Physics of low-dimensional structures and quantum devices,

Lund University

Project 5:
Coulomb blockade with rate equation

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1 Intoduction

In this project, the current through a single electron transistor (SET) will be calculated using a rate equation model. For simplicity, only one spin-degenerate orbital in the QD will be considered. After setting up the program, the influence of differnt parameters (mainly the magnetic field and the tunnel couplings) on the current will be studied.

2 Theory

A SET consists of a quantum dot (QD) which is capacitively coupled to a source and a drain contact (leads) and the current through the transistor can be controlled by a third electrode, the gate.
In contrast to the approach we used in the lecture, we here calculate the current through the device using a rate equation.
At finite source-drain bias, electrons can tunnel into and out of excited states. It is therefore necessary to define an extended dot chemical potential [2]:

$$\mu_N^{ij} = E_i(N) - E_j(N-1),$$

where $E_i(N)$ is the energy of the ith excited N-electron state[1]. In the following considerations, many-body states $|N,i\rangle$ will be called 'states' and single-particle orbitals with energy ε_k 'orbitals'. Unless a magnetic field is applied all orbitals come in pairs with the same energy due to spin degeneracy.
When a current is flowing through the SET, the many-body state in the QD will change as electrons tunnel on and off the dot. To calculate the current through the SET, the probability P_{N_i} for the dot being in state $|N,i\rangle$ is needed. For finding P_{N_i}, the tunneling rates on and off the dot have to be determined.
The total rate for a tunneling process on the dot, which changes its initial state from $|N-1,j\rangle$ to $|N,i\rangle$, is given by [2]:

$$W_{Ni,(N-1)j} = \sum_{r=L,R} \Gamma^r_{Ni,(N-1)j} f_r\left(\mu_N^{ij}\right), \tag{2.1}$$

where $f_r\left(\mu_N^{ij}\right)$ is the Fermi-Dirac function of the left ($r = L$) or of right ($r = R$) electrode and it is included in equation 2.1 because there has to be an available electron in the lead which can tunnel on the dot.
$\Gamma^r_{Ni,(N-1)j}$ is the tunnel coupling between the dot and one of the leads and $\Gamma^r_{Ni,(N-1)j} = \gamma^r_k$ if the states $|N-1,j\rangle$ and $|N,i\rangle$ are connected by a single tunnel event into orbital k. Otherwise, $\Gamma^r_{Ni,(N-1)j} = 0$.
The rate for tunneling off the QD, changing its state from $|N+1,j\rangle$ to $|N,i\rangle$, is [2]:

$$W_{Ni,(N+1)j} = \sum_{r=L,R} \Gamma^r_{Ni,(N+1)j} \left(1 - f_r\left(\mu_N^{ji}\right)\right), \tag{2.2}$$

[1] The index i is completely arbitrary.

where a hole instead of an electron is needed in the lead.
The change of the probability of the SET being in state $|N,i\rangle$ with time is given by the sum of all tunnel processes leading to an occupation of the state, weightend by the probability $P_{N'j}$ of the corresponding initial state being occupied, minus the sum of all tunnel processes depopulating state $|N,i\rangle$, weightend by P_{Ni} [3]:

$$\dot{P}_{Ni} = \sum_{N'=N\pm 1} \sum_{j} W_{Ni,N'j} P_{N'j} - \sum_{N'=N\pm 1} \sum_{j} W_{N'j,Ni} P_{Ni}.$$

If the applied voltages are time-independent, the probabilities approach a steady state value in the long-time limit, so $\dot{P}_{Ni} = 0$. Together with the probability normalization condition $\sum_{Ni} P_{Ni} = 1$, all occupation probabilities can be calculated.
The current flowing out of electrode r is then simply given by counting the electrons tunneling out of that electrode, minus the electrons tunneling in, which is given by a similar rate as above, weightend by the probability that the quantum dot is in the corresponding initial state.

2.1 One spin-degenerate orbital

In this project, a single-level QD will be considered. Including spin, there are two orbitals with energies ε_1 and ε_2, which are only different if a magnetic field B is applied. In that case the orbitals split by an amount of $\Delta E = g\mu_B B$ (Zeeman splitting) [1], where g is the g-factor ($g = 2.002$ in vacuum) and μ_B is the Bohr magneton. Figure 2.1 shows the states (a magnetic field is applied) and the possible tunnel events between them.

