Confusion about capacity matrices

Motivation

In this note we finally solve the problem with the capacity matrices. We will distinguish between the capacity matrix and Maxwell capacitance matrix, and use the latter to calculate the charging energy, lever arms and other measurable quantities.

Example system

Task: We want to find a occupation of the quantum dots that minimizes the energy of the system at finite temperature and voltage on the gate.

However in this setup we keep temperature constant (T) and apply a constant voltage. The constant voltage multiplied by charge on the gates is the work done on the dot system $W = V_G Q_G$. However in this setup we keep the voltage constant, which playes the similair role as constant pressure in case of the gas container with movable piston (Note that mechanical work is $W = pV$, and p is also intensive quantity just like V_G). As a result we are looking for the minimum of the Gibbs free energy

$$G = U + W - TS + = E_{\text{dot}} - W_{gate-dot} - TS.$$

Where we are not sure about the sign of $W_{gate-dot}$, but we will see that it is negative.

1. Define the System

We have two types of components:

- **Quantum Dots**: Q_D denotes the charges on the dots, and V_D denotes the voltages on the dots. The number of dots is N_d.
- **Gates**: Q_G denotes the charges on the gates, and V_G denotes the externally controlled voltages on the gates. The number of gates is N_g.

The system can be described using the capacitance matrix, which captures the relationship between charges and voltages on the dots and gates (analogous to $Q = CV$). It is convinient to use capacitance matrix in a **block form**:

$$\begin{pmatrix} Q_D \\ Q_G \end{pmatrix} = \begin{pmatrix} C_{DD} & C_{DG} \\ C_{DG}^T & C_{GG} \end{pmatrix} \begin{pmatrix} V_D \\ V_G \end{pmatrix}$$

Where:

- C_{DD} is the dot-dot capacitance matrix (size $N_d \times N_d$).
- C_{DG} is the dot-gate cross-capacitance matrix (size $N_d \times N_g$).
- C_{GG} is the gate-gate capacitance matrix (size $N_g \times N_g$).
- Q_D, V_D, Q_G, and V_G are vectors of size N_d and N_g for dots and gates, respectively.

2. Voltage on the Dots

Task: We want to express the free energy as a function of the charge on the dots Q_D and the gate voltages V_G only, as the first one is the variable we want to minimize and the second one is the control parameter.

As a result we eliminate the voltages on the dots
V_D, using equation above, i.e.:

$$Q_D = C_{DD}V_D + C_{DG}V_G$$

Solving for V_D:

$$V_D = C_{DD}^{-1}Q_D - C_{DD}^{-1}C_{DG}V_G$$

This expresses the dot voltages V_D as a function of the charge on the dots Q_D and the applied gate voltages V_G as intended

3. Energy of the Dots

We compute the total energy stored in the dots. Using the electrostatic energy formula $E = \frac{1}{2}Q^T V$, the total energy associated with the dots and their interaction with the gates is:

$$E_{\text{dot}} = \frac{1}{2}Q_D^T V_D$$

Substitute the expression for V_D from Step 2:

$$E_{\text{dot}} = \frac{1}{2} Q_D^T \left(C_{DD}^{-1} Q_D - C_{DD}^{-1} C_{DG} V_G \right)$$

gives:

$$E_{\text{dot}} = \frac{1}{2} Q_D^T C_{DD}^{-1} Q_D - \frac{1}{2} Q_D^T C_{DD}^{-1} C_{DG} V_G$$

The first term $\frac{1}{2} Q_D^T C_{DD}^{-1} Q_D$ is the standard charging energy of the dots. The second term represents the coupling energy due to the gate voltages V_G.

