Department of Physics

Universität Regensburg

Bachelorthesis

Coulomb blockade effects in semi-conductive islands

submitted by: Susanne Candussio
Matriculation number: 1624007
Course of studies: Physics
University of Regensburg

adviced by: PD Dr. Andrea Donarini
Institute of Theoretical Physics
University of Regensburg

Regensburg, August 31, 2015

Contents

List of Figures

1 Introduction

Since 1978 many theoretical and experimental advances in mesoscopic physics were recorded. This branch of condensed matter physics describes systems with intermediate sizes. Since the 1980s M. A. Kastner and his group have been studying narrow transistors[1]. He describes his discovery in an article in Reviews of Modern Physics (1992). Several years before this article was published he and his group accidentally discovered the so called single-electron transistor and they studied how to control its behaviour. First they saw oscillations of the conductance in narrow Si-transistors like in Fig.1. To understand the dependence of the period of the oscillations they made many experiments with GaAs transistors, which Meirav et. al [2] had discovered at that time and they came to the result that each oscillation stands for adding one electron.[1] Thus Kastner et al. conclude that submicronsize transistors, which are

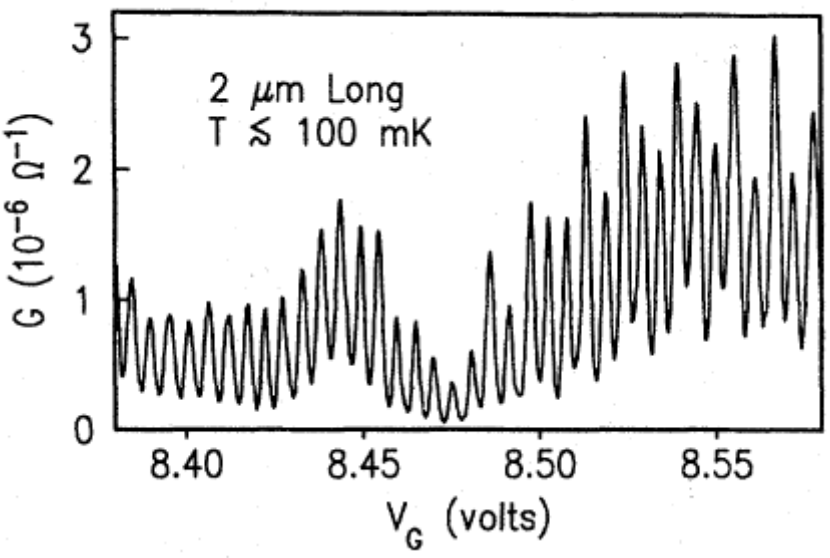


Figure 1: Coulomb oscillations for a symmetric Si-transistor ([1])

connected to their lead electrodes via tunnel junctions, turn on and off again every time an electron is added. This was different from the transistors, which were usually used at that time. They only turn on once as electrons are added.[1] L.Sohn, L. Kouwenhoven and G. Schön describe in their work about the mesoscopic electron transport([3]) the theory of single-electron tunnelling, with emphasis on the Coulomb blockade effects. They studied the current in a symmetric single-electron transistor.[3] In these devices the metallic island, which has a capacitance in the range of 10^{-15}F or smaller, is separated by tunnelling barriers with the tunnelling resistance $R_T > (\frac{h}{e^2})$. [4] Such systems are in a regime where the charging energy E_c is larger than the ther-

mal energy kT. [5] Sohn et. al describe the so called Coulomb oscillations, where the current (and the differential conductance) oscillates with the gate voltage, which controls the additional energy of the metallic island. [3][4] This effect can be exploited to control the transfer of a single charge from one island to another. [4]

S. Geißler et al. [6] studied Coulomb blockade effects in nano fabricated narrow constrictions in thin (Ga,Mn)As films. They observed nested Coulomb diamonds and anomalous conductance suppression in the vicinity of charge degeneracy points. They analyzed the transport characteristics of the system with a modified orthodox theory of Coulomb blockade which takes into account the energy dependence of the density of states in the metallic island. They assumed a density of states with an upward shift in energy of the minority spin band with respect to the majority spin band and saw that there is a conductance suppression for tunnelling if the chemical potential lies between the bottom of the majority and of the minority spin band for low bias voltages. But this does not describe the fact that there is a full suppression of the conductance peaks.[6] Because of this we want to consider conductance suppression for another density of states.

The aim of this work is to study the Coulomb blockade effects in semi-conductive islands. We calculate the characteristics for tunnelling processes with a energy-dependent density of states and compare this with the results of the energy-independent density of states.

The thesis is structured as follows: Sec. 2 explains the building and functionality of the single-electron transistor. In Sec. 3 we briefly outline the calculations of the characteristics of the transport theory. The framework is the orthodox theory of coulomb blockade. To get a final analytical equation for the transition rates we first evaluate the master equation for the reduced density matrix. Then the resulting current can be evaluated with the calculated tunnelling rates. In Sec. 4 we present the results of the transport theory with an energy-dependent density of states of the island. The conclusion is written in Sec. 5.

2 Single-Electron Transistor

An elementary Coulomb blockade circuit is the so called single-electron box. It consists of a small metallic island, which is coupled via a tunnel junction to a source electrode. There is also a gate connected via a capacitor to the system. The number of excess electrons in the island can be varied by changing the gate voltage, due to the change of the electrochemical potential of the island. The latter helps the electrons from the source to tunnel in the island in discrete steps.[3][7] The single-electron-transistor, or the SET, is very similar to the single-electron box. It has though three electrodes. The island is coupled via two tunnel junctions to the the transport electrodes source and drain. Furthermore, as well as in the single-electron box it is capacitively connected to the gate.[3] The structure is sketched in Fig. 2. The charging energy is given as a function of the integer number n of excess electrons and of the gate charge.

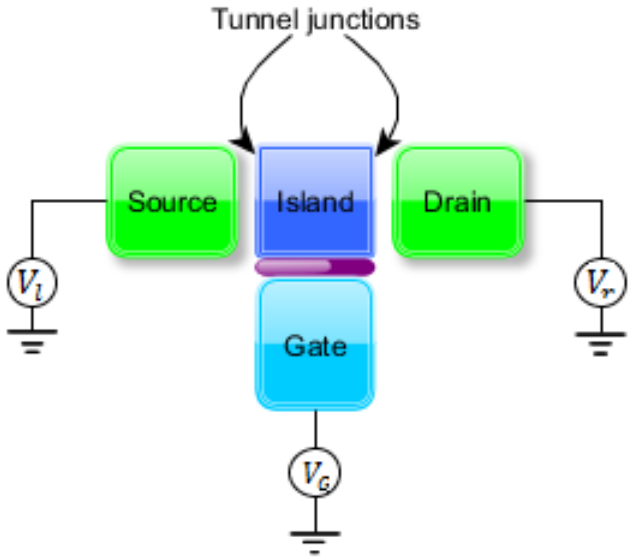


Figure 2: Schematics of a single-electron transistor. The island is coupled via a capacitor(purple) to the gate and via tunnel junctions to source and drain.

$$E_{\mathrm{ch}}(n, Q_{\mathrm{G}}) = \frac{(ne - Q_{\mathrm{G}})^2}{2C} \tag{1}$$

The total capacitance C is expressed as the sum of the junction capacitances and the gate capacitance. To calculate the gate charge we require also the three voltages, V_{G} for the gate, V_{R} for the right lead and V_{L} for the left lead.[3]

$$Q_{\mathrm{G}} = C_{\mathrm{G}} V_{\mathrm{G}} + C_{\mathrm{L}} V_{\mathrm{L}} + C_{\mathrm{R}} V_{\mathrm{R}} \tag{2}$$

We assume that there are N extra electrons in the island. There are four possible tunnelling processes, which change the current charge state. They are all depending on the energy difference between the final and the initial state ΔE_{ch}. One possible electron transfer, which replaces $N \to N+1$ is characterized by the energy difference $E_{\mathrm{ch}}(N+1, Q_{\mathrm{G}}) - E_{\mathrm{ch}}(N, Q_{\mathrm{G}})$. It occurs when the electrochemical potential in the left or in the right lead is high enough to compensate ΔE_{ch}. Thus an electron can tunnel in the island. After the increase of the electron number in the island due to an electron transfer from i.e. the left lead to the island, it is possible that an electron of the island tunnels to the right lead. Thus the island is again in charge state N. This hole process runs if both

$$eV_{\mathrm{L}} > E_{\mathrm{ch}}(N+1, Q_{\mathrm{G}}) - E_{\mathrm{ch}}(N, Q_{\mathrm{G}}) \tag{3}$$

for the transition from $N \to N+1$ and

$$eV_{\mathrm{R}} < E_{\mathrm{ch}}(N+1, Q_{\mathrm{G}}) - E_{\mathrm{ch}}(N, Q_{\mathrm{G}}) \tag{4}$$

for $N+1 \to N$ are concurrently valid. This way a current flows through the transistor. The electrons are transferred one-by-one, due to the fact, that the number of excess electrons, so the charge state, is an integer number.[7] One speaks of a Coulomb blockade if none of the above equations Eq. (3) and Eq. (4) is satisfied. The charge state can be shifted by varying the gate voltage.[8] The quantum fluctuations in the particle number N should be sufficiently small that the charge is well localized on the island. We consider the uncertainty relationship $\Delta E \Delta t \geq \hbar$, where t gives the time to transfer charge into and out of the island: $\Delta t \approx R_t C$ and $\Delta E \propto \frac{e^2}{C}$. Combining these two equations gives that the tunnel resistance should be sufficiently large:

$$R_t > \frac{h}{e^2}.$$

In Fig 3 the voltage for the left electrode is above the threshold voltage to overcome Coulomb blockade. Thus one electron can tunnel in the island. After this process the island is in charge state N+1 and the fermi energy of the island is raised by E_{ch}. There will be a gap that prohibits a second electron from tunnelling into the island from the left lead. No further charge flows until the extra electron on the island tunnels into the right electrode, taking it back to the N state. This process lowers the Fermi energy in the dot and allows another electron to tunnel from the left electrode inside and then the process repeats itself.[8]

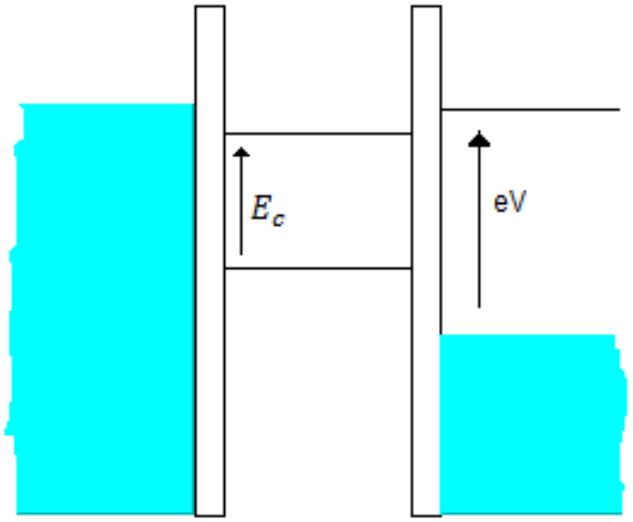


Figure 3: Band diagram of a single-electron transistor, illustrating the Coulomb blockade effect for a applied bias voltage.

