

Assignments to Condensed Matter Theory I
Sheet 8

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sheet online: <http://www-MCG.uni-R.de/teaching/>

Problem set: Single electron transistor (SET)

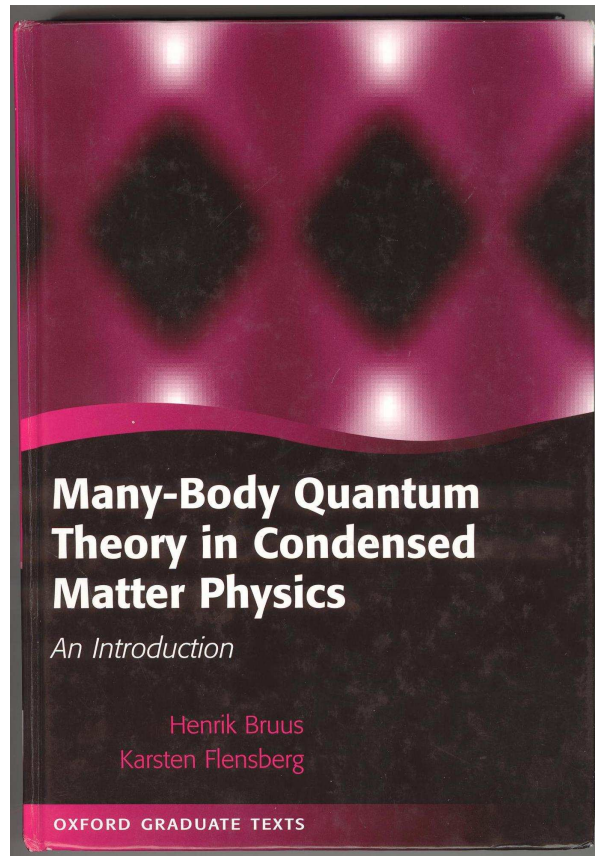
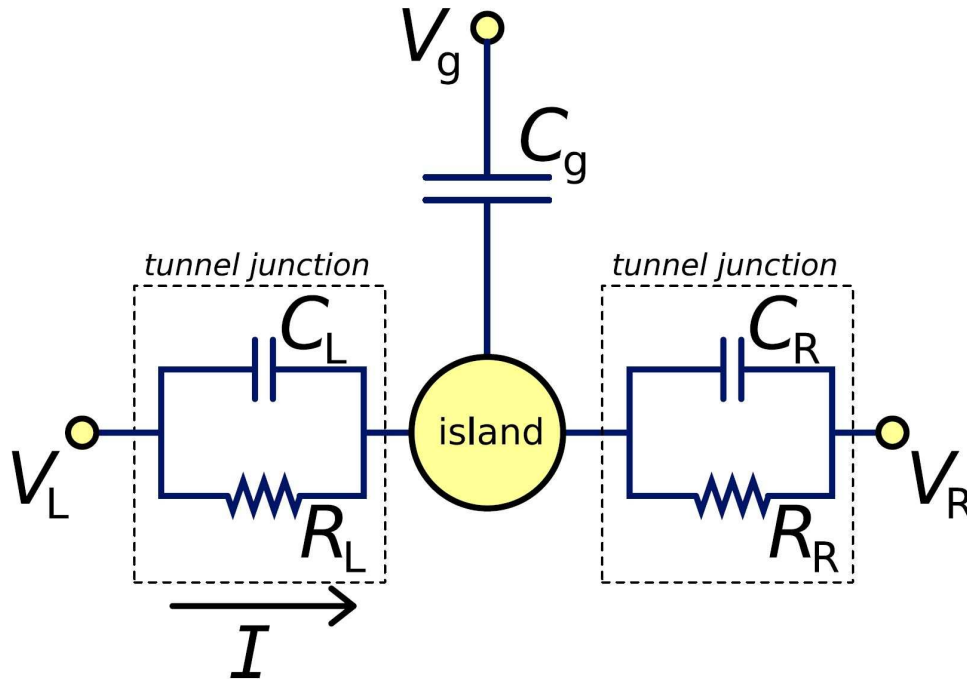


Figure 1: The cover picture of this book (a so-called SET stability diagram) is what you should reproduce and understand in this Sheet.

