**Introduction to *"Coulomb Blockade Lab"***

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## INTRODUCTION:

Electronic charge is well recognized to be discrete, a fact well noted by any high school physics student. Yet, no such well known signatures of this concept appear within the present electronic device context. One always measures a smooth, continuous capacitance, resistance and Current-Voltage characteristic. So, how can we measure a discrete effect due to discrete charge? One might have always questioned why the charge does not increase in steps in a capacitor by an amount equal to the charge quantum, rather than exhibiting a linear relationship with respect to applied voltage. The answer lies in a phenomenon called Coulomb Blockade that was discovered and experimented in the late 1980s. This phenomenon and its implication is much far outreaching than just a physical curiosity, but bear fundamental concepts as well as potential applications.. The main players of the game are artificially fabricated devices called Quantum Dots. The advantage of course is the creation of artificial atomic entities that can be tailored for study. In other words, the development of mesoscopic physics and microelectronic fabrication techniques led to the discovery of Coulomb Blockade-a straightforward reconfirmation of the fact that electron charges are actually added one after the other. But this is not where the story ends. Quantum dots, or artificial atoms, are islands of confined zero-dimensional devices – or quantum confinement taken to the extreme. It is amazing that artificial atoms and molecules could be fabricated right in the laboratory, and basics of quantum physics can be probed by man made structures. The most important aspect of course is to understand the fundamentals of electrons interact with one another. The object of this tutorial is to simulate quantum dots via simple phenomenological modes and display the plethora of interesting electron transport effects that can arise simply out of charge and size quantization.

## QUANTUM DOT TRANSPORT:

What follows now is a brief description of how to use this tutorial. To get started let us begin with a single quantum dot. It is an island formed due to confinement of electrons in three dimensions. This confinement can be achieved at will. Some typical confinement geometries are shown in Fig. 1

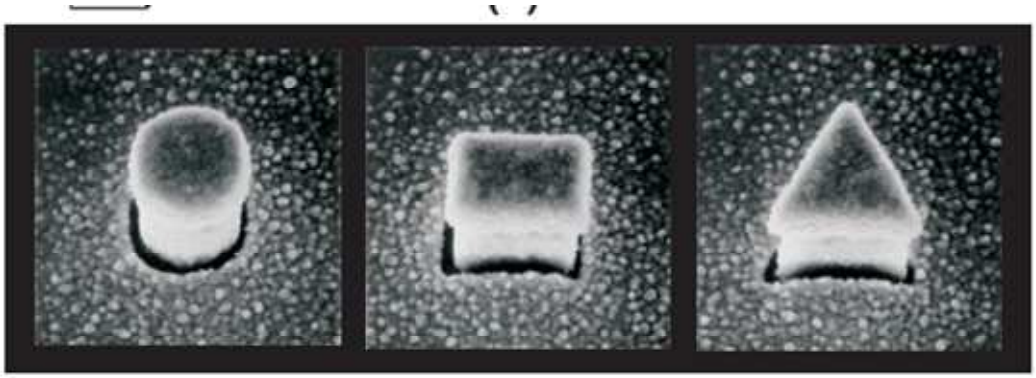

Fig.1: Examples of confinement types resulting in quantum dots [1].

For experimental purposes the cylindrical confinement possesses the highest symmetry. Transport measurements are made when these confined structures are sandwiched between electrodes, much like conventional device geometries [1-2].

Regardless of the device geometry or the confinement type, it is easy to abstract these into a simpler and yet powerful schematic. The transport situation is nothing but a bunch of quantized levels (fig.2) depicting the quantum dot island, tunneling barriers connected to macroscopic contacts from which electrons hop into available energy levels. But the electrons hardly zip through the available energy levels. An interesting interplay between different time scales is possible resulting in curious and potentially useful applications. It is more instructive to consider the time scales as being translated into their inverses – transition rates or interaction energies. The rate of in- and out tunneling into the structure translates into the broadening or energetic uncertainty of the localized quantum states. The separation of the localized states due to quantum confinement is another relevant energy scale. The Charge interaction energy is the third relevant energy scale. For double quantum dots a forth energy scale, the inter-dot coupling energy / rate. Interesting phenomena appear when two or more of these energy / rate scales are comparable in size. The simplest and well understood one is Coulomb Blockade. This tutorial is intended to provide as a primer for various phenomena associated with Coulomb Blockade.

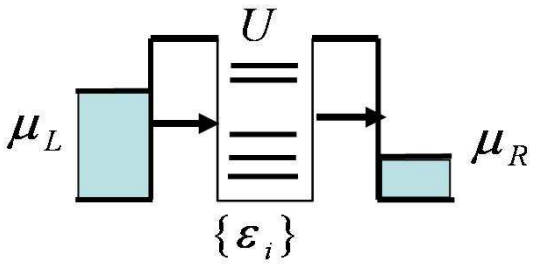


Fig. 2: Schematic representation of quantum dot transport. The quantum dot device is a bunch of discrete energy levels, coupled to the electrodes acting as reservoirs. Electrons hop on to available energy levels and interact with each other strongly within the device.

