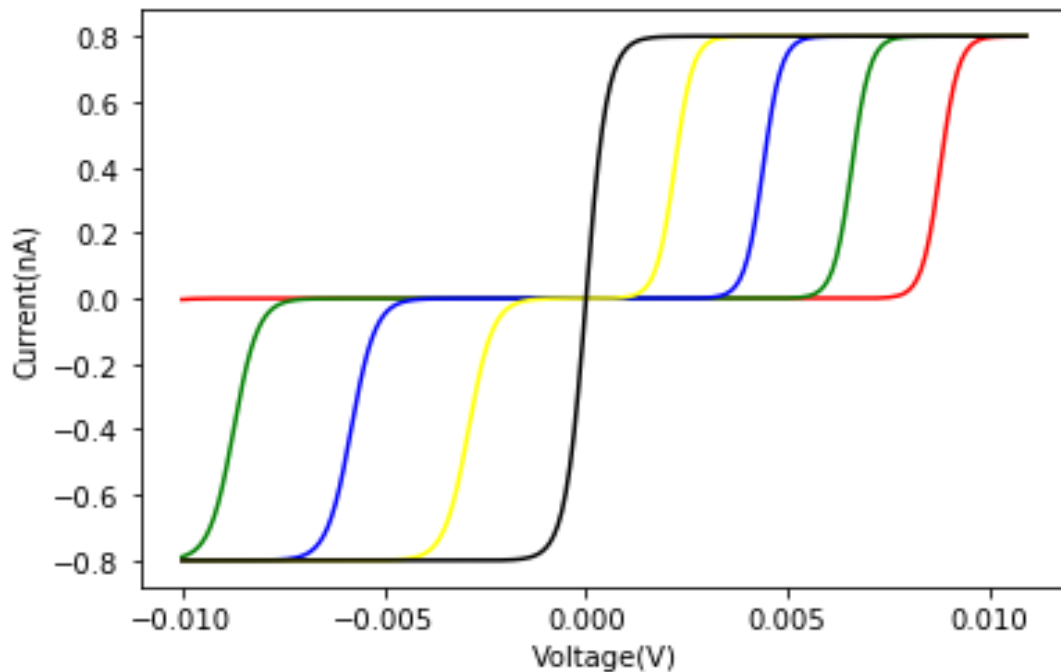


Figure 4.1: Five I-V curves at $T = 1.5K$ at different V_G where the red line is for $V_G = -100mV$, the green line is for $V_G = -75mV$, the blue line is for $V_G = -50mV$, the yellow line is for $V_G = -25mV$ and the black line is for $V_G = 0V$

Each curve in above mentioned figure shows a non-conducting region up to a certain bias until it starts conducting again. This de-escalation of conductance at low biases is a direct result of the Coulomb blockade theory which results due to the effect of charge addition energy.