3 Orthodox theory of Coulomb blockade

The above introduced device consists of an island in tunnelling contact with source and drain leads (see Fig. 4). To shift the energy level in the island, it also interacts capacitively with a nearby metallic gate. To study this problem we use the orthodox theory of Coulomb blockade. The theory is based on the master equation for the reduced density matrix.[3][5][7][9][10] To analyze the tunnelling processes in the transistor we will calculate the transition rates and the current. The time to tunnel from one side of the barrier to the other is on the order of 10^{-14}s, whereas the actual time between tunnelling events themselves is on the order of 10^{-12}s. The time for charge to rearrange itself on the electrodes due to the transition of one particle is also very short. Therefore we can consider that the junctions act as ideal capacitors which charge is slowly gone through.[8] The hole system can be described by the Hamiltonian

$$H = H_{\text{sys}} + H_{\text{ext}} + H_{\text{tun}} + H_{\text{leads}}. \tag{5}$$

We assume, that the island is large enough to have a quasi continuous single-particle spectrum, but small enough that their charging energy dominates the transition process.[6] Hence the Hamiltonian for the island reads

$$H_{\text{sys}} = \sum_{i,\sigma} \epsilon_i d^\dagger_{i\sigma} d_{i\sigma} + \frac{U}{2}\hat{N}(\hat{N}-1). \tag{6}$$

It describes the island with many-body eigenstates, where ϵ_i gives the single particle energy, $d^\dagger_{i\sigma}$ creats a particle in the island and $d_{i\sigma}$ annihilates one. U labels the charging energy of the island and $\hat{N} = \sum_{i\sigma} \hat{n}_{i\sigma}$ is the number operator.[11] The Hamiltonian for the metallic leads

$$H_{\text{leads}} = \sum_{\alpha,k,\sigma} \epsilon_k c^\dagger_{\alpha k\sigma} c_{\alpha k\sigma} \tag{7}$$

describes them as a Fermi-gas of noninteracting particles. The operator $c^\dagger_{\alpha k\sigma}$ creates a quasi-particle with spin σ and energy ϵ_k.[11] The index k labels the momentum of the electrons in the source and drain contacts and $\alpha = l, r$, for the left (source) and the right lead (drain). The effects on the system caused by the gate voltage V_g are described by the Hamiltonian:

$$H_{\text{ext}} = eV_g\hat{N}. \tag{8}$$

To study the electron transfer between the leads and the system the tunnelling Hamiltonian is introduced. It depends on the tunnel matrix elements T_{ki}, which now can be considered as a constant $T_{ki} = T$:

$$H_{\text{tun}} = |T| \sum_{\alpha,i,k,\sigma} \left(c^\dagger_{\alpha k\sigma} d_{i\sigma} + d^\dagger_{i\sigma} c_{\alpha k\sigma} \right). \tag{9}$$

3.1 Calculation of the transition rates

For the following calculations H_{tun} is treated like a perturbation, because we assume a weak coupling between leads and island.[11] The density matrix plays an important role in the quantum statistic. It can deliver all informations about a system. The equation of motion for the density matrix in the interaction picture can be calculated with the quantum mechanical Liouville-equation:

$$\frac{\partial \rho_{\mathrm{I}}(t)}{\partial t} = -\frac{i}{\hbar}\left[H_{\mathrm{tun,I}}(t), \rho_{\mathrm{I}}(t)\right]. \tag{10}$$

Integration after t and reinserting in Eq. (10) gives an integral over a double-commutator. Since we are not interested in the details of the dynamics of the leads, we trace over the corresponding degrees of freedom. This gives for the equation of motion of the reduced density matrix, approximated to second order:

$$\dot{\rho}_{\mathrm{I,red}}(t) = -\frac{1}{\hbar^2}\int_{t_0}^{t} \mathrm{dt'Tr}_{\mathrm{leads}}\{[H_{\mathrm{tun,I}}(t), [H_{\mathrm{tun,I}}(t'), \rho_{\mathrm{I}}(t')]]\}. \tag{11}$$

To bring this into a time-local form, we replace $\rho_{\mathrm{I}}(t')$ by $\rho_{\mathrm{I}}(t)$, which is allowed to lowest order in the tunnelling coupling. The leads can be considered as thermal reservoirs which stay in thermal equilibrium. We also assume that the influence of the island on the system is weak.[11] Because of this the statistic operator can be factorised: $\rho_{\mathrm{I}}(t) = \rho_{\mathrm{red,I}}(t) \otimes \rho_{\mathrm{leads}}$, where ρ_{leads} gives the density operator for the leads in thermal equilibrium. The general transformation from the interaction picture to the Schrödinger picture is given by the equation:$\rho_{\mathrm{I}}(t) = e^{\frac{i}{\hbar}H_0 t}\rho_{\mathrm{I}} e^{-\frac{i}{\hbar}H_0 t}$. To apply this on Eq. (11) this term has to be derived and changed. We substitute the time $t'' = t - t'$ and say $t'' = t'$. In the introduced problem we find: $H_0 = H_{\mathrm{sys}} + H_{\mathrm{ext}}$. Hence the equation of motion for the reduced density matrix in the Schrödinger picture reads

$$\begin{aligned} \dot{\rho}_{\mathrm{red}}(t) = -\frac{i}{\hbar}\left[H_{\mathrm{sys}} + H_{\mathrm{ext}}, \rho_{\mathrm{red}}(t)\right] - \\ \frac{1}{\hbar^2}\int_0^{\infty} \mathrm{dt'Tr}_{\mathrm{leads}}\{[H_{\mathrm{tun}}, [H_{\mathrm{tun,I}}(-t'), \rho_{\mathrm{red,I}}(t) \otimes \rho_{\mathrm{leads}}]]\}. \end{aligned} \tag{12}$$

The metallic island relaxes to equilibrium after each tunnelling process, because of its continuous spectrum and to the action of additional sources of dissipation. Thus the shape of the density matrix is: $\rho_{\mathrm{red}} = \sum_N P_N(t)\rho_{\mathrm{th},N}$. P_N is the probability for the island to be in charge state N and $\rho_{\mathrm{th},N}$ represents the system in the local thermal equilibrium. We define

$$\rho_{\mathrm{th},N} = \frac{1}{Z_N}\exp\left[-\beta(H_{\mathrm{sys}} + H_{\mathrm{ext}})\right]\mathcal{P}_N, \tag{13}$$

where Z_N gives the partition function $Z_N = \mathrm{Tr}_{\mathrm{sys}}\{\exp\left[-\beta(H_{\mathrm{sys}} + H_{\mathrm{ext}}\right]\mathcal{P}_N\}$, $\beta = \frac{1}{kT}$ and $\mathcal{P}_N$ is the projector on the subspace with N particles, which can be written as

$$\mathcal{P}_N = \sum_N = |N\rangle \langle N| . \tag{14}$$

After inserting Z_N in Eq. (13) and making use of the properties of the trace, the density operator in the thermal equilibrium becomes

$$\rho_{\mathrm{th},N} = \frac{e^{-\beta(\sum_{i\sigma} \epsilon_i \hat{n}_{i\sigma})} \mathcal{P}_N}{\sum_{\{n_{i\sigma}\}_N} \langle \hat{n}_{i\sigma} | e^{-\beta(\sum_{i\sigma} \epsilon_i \hat{n}_{i\sigma})} | \hat{n}_{i\sigma} \rangle}. \tag{15}$$

The approach for the normalization $\mathrm{Tr}_{\mathrm{sys}} \rho_{\mathrm{sys}}(t) = 1$ gives the result:

$$\begin{aligned} \mathrm{Tr}_{\mathrm{sys}} \{ \sum_N P_N(t) \rho_{\mathrm{th},N} \} &= \sum_N P_N \frac{\sum_{\{n_{i\sigma}\}_{N'}} \langle \hat{n}_{i\sigma} | e^{-\beta(\sum_{i\sigma} \epsilon_i \hat{n}_{i\sigma})} \mathcal{P}_N | \hat{n}_{i\sigma} \rangle}{\sum_{\{n_{i\sigma}\}_N} \langle \hat{n}_{i\sigma} | e^{-\beta(\sum_{i\sigma} \epsilon_i \hat{n}_{i\sigma})} | \hat{n}_{i\sigma} \rangle} \\ &= \sum_N P_N . \end{aligned}$$

This result confirmed that P_N is a probability. From that the equation of motion for $P_N(t)$ can be calculated. Because of the previous calculations it is known, that $\dot{P}_N = \mathrm{Tr}_{\mathrm{sys}} \{ \dot{\rho}_{\mathrm{red}}(t) \mathcal{P}_N \}$. Thus with Eq. (9) follows

$$\begin{aligned} \dot{P}_N(t) = -\frac{1}{\hbar^2} |T|^2 \mathrm{Tr}_{\mathrm{sys}} \Bigg\{ \mathcal{P}_N \int_0^\infty \mathrm{d}t' \mathrm{Tr}_{\mathrm{leads}} \Bigg\{ \Bigg[\sum_{\alpha,i,k,\sigma} (c^\dagger_{\alpha k\sigma} d_{i\sigma} + d^\dagger_{i\sigma} c_{\alpha k\sigma}) \\ , \Big[(c^\dagger_{\alpha k\sigma}(-t') d_{i\sigma}(-t') + d^\dagger_{i\sigma}(-t') c_{\alpha k\sigma}(-t')), \sum_{N'} P_{N'} \rho_{\mathrm{th},N'} \otimes \rho_{\mathrm{leads}} \Big] \Bigg] \Bigg\} \Bigg\}. \end{aligned}$$