The many-body system and transport calculations are based on configuration interaction calculations and rate equations. Details of these formalisms that are implemented in the Coulomb Blockade Lab are given in references [3-6]. Reference [5] in particular contains tutorial-like material on the approach in the form of a Ph.D. thesis that is available on the nanoHUB.

## COULOMB BLOCKADE

This tutorial is graded in its complexity. We first begin with simple examples to elucidate Coulomb Blockade effects. This section basically serves as a guide so that more complex examples can be tested out after systematically going through this material.

The components of this lab are:

1) Single quantum dot: Here we explore the transport through the simplest example, a single spin degenerate level quantum dot. We can hypothetically call this a

hydrogen-like artificial atom with only an s-type orbital. Here we will briefly play around and explore as to what Coulomb Blockade really means. Once the user is comfortable with the idea, we will try out more exotic examples such as negative differential resistance (NDR), i.e., a decreasing current with increasing voltage bias.

2) Double quantum dots: Here we will explore a slightly more interesting device type: two serially coupled quantum dot islands sandwiched between electrodes. We can call this an artificial hydrogen-molecule with an s-type orbital on each atom. Here there are more interesting effects such as formation of interesting many-body states which results to intense excitation spectra all of which can be mapped through the I-V characteristics. We will further see how recent experiments such as Pauli-spin blockade [7] can be easily understood from these simple models.

Once the user is comfortable with these, please try out the multi-orbital case for both single and double quantum dots.

***Single Quantum Dot:***

To get started four simple steps shown in fig.3 will simulate the I-V characteristics.

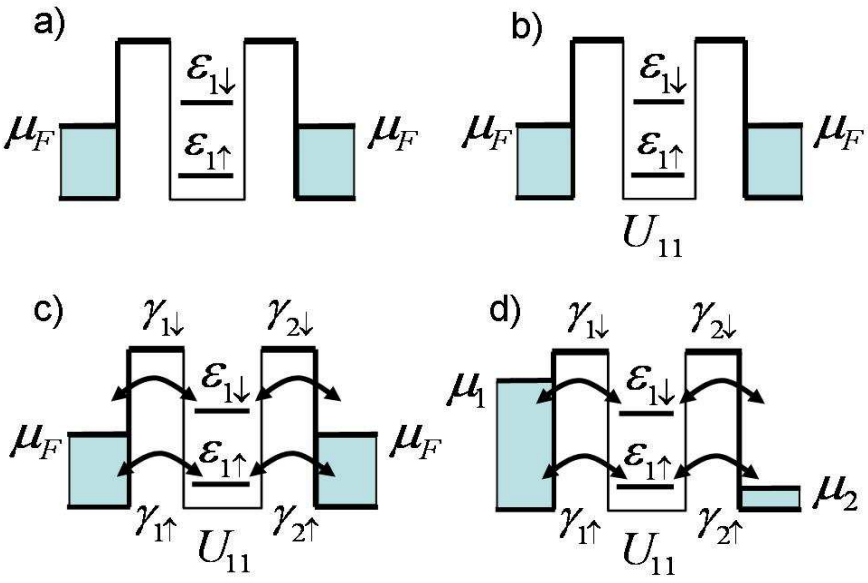


Fig.3: Input Stages a) position the energy levels with respect to contact Fermi level, b) Add the charging parameter c) add contact couplings and d) input the voltage bias range.

The four simple steps are:

1) Placement of Energy levels: The relative position of the energy levels with respect to equilibrium Fermi potential decides how many electrons are in the quantum dot to begin with. For example when $\mu_F > \varepsilon_{1\uparrow}$, and $\mu_F < \varepsilon_{1\downarrow}$, there is only one electron in the dot to begin with.

2) The charging parameter: This parameter dictates how much repulsion is there in the system. After all it is the repulsion that causes Coulomb Blockade.

3) Contact Couplings: Tell us how strongly or weakly coupled each energy level is to either contact, left or right. The coupling parameter physically is the inverse of the transit time that the electron needs to tunnel from the electrode on to the device.

4) Voltage Range: When a bias is applied the contacts are no longer pinned to the Fermi level. The voltage range is basically upto how much bias your I-V characteristics must be taken.

***Some Examples to get Started:***

1) Lets now get started. Say fix $\mu_F = 0$, , $\varepsilon_{1\uparrow} = \varepsilon_{1\downarrow} = 0.1meV$ , and U=0.
   How many electrons do you think are there in the system at equilibrium?

2) Lets fix $\gamma_{L\uparrow} = \gamma_{R\uparrow} = \gamma_{L\downarrow} = \gamma_{R\downarrow} = 1meV$ , and the bias range to be -10mV to 10mV

How many plateaus does the I-V have in the positive bias direction and why?

Try steps 1 and 2 but now change to U=0.1 meV, now how many plateaus does the I-V have in the positive bias direction? How different is this from the first case? Next put $\varepsilon_{1\uparrow} = -0.1meV$ $\varepsilon_{1\downarrow} = 0.1meV$ . How many plateaus now? What is the difference between the three cases?

Now try out different cases by varying positions of energy levels with respect to Fermi levels and note what happens and why?

