Coulomb blockade theory with rate equations

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1 Introduction

In this project we model the current through a quantum dot using rate equations. The model is based on a theoretical Single Electron Transistor (SET) which means that the quantum dot can be influenced by a gate and source drain voltages. The rate of tunneling, which is connected to the chemical potentials in the system, gives the probability of quantized states being occupied in the quantum well (QW) [1] [3]. To calculate the chemical potential inside the QW we have to take into account that the electron configuration does not have to be in the ground state. The chemical potential with excited states is given by

$$\mu_N^j = E_i(N) - E_j(N - 1),$$  \hspace{1cm} (1)

where $E_i(N)$ is the energy of the $i$th excited $N$-electron state. We define the many-body states $|N, i\rangle$ and the single-particle orbitals $k$ with energies $\epsilon_k$ as shown in figure 1. The numbering of the states $i$ is arbitrary.

![Figure 1: A few examples of naming of energy states and transitions.](image)

To simplify the system we approximate only one tunneling event to happen at a time. The tunneling of a single electron into orbital $\epsilon_4$ and out of orbital $\epsilon_6$. These are multiple tunneling events and thus this transition is forbidden.

To calculate the chemical potential inside the QW we have to take into account that the electron rate equations in and out the dot. The rate of a electron tunneling into the dot, changing its state from $|\epsilon_6\rangle$, $|\epsilon_4\rangle$, and $|\epsilon_5\rangle$ to $|4,1\rangle$, $|4,2\rangle$, $|4,3\rangle$, $|5,1\rangle$, and $|5,2\rangle$. If the states are connected by multiple tunnelings $\Gamma_{N1,(N-1)j}^r = 0$. An example of these transitions is shown in figure 1.

1.1 Rate equations

With a current going through a dot the state of the dot changes continuously. The chance that the dot is in state $|N, i\rangle$ is given by the probability $P_{Ni}$. To calculate these probabilities we need the tunneling rates in and out the dot. The rate of a electron tunneling into the dot, changing its state from $|N - 1, j\rangle$ to $|N, i\rangle$ is given by

$$W_{N1,(N-1)j} = \sum_{r=L,R} \Gamma_{N1,(N-1)j}^r f_r(\mu_N^j),$$  \hspace{1cm} (2)

where

$$f_r(\mu) = \frac{1}{1 + \exp[\frac{\mu - \mu_r}{k_BT}]}$$  \hspace{1cm} (3)

is the Fermi function of the electrode $r$, with $\mu_r$ the chemical potential in the electrode, which is affected by the bias voltage according to $-eV = \mu_L - \mu_R$. The Fermi function predicts the available electrons in the lead with energy $\mu$ that can tunnel through.

The rate of electrons tunneling out of the dot, changing its state from $|N + 1, j\rangle$ to $|N, i\rangle$ is given by

$$W_{N1,(N-1)j} = \sum_{r=L,R} \Gamma_{N1,(N+1)j}^r \left(1 - f_r(\mu_{N+1}^j)\right),$$  \hspace{1cm} (4)

where a hole instead of an electron is needed in the lead.

In a steady-state system the probability of a state $|N, i\rangle$, $P_{Ni}$, does not change in time. In that case the individual probabilities can be calculated by

$$\dot{P}_{Ni} = \sum_{N' = N \pm 1} \sum_j W_{N1,N'j} P_{N'j} - \sum_{N' = N \pm 1} \sum_j W_{N'j,Ni} P_{Ni} = 0.$$  \hspace{1cm} (5)
This are all tunneling processes populating the state \( |N,i⟩ \), weighted with the probability \( P_{N′j} \), minus all the processes that depopulate \( |N,i⟩ \), weighted with \( P_{Ni} \). This system of equations is not complete: any equation can be written as a linear combination of the others. This means one equation can be discarded and the system can not be solved. Luckily, in addition to the equations in 5 we know the normalisation condition, \( \sum_{N,i} P_{Ni} = 1 \), must hold, making the system solvable again.

In matrix form this would be written as

\[
\tilde{W} P = R
\]

where \( \tilde{W} \) is the normalizing rate matrix with the diagonal

\[
\tilde{W}_{mm} = -\sum_{m′} \tilde{W}_{mm′}
\]

and a row \( M \) replaced with a row with 1 on every element. The vector \( R \) is a vector with 1 on row \( M \) and zeros on other positions.