This double-commutator can be figured out. The outcome terms are separated in two trace-parts. We also exploit the possibility to change the trace cyclical. Hence

$$\dot{P}_N(t) = -\frac{1}{\hbar^2}\sum_{N'}\int_0^\infty \mathrm{d}t' \sum_{\alpha,j,i,k,\sigma} |T|^2 \Bigg[$$
$$\mathrm{Tr}_{\mathrm{leads}}\{c_{\alpha k\sigma}c^\dagger_{\alpha k\sigma}(-t')\rho_{\mathrm{leads}}\}\mathrm{Tr}_{\mathrm{sys}}\{\mathcal{P}_N d^\dagger_{i\sigma}d_{j\sigma}(-t')\rho_{\mathrm{th},N'}\}P_{N'} -$$
$$\mathrm{Tr}_{\mathrm{leads}}\{c_{\alpha k\sigma}c^\dagger_{\alpha k\sigma}(-t')\rho_{\mathrm{leads}}\}\mathrm{Tr}_{\mathrm{sys}}\{d^\dagger_{i\sigma}\mathcal{P}_N d_{j\sigma}(-t')\rho_{\mathrm{th},N'}\}P_{N'} +$$
$$\mathrm{Tr}_{\mathrm{leads}}\{c^\dagger_{\alpha k\sigma}c_{\alpha k\sigma}(-t')\rho_{\mathrm{leads}}\}\mathrm{Tr}_{\mathrm{sys}}\{\mathcal{P}_N d_{i\sigma}d^\dagger_{j\sigma}(-t')\rho_{\mathrm{th},N'}\}P_{N'} -$$
$$\mathrm{Tr}_{\mathrm{leads}}\{c^\dagger_{\alpha k\sigma}c_{\alpha k\sigma}(-t')\rho_{\mathrm{leads}}\}\mathrm{Tr}_{\mathrm{sys}}\{d_{i\sigma}\mathcal{P}_N d^\dagger_{j\sigma}(-t')\rho_{\mathrm{th},N'}\}P_{N'} -$$
$$\mathrm{Tr}_{\mathrm{leads}}\{c^\dagger_{\alpha k\sigma}(-t')c_{\alpha k\sigma}\rho_{\mathrm{leads}}\}\mathrm{Tr}_{\mathrm{sys}}\{d_{j\sigma}(-t')\mathcal{P}_N d^\dagger_{i\sigma}\rho_{\mathrm{th},N'}\}P_{N'} +$$
$$\mathrm{Tr}_{\mathrm{leads}}\{c^\dagger_{\alpha k\sigma}(-t')c_{\alpha k\sigma}\rho_{\mathrm{leads}}\}\mathrm{Tr}_{\mathrm{sys}}\{d_{j\sigma}(-t')d^\dagger_{i\sigma}\mathcal{P}_N\rho_{\mathrm{th},N'}\}P_{N'} -$$
$$\mathrm{Tr}_{\mathrm{leads}}\{c_{\alpha k\sigma}(-t')c^\dagger_{\alpha k\sigma}\rho_{\mathrm{leads}}\}\mathrm{Tr}_{\mathrm{sys}}\{d^\dagger_{j\sigma}(-t')\mathcal{P}_N d_{i\sigma}\rho_{\mathrm{th},N'}\}P_{N'} +$$
$$\mathrm{Tr}_{\mathrm{leads}}\{c_{\alpha k\sigma}(-t')c^\dagger_{\alpha k\sigma}\rho_{\mathrm{leads}}\}\mathrm{Tr}_{\mathrm{sys}}\{d^\dagger_{j\sigma}(-t')d_{i\sigma}\mathcal{P}_N\rho_{\mathrm{th},N'}\}P_{N'}\Bigg].$$

In the next step we are making use of the following terms for the trace over the lead degrees of freedom, where f gives the Fermi function which is defined as: $f(\epsilon_k-\mu_\alpha) = \frac{1}{1+e^{\beta(\epsilon_k-\mu_\alpha)}}$. This describes the occupation probability for a state with energy ϵ_k.

$$\mathrm{Tr}_{\mathrm{leads}}\{c^\dagger_{\alpha k\sigma}c_{\alpha k\sigma}(-t')\rho_{\mathrm{leads}}\} = f(\epsilon_k-\mu_\alpha)e^{i\epsilon_k\frac{t'}{\hbar}} \tag{16}$$
$$\mathrm{Tr}_{\mathrm{leads}}\{c_{\alpha k\sigma}c^\dagger_{\alpha k\sigma}(-t')\rho_{\mathrm{leads}}\} = [1-f(\epsilon_k-\mu_\alpha)]e^{-i\epsilon_k\frac{t'}{\hbar}} \tag{17}$$
$$\mathrm{Tr}_{\mathrm{leads}}\{c_{\alpha k\sigma}(-t')c^\dagger_{\alpha k\sigma}\rho_{\mathrm{leads}}\} = [1-f(\epsilon_k-\mu_\alpha)]e^{i\epsilon_k\frac{t'}{\hbar}} \tag{18}$$
$$\mathrm{Tr}_{\mathrm{leads}}\{c_{\alpha k\sigma}(-t')c^\dagger_{\alpha k\sigma}\rho_{\mathrm{leads}}\} = f(\epsilon_k-\mu_\alpha)e^{-i\epsilon_k\frac{t'}{\hbar}} \tag{19}$$

The only statistically relevant term of H_{sys} is $\sum_{i,\sigma}\epsilon_i d^\dagger_{i\sigma}d_{i\sigma}$.[6] Under this assumptions we can continue with the terms, where we take the trace over the leads in Eq. (16). For this the explicit time evolution of the system operator should be calculated. The time evolution operator is:

$$U_0(t) = e^{\frac{i}{\hbar}\sum_{i,\sigma}\epsilon_i d^\dagger_{i\sigma}d_{i\sigma}t'}e^{\frac{i}{\hbar}(eV_g\hat{N}+\frac{U}{2}\hat{N}(\hat{N}-1))t'}. \tag{20}$$

The external and interacting components become numbers and can be evaluated immediately. Now using the description of the projection operator in Eq. (14) and inserting two identities with M and M': $\sum_M |M\rangle\langle M|$ in front of the left and after the right exponential function gives for the third term:

$$\begin{aligned}&\mathrm{Tr}_{\mathrm{sys}}\{\mathcal{P}_N d_{i\sigma}d^\dagger_{j\sigma}(-t')\rho_{\mathrm{th},N'}\} = \\ &e^{-\frac{i}{\hbar}(eV_g+U\hat{N})t'}\mathrm{Tr}_{\mathrm{sys}}\left\{\mathcal{P}_N d_{i\sigma}e^{-\frac{i}{\hbar}\sum_{i\sigma}\epsilon_i\hat{n}_{i\sigma}t'}d^\dagger_{j\sigma}e^{\frac{i}{\hbar}\sum_{i\sigma}\epsilon_i\hat{n}_{i\sigma}t'}\rho_{\mathrm{th},N'}\right\}.\end{aligned} \tag{21}$$

Moreover, we calculate the time evolution with the left exponential-function in Eq. (21):

$$\frac{\mathrm{d}}{\mathrm{dt}} d^\dagger_{j\sigma}(-t') = \frac{i}{\hbar} e^{-\frac{i}{\hbar}\epsilon_i \hat{n}_{i\sigma} t'} \left[d^\dagger_{j\sigma}, \epsilon_i \hat{n}_{i\sigma} \right] e^{\frac{i}{\hbar}\epsilon_i \hat{n}_{i\sigma} t'}. \tag{22}$$

The commutator gives $\left[d^\dagger_{j\sigma}, \epsilon_i \hat{n}_{i\sigma} \right] = -\epsilon_i d^\dagger_{j\sigma} \delta_{ij}$. This yields a differential equation, which can be easily solved: $d^\dagger_{i\sigma}(-t') = e^{-\frac{i}{\hbar}\epsilon_i t'} \cdot d^\dagger_{i\sigma}$. Putting all results together gives

$$\mathrm{Tr}_{\mathrm{sys}}\{\mathcal{P}_N d_{i\sigma} d^\dagger_{j\sigma}(-t') \rho_{\mathrm{th},N'}\} = e^{-\frac{i}{\hbar}(\epsilon_i + eV_g + UN)t'} \cdot \delta_{ij} \cdot \delta_{NN'} \mathrm{Tr}_{\mathrm{sys}} \left\{ d_{i\sigma} d^\dagger_{i\sigma} \rho_{\mathrm{th},N'} \right\}. \tag{23}$$

These are behaving a little bit different, if the order of the operator in the trace is another. I.e.:

$$\mathrm{Tr}_{\mathrm{sys}}\{d_{j\sigma}(-t') \mathcal{P}_N d^\dagger_{i\sigma} \rho_{\mathrm{th},N'}\} = e^{\frac{i}{\hbar}(\epsilon_i + eV_g + U(N-1))t'} \cdot \delta_{ij} \cdot \delta_{N'N-1} \mathrm{Tr}_{\mathrm{sys}} \left\{ d_{i\sigma} d^\dagger_{i\sigma} \rho_{\mathrm{th},N'} \right\}. \tag{24}$$

The left terms can be evaluated in the same way. Here we see the difference of the charging energy ΔE_{ch} in the exponential function. The form of the delta-function depends on the position of the projection operator. The problem now is, that $\hat{\rho}_{\mathrm{th},N}$ fixes the total particle number of the system to N. In the limit of large particle numbers the canonical and the grand canonical ensembles coincide. Thus we can make the approximation:

$$\mathrm{Tr}_{\mathrm{sys}} \left\{ d_{i\sigma} d^\dagger_{i\sigma} \hat{\rho}_{\mathrm{th},N} \right\} \approx \mathrm{Tr}_{\mathrm{sys}} \left\{ d_{i\sigma} d^\dagger_{i\sigma} \hat{\rho}_{\mu_N} \right\}, \tag{25}$$

where

$$\hat{\rho}_{\mu_N} = \frac{\exp -\beta[\sum_{i\sigma}(\epsilon_i - \mu_N)\hat{n}_{i\sigma}]}{\mathrm{Tr}_{\mathrm{sys}}\{\exp -\beta[\sum_{i\sigma}(\epsilon_i - \mu_N)\hat{n}_{i\sigma}]\}}.$$

Under these assumptions the trace in Eq. (23) can be evaluated. We use the abbreviations: $f(\epsilon_k - \mu_\alpha) = f^+_\alpha(\epsilon_k)$ and $[1 - f(\epsilon_k - \mu_\alpha)] = f^-_\alpha(\epsilon_k)$. Furthermore, we introduce $\mu_N = \mu_{\mathrm{sys}}$. The above assumption in Eq. (25) carries

$$\mathrm{Tr}_{\mathrm{sys}} \left\{ d_{i\sigma} d^\dagger_{i\sigma} \hat{\rho}_{\mu_N} \right\} = 1 - f(\epsilon_i - \mu_{\mathrm{sys}}). \tag{26}$$

The other system traces can be evaluated in complete analogy. Now we use these results and the equations for the trace over the lead degrees of freedom and combine them in Eq. (16). Thus we can write $\dot{P}_N(t)$ as

$$
\begin{aligned}
&\dot{P}_N(t) = -\frac{1}{\hbar}\int_0^\infty \mathrm{dt}' \sum_{\alpha\sigma}\sum_{ik}|T|^2 \\
&f_\alpha^+(\epsilon_k) f_{\mathrm{sys}}^-(\epsilon_i) \exp\left[-\frac{i}{\hbar}(\epsilon_i + eV_g + UN - \epsilon_k)t'\right] P_N(t) + \\
&f_\alpha^-(\epsilon_k) f_{\mathrm{sys}}^+(\epsilon_i) \exp\left[\frac{i}{\hbar}(\epsilon_i + eV_g + U(N-1) - \epsilon_k)t'\right] P_N(t) - \\
&f_\alpha^-(\epsilon_k) f_{\mathrm{sys}}^+(\epsilon_i) \exp\left[-\frac{i}{\hbar}(\epsilon_i + eV_g + UN - \epsilon_k)t'\right] P_{N+1}(t) - \\
&f_\alpha^+(\epsilon_k) f_{\mathrm{sys}}^-(\epsilon_i) \exp\left[\frac{i}{\hbar}(\epsilon_i + eV_g + U(N-1) - \epsilon_k)t'\right] P_{N-1}(t) - \\
&f_\alpha^-(\epsilon_k) f_{\mathrm{sys}}^+(\epsilon_i) \exp\left[\frac{i}{\hbar}(\epsilon_i + eV_g + UN - \epsilon_k)t'\right] P_{N+1}(t) - \\
&f_\alpha^+(\epsilon_k) f_{\mathrm{sys}}^-(\epsilon_i) \exp\left[-\frac{i}{\hbar}(\epsilon_i + eV_g + U(N-1) - \epsilon_k)t'\right] P_{N-1}(t) + \\
&f_\alpha^+(\epsilon_k) f_{\mathrm{sys}}^-(\epsilon_i) \exp\left[\frac{i}{\hbar}(\epsilon_i + eV_g + UN - \epsilon_k)t'\right] P_N(t) - \\
&f_\alpha^-(\epsilon_k) f_{\mathrm{sys}}^+(\epsilon_i) \exp\left[-\frac{i}{\hbar}(\epsilon_i + eV_g + U(N-1) - \epsilon_k)t'\right] P_N(t).
\end{aligned}
$$