4. Energy of the Gates

To compute the work done by the gates on the dots we first compute the energy of the gates, i.e.

$$E_{\text{gate}} = \frac{1}{2} Q_G^T V_G$$

where after substitution of:

$$Q_G = C_{DG}^T V_D + C_{GG} V_G$$

and V_D from the above, reads:

$$Q_G = C_{DG}^T \left(C_{DD}^{-1} Q_D - C_{DD}^{-1} C_{DG} V_G \right) + C_{GG} V_G.$$

Substituting to $\frac{1}{2} Q_G^T V_G$ we separate the only term dependent on Q_D, and identify that as work done by the gates on the dots:

$$W_{\text{gate-dot}} = \frac{1}{2} Q_D^T [C_{DD}^{-1}]^T C_{DG} V_G$$

5. Full Gibbs Free Energy

Note that the second term in the energy of the dots and the work done by the gates on the dots are the same. As a result, the Gibbs free energy of the system is:

$$G(N_D, V_G) = \frac{e^2}{2} N_D^T C_{DD}^{-1} N_D + e N_D^T C_{DD}^{-1} C_{DG} V_G$$

where we use the fact that C_{DD} is symmetric, i.e. $[C_{DD}^{-1}]^T = C_{DD}^{-1}$, and replaced Q_D with N_D e, where e is the elementary charge.

6. Alternative derivation

According to many references, the free energy of the dots can be computed directly from the generalisation of the formula $E = \frac{1}{2} Q^2 / C$, which for the matrix form reads:

$$E = \frac{1}{2} \begin{bmatrix} Q_D \\ V_G \end{bmatrix}^T C^{-1} \begin{bmatrix} Q_D \\ V_G \end{bmatrix}$$

which leads to exactly the same formula as above.

7. Chemical potential

The chemical potential of the dot i is defined as the change in the energy of the dot i with respect to the change in the charge on the dot i. It is given by:

$$\mu_i(N_D, V_G) = G(N_D, V_G) - G(N_D - e_i, V_G)$$

the transition takes place where μ_i is 0, i.e. the cost of adding a pariticle is 0.

8. Size of Coulomb diamond

The size of the Coulomb diamond $\Delta V_\diamond[i]$ along e_i is related to charging energy. To get the size of the Coulomb diamond we need to measure the voltage distance between the two points where the chemical potential is 0.

$$\mu_i(N_D, V_G) = \mu_i(N_D + e_i, V_G + \Delta V_\diamond[i] e_i)$$

which after some computation gives:

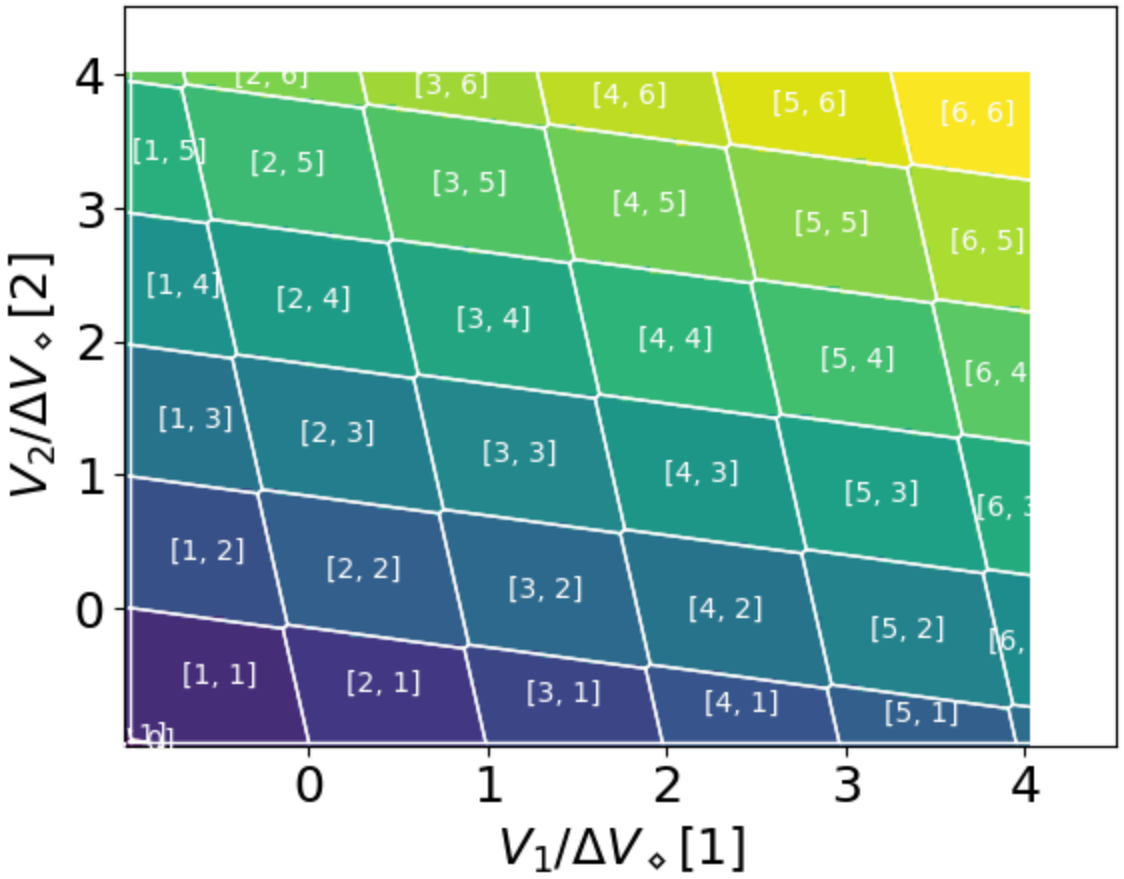
$$e_i^T C_{DD}^{-1} \left(|e| e_i - C_{DG} e_i \Delta V_\diamond[i] \right) = 0$$