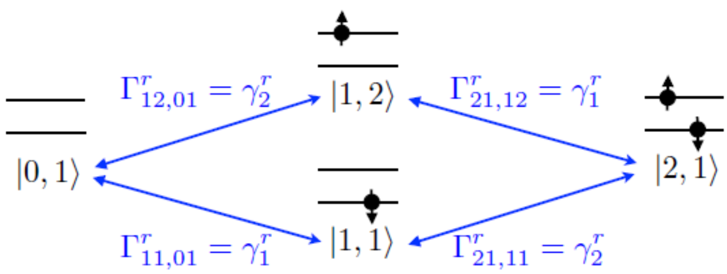

Figure 2.1: States and possible tunnel events in a system with one spin-degenerate orbital. Figure taken from [3].

In our calculations we assume that source-drain voltage is applied symmetrically. We also set the following parameters (unless otherwise stated): $T = 0.3\,\mathrm{K}$, $\gamma^L = \gamma^R = 5 \cdot 10^9$, $C_\Sigma = 1.5 \cdot 10^{-16}\,\mathrm{F}$ and $B = 0\,\mathrm{T}$.

3 Results and Discussion

In this section, we analyse the impact of different parameters on the performance of the SET. We qualitatively discuss how a magnetic field, a higher or lower total capacitance of the QD and a different tunnel coupling in the left and in the right barrier change the current through the SET. Finally, we also comment on the importance of a low temperature when operating a SET.

3.1 Coulomb diamonds

First of all, we consider the case where no magnetic field is applied, the total capacitance of the QD is set to a fixed value ($C_\Sigma = 1.5 \cdot 10^{-16}\,\mathrm{F}$), the tunnel coupling in the left and in the right barrier is the same and the temperature is low ($T = 0.3\,\mathrm{K}$).
Figure 3.1 a) shows the stability diagram of the SET. A characteristic Coulomb diamond is clearly visible in the middle of the figure. In the left green area no electron is on the QD, in the Coulomb diamond one electron is on the QD and in the right green area two electrons are on the QD.
As soon as the two-electron state is accessible, a higher current (yellow/darkblue area) can flow through the device compared to the case where only the one-electron state lies in the transport window (orange/light-blue area).
Figure 3.1 b) shows the conductance of the SET. Regions where I_{sd} changes with respect to V_{sd} are indicated in light-blue whereas regions where I_{sd} is constant are depicted in dark-blue.
In figure 3.1 c), I_{sd} is plotted against V_{sd} at a fixed gate voltage of $V_g = -1\,\mathrm{mV}$ (this corresponds to a cross-section through figure 3.1 a)). For small source-drain voltages, the SET is in a blocked state. At some point however, V_{sd} will be large enough so that the one-electron state is accessible and the current starts to flow. If we increased V_{sd} even more, the two-electron state would also lie in the transport window giving rise to another increase/decrease in the current. In figure 3.1 d) ($I_{sd}V_{sd}$-curve at a fixed gate voltage of $V_g = -1\,\mathrm{mV}$), this second increase/decrease can be seen.