In the next step we can combine respectively two terms: The first and the seventh, the second and the eight, the third and the fifth and the fourth and the sixth. This process results in four terms. Each of them can be written as two times the real part of the exponential function. Substituting $\frac{t'}{\hbar} = x$ and using $2\hbar \mathrm{Re}\int_0^\infty \mathrm{dx} e^{i\Delta E x} = 2\pi\hbar\delta(\Delta E)$ yields

$$
\begin{aligned}
\dot{P}_N = -\frac{1}{\hbar^2}\sum_{\alpha\sigma}\sum_{ik}|T|^2 \Big[& f_\alpha^+(\epsilon_k) f_{\mathrm{sys}}^-(\epsilon_i) 2\pi\hbar\delta(\epsilon_i + eV_g + UN - \epsilon_k) P_N(t) + \\
& f_\alpha^-(\epsilon_k) f_{\mathrm{sys}}^+(\epsilon_i) 2\pi\hbar\delta(\epsilon_i + eV_g + U(N-1) - \epsilon_k) P_N(t) - \\
& f_\alpha^-(\epsilon_k) f_{\mathrm{sys}}^+(\epsilon_i) 2\pi\hbar\delta(\epsilon_i + eV_g + UN - \epsilon_k) P_{N+1}(t) - \\
& f_\alpha^+(\epsilon_k) f_{\mathrm{sys}}^-(\epsilon_i) 2\pi\hbar\delta(\epsilon_i + eV_g + U(N-1) - \epsilon_k) P_{N-1}(t) \Big].
\end{aligned} \tag{27}
$$

Next we transform: $\sum_{ik} \longrightarrow \int_{-\infty}^{\infty} \mathrm{d}\epsilon_\mathrm{i} D_{sys} \int_{-\infty}^{\infty} \mathrm{d}\epsilon_\mathrm{k} D_\alpha$, where the density of states D_α and D_{sys} were introduced. This defines the number of states per energy interval. In this chapter we assume that the density of states for both, the island and the leads is constant.

Thus

$$\begin{aligned}
\dot{P}_N = -\sum_{\alpha\sigma} \frac{1}{\hbar}|T|^2 2\pi D_\alpha D_{sys} \int_{-\infty}^{+\infty} \mathrm{d}\epsilon_i \int_{-\infty}^{+\infty} \mathrm{d}\epsilon_k \Big[\\
f_\alpha^+(\epsilon_k) f_{\mathrm{sys}}^-(\epsilon_i) 2\pi\delta(\epsilon_i + eV_g + UN - \epsilon_k) P_N(t) + \\
f_\alpha^-(\epsilon_k) f_{\mathrm{sys}}^+(\epsilon_i) 2\pi\delta(\epsilon_i + eV_g + U(N-1) - \epsilon_k) P_N(t) - \\
f_\alpha^-(\epsilon_k) f_{\mathrm{sys}}^+(\epsilon_i) 2\pi\delta(\epsilon_i + eV_g + UN - \epsilon_k) P_{N+1}(t) - \\
f_\alpha^+(\epsilon_k) f_{\mathrm{sys}}^-(\epsilon_i) 2\pi\delta(\epsilon_i + eV_g + U(N-1) - \epsilon_k) P_{N-1}(t) \Big].
\end{aligned} \tag{28}$$

These terms can be interpreted as transition rates. They describe the tunnelling of one particle of the states k in the leads to one of the free states i in the island. The first term characterizes the transition from the state with N particles to N+1. The second one describes the change of N to N-1 and the last two terms describe the tunnelling process from N+1 and N-1 to N. The energy conservation is expressed by the δ-function. It contains the change of the charging energy, which is required for the transition and also for the energies of the particle states $\epsilon_{k,i}$. Now we can make the final integrations. First we substitute the constant $\gamma_\alpha = 2\frac{2\pi}{\hbar} D_\alpha D_{sys}|T|^2$ and then continue with the integration over ϵ_k. Exploiting the properties of the delta function carries

$$\begin{aligned}
\dot{P}_N(t) = \sum_\alpha \gamma_\alpha \int_{-\infty}^{+\infty} \mathrm{d}\epsilon_i \Big[- \\
\left(f_\alpha^+(\epsilon_i + eV_g + UN) f_{\mathrm{sys}}^-(\epsilon_i) + f_\alpha^-(\epsilon_i - eV_g + U(N-1)) f_{\mathrm{sys}}^+(\epsilon_i) \right) P_N(t) + \\
f_\alpha^-(\epsilon_i + eV_g + UN) f_{\mathrm{sys}}^+(\epsilon_i) P_{N+1}(t) + f_\alpha^+(\epsilon_i + eV_g + U(N-1)) f_{\mathrm{sys}}^-(\epsilon_i) P_{N-1}(t) \Big].
\end{aligned} \tag{29}$$

For solving the last integral we want to rewrite the above equation. We make a partial fraction expansion for $f^+(\epsilon_1) f^-(\epsilon_2)$. This results in

$$f^+(\epsilon_1) f^-(\epsilon_2) = n_B(\epsilon_1 - \epsilon_2)[f^+(\epsilon_2) - f^+(\epsilon_1)]. \tag{30}$$

Furthermore, we can make use of the following relation:

$$\int_{-\infty}^{+\infty} \mathrm{d}\epsilon \left[f^+(\epsilon) - f^+(\epsilon + \omega) \right] = \omega, \tag{31}$$

where $n_B(\epsilon_1 - \epsilon_2) = \frac{1}{e^{\beta(\epsilon_1 - \epsilon_2)} - 1}$ defines the Bose-Einstein function. Using the first identity (Eq. (30)) gives

$$\dot{P}_N(t) = \sum_\alpha \gamma_\alpha \int \mathrm{d}\epsilon_\mathrm{i} \Big[-$$
$$\left[n_B(-\mu_\alpha + eV_g + UN + \mu_\mathrm{sys})(f^+_\mathrm{sys}(\epsilon_i) - f^+_\alpha(\epsilon_i + eV_g + UN))\right] P_N(t) -$$
$$\left[n_B(\mu_\alpha - eV_g - U(N-1) - \mu_\mathrm{sys})(f^+_\alpha(\epsilon_i + eV_g + U(N-1)) - f^+_\mathrm{sys}(\epsilon_i)\right] P_N(t) +$$
$$\left[n_B(\mu_\alpha - eV_g - UN - \mu_\mathrm{sys})(f^+_\alpha(\epsilon_i + eV_g + UN) - f^+_\mathrm{sys}(\epsilon_i)\right] P_{N+1}(t) +$$
$$\left[n_B(-\mu_\alpha + eV_g + U(N-1) + \mu_\mathrm{sys})(f^+_\mathrm{sys}(\epsilon_i) - f^+_\alpha(\epsilon_i + eV_g + U(N-1))\right] P_{N-1}(t) \Big]. \tag{32}$$

Now we can apply the second relation on Eq. (29) and obtain

$$\begin{aligned}\dot{P}_N(t) = \sum_\alpha \gamma_\alpha \Big[& - \\ & n_B(-\mu_\alpha + eV_g + UN + \mu_\mathrm{sys}) \left[-\mu_\alpha + eV_g + UN + \mu_\mathrm{sys}\right] P_N(t) - \\ & n_B(\mu_\alpha - eV_g - U(N-1) - \mu_\mathrm{sys}) \left[\mu_\alpha - eV_g - U(N-1) - \mu_\mathrm{sys}\right] P_N(t) + \\ & n_B(\mu_\alpha - eV_g - UN - \mu_\mathrm{sys}) \left[\mu_\alpha - eV_g - UN - \mu_\mathrm{sys}\right] P_{N+1}(t) + \\ & n_B(-\mu_\alpha + eV_g + U(N-1) + \mu_\mathrm{sys}) \left[-\mu_\alpha + eV_g + U(N-1) + \mu_\mathrm{sys}\right] P_{N-1}(t) \Big].\end{aligned} \tag{33}$$

With Fermi's golden rule we can identify the tunnelling rates, so we can present the master equation for the orthodox theory of coulomb blockade:

$$\begin{aligned}\dot{P}_N(t) = & - \\ & \left[\Gamma_\mathrm{l}^{N\to N+1} + \Gamma_\mathrm{r}^{N\to N+1} + \Gamma_\mathrm{l}^{N\to N-1} + \Gamma_\mathrm{r}^{N\to N-1}\right] P_N(t) + \\ & \left[\Gamma_\mathrm{l}^{N+1\to N} + \Gamma_\mathrm{r}^{N+1\to N}\right] P_{N+1}(t) + \left[\Gamma_\mathrm{l}^{N-1\to N} + \Gamma_\mathrm{r}^{N-1\to N}\right] P_{N-1}(t),\end{aligned} \tag{34}$$

where we have introduced the equations for the transition rates, which describe the tunnelling processes in and out of the island. In the following calculations we only consider the transitions from the state with N excess electrons to N+1 and the reverse process (compare with Fig. 4).