solving which gives:

$$\Delta V_\diamond[i] = \frac{|e| e_i^T C_{DD}^{-1} e_i}{e_i^T C_{DD}^{-1} C_{DG} e_i} \rightarrow |e| C_{DD}^{-1}[i,i] / (C_{DD}^{-1} C_{DG})[i,i]$$

as both are the scallars.

Proof it works:



9. Lever arm

In the previous equation, we used the relation between the change in dot voltage and gate voltage, which for constant N_D:

$$|\Delta V_D| = C_{DD}^{-1} C_{DG} \Delta V_G$$

For instance if we would be interested how the ith gate affects the jth dot we would look at the lever arm:

$$|\Delta V_D|_i = C_{DD}^{-1}[i,k] C_{DG}[k,j] \Delta V_G[j] = \alpha_{ij} \Delta V_G[j]$$

from which the lever arm matrix is defined as:

$$\alpha = C_{DD}^{-1} C_{DG}.$$

Virtual gates

The lever-arm matrix can be used to virtualise the gates, i.e.

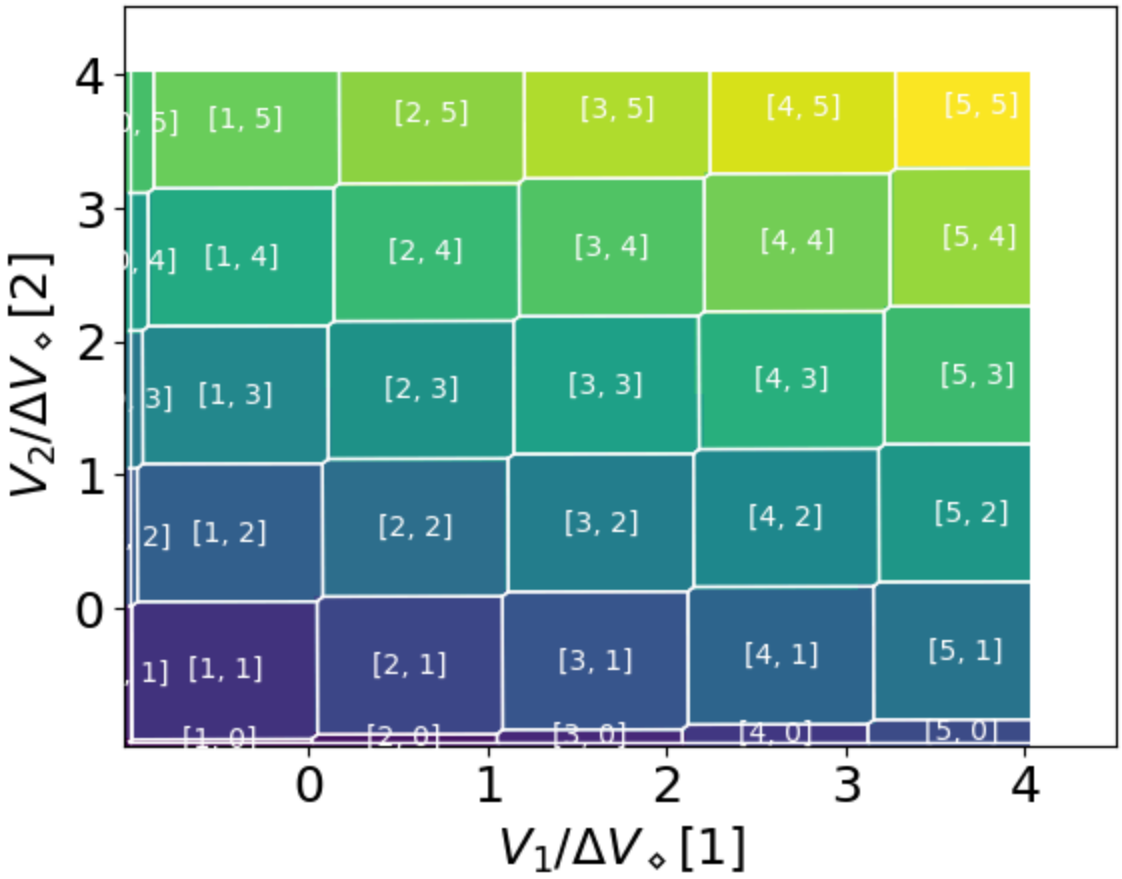
$$\Delta V_D = \alpha \Delta V_G \implies \Delta V_G = \alpha^{-1} \Delta V_D$$