4.2 Differential conductance versus source drain voltage graph for different gate voltages

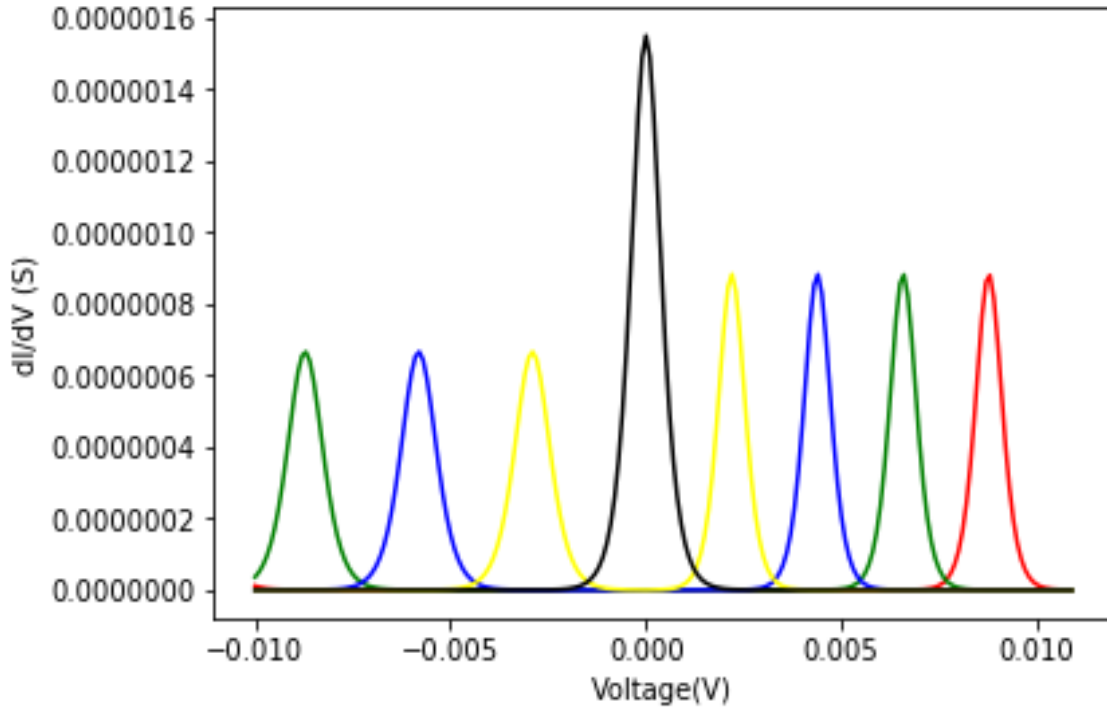


Figure 4.2: $\frac{dI}{dV}$ as a function of V at different V_G at $T = 1.5K$. They show peaks corresponding to the current steps I - V curves.

The overall conductance of the single molecule transistor had the max *value* $= 1.5 \times 10^{-6}$ which is significantly lower than the conductance quantum, $\frac{e^2}{h} = 3.874 \times 10^{-5}$. This is due to a large tunnel contact resistance between the molecule and the electrodes, which is consistent with the formation of a single electron transistor.

Each dI/dV - V curve shows a peak near each current step present in the corresponding I - V curve.

Since the equation used was

$$\frac{dI}{dV} = \frac{e^2\Gamma}{k_B T} \left[(1 - f_D) f_D \frac{C_S}{C_{total}} + (1 - f_S) f_S \left(\frac{C_D - C_G}{C_{total}} \right) \right]$$

It is evident from here that by varying the voltages V_G and V thereby changing the corresponding μ_S and μ_D the value of $\mu_{(N+1)}$ can be calculated by using the workings done in section 2.7.

4.3 Differential conductance versus voltage graph for different temperature, T

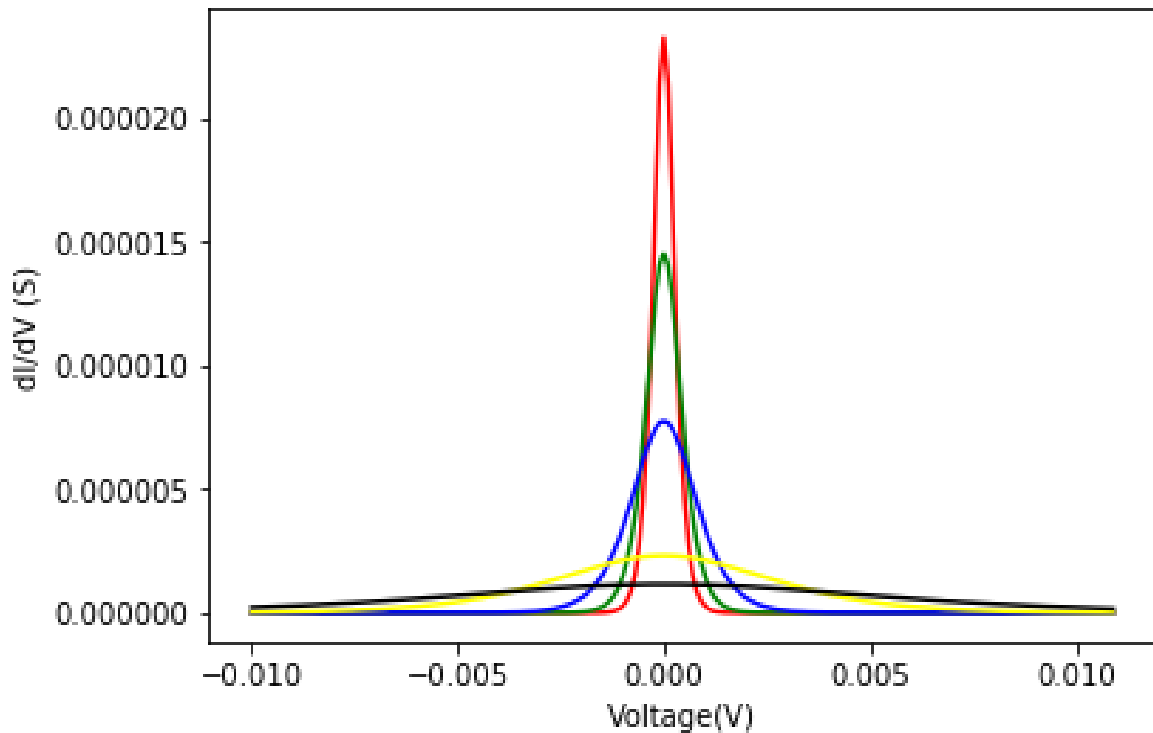


Figure 4.3: Five $\frac{dI}{dV}$ curves at different T where the red line is for $T = 100mK$, the green line is for $T = 160mK$, the blue line is for $T = 300mK$, the yellow line is for $T = 1K$ and the black line is for $T = 2K$

The graph obtained clearly depicts the temperature being inversely proportional to the differential conductance, i.e. as the temperature decreases the differential conductance increases. The temperature dependence of a Coulomb oscillation peak is one of the signature behaviours of a quantum dot as opposed to a classical dot because when it comes to classical dots its peak height does not change with increasing temperatures. This temperature dependence of a Coulomb oscillation peak can be used for measuring quantum dot parameters

like intrinsic broadening, α which is the ratio of gate capacitance to total capacitance, crossing potential which is V_C , etc.