For the left lead we define

$$\Gamma_\mathrm{l}^\pm = \gamma_l \frac{\pm(eV_g + UN - \frac{e}{2}V_b)}{e^{\pm(eV_g + UN - \frac{e}{2}V_b)} - 1}. \tag{35}$$

Here we assume a junction with symmetric bias voltage. Such that we can define the chemical potential for the leads as $\mu_l = \mu_0 + \frac{eV_b}{2}$ and $\mu_r = \mu_0 - \frac{eV_b}{2}$. We introduce

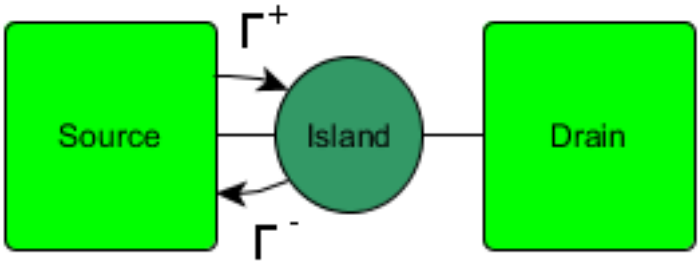
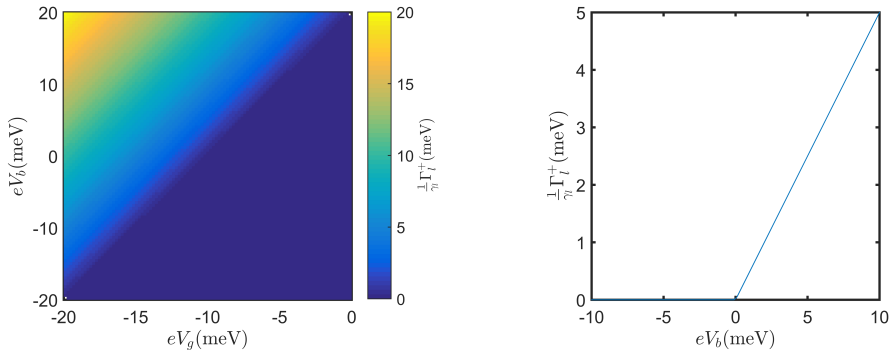


Figure 4: Schematics of the island with source and drain leads. The island is capacitively coupled to the leads. Transitions from N to N+1 and from N+1 to N for the source lead are also sketched.

μ_0, which gives the chemical potential for the leads at zero bias voltage and we also assume, that $\mu_{sys} = \mu_0$. In analogy to Eq. (35) we obtain

$$\Gamma_{\mathrm{r}}^{\pm} = \gamma_r \frac{\pm(eV_g + UN + \frac{e}{2}V_b)}{e^{\pm(eV_g+UN+\frac{e}{2}V_b)} - 1}. \tag{36}$$

In this two equations we use the short-cut for the transition from N to N+1 (+) and N+1 to N (-). Looking at Fig. 5a), which represents the transition rate for the process, where one particle tunnels from the left lead into the island, one can see the positive slope. There is almost no suppression of the transition at low gate voltages. The transition is getting higher with the bias voltage. Looking at bigger gate voltages the linear increase of the region where no transition takes place is good to see. Thus the transition rate is very small at zero gate voltage. This information can be compared with Eq. (36). At constant bias voltage we can see on Fig. 5b), that the transition starts suddenly at one point. This happens if the chemical potential of the lead is big enough to compensate the difference of the charge energies. In the example of our plot, we assumed that $eV_g = -U$, so that the transition starts at zero bias. Eq. (33) reveals that there is a Coulomb blockade, if $\Delta E_{ch} - \mu_\alpha = 0$. The pre factor γ_α can be written as $\gamma_\alpha = \frac{1}{e^2 R_{t,\alpha}}$, where R_t gives the tunnel resistance.



(a) (b)

Figure 5: Tunnelling rate for the transition from state N to N+1 for the source electrode: a) Depending on bias and gate-voltage. b)With constant gate voltage. The rate was plotted for the source electrode an with following parameters: $U = 10\text{meV}$, $N = 1$, $kT = 0.01\text{meV}$, $eV_g = -10\text{meV}$.

3.2 Calculation of the current

The above results also determine the current. Considering the latter example for the left lead, we we find the equation:

$$I_l(t) = -e \sum_N \left[\Gamma_l^{N\to N+1} P_N(t) - \Gamma_l^{N+1\to N} P_{N+1}(t)\right]. \tag{37}$$

Taking into account that we are talking about a stationary state, we exploit the principle of detailed balance. This expresses

$$P_N(\Gamma_l^{N\to N+1} + \Gamma_r^{N\to N+1}) = P_{N+1}(\Gamma_l^{N+1\to N} + \Gamma_r^{N+1\to N}). \tag{38}$$

To get the final equation for the current we also use that the sum over all probabilities is equal to one and at low bias voltages only two charge states play a role: $P_N(t) + P_{N+1}(t) = 1$. Putting this two identities together gives expressions for the probabilities.

$$P_N = \sum_\alpha \frac{\Gamma_\alpha^{N+1\to N}}{\left(\Gamma_\alpha^{N\to N+1} + \Gamma_\alpha^{N+1\to N}\right)}, \tag{39}$$

$$P_{N+1} = \frac{\Gamma_l^{N\to N+1} + \Gamma_r^{N\to N+1}}{\sum_\alpha \left(\Gamma_\alpha^{N\to N+1} + \Gamma_\alpha^{N+1\to N}\right)}. \tag{40}$$

Inserting this in Eq. (37), we find

$$I_l(t) = -e \sum_N \frac{\left[\Gamma_l^{N\to N+1}\Gamma_r^{N+1\to N} - \Gamma_l^{N+1\to N}\Gamma_r^{N\to N+1}\right]}{\Gamma_l^{N\to N+1} + \Gamma_r^{N+1\to N} + \Gamma_l^{N+1\to N} + \Gamma_r^{N\to N+1}}, \tag{41}$$

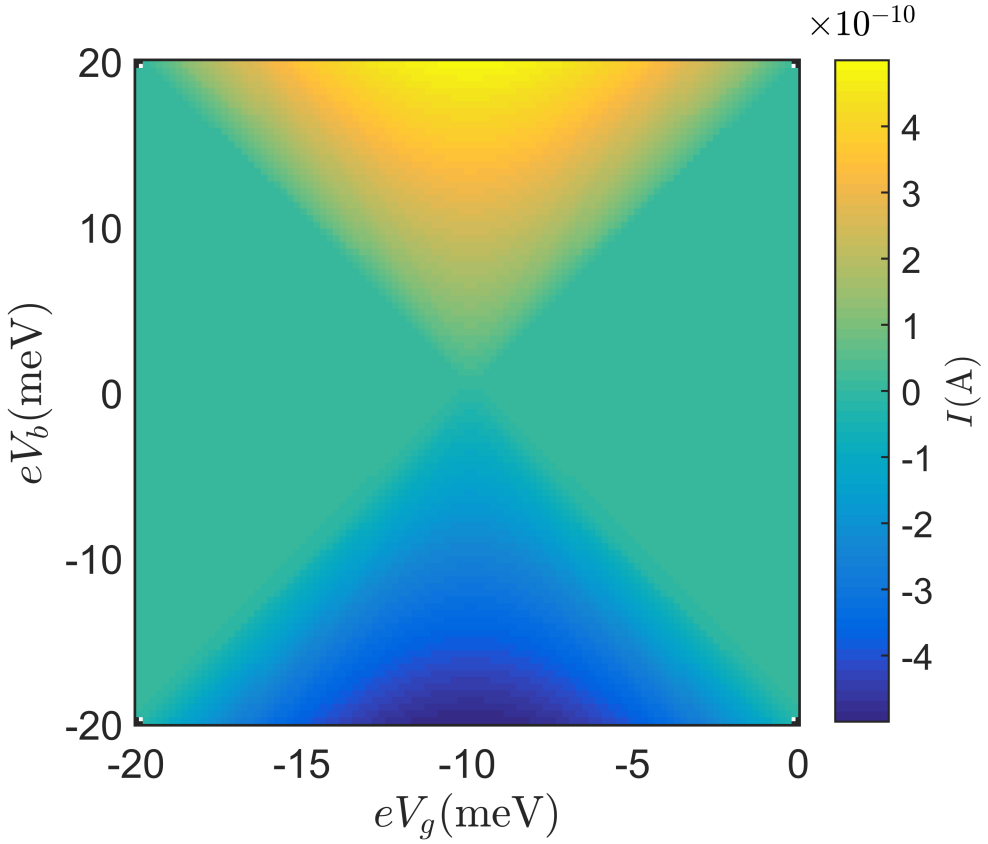


Figure 6: The resulting current for the left lead for the transition from N to N+1 and from N+1 to N. Following parameters were assumed: $U = 10$ meV, N=1, $kT = 0.01$ meV, $\gamma_l = \gamma_r = 10^{12} \frac{1}{\text{Js}}$

which gives us Fig. (6). This shows the current, depending on gate-and bias-voltage, where the slopes of the plot provides informations on source- and drain leads. There are two different slopes. The negative slope represents transitions from or in the drain, where the upper part determines a process where one particle goes into the drain, the lower stands for the reverse process. The positive inclination provides informations about the transition processes in the source lead. The upper slope can be compared with Fig. 5a), thus we find that this is related to the transition from N to N+1 and the lower is again the reverse process.

4 Calculations with a energy-dependent density of states of the island

In the previous chapter, it was assumed, that the density of states is independent of the energy. But especially in semiconducting islands the energy dependence of the density of states of the island should also be taken into account. In our following calculations we want to consider a density of state of the island which has got a gap between two different band edges (see Fig. 7). The two edges can be interpreted as the valence- and the conduction band in semi-conductive materials. We first assume a symmetric distribution and define the size of the gap as Δ. In the middle of the gap lies the chemical potential of the lead, so that there should be no transition. In the following calculations we want to check if increasing the voltage enforces transition processes. The density of states of the island is given by

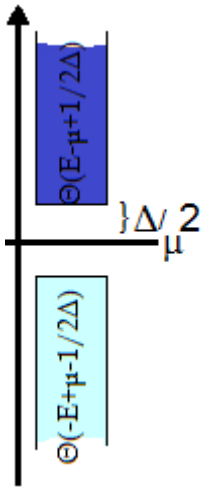


Figure 7: Sketch of the density of states of the island.

$$D_{sys}(\epsilon_i) = \tilde{D}_{sys}\left(\Theta(\epsilon_i - \mu_{sys} - \frac{\Delta}{2}) + \Theta(-\epsilon_i + \mu_{sys} - \frac{\Delta}{2})\right). \tag{42}$$

Here the constant $\tilde{D}_{sys}$ defines the strength of the density of states. The step functions can be approximated as Fermi functions, because the upper one goes to infinity and the limit of the lower one is minus infinity. This yields

$$D_{sys}(\epsilon_i) = \tilde{D}_{sys}\left(f^-(\epsilon_i - \mu_{sys} - \frac{\Delta}{2}) + f^+(\epsilon_i - \mu_{sys} + \frac{\Delta}{2})\right) = \tilde{D}_{sys}\sum_\tau f^\tau(\epsilon_i - \mu_{sys} + \tau\frac{\Delta}{2}), \tag{43}$$

where we have defined $\tau = \pm 1$.