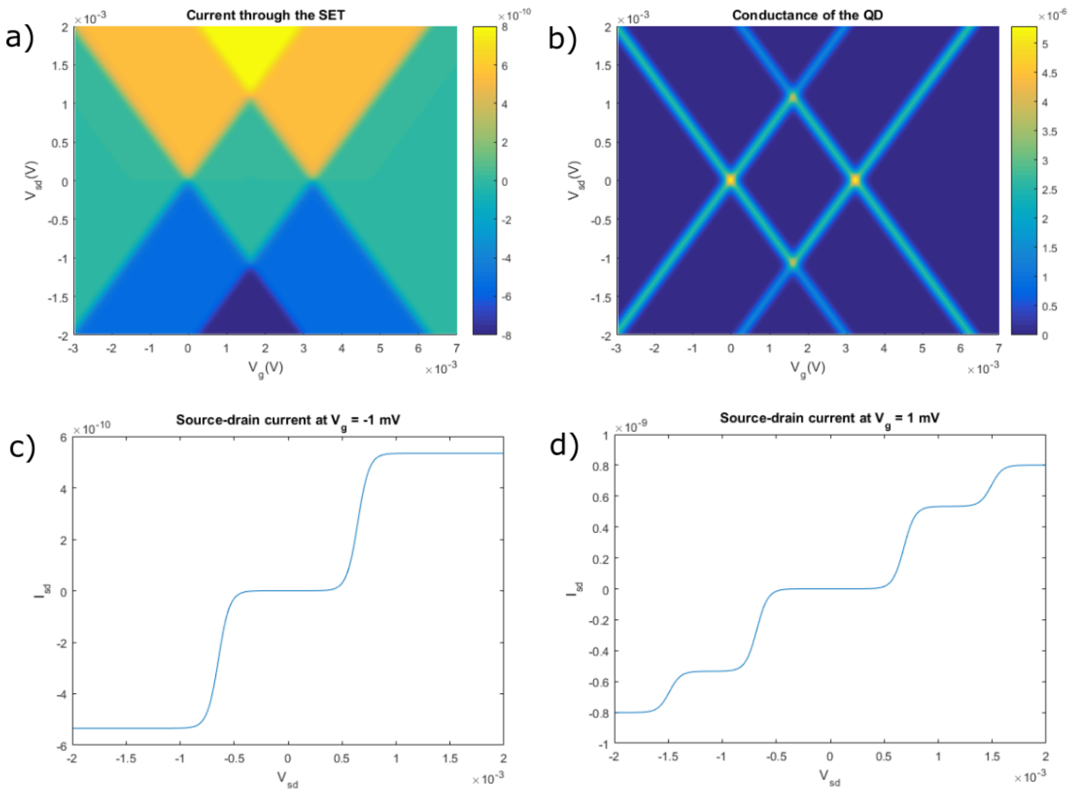

Figure 3.1: a) Stability diagram and b) conductance plot of the SET at $T = 0.3\,\mathrm{K}$, $B = 0\,\mathrm{T}$ and $\gamma_L = \gamma_R$. Figure c) shows a cross-section of figure a) at a fixed gate voltage of $V_g = -1\,\mathrm{mV}$ and figure d) shows the $I_{sd}V_{sd}$-curve at $V_g = 1\,\mathrm{mV}$.

3.2 Application of a magnetic field

As mentioned in the theory section, under the presence of a magnetic field B, orbital energies are no longer the same for spin up and spin down electrons, but will differ from the zero field level by $\Delta E = g\mu_B B$.

The splitting of the energy levels associated with the different spins becomes apparent in the conductance plot (figure 3.2 a)) as well as in the $I_{sd}V_{sd}$-curve (figure 3.2 b)).

In figure 3.2 b), the Zeeman splitting is clearly visible since there are two increases/decreases in the current instead of only one, which was the case without applied magnetic field (compare to figure 3.1 c)). When the source-drain voltage is high enough to include the one-electron spin-up state in the transport window, we get the mentioned second increase/decrease in the current. For even higher source-drain voltages, there would be two more increases/decreases visible (for the possible

two-electron states).
The maximum (saturation) source-drain current should be unaffected by the magnetic field, since it is only dependent on the tunneling rates.

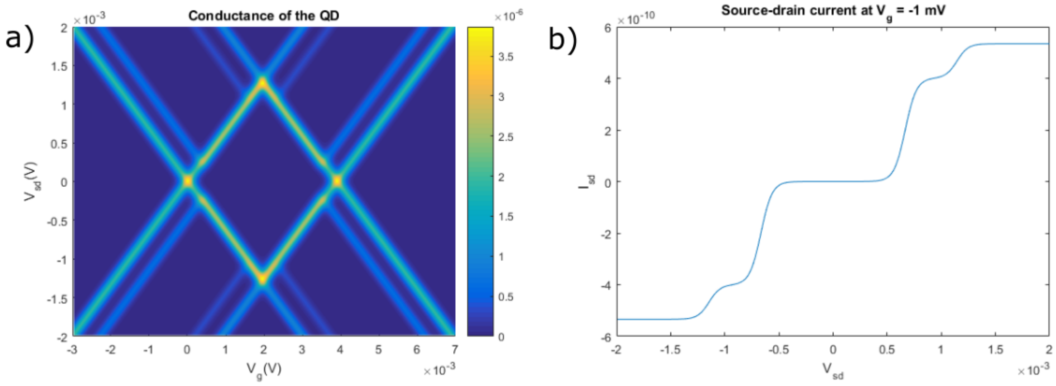

Figure 3.2: a) Conductance plot and b) $I_{sd}V_{sd}$-curve at $V_g = -1\,\mathrm{mV}$ if a magnetic field of $B = 2\,\mathrm{T}$ is applied.

3.3 Different total capacitances

Figure 3.3 shows that changing the total capacitance C_Σ leads to a change in the Coulomb diamond's width and height. This is due to the fact that both, the width and the height are proportional to the charging energy which is in turn inversely protortional to the total capacitance: $E_C = e^2/C_\Sigma$.