Hence if we want to change the voltage of ith dot, i.e. $\Delta V_D = e_i$ we can compute combination of the gate voltages that would do that:

$$\Delta V_{G,i} = \alpha^{-1} e_i$$

which is the ith column of the inverse of the lever arm matrix.

To test that we take a random 2-dot system and plot CSD with plane axes = $[[1,0],[0,1]]$ (above) and compare the one with transformed plane axes $[\Delta V_{G,0}, \Delta V_{G,1}]$ (right). The latter should be a straight line, which is the case.



10. Charging energy

We finally compute the charging energy, which is the energy required to add one electron to the dot, i.e. the energy required to increase the charge on the dot by one elementary charge. We use the previous result and first compute the voltage on the dot resulting from pulsing the plunger gate by $V_\diamond[i]$, i.e.

$$\Delta V_{D,\diamond}[i] = \alpha[i,i]\Delta V_\diamond[i] = |e|(C_{DD}^{-1})[i,i]$$

which can be easily converted in energy needed to add an electron, i.e. $E = QV/2$, i.e.

$$E_c[i] = \frac{1}{2}|e|\Delta V_{D,\diamond}[i] = \frac{1}{2}|e|^2(C_{DD}^{-1})[i,i]$$

which can be alternatively obtained by comparing the energy of the dot with N_D and $N_D + e_i$:

$$E_c[i] = \mu_i(N_D, 0) - \mu_i(N_D - e_i, 0)$$

11. QDarts implementation

In QDarts, instead of Maxwell capacitance matrix C_{DD}, C_{DG}, we use the canonical capacity matrix $\tilde{C}_{DD}$ and $\tilde{C}_{DG}$.

We have procedure to generate $\tilde{C}_{DD}$, $\tilde{C}_{DG}$ i.e.

$$\tilde{C}_{DD}[i,i] \sim c_{dot}$$
$$\tilde{C}_{DD}[i,j] = \sqrt{\tilde{C}_{DD}[i,i]\tilde{C}_{DD}[j,j]}\exp\left(-\frac{d_{ij}}{\lambda_d}\right)$$
$$\tilde{C}_{DG}[i,i] \sim c_{gate}$$
$$\tilde{C}_{DG}[i,j] = \sqrt{C_{DD}[i,i]C_{DG}[j,j]}\exp\left(-\frac{d_{ij}}{\lambda_{dg}}\right)$$

where $c_{dot} \sim \mathcal{N}(\bar{c}_{dot}, \sigma_{dot})$, $c_{gate} \sim \mathcal{N}(\bar{c}_{gate}, \sigma_{gate})$, and d_{ij} is the distance between the ith and jth dot/gate.