4.1 Calculation of the transition rates

For the following calculations we take Eq.(28) and replace D_{sys} by $D_{sys}(\epsilon_i)$. Thus Eq.(29) becomes

$$\begin{aligned}\dot{P}_N = \sum_{\alpha\tau} \tilde{\gamma}_\alpha \int \mathrm{d}\epsilon_\mathrm{i} f^\tau(\epsilon_i - \mu_{sys} + \tau\frac{\Delta}{2})\Big[\\ - \left(f^+_\alpha(\epsilon_i + eV_g + UN) f^-_{\mathrm{sys}}(\epsilon_i) + f^-_\alpha(\epsilon_i - eV_g + U(N-1)) f^+_{\mathrm{sys}}(\epsilon_i)\right) P_N(t) \\ + f^-_\alpha(\epsilon_i + eV_g + UN) f^+_{\mathrm{sys}}(\epsilon_i) P_{N+1}(t) + f^+_\alpha(\epsilon_i + eV_g + U(N-1)) f^-_{\mathrm{sys}}(\epsilon_i) P_{N-1}(t)\Big],\end{aligned} \tag{44}$$

where $\tilde{\gamma}_\alpha$ is given as: $\tilde{\gamma}_\alpha = 2\frac{2\pi}{\hbar} D_\alpha \tilde{D}_{sys}|T|^2$. The difference to Eq. (29) is, that when we sum over τ we have one part (for $\tau = -1$) where the integrals look like: $\int_{-\infty}^{+\infty} f^+(x+a) f^-(x+b) f^-(x+c)\,\mathrm{d}x$ and the others ($\tau = +1$) have the shape of: $\int_{-\infty}^{+\infty} f^+(x+a) f^-(x+b) f^+(x+c)\,\mathrm{d}x$. First we make the integration over the terms with $\tau = -1$:

$$\begin{aligned}&\int_{-\infty}^{+\infty} \mathrm{d}x\, f^+(x+a) f^-(x+b) f^-(x+c) = \\ &\int_{-\infty}^{+\infty} \mathrm{d}x\, n_B(a-b)\Big(f^+(x+b) - f^+(x+a)\Big) f^-(x+c) = \\ &n_B(a-b)\Big[n_B(b-c)\int_{-\infty}^{\infty} \mathrm{d}x \left(f^+(x+c) - f^+(x+b)\right) \\ -&n_B(a-c)\int_{-\infty}^{+\infty} \mathrm{d}x \Big(f^+(x+c) - f^+(x+a)\Big)\Big] = \\ &n_B(a-b)\Big(F(b-c) - F(a-c)\Big).\end{aligned} \tag{45}$$

Here for the first two steps we made use of Eq. (30) and in the last step we exploited Eq. (31). Like in Eq. (31) n_B defines the Bose-Einstein function and $F(x)$ reads: $F(x) = x * n_B(x) = \frac{x}{e^{\beta x}-1}$.
For the remaining integration for $\tau = +1$ we use: $f^+(x) = 1 - f^-(x)$. This results in

$$\begin{aligned}&\int_{-\infty}^{+\infty} \mathrm{d}x\, f^+(x+a) f^-(x+b) f^+(x+d) = \\ &\int_{-\infty}^{+\infty} \mathrm{d}x \left[f^+(x+a) f^-(x+b) - f^+(x+a) f^-(x+b) f^-(x+d)\right].\end{aligned} \tag{46}$$

The first term can be calculated in the same way as we did in the previous chapter and the last product is the same as for $\tau = -1$, hence Eq.(46) reads

$$F(a-b) - n_B(a-b)\Big(F(b-d) - F(a-d)\Big). \tag{47}$$

With this considerations we arrive at the final equation for $\dot{P}_N$:

$$\begin{aligned}
\dot{P}_N = \sum_{\alpha\tau} \tilde{\gamma}_\alpha \Bigg[& \\
& - \Big\{ F(-\mu_\alpha + \mu_{\rm sys} + eV_g + UN) + n_B(-\mu_\alpha + \mu_{\rm sys} + eV_g + UN)\Big(\\
& - \tau F(-\tau\frac{\Delta}{2}) + \tau F(-\mu_\alpha + eV_g + UN + \mu_{\rm sys} - \tau\frac{\Delta}{2})\Big) \\
& + F(\mu_\alpha - \mu_{\rm sys} - eV_g + U(N-1)) + n_B(\mu_{\rm sys} + \mu_\alpha + eV_g - U(N-1))\Big(\\
& - \tau F(-\mu_\alpha + \mu_{\rm sys} - eV_g + U(N-1) - \tau\frac{\Delta}{2}) + \tau F(-\tau\frac{\Delta}{2})\Big)\Big\} P_N \\
& + \Big\{ F(\mu_\alpha - \mu_{\rm sys} - eV_g - UN) + n_B(\mu_\alpha - \mu_{\rm sys} - eV_g - UN)\Big(\\
& - \tau F(-\mu_\alpha + \mu_{\rm sys} + eV_g + UN - \tau\frac{\Delta}{2}) + \tau F(-\tau\frac{\Delta}{2})\Big)\Big\} P_{N+1} \\
& + \Big\{ F(-\mu_\alpha + eV_g + U(N-1) + \mu_{\rm sys}) + n_B(-\mu_\alpha + eV_g + U(N-1) + \mu_{\rm sys})\Big(\\
& - \tau F(-\tau\frac{\Delta}{2}) - F(-\mu_\alpha + \mu_{\rm sys} + eV_g + U(N-1) - \tau\frac{\Delta}{2})\Big)\Big\} P_{N-1}\Bigg].
\end{aligned} \tag{48}$$

Comparing this with Eq. (34) gives the transition rates. We again assume a symmetric bias voltage and that the chemical potential of the island is μ_0. Hence we find

$$\begin{aligned}
\Gamma^{\pm}_{\alpha} = \tilde{\gamma_\alpha} \Bigg[& F(\pm(-k\frac{e}{2}V_b + eV_g + UN)) + n_B(\pm(-k\frac{e}{2}V_b + eV_g + UN))\cdot \\
& \Big(\pm \Big(F(\frac{\Delta}{2}) - F(-k\frac{e}{2}V_b + eV_g + UN + \frac{\Delta}{2}) \\
& - F(-\frac{\Delta}{2}) + F(-k\frac{e}{2}V_b + eV_g + UN - \frac{\Delta}{2})\Big)\Big)\Bigg],
\end{aligned} \tag{49}$$

where k is +1 for α =l and -1 for α =r. To see the behaviour of the particles we plot the tunnelling rates for the left lead (see Fig. 8), where the system in charge state N proceeds in charge state N+1.

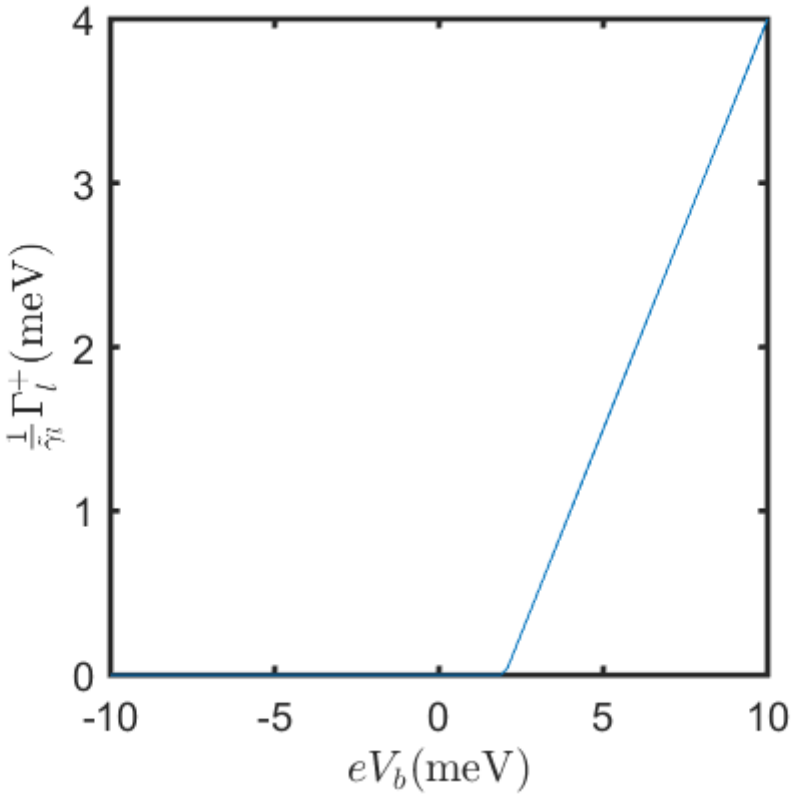


Figure 8: Transition rate for constant gate voltage and with following parameters: U=10meV, kT=0.01meV, N=1, Δ=2meV, eV_g=-10meV

The transitions begin when our bias voltage is about 2 mV. This reveals that the gap between the two bands of our density of states prevents electron tunnelling. In our example we have chosen Δ=2 meV and $eV_g = -U$ and it's revealing to see that with eV_B=2 meV we can counteract the blockade.

4.2 Calculations of the current

The current can be evaluated in the same way as we did in the previous chapter. Inserting the transition rates from Eq. (49) in Eq. (41) gives the final equation for the current for the processes N to N+1 and N+1 to N. The resulting plot can be seen in Fig. 9. Different to our first current there is a gap in Fig. 9, due to the gap in our density of states. The equation for the current (see Eq.(41)) can be used to calculate de conductance $G = \frac{dI}{dV_b}$. The plot of G in the V_b-V_g-plane shows stable

regions corresponding to each N for which no tunnelling may occur (see in Fig. 10). These structures are called Coulomb diamonds. The dark areas correspond to regions where the current vanishes and hence where Coulomb blockade exists. The brighter the areas are, the higher the conductance is. Since there is a gap in the current, there is also no conductance at the edges of our coulomb diamonds, thus there would be no peak in a plot for the conductance at zero bias. Hence the tunnelling of a source electron into the island is highly suppressed for low bias voltages, because no states are available near the Fermi level. Only after the bias voltage exceeds the gap, the suppression is lifted and the current increases.