4.4 Maximum conductance versus temperature graph

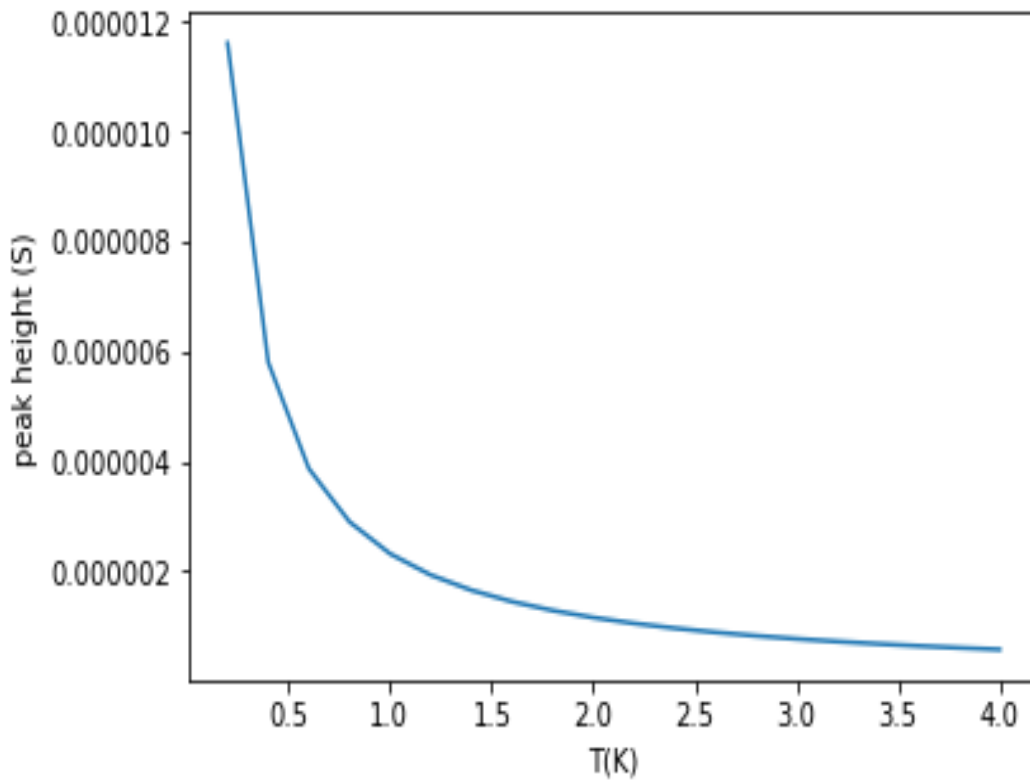


Figure 4.4: Temperature dependence of the Coulomb oscillation peak

The graph given above clearly depicts that the peak height, G_{max} decreases with an increasing temperature.

Chapter 5

Conclusion

Single molecule devices consisting of quantum dots formed due to a large charging energy and energy level quantization tend to show similar electronic transport properties despite of their differences in chemical compositions. As seen in the preceding chapters the electron number on the dot oscillates between N and $N+1$ during the on-state due to Coulomb oscillation. Also the differential conductance displays two different peaks for the same I-V graph due to the Coulomb oscillation. The discrete conductance peak indicates different atomic states. In addition to all these the differential conductance increases with the decrease in temperature. The temperature dependence of a Coulomb oscillation peak is one of the signature behaviours of a quantum dot. This means the approach adopted to decipher the transport mechanism and characteristic behaviours due to physical variables like gate voltage and temperature can be expanded to an array of different molecules to study their electron transport properties and in turn investigate the coupling between various quantum excitations of a molecule and its electronic degree of freedom. All these molecular level understanding can hence be used to create newer devices with desirable characteristics and outputs. Since well-equipped laboratories with optimum working environment are somewhat a luxury that is difficult to avail simulating the findings to artificially visualize the expected experimental outcomes can prove to be second best option. It also minimizes the window of error since the numerical calculations and characteristics graph are computer generated and handled. However the drawback of this methodology is that it is assumption and approximation laden which means real life outputs might be way off from the simulated ones. Though the risk is worth it since the understanding might very as well lead to greater discoveries.

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