We can use them as the input for QDarts the generate CSD and sensor signals.

However to estimate the charging energy, lever arms and other quantities we need to convert them to Maxwell capacitance matrix using:

$$C_{DD}[i,j] = -(1-\delta_{ij})\tilde{C}_{DD}[i,j] + \delta_{ij}\sum_k \tilde{C}_{DD}[i,k]$$
$$C_{DG} = \tilde{C}_{DG}$$

where the constructed C_{DD} and C_{DG} are used in all analytical above formulas.

Summary

To make our work more impactful, one could just learn:

- Vector $E_c[i] = 1/2|e|^2(C_{DD}^{-1})[i,i]$ - N numbers
- Matrix $\alpha^{-1} = [C_{DD}^{-1}C_{DG}]^{-1}$ - NxN numbers
    - Possibly starting with the diagonal elements of the matrix, which are the lever arms of the dots.

Bonus considerations

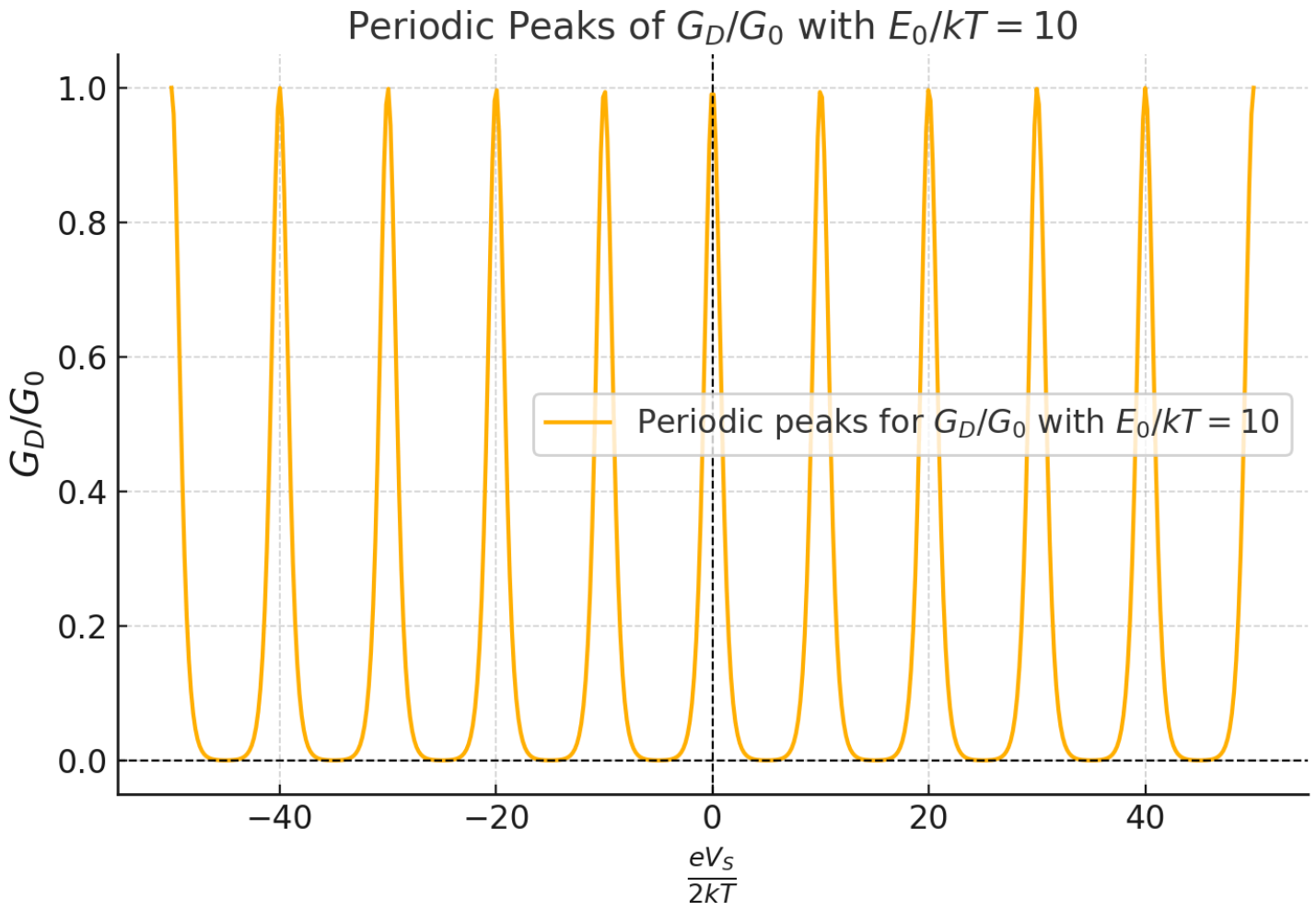
Why the sensor dot conductance experiences a shift at transition and shows a smooth drift in between?