This Sheet will present the physics of the “Coulomb Blockade” effect. Differently from the other assignments you will be asked to solve this sheet by means of numerical techniques. By connecting a single metallic island to two electronic contacts and capacitively to a back-gate, one can realize a transistor-like device that allows the switching of a current electron by electron. This device is commonly known as a single electron transistor (SET). Its realization was made possible by fabricating ultrasmall capacitances (order 10^{-16} F) A comprehensive introduction to the SET can be found in: Electron transport in quantum dots by L. P. Kouwenhoven et al., published in Mesoscopic Electron Transport, edited by L. L. Sohn, L. P. Kouwenhoven and G. Schön (Kluwer, 1997), available online at <http://marcuslab.harvard.edu/papers/KouwenhovenReview.pdf>. Please download and read this introduction as a background for this project.

8.1. Coulomb blockade in a nutshell

A single electron transistor (SET) is described by the following diagram:¹



Here we have labelled the two tunnel junctions as L and R and the back-gate as g. The equilibrium charge Q_0 of the island can be determined classically by:

$$Q_0 = C_L V_L + C_R V_R + C_g V_g \quad (1)$$

The total energy of the island charged with n electrons is given by:

$$E_{\text{ch}}(Q) = (Q - Q_0)^2 / 2C_{\Sigma} \quad (2)$$

with $C_{\Sigma} = C_L + C_R + C_g$. You can now appreciate that if C_{Σ} is extremely small, the energy E_c necessary to add a single electron to the island can be much larger than $k_B T$ and become observable. Considering a discrete number of electrons n on the island (i.e. $Q = -en$ and $Q_0 = -en_0$), one has alternatively $E_{\text{ch}}(n) = E_c (n - n_0)^2$ where $E_c = \frac{e^2}{2C_{\Sigma}}$. If $k_B T \ll E_c$, the system is electronically blocked. No extra electron can be allocated without paying an energy cost of E_c . This is the so-called Coulomb blockade phenomenon. When moving one electron from the left/right reservoir to the island (raising the number of electrons on the island from n to $n + 1$), the total

¹This Sheet is based on scripts and assignments of previous courses 2004 SS: 52251 and 2005 WS: 52853.

energy of the system changes by:

$$\begin{aligned}\Delta E_{L/R}(n) &= E_{\text{ch}}(n+1) - E_{\text{ch}}(n) - (-e)V_{L/R} \\ &= \frac{e^2}{C_{\Sigma}} \left(n - n_0 + \frac{1}{2} \right) + eV_{L/R}\end{aligned}\quad (3)$$

The rate for this process at a temperature T is then determined by the Fermi golden rule:

$$\Gamma_{n \rightarrow n+1}^L = \frac{1}{e^2 R_L} \int d\epsilon_L \int d\epsilon_{\text{dot}} f_L(\epsilon_L) (1 - f_{\text{dot}}(\epsilon_{\text{dot}})) \delta(\Delta E_L + \epsilon_L - \epsilon_{\text{dot}}) \quad (4)$$

which can be integrated out via $\int d\epsilon f(\epsilon)(1 - f(\epsilon - E)) = E/(\exp(E/k_B T) - 1)$ to obtain:

$$\Gamma_{n \rightarrow n+1}^{L/R} = \frac{1}{e^2 R_L} \frac{\Delta E_{L/R}(n)}{\exp(\beta \Delta E_{L/R}(n)) - 1} \quad (5)$$

where $\beta = 1/k_B T$. Analogously, one can find:

$$\begin{aligned}\Gamma_{n+1 \rightarrow n}^{L/R} &= \frac{1}{e^2 R_L} \frac{-\Delta E_{L/R}(n)}{\exp(-\beta \Delta E_{L/R}(n)) - 1} \\ \Gamma_{n \rightarrow n-1}^{L/R} &= \frac{1}{e^2 R_L} \frac{-\Delta E_{L/R}(n-1)}{\exp(-\beta \Delta E_{L/R}(n-1)) - 1} \\ \Gamma_{n-1 \rightarrow n}^{L/R} &= \frac{1}{e^2 R_L} \frac{\Delta E_{L/R}(n-1)}{\exp(\beta \Delta E_{L/R}(n-1)) - 1} \\ \Gamma_{i \rightarrow j} &= \Gamma_{i \rightarrow j}^L + \Gamma_{i \rightarrow j}^R\end{aligned}\quad (6)$$