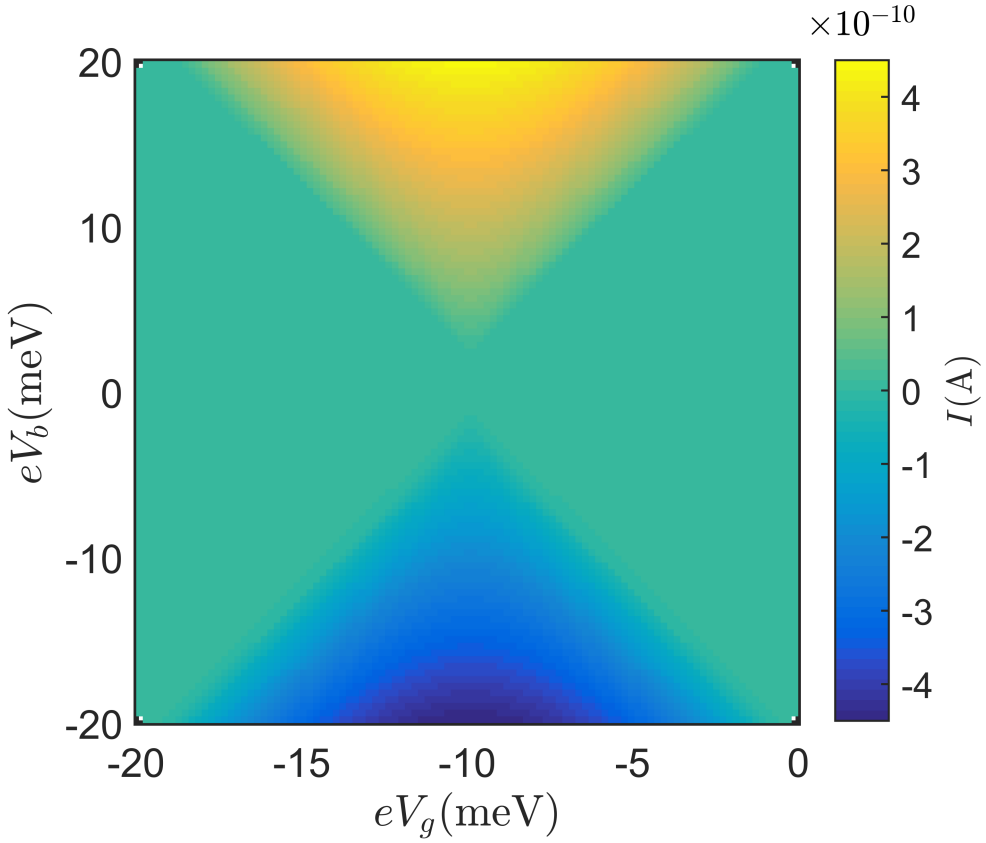


Figure 9: Current for the left lead, depending on bias-and gate-voltage with following parameters: U=10meV, kT=0.01meV, N=1, Δ=2meV, $\gamma_l = \gamma_r = 10^{12}\frac{1}{\mathrm{Js}}$

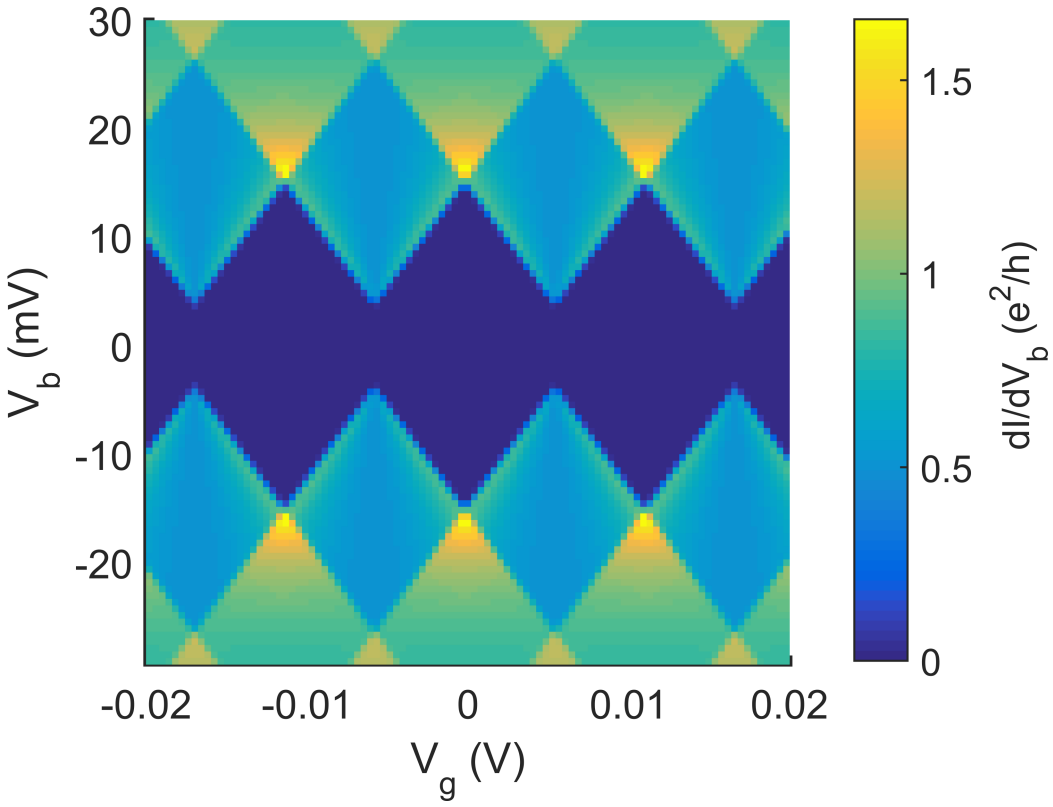


Figure 10: Conductance plotted as a function of gate- and bias- voltage with following parameters: kT= 0.07 meV, U=11.2 meV, μ_{sys}=-3.5U, μ_0=0, $\tilde{\gamma}_l = \tilde{\gamma}_r = \frac{1}{h}$

4.3 Variation of the density of states

Further we want to understand more about the behaviour of the conductance dependent on the density of states. We first assume that the density of state is spin dependent and there is a shift between spin-up and spin-down band. This assumption modifies Eq. (49). We assume that the density of state is not symmetric around μ_{sys}. Because of this we set $\frac{\Delta}{2} = B1_{up}$, $\frac{-\Delta}{2} = B2_{up}$ for spin up and $\frac{\Delta}{2} = B1_{down}$, $\frac{-\Delta}{2} = B2_{down}$ for spin down. Moreover, there should be a pre factor of $\frac{1}{2}$ in $\tilde{\gamma}_\alpha$. In our first calculation the energy bands are shifted, such that the top of the spin down band is above the chemical potential (see in Fig. 11). The result is plotted in Fig. 12. It shows the Coulomb diamonds without suppression at the charge degeneracy points around $V_b = 0$. This is fascinating, because despite the gap around μ_{sys}, there is no current suppression. The reason for this is, that there is no full gap around Fermi level, because the top of the lower spin-down band is on the height of the bottom of

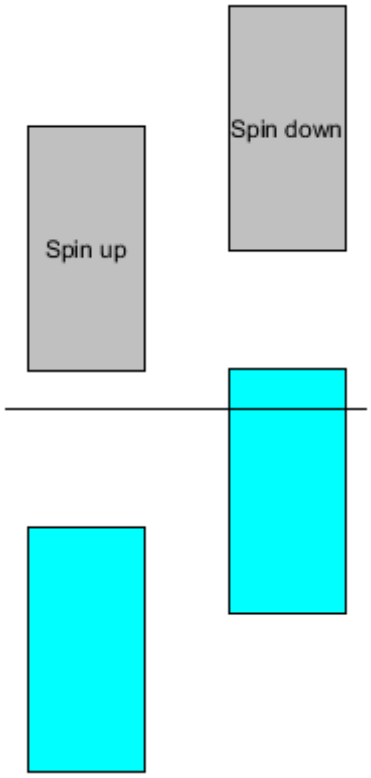


Figure 11: Sketch of the density of state with shifted spin-up and spin-down bands.

the upper spin-up band. According to this there are available states for an incoming electron near the chemical potential. Further we assume to have an asymmetric bias voltage, such that the potentials of the leads are:

$$\mu_l = \mu_0 + e\frac{1}{3}V_b$$
$$\mu_r = \mu_0 - e\frac{2}{3}V_b.$$

With the same band splitting as in the above example we get asymmetric coulomb diamonds in Fig. 14, due to the unequal voltage input of source and drain. Further thinking of a density of states, where the shift of spin-up structure to spin-down structure is such, that there is again a gap around the chemical potential (see Fig. 13). We can observe asymmetric coulomb diamonds with current suppression around zero bias (compare Fig. 15). That is how we have expected, because there are again no available states around μ_{sys}.

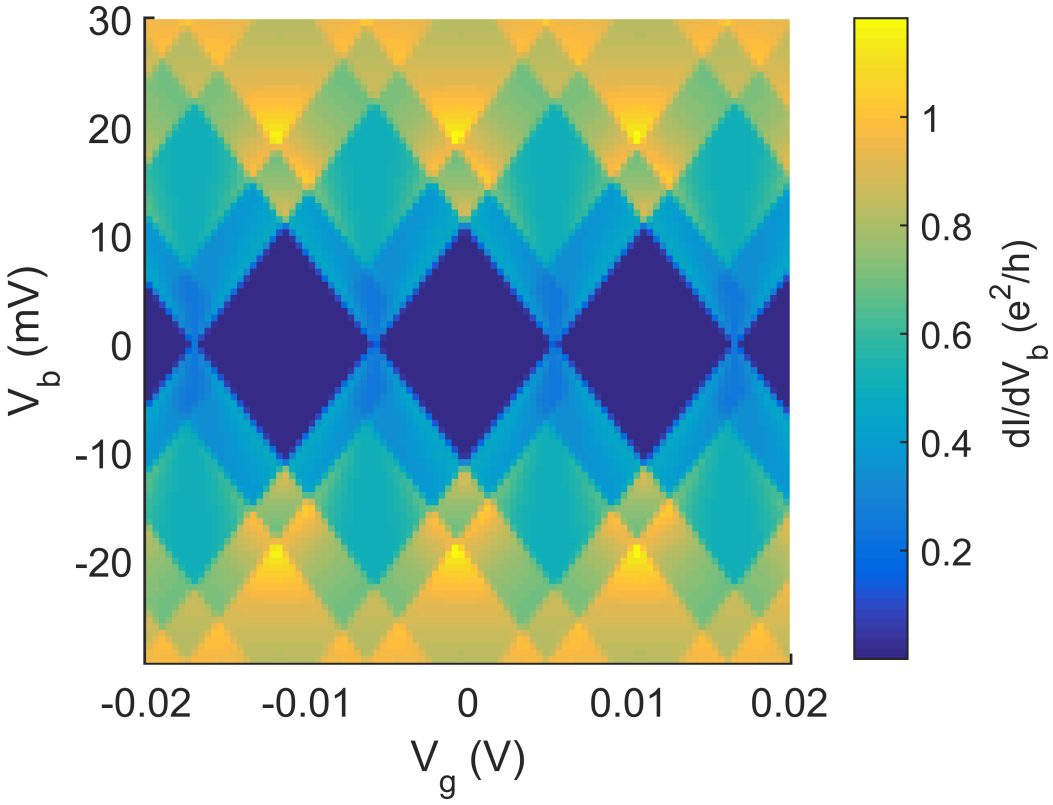


Figure 12: Conductance plotted as a function of gate- and bias- voltage with shifted spin-up and spin-down band. Including following parameters: $kT = 0.07$ meV, $U = 11.2$ meV, $\mu_{sys} = -3.5U$, $\mu_0 = 0$, $B1_{up} = 1$, $B2_{up} = -4$, $B1_{down} = 3$, $B2_{down} = 1$, $\tilde{\gamma}_l = \tilde{\gamma}_r = \frac{1}{h}$

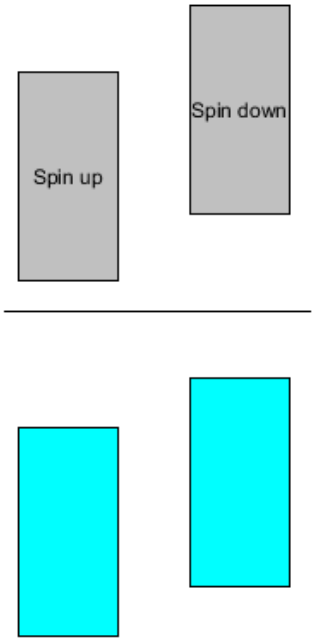


Figure 13: Schematics of a density of states with shifted spin-up and spin-down bands. There are no available states around the Fermi level