Once the probabilities are calculated the current in one of the leads is given by all the tunneling processes from and to the lead:

\[
I_r = -e \sum_{N} \sum_{i} \sum_{N′=N±1} W_{Ni,N′j}^I P_{N′j}
\]

with

\[
W_{Ni,(N-1)j}^I = \Gamma_{Ni,(N-1)j}^r (\mu_{Ni}^{ji})
\]

\[
W_{Ni,(N+1)j}^I = -\Gamma_{Ni,(N+1)j}^r \left(1 - f_r(\mu_{Ni}^{ji})\right).
\]

### 1.2 Zeeman splitting

Without a magnetic field every quantum dot energy level is spin degenerate. In a magnetic field however the energy levels of spin up and spin down split with a factor\(^2\)

\[
E_B = g\mu_B B
\]

where

\[
\mu_B = \frac{e\hbar}{2m_e}
\]

is the Bohr magnetron and \( B \) is the magnetic field in Tesla. \( g \) is a correction factor for the magnetic moment, or \( g \)-factor, which has a value of \( g = 2.002 \) in vacuum. In solids this \( g \)-factor can take on different values, that can vary with the shape of the dot, but in our model the value for vacuum is used. This splitting of the energies in a quantum dot causes excited states to be accessible when tunneling.

### 2 Theoretical system setup

In our system, we model a single-level quantum dot containing four states with spin. Unless applying a magnetic field, the two orbitals have the same energy which means \( \epsilon_1 \) and \( \epsilon_2 \) are equal. When applying a magnetic field, the energy difference for splitting of levels can be calculated with equation 10.

In the setup we base certain values on earlier lab-results (Coulomb Blockade lab) such as the total capacitance of the island, \( C_Σ = 1 \cdot 10^{-17} \) F, and gate capacitance ratio \( \alpha_g = 1/20 \). All values used are shown in the table 1. Another assumption is that the bias is applied symmetrically as \( \mu_L = +eV/2 \), \( \mu_R = -eV/2 \).

As shown in figure 2, there are two types of tunneling that are forbidden in our approximation. For the tunneling event between two states with different number of electrons, for instance \( |0,1⟩ \) and \( |2,1⟩ \), two electrons need to tunnel at the same time, which we approximated to be impossible. For the states \( |1,2⟩ \) and \( |1,1⟩ \), the electrons with different orbitals also make it impossible to achieve by only one process.

In the used model the tunnel rates \( \gamma_L^r \) are the same, which means there is no difference in tunnel rate between the spin orbitals or the leads.

The temperature of the system defines the energy spread of the electrons in the leads. For the simulations the temperature of the dot is set to be 4K, the temperature of liquid helium. In experiments on quantum dots the temperature is often even lower.
3 Results & Discussion

All the results are based on the calculations of rate-equations via MATLAB, see APPENDIX.

3.1 Diamond structure

The characteristic diamond structures are shown above with both the conductance- and current-landscape in the $V_g$-$V_{sd}$-plane. In figure 3 the current and conductance of the dot without a magnetic field is shown. The Coulomb blockade region is visible as a diamond shaped region without current. In figure 3b the sharp conducting lines indicate that the current outside the blockade regions is well defined and does not vary within a region until the charging energy is surpassed and the dot can vary between the three occupation levels $|0, 1\rangle$, $|1, i\rangle$ and $|2, 1\rangle$ instead of only two. In this case a larger current is possible.

In figure 4 the current and conductance of the dot with a applied magnetic field of 20T is shown. The plots look similar to the figure 3, but additional conductance lines are visible parallel to the edges of the diamond. The splitting of the lines is due to the fact that the bound states are not spin degenerate in a magnetic field. In other words this gives us two possibilities for electron tunneling. The splitting between these energies is controlled by the Zeeman splitting which states that a stronger B-field gives a bigger energy split $E_B$ between spin-states according to equation 10.

3.2 $I$-$V_{sd}$-curve

When setting the gate-voltage $V_{sd}$ to a certain value in the non-conducting state and varying the source-drain-bias $V_{sd}$ we get figures 5a and 5b. In other words they are just plots along the cross-section down the middle of the diamonds in figures 3a & 4a.
(a) The color-coding for the current is according to
the scale and goes from -150 to 150 pA.

(b) The color-coding for the conductance is ac-
cording to the scale and goes from $0$ to $-8 \times 10^{-8}$
$m^{-1} \Omega^{-1}$. Observe the splitting of the lines.

Figure 4: A diamond pattern, applied B-field of 20 T, showing the landscape of current[A](left) and conductance[$\Omega^{-1}m^{-1}$](right) in the $V_g$-$V_{sd}$-plane.

(a) No applied B-field.

(b) Applied B-field of 20T.

Figure 5: A cross section, down the middle, of the diamond pattern in figure 3a(left) and 4a(right). In other words, showing the current fluctuation when changing the source-drain-voltage $V_{sd}$ at a constant gate-voltage $V_g$.

When sweeping the $V_{sd}$ over the theoretical SET, with applied B-field, the difference between the fermi-levels will first include only one of the two states until its increased to include both, so therefore we get this very characteristic look of two plateaus in the conducting state, see figure 5b. When the quantum well is fully conducting both spin-up and spin-down electrons are able to tunnel.