A very interesting case: With $\varepsilon_{1\uparrow} = 0meV$ $\varepsilon_{1\downarrow} = 0.05meV$ , U=0.1 meV let us keep assume the down spin level is badly coupled to the right contact, .i.e., $\gamma_{L\uparrow} = \gamma_{R\uparrow} = \gamma_{L\downarrow} = 1meV, \gamma_{R\downarrow} = 0.01meV$ , what happens now?. The current falls down with increasing voltage!. This is called Negative differential resistance. Now try the same with U=0. Do you see this phenomena?. If not why?. Some answers can be found in [6]. Try out various combinations and once comfortable lets try the next example: the double quantum dot.

***Double Quantum Dots:***

This case is almost the same as the previous one, except that there are two quantum dots forming the device, and thus more parameters to be input. The four basic steps are really the same.

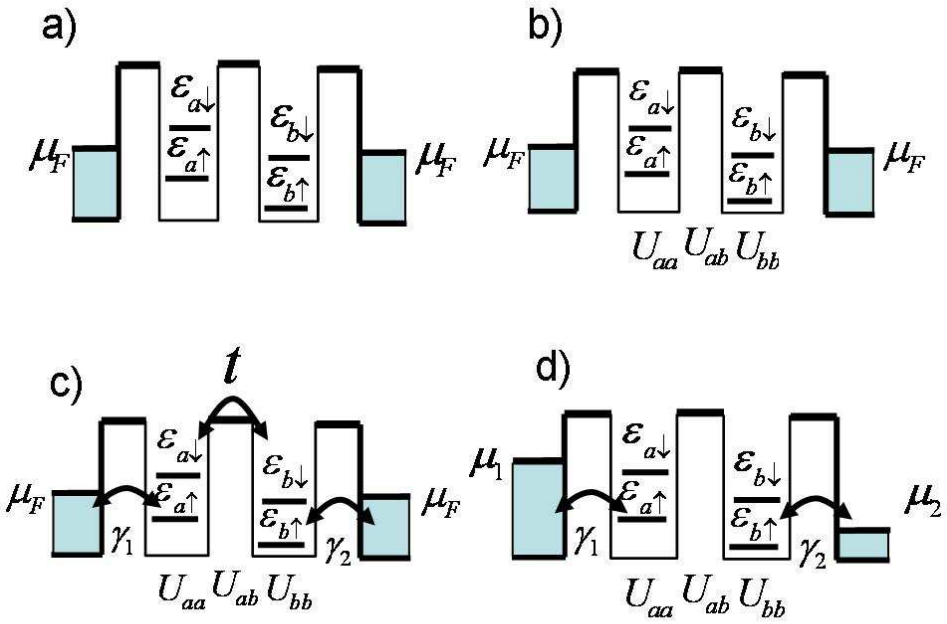


Fig.4: Input stages: a) position the energy levels with respect to contact Fermi level, b) Add the charging parameters c) add contact couplings, and tunnel coupling between the two dots and d) input the voltage bias range.

But now there are more parameters involved, such as the energy levels in both dots, coupling between the two dots t, and various charging parameters. Let us try out some examples:

***Some Examples to get Started:***

1) Take $\mu_F = 0$ $\varepsilon_{1\uparrow} = \varepsilon_{1\downarrow} = \varepsilon_{2\uparrow} = \varepsilon_{2\downarrow} = 0.1meV$ ,with
   $U_{aa} = U_{bb} = 0.2meV, U_{ab} = 0.1meV$
   With $\gamma_{L\uparrow} = \gamma_{R\uparrow} = \gamma_{L\downarrow} = \gamma_{R\downarrow} = 1meV$ , and t=0.1 meV
   and the bias range to be -10mV to 10 mV

Notice how the I-V characteristics look?. Notice the number of plateaus? For more reasoning on DQD spectrum, go through [1].

Now play around with various positions of energy levels, and notice how the I-Vs change.

2) Interesting Example: In this example we will note that NDR can occur in double quantum dot transport. The physics of how this NDR happens is called Pauli spin blockade [3]. The origin of NDR is an excited triplet state that blocks current flow due to other conducting states. This mechanism has been described in great detail in Ref. [6].

   Take $\mu_F = 2.0meV$ $\varepsilon_{1\uparrow} = \varepsilon_{1\downarrow} = 0meV \varepsilon_{2\uparrow} = \varepsilon_{2\downarrow} = -2meV$ ,with

   $U_{aa} = U_{bb} = 4meV, U_{ab} = 2meV$

   With $\gamma_{L\uparrow} = \gamma_{R\uparrow} = \gamma_{L\downarrow} = \gamma_{R\downarrow} = 1meV$ , and t=0.1 meV

   and the bias range to be -5mV to 5 mV.

   Notice carefully that current collapses in certain regions causing NDRs, What else do you observe?. Do you notice the asymmetry between positive and negative bias directions? Try varying the position of $\varepsilon_{2\uparrow}$ and $\varepsilon_{2\downarrow}$ and see how NDR critically depends on the relative position of energy levels between the two dots. Now vary the charging parameters and notice what else happens? Interested readers can go through reference [5] to get a general idea of how this NDR is caused.

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