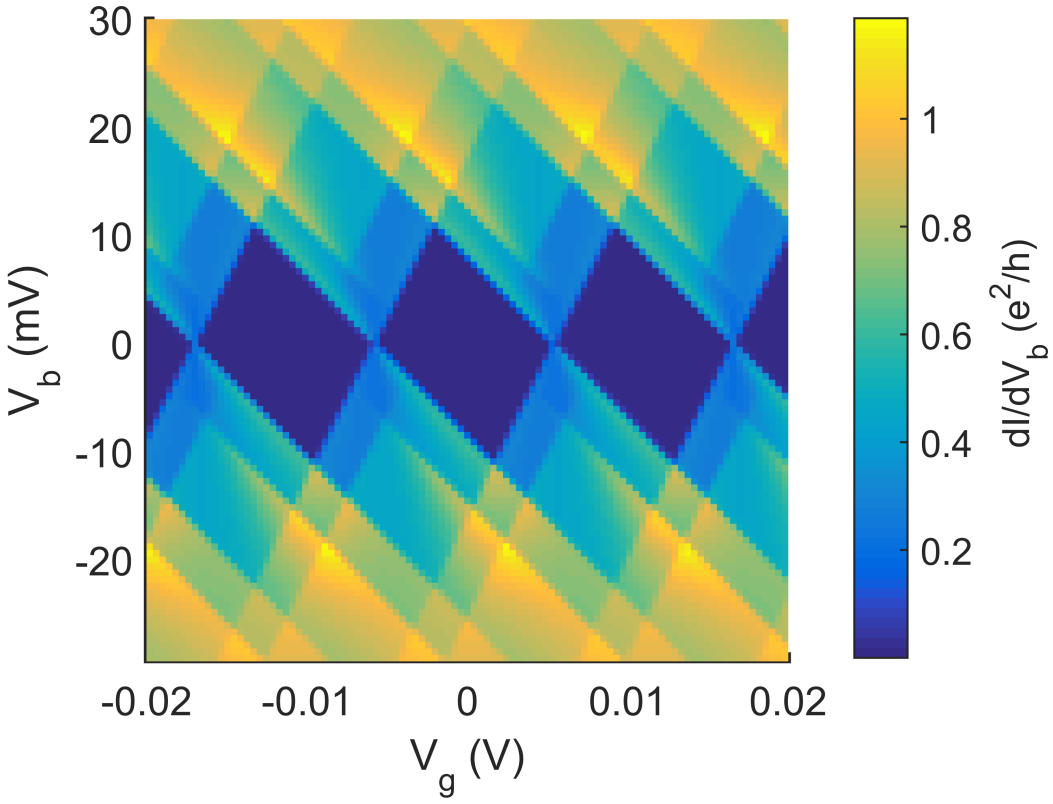


Figure 14: Conductance, depending on bias- and gate-voltage with its characteristics, the coulomb diamonds. The plot is for an asymmetric bias voltage and shifted spin-up and spin-down band($B1_{up}$=1, $B2_{up}$=-4, $B1_{down}$=3, $B2_{down}$=1), with following parameters: $kT = 0.07$ meV, $U = 11.2$ meV, $\mu_{sys} = -3.5U$, $\mu_0 = 0$, $\tilde{\gamma}_l = \tilde{\gamma}_r = \frac{1}{h}$.

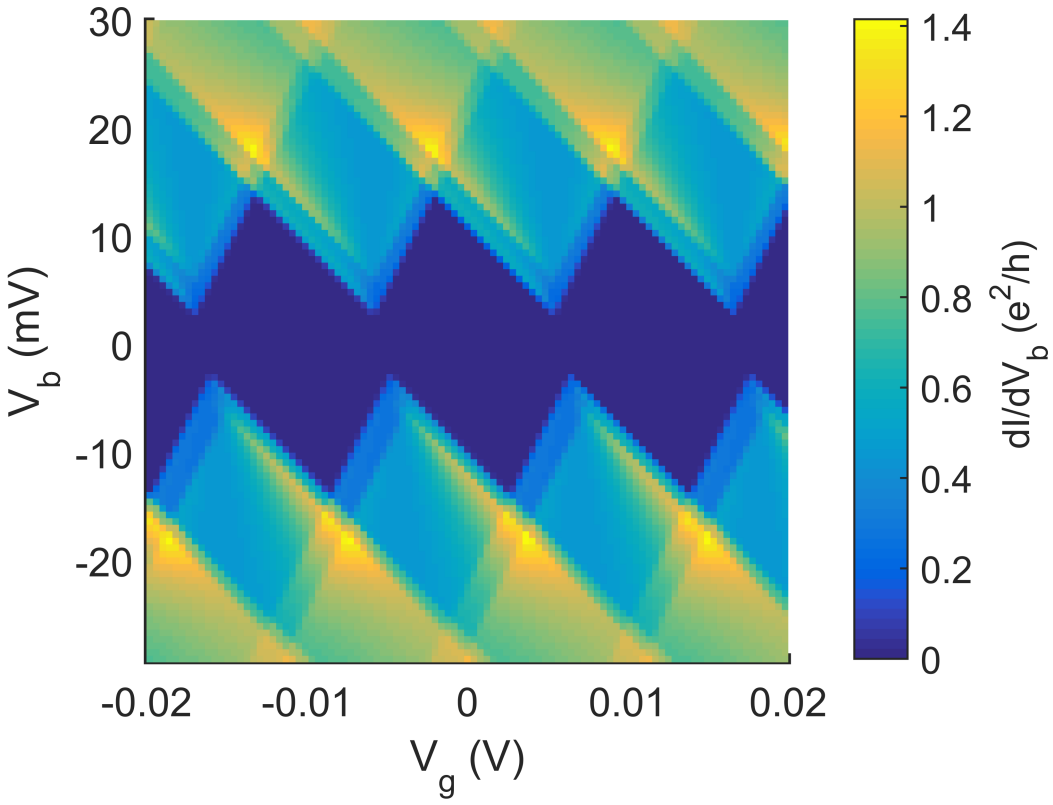


Figure 15: Conductance for a asymmetric bias voltage and shifted spin-up and spin-down band ($B1_{up} = 2$, $B2_{up} = -2$, $B1_{down} = 3$, $B2_{down} = 1$). The plot has following parameters: $kT = 0.07$ meV, $U = 11.2$ meV, $\mu_{sys} = -3.5U$, $\mu_0 = 0$, $\tilde{\gamma}_l = \tilde{\gamma}_r = \frac{1}{h}$.

5 Conclusion

After a short introduction on the Coulomb blockade effects (Sec. 1), we introduce the single-electron transistor. In the third section we have calculated the characteristics of tunnelling with the orthodox theory of coulomb blockade. First we have evaluated the equation of motion for the reduced density matrix. The density matrix is very important for a system, because all physical observables can be calculated with it. Furthermore, we have calculated the master equation, which is characteristic for the orthodox theory of Coulomb blockade. Hence we got the transition rates for the tunnelling processes. In Fig. 5b) we observed that if we choose: $V_g = -U$, the transition begins when we switch on the bias voltage. This is according to Eq. (35). The aim of this work was to study the causes for current suppression, which Geißler et al. found in their work [6]. First we have assumed a density of states, which is energy-dependent and has a structure where the chemical potential lies in a gap between the lower and the upper band of the density of states (see Fig. 7). The resulting conductivity-plot shows suppressions at the degeneracy points around zero bias. We again considered the transition rate at $V_g = -U$ in Fig. 49 and saw that there is no tunnelling until the bias voltage exceeds the gap-width (in our example 2 meV). We plotted the conductance for a shifted density of states, under the assumption that the density of state is spin-dependent. There is a shift between the spin-up bands and the spin-down bands. With this modelling the suppression at the charge degeneracy points can be prevented, like we did in the first example. We also took into account that a symmetric bias voltage is not realistic. The pre factor of the bias voltage normally depends on the capacitances of the leads and of the gate. We saw that with an asymmetric bias voltage the coulomb diamonds also get asymmetric, as one can see in Fig. 14. In the last consideration we assumed an asymmetric bias voltage and again a shifted density of states. We kept an eye on the vicinity of the Fermi level, so that there is a full gap. Like expected there‘s again no conductance at the degeneracy points around zero bias.
The main result of this work is that with a gap in our density of states we can explain current suppression at charge degeneracy points. In this work we used a very simplified model. We neglected the dependence of the density of states of the leads and other spin effects. To understand the results of the experiments [6] better, there should be a more realistic description of the density of states of the island.

References

[1] M. A. Kastner, Rev. Mod. Phys., (64), No. 3,(1992)

[2] U. Meirav, M. Heiblum and F. Stern, Appl. Phys. Lett. 54, (1988)

[3] L. Kouwenhoven, G. Schön and L. Sohn,eds., Introduction to mesoscopic electron transport, NATO ASI Series (Springer US, 1992).

[4] H. Grabert, Z. Phys. B - Condensed Matter 85, 319-325 (1991)

[5] G.-L. Ingold, Yu. V. Nazarov, Single Charge Tunneling, NATO ASI Series B, (294), pp. 21-107 (1992)

[6] S. Geißler, S. Pfaller, M. Utz, D. Bougeard, A. Donarini, M. Grifoni and D. Weiss, Double island Coulomb blockade in (Ga,Mn)As-nanoconstrictions (2015)

[7] Nazarov, Yuli/Blanter, Yaroslav (2009), Quantum Transport, Cambridge.

[8] Ferry, David/Goodnick, Stephen/Bird, Jonathan (2009), Transport in Nanostructures, second Edition, Cambridge.

[9] D.V. Averin and K.k. Likharev, Mesoscopic Phenomena in Solids (Elsevier Science, Amsterdam, 1991)

[10] H.Grabert and M.H. Devoret, eds., Single Charge Tunnelling, NATO ASI Series (Springer US, 1992).

[11] L. Mayrhofer, Spectrum and Transport Properties of interacting Carbon Nanotubes (2007).

[12] Nolting, Wolfgang (2013) Grundkurs Theoretische Physik 6, Statistische Physik, Springer: Braunschweig/Wiesbaden.

Erklärung

Ich habe die Arbeit selbständig verfasst, keine anderen als die angegebenen Quellen und Hilfsmittel benutzt und bisher keiner anderen Prüfungsbehörde vorgelegt. Außerdem bestätige ich hiermit, dass die vorgelegten Druckexemplare und die vorgelegte elektronische Version der Arbeit identisch sind, dass ich über wissenschaftlich korrektes Arbeiten und Zitieren aufgeklärt wurde und dass ich von den in § 24 Abs. 5 vorgesehenen Rechtsfolgen Kenntnis habe.

Susanne Candussio, August 31, 2015