(a) Diamond structure with uneven barriers. Color
scale showing current[A].

(b) A cross section of the diamond pattern, slightly
off centre.

Figure 6: The Coulomb diamonds and a $I$-$V_{sd}$-curve of a dot with $\gamma^R = 10 \gamma^L$ and no applied B-field.
Another possible scenario is that the tunnel couplings, $\gamma$, between the two barriers of the quantum dot are not equal, see figure 6. It means that the widths of the barriers are different, which makes the rate of tunneling vary between the two sides. In this case $\gamma^R = 10\gamma^L$, so the left barrier is thicker than the right barrier.

As visible in figure 6b this results in an asymmetric $I-V$ curve. When $V_{sd}$ is applied such that $\mu_L$ is above $\mu(N)$ on the dot, an electron has to pass a thick barrier to populate the dot. However, the electron on the dot can tunnel through the right barrier very easily, so the probability of the dot being empty, $P_{0,1} \approx 1$. Current going through the dot is high and does not change much when the two electron state is accessible, since any electron on the dot will not stay long enough for a second electron to join him. However, if $V_{sd}$ is applied such that $\mu_R$ is above $\mu(N)$ on the dot, the current is limited by an electron tunnelling out of the dot through the thick left barrier. The probabilities $P_{1,1} = P_{1,2} \approx 1/2$ so the current is limited. When the applied bias is large enough to access the two electron state as well the current will approximately double. The total current at large $\pm V_{sd}$ is equal except for a minus sign.

### 3.3 Data

Table 1 shows some results and used values of our system. The chosen values are the island capacitance $C_\Sigma$, the gate capacitance ratio $\alpha_g$, and tunneling rate $\gamma^r$. These are chosen based on real results from a nanowire based SET. The rest of the values are calculated.

<table>
<thead>
<tr>
<th>DATA</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_\Sigma$ gate capacitance</td>
<td>$10^{-17}$</td>
<td>F</td>
</tr>
<tr>
<td>$\alpha_g$ ratio</td>
<td>1/20</td>
<td>-</td>
</tr>
<tr>
<td>$E_c$ charging energy</td>
<td>16</td>
<td>meV</td>
</tr>
<tr>
<td>$\gamma^r$ tunneling rate</td>
<td>$10^9$</td>
<td>Hz</td>
</tr>
</tbody>
</table>

### 4 Conclusions

Figure 3 shows the expected Coulomb diamond plot of a SET. The current through the dot is dependent of the gate voltage and the source-drain bias in a way that has been calculated before and is zero in the diamond shaped blockade regions.

In a magnetic field the spin levels split due to the Zeeman effect, which causes the current increase stepwise when the excited state is accessible. This is visible in figure 5b.

In addition, if we change the temperature from 4.2K to 20K, the thermal energy of the electron is becoming higher which gives them enough energy to tunnel even if the energy level on the island is above the chemical potential on the lead. The edge of the diamond structure is not well defined.

In this project, our simulating programme works well in the single-level system via the 4x4 rate matrix. If we turn to many-level system, for instance two levels, the complexity of the rate matrix, as well as the feasible states and the interaction of electrons will increase rapidly. They will contribute to additional currents which give rise to multiple conductance lines like the Zeeman splitting does in our simple case. The Coulomb diamond plot will still show the Coulomb blockade regions, but more diamonds will be visible.
APPENDIX

The MATLAB code for creating the figures 3a, 3b, 4a and 4b in the result part is shown below. The code is based on the theory of the rate-equations for an SET and with a simplified setup of a single energy-level.

%rate equations

%mu_N_ij
%N number of e-
%ij the different states

clear all

resolx = 300 % resolution in x-direction
resoly = 300 % resolution in y-direction
e = 1.602*10^-19; %elementary [C]
C_sum = 1*10^(-17); %capacitance in island [F]
g = 2.002319; %unitless g-factor for zeeman
mu_B = 9.27400968 * 10^(-24); %bohr magnetron [J/T]
B = 20; %magnetic field [T]
alpha_g=1/20;
delta_E_b = B * mu_B * g; %splitting of levels [J]
E_c = e^2 / C_sum; %charging energy [J]
V = linspace(-25*10^(-3),25*10^(-3),resoly); %source-drain-bias [V]
Vg=linspace(-0.6,0.3,resolx); %gate voltage [V]
I_L=zeros(numel(V),numel(Vg));
gamma=10^9;

for k=1:numel(V)
    for i=1:numel(Vg)
        mu_L = e*V(k)/2; % chemical potential in lead left [J]
        mu_R = -e*V(k)/2; % chemical potential in lead right [J]

        % ---------Chemical potentials in island-----------------------
        mu_1_11 = Vg(i)*e*alpha_g;
        mu_1_21 = Vg(i)*e*alpha_g+delta_E_b;
        mu_2_12 = Vg(i)*e*alpha_g+E_c;
        mu_2_11 = Vg(i)*e*alpha_g+E_c + delta_E_b ;