Now we define p_n as the probability to find the system in a state with n electrons on the island. This probability evolves in time due to a balance of outgoing and incoming tunnelling processes. Using the rates for these processes (just calculated) one can easily set up the equation

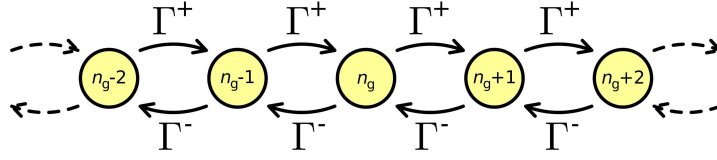
$$\frac{d}{dt} p_n = \Gamma_{n+1 \rightarrow n} p_{n+1} + \Gamma_{n-1 \rightarrow n} p_{n-1} - (\Gamma_{n \rightarrow n+1} + \Gamma_{n \rightarrow n-1}) p_n \quad (7)$$

for the *classical* occupation probabilities in the lattice network. Such equation is known in statistical mechanics as **master equation**. It is basically a first order differential equation describing the time-evolution of the probability of the system to occupy each one of a discrete set of states.² The only quantum content here is the derivation of the rates Γ 's.

One can visualize this dynamical system as a chain of states with probability flowing in both directions:

Now, we want to find the **steady state where** the probabilities do not change with time. To achieve this, it is clear that each pair of arrows in the diagram has to cancel out exactly. This condition is called **detailed balance** and can be written as:

²See *e.g.* K. Huang, Statistical Mechanics, Wiley, 2nd edition, (1987) end of chap. 8



$$\Gamma_{n \rightarrow n+1} p_n = \Gamma_{n+1 \rightarrow n} p_{n+1} \quad (8)$$

With this, we can find a simple algorithm to find all the p_n :

- (a) choose $n_g \in \mathbb{Z}$ as starting point such that $n_g \approx n_0$ (round to nearest integer)
- (b) set $p_{n_g} = 1$
- (c) use the detailed balance to find recursively all other p_n one by one, stopping when $p_n < \varepsilon$ for some small predefined ε
- (d) correct the normalization: $p_n \rightarrow p_n / \sum_n p_n$

Finally, the current from left to right through the dot can be defined by:

$$I = -e \sum_n p_n (\Gamma_{n \rightarrow n+1}^L - \Gamma_{n \rightarrow n-1}^L) \quad (9)$$

For a thorough theoretical introduction, see also: Single electron tunneling, Ch. 3 of Quantum transport and dissipation, T. Dittrich, et al., (Wiley-VCH, 1998), online at <http://marcuslab.harvard.edu/papers/KouwenhovenReview.pdf>

8.2. SET routine

Write a function that calculates the current I as a function of C_L , C_R , C_g , V_L , V_R , V_g , R_L , R_R and the temperature T . Take special care about the units involved in the calculations. Remember the best practice introduced before: stick to SI units internally everywhere, define the constants once and use them everywhere explicitly. If you find at input or output that non-SI units are more appropriate, do the conversion right at that point and document in place what the unit is.

8.3. Test cases: $I-V$ -characteristics

For a starting point choose the default values:

$$C_L = C_R = 653e/V (\approx 105aF); C_g = 145e/V$$

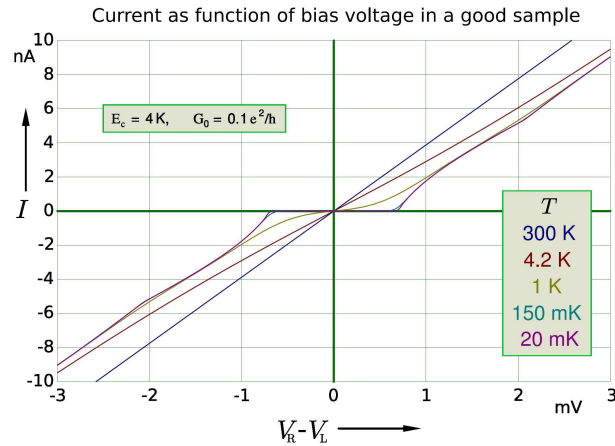
$$V_g = 0V$$

$$R_L = R_R = 10h/2e^2 (\approx 129k)$$

$$T = 0.1E_c/k_B (\approx 0.4K)$$

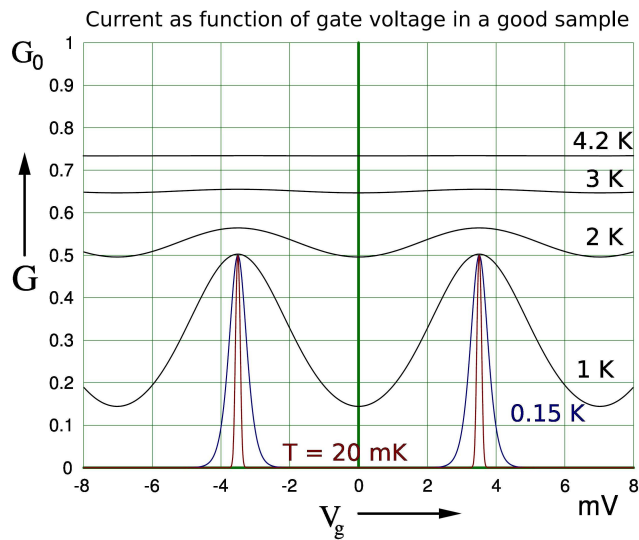
and do the following calculations to check the program for correctness:

- Scan along $V \in [-3\text{ mV}, 3\text{ mV}]$ with $V_R = V/2$, $V_L = -V/2$ for various temperatures. You should get the following graph:



8.4. Coulomb oscillations

- Scan along $V_g \in [-8\text{ mV}, 8\text{ mV}]$ and plot the linear conductance $G = I/(V_R - V_L)$ for the small voltages $V_L = -0.5\text{ nV}$; $V_R = 0.5\text{ nV}$. You should get the following graph:

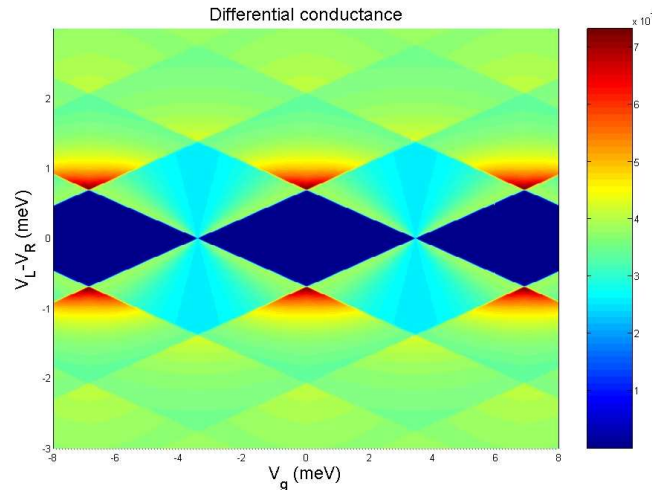


8.5. Stability Diagrams

The figure that opens this sheet is a **stability diagram** i.e. a surface plot of the differential conductance as a function of the gate voltage V_g (x axis) and bias voltage V (y axis). It appears as tiling of diamond-shape regions at almost constant conductance. The differential conductance is defined as:

$$G(V_g, V) = \frac{\partial I}{\partial V} \quad (10)$$

- Scan along $V_g \in [-8 \text{ mV}, 8 \text{ mV}]$ and $V_L - V_R \in [-3 \text{ mV}, 3 \text{ mV}]$ at $T = 20 \text{ mK}$
You should get the following graph:



- [Kür] What is the meaning of the blue diamonds? Can you count the number of electrons in the metallic island? How does the stability diagram changes by raising the temperature, why? Often in experiments the tunneling rate to the left or right electrodes can be very different. Can you predict how the stability diagram will change for example if $R_L \ll R_R$?