Dot conductance

One can derive that the dot conductance is given by the cosh function, and is periodic due to different number of

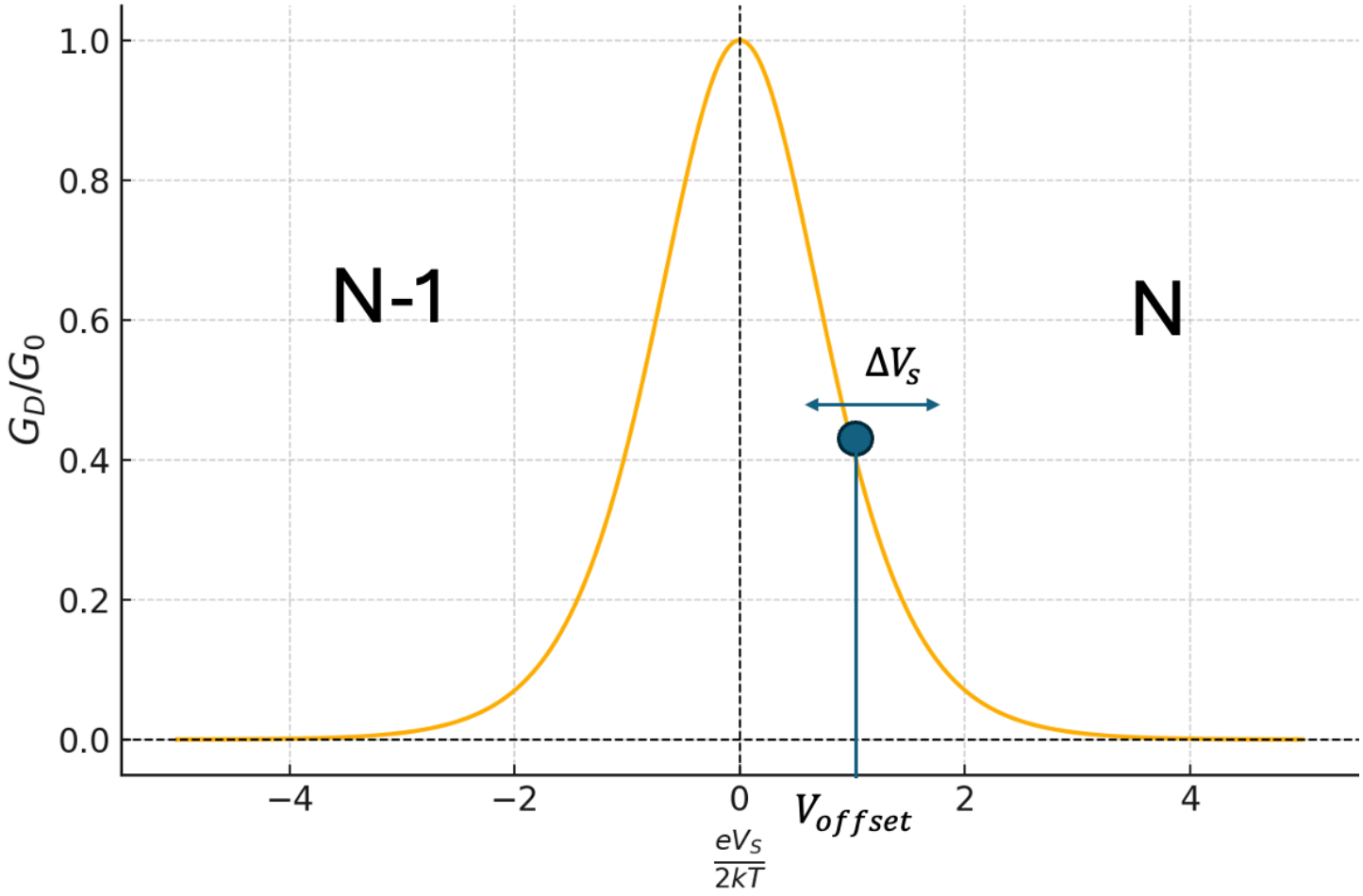
$$G_D = G_0 \sum_n \frac{1}{\cosh^2\left(\frac{eV_S - E_n}{2kT}\right)}$$