        % ---------Rate of tunneling-----------------------------------
        % gamma_k_r = 10^9 in this simplified case
        T = 4; %temperature [K]

        %tunnel in

        W_11_01 = [f(mu_1_11,mu_L,T) f(mu_1_11,mu_R,T)];

References

\[
W_{12\_01} = \begin{bmatrix} f(\mu_{1\_21}, \mu_L, T) & f(\mu_{1\_21}, \mu_R, T) \end{bmatrix} ;
\]
\[
W_{21\_12} = \begin{bmatrix} f(\mu_{2\_12}, \mu_L, T) & f(\mu_{2\_12}, \mu_R, T) \end{bmatrix} ;
\]
\[
W_{21\_11} = \begin{bmatrix} f(\mu_{2\_11}, \mu_L, T) & f(\mu_{2\_11}, \mu_R, T) \end{bmatrix} ;
\]
% tunnel out
\[
W_{01\_11} = \begin{bmatrix} (1-f(\mu_{1\_11}, \mu_L, T)) & (1-f(\mu_{1\_11}, \mu_R, T)) \end{bmatrix} ;
\]
\[
W_{01\_12} = \begin{bmatrix} (1-f(\mu_{1\_21}, \mu_L, T)) & (1-f(\mu_{1\_21}, \mu_R, T)) \end{bmatrix} ;
\]
\[
W_{11\_21} = \begin{bmatrix} (1-f(\mu_{2\_11}, \mu_L, T)) & (1-f(\mu_{2\_11}, \mu_R, T)) \end{bmatrix} ;
\]
\[
W_{12\_21} = \begin{bmatrix} (1-f(\mu_{2\_12}, \mu_L, T)) & (1-f(\mu_{2\_12}, \mu_R, T)) \end{bmatrix} ;
\]

% ---------Final matrix---------------------------------------
WMAT = \[
\begin{bmatrix} 1 & 1 & 1 & 1; \\
\text{sum}(W_{11\_01}) & -\text{sum}(W_{01\_11}) & -\text{sum}(W_{21\_11}) & 0 & \text{sum}(W_{11\_21}); \\
\text{sum}(W_{12\_01}) & 0 & -\text{sum}(W_{01\_12}) & -\text{sum}(W_{21\_12}) & \text{sum}(W_{12\_21}); \\
0 & \text{sum}(W_{21\_11}) & \text{sum}(W_{21\_12}) & -\text{sum}(W_{11\_21}) & -\text{sum}(W_{12\_21}) \\
\end{bmatrix};
\]

% ---------Calculation of probabilities and current-----------
\[
R = [1; 0; 0; 0];
\]
\[
P = \text{WMAT}\text{\(R\)}; \text{\(\%\) P(1) 01; P(2) 11; P(3) 12; P(4) 21}
\]
\[
I_L(k,i) = -e\gamma(-W_{01\_11}(1)*P(2)-W_{01\_12}(1)*P(3)+W_{11\_01}(1)*P(1)-W_{11\_21}(1)*P(4)+W_{12\_01}(1)*P(1)-W_{12\_21}(1)*P(4)+W_{21\_11}(1)*P(2)+W_{21\_12}(1)*P(3));
\]
\[
% I_R = -e(-W_{01\_11}(2)*P(2)-W_{01\_12}(2)*P(3)+W_{11\_01}(2)*P(1)-W_{11\_21}(2)*P(4)+W_{12\_01}(2)*P(1)-W_{12\_21}(2)*P(4)+W_{21\_11}(2)*P(2)+W_{21\_12}(2)*P(3))
\]
end

disd= []; 
\[
dV = V(2)-V(1);
\]

% ---------Calculation of conductance----------------------------
\[
\text{for } n=1:\text{numel}Vg.
\]
\[
disd=\text{dird)} \text{diff}(I_L(:,n))/dV ;
\]
end

figure(1)
surf(Vg, V, I_L, 'EdgeColor', 'none', 'LineStyle', 'none', 'FaceLighting', 'phong')
view(2)
xlabel('Gate Bias V_G')
ylabel('source drain bias V_{sd}')
title('Diamond structure for singe electron transistor InP/InAs')

figure(2)
plot(V, I_L(:, round(numel(V)/2)))
xlabel('Bias V_{sd}')
ylabel('current I')
title('Conductivity: sweeping V_{sd} over diamond mid-section')

figure(3)
surf(Vg, V(1:end-1), disd, 'EdgeColor', 'none', 'LineStyle', 'none', 'FaceLighting', 'phong')
view(2)
xlabel('Gate Bias V_G')
ylabel('source drain bias V_{sd}')
title('Diamond structure for singe electron transistor InP/InAs')