8.6. Examples of codes

- A possible code is listed at the end of this Sheet. Additionally it is also available at the url:
http://www-mcg.uni-r.de/downloads/QTKM1/SET_ME.mb.
Try to understand it, to use it in the different parameter regimes and finally to improve it!
- An example code is also offered in "ansi c". But please note that class assistance is only guaranteed for MATLAB coding.
http://www-mcg.uni-r.de/downloads/QTKM1/SET_ME.c

8.7. Presentation

- You will be asked to give a presentation about the numerical work and the results on Tuesday the 27th. A central aspect of scientific work is the interpretation and presentation of results. You will be asked to show the results of this sheet in a short, informal presentation. To give you a smooth start, we have prepared a first sample presentation for download at

<http://www-mcg.uni-r.de/downloads/CNS/dummy-presentation.tar.gz>

Download and unpack the archive. To compile the source into a PDF file:

```
pc12345:... make
```

Now modify the file to place your own results inside. Get comfortable editing the file. The presentation uses latex-beamer, which is installed on our machines. Download and documentation at: <http://latex-beamer.sourceforge.net/>. Of course you are free to choose other presentation tools, but assistance cannot be promised. Whatever program you choose to use, make sure that you can create a PDF. Come to the Tuesday 27.06. lecture with your presentation on a memory stick.

8.8. Appendix: MATLAB code

```
clear all
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%Program to calculate the stability diagram in orthodox theory
%(the theory schematically presented in the Sheet number 8 of
%the course Condensed Matter Theory 1)
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
Vgvet = [-8:0.01:8]*10^-3;
Vvet = [-3:0.01:3]*10^-3;
for k =1:length(Vgvet);
for j = 1:length(Vvet);
V = Vvet(j); % V

%minimum probability accepted as different from 0
eps = 10^-6;
CL=653; % e/V
VL=V/2; % V
CR=653; % e/V
```

```

VR=-V/2;% V
Cg=145; % e/V
Vg=Vgvet(k);% V

RL=10; % h/2e^2
RR=10; % h/2e^2
T = 20*10^-3*(0.0258/300); %temperature in kelvin transformed in eV

Ec = 1/(2*(CL+CR+Cg)); % eV

%equilibrium charge on the island
%(approximated to the clsest integer, well, charge is quantized)

n0 = CL*VL+CR*VR+Cg*Vg;
%I reset to 0 the vectors I have (eventually) used in the previous loops;
GammaLin = 0;
GammaLout = 0;
Ppos = 0;
Ptemp=1;
%evaluation of the probabilities for P(n) for n>n0 of occupation of the
%island
i = 1;
while Ptemp>eps
  %N.B. for i=1 n = floor(n0)!!!
  %energy to pay to pass from n to n+1 electrons in the island entering
  %from the Left
  DeltaE_L = 2*Ec*(floor(n0)+i-1-n0+1/2)+VL;
  %from the Right
  DeltaE_R = 2*Ec*(floor(n0)+i-1-n0+1/2)+VR;
  %
  %Rate to go from n to n+1 electrons in the island entering
  %from the Left
  GammaLin(i)= 1/RL*DeltaE_L/(exp(DeltaE_L/T)-1);
  %from the right
  GammaRin=1/RR*DeltaE_R/(exp(DeltaE_R/T)-1);
  %Rate to go from n+1 to n electrons in the island leaving
  %to the Left
  GammaLout(i)=1/RL*(-DeltaE_L)/(exp(-DeltaE_L/T)-1);
  %to the Right
  GammaRout=1/RR*(-DeltaE_R)/(exp(-DeltaE_R/T)-1);
  %Total rates in and out
  Gammain = GammaLin(i)+GammaRin;
  Gammaout = GammaLout(i) + GammaRout;
  %Probability P(n+1);
  Ptemp = Ptemp*Gammain/Gammaout;