where E_n is the location of the nth peak, typically $E_n = nE_{c,s}$.



In the figure we have the conductance as a function of V_s. Each playeau corresponds to different occupation of a sensor dot (0,1,2,3,4,5,6,7,8,9,10). The peaks are separated by the charging energy of the sensor dot $E_{c,s}$, and the width of the peak is given by the temperature.

When coupling between the sensor and the dot is weak (typically) we are operating within a single peak.



Smooth drift

The smooth drift is caused by the coupling between the dots and the sensor, which could be understood by the equation:

$$\Delta V_D[i] = \alpha[i,j]\Delta V_G[j]$$

where the $\alpha = C_{DD}^{-1}C_{DG}$ is the lever arm matrix. For the set of a single dot and a sensor we have the C_DD of the form:

$$C_{DD} = \begin{bmatrix} c_m + c_{gd} & -c_m \\ -c_m & c_S \end{bmatrix}$$

and

$$C_{DG} = \begin{bmatrix} c_{gd} & 0 \\ 0 & c_{gs} \end{bmatrix}$$

The inverse is given by

$$C_{DD}^{-1} = \begin{bmatrix} \frac{c_S}{c_S c_{gd} + c_S c_m - c_m^2} & \frac{c_m}{c_S c_{gd} + c_S c_m - c_m^2} \\ \frac{c_m}{c_S c_{gd} + c_S c_m - c_m^2} & \frac{c_{gd} + c_m}{c_S c_{gd} + c_S c_m - c_m^2} \end{bmatrix}.$$

which for our toy model gives:

$$\Delta V_S(\text{smooth}) = \frac{c_{gd} c_m}{c_S c_{gd} + c_S c_m - c_m^2} \Delta V_G[1] \approx \frac{1}{c_S} \frac{c_{gd} c_m}{c_{gd} + c_m} \Delta V_G[1]$$

this is why large c_S is good to prevent the drift of the sensor due to pulsing plnugers.

Rapid jump at transitions

The rapid jump at transitions is due to the fact that the central dots are chging their occuption.

This can be understood by considering the equation for the dot potential:

$$V_D = C_{DD}^{-1} Q_D - C_{DD}^{-1} C_{DG} V_G$$

NOTE the minus sigh that we ignored in the above analysis. It does not matter, as we could be on the other side of the transition.

Anyway clearly the addition of one electron to central dot changes the potential of the sensor by:

$$\Delta V_S(\text{jump}) = -C_{DD}^{-1}[s, :] \Delta Q$$

where $[s, :]$ denotes the row of the sensor in the C_{DD}^{-1} matrix. For the toy model and for a single electron transition $\Delta Q = [1, 0]^T$ we have:

$$\Delta V_S(\text{jump}) = -\frac{c_m e}{c_S c_{gd} + c_S c_m - c_m^2}$$

where the $-$ sign highlights that the change of the potential (and hence) condutance of the sensor is opposite to drift contribution.

Additionally for no sensor gate cross-talks one check that: $c_{dg} V_\diamond[1] = e$ meaning that $\Delta V_S(\text{jump}) = -\Delta V_S(\text{drift})$ when the latter is pulsed through the whole coulomb diamond. This

is why the colors change approximately periodically. It will be not the case if the cross-talk is high.