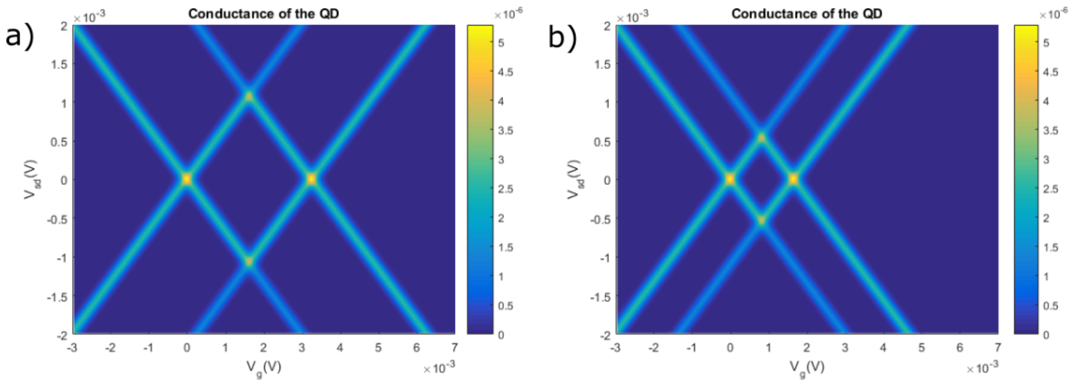

Figure 3.3: a) Conductance plot for a total capacitance of the QD of $C_\Sigma = 1.5 \cdot 10^{-16}\,\mathrm{F}$. b) Conductance plot for $C_\Sigma = 3 \cdot 10^{-16}\,\mathrm{F}$.

3.4 Different tunnel couplings

Next, a different tunnel coupling in the left and in the right barrier will be considered ($B = 0\,\mathrm{T}$, $C_\Sigma = 1.5 \cdot 10^{-16}\,\mathrm{F}$, $T = 0.3\,\mathrm{K}$). As an example, we set $10\gamma^L = \gamma^R$, which means that the left barrier is thicker (or higher) than the right barrier.
Figure 3.4 a) shows the conductance in the $V_{sd}V_g$-plane and in figure 3.4 b), I_{sd} is plotted against V_{sd} at a fixed gate voltage of $V_g = 1\,\mathrm{mV}$.

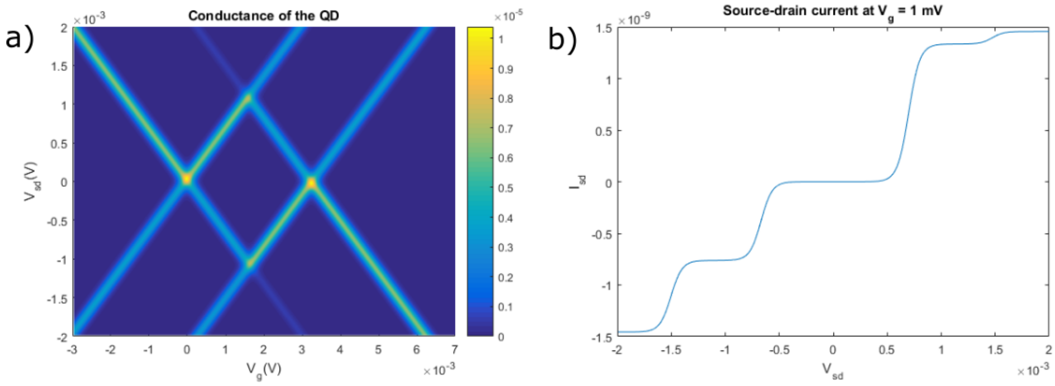

Figure 3.4: a) Conductance plot and b) $I_{sd}V_{sd}$-curve at $V_g = 1\,\mathrm{mV}$, if $10\gamma^L = \gamma^R$.

As shown in figure 3.4 b), the current is asymmetric now.
When a positive source-drain voltage is applied so that the chemical potential of the left lead is above the one-electron orbital in the QD, an electron can tunnel through the thick barrier on the dot. Since the right barrier is so small the electron will leave the dot immediately which means that the probability of the dot being empty is close to one. The current through the SET is high and does not change much when the two-electron orbital is accessible.
When a negative source-drain voltage is applied so that the chemical potential of the right lead is above the one-electron orbital in the QD, an electron can tunnel on the dot quite easily but the current is limited by an electron tunneling off the dot through the thick right barrier. When the two-electron orbital is accessible, the current will approximately double.
For large source-drain voltages, the current is the same.

3.5 Temperature

The last parameter we want to focus on is the temperature. When the thermal energy of the electrons is in the range of the charging energy, the two-electron state in the QD is accessible independent of the applied gate voltage. This is to say that the gate loses the control over the source-drain current.

Bibliography

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[3] M. Leijnse. *Coulomb blockade with rate equations*, 2014.