```



```

Ppos(i) = Ptemp;
i = i+1;
end
%contribution to the current of the states with n>n0
Ipos = -[1,Ppos(1:end-1)]*GammaLin' + Ppos*GammaLout';
%evaluation of the probabilities for P(n) for n<n0 of occupation of the
%island
%I reset to 0 the vectors I have used in the previous while loop;
GammaLin = 0;
GammaLout = 0;
Pneg = 0;
Ptemp = 1;
i = 1;
while Ptemp>eps
  %N.B. for i=1 n = floor(n0)!!!
  %energy to "pay" (it can be negative and you gain!)
  %to pass from n-1 to n electrons in the island entering
  %from the Left
  DeltaE_L = 2*Ec*(floor(n0)-i-n0+1/2)+VL;
  %from the Right
  DeltaE_R = 2*Ec*(floor(n0)-i-n0+1/2)+VR;
  %
  %Rate to go from n-1 to n electrons in the island entering
  %from the Left
  GammaLin(i)= 1/RL*DeltaE_L/(exp(DeltaE_L/T)-1); %2eV/h
  %from the right
  GammaRin=1/RR*DeltaE_R/(exp(DeltaE_R/T)-1);
  %Rate to go from n to n-1 electrons in the island leaving
  %to the Left
  GammaLout(i)=1/RL*(-DeltaE_L)/(exp(-DeltaE_L/T)-1);
  %to the Right
  GammaRout=1/RR*(-DeltaE_R)/(exp(-DeltaE_R/T)-1);
  %Total rates in and out
  Gammain = GammaLin(i)+GammaRin;
  Gammaout = GammaLout(i) + GammaRout;
  %Probability P(n+1);
  Ptemp = Ptemp*Gammaout/Gammain;
  Pneg(i) = Ptemp;
  i = i+1;
end
%contribution to the current of the states with n<n0
Ineg = -Pneg*GammaLin'+[1,Pneg(1:end-1)]*GammaLout';
% construction of the probability distribution P(n)
P = [fliplr(Pneg),1,Ppos];
%definition of the unit conversion for the current. it is in the end
%expressed in Ampere. Notice also the normalization /sum(P)
Unitconv = 1.602*10^-19/(pi*0.6582*10^-15);
IL(j,k) = (Ipos+Ineg)/sum(P)*Unitconv;

```

```

P = P/sum(P);
end
end
%calculation of the differential conductance
G = diff(IL,1,1)/diff(Vvet(1:2));

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% Graphical section
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%Plot of the current as a function of the bias at zero gate voltage
figure(1)
%subplot(2,2,1)
plot(Vvet*10^3,IL(:,floor(length(Vvet)/2))*10^9)
xlabel('V_L-V_R (meV)', 'FontSize',18)
ylabel('I (nA)', 'FontSize',18)
title('Current (V_g=0 V)', 'FontSize',18)
%Plot of the differential conductance as a function of the gate volage
%at 0 bias.
figure(2)
%subplot(2,2,2)
plot(Vgvet*10^3,G(floor(length(Vvet)/2),:)*10^6)
xlabel('V_g (meV)', 'FontSize',18)
ylabel('G (\muS)', 'FontSize',18)
%ylim([0 2*max(max(G))*10^6])
title('Differential conductance (V=0 V)', 'FontSize',18)

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%Plot of the stationary current as a function of the bias voltage and
%of the gate voltage (the so called stability diagram)
figure(3)
%subplot(2,2,3)
surf(Vgvet*10^3,Vvet*10^3,IL)
%note the conversion to meV. For some funny reason
%Matlab wants the input of the surf comand like (X,Y,f(Y,X))!!!!
xlabel('V_g (meV)', 'FontSize',18)
ylabel('V_L-V_R (meV)', 'FontSize',18)
title('Current', 'FontSize',18)
box on
axis tight
shading flat
view([0 90])
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%Plot of the differential conductance as a function of the bias voltage

```

```
%and of the gate voltage (the so called stability diagram)
figure(4)
%subplot(2,2,4)
surf(Vgvet*10^3,Vvet(1:end-1)*10^3,G)
%note the conversion to meV. For some funny reason
%Matlab wants the input of the surf comand like (X,Y,f(Y,X))!!!!
xlabel('V_g (meV)', 'FontSize',18) ylabel('V_L-V_R
(meV)', 'FontSize',18) title('Differential
conductance', 'FontSize',18) box on axis tight shading flat view([0
90])
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
```