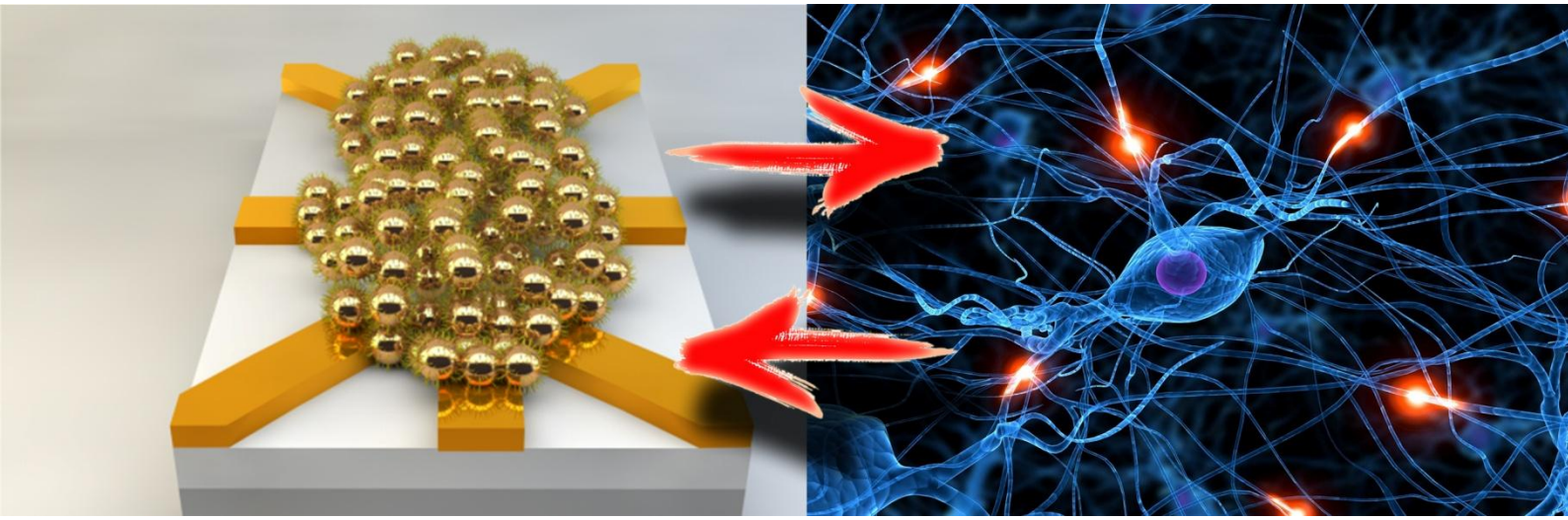
Nanoelectronics group

Mapping electron tunnelling in a nanoparticle network to a cellular neural network

University of Twente



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Chapter 1: Introduction

Today's scientists are looking for new ways to do computations faster, more efficiently and to master more complex computations like pattern recognition. Especially pattern recognition is for conventional computers a very difficult and a time consuming task. To improve upon doing these sorts of computations new concepts must be developed.

An example of such a new concept is for instance the recent work of S.K. Bose and C.P. Lawrence, in which a designless nanoparticle network is turned into reconfigurable Boolean logic by evolution[1]. These networks of interconnected metal nanoparticles act as strongly nonlinear single-electron transistors[2], [3] and can be turned into any Boolean logical gate. This concept is very interesting for further research to see if more advanced tasks like pattern recognition can be handled.

Looking into the behaviour of these networks before fabricating them requires an appropriate computer model. At this moment circuits built of single-electrons can be modelled by a simulator for single-electron tunnel devices and circuits called SIMON 2.0 [4],[5]. However, SIMON is only suitable for simulating small amounts of nanoparticles, because for large systems the computation time becomes too large, due to the use of Monte Carlo simulations [3]. Therefore, another model must be found to simulate the behaviour of larger systems.

In this report will be investigated if it is possible to map a nanoparticle network to a cellular neural network (CNN) and discover the behaviour of such networks. The advantages of CNNs are [6],[7]:

- Scalability
- High-speed parallel signal processing
- Local dynamics, local feedback and local feedforward

To check if the adopted CNN model is valid, the results of the CNN model will be compared with the results of SIMON which is proven to be realistic for small networks. Later on, if the CNN model matches with SIMON, the model can be tested for bigger networks. The CNN model will be made in Wolfram Mathematica [8].

The first goals will be to simulate the basics: a one nanoparticle system. Later on, a parallel two nanoparticle network will be considered.

Chapter 2: Theory

The basics of single-electron tunnelling (SET) will be discussed in this subsection. First the basic concept of SET will be explained. Secondly the simplified theory used to describe SET will be introduced. Then the special behaviour of SET will be discussed, further more the voltage relations in a basic network and energy levels are explained. Finally, the working principle of the simulation software SIMON is presented.

2.1 Single-electron tunnelling (SET)

2.1.1 Basic concept

First of all, a conducting island or nanoparticle is needed for SET. At the right conditions, which will be introduced next, SET has a very interesting behaviour. Under these conditions the tunnelling of individual electrons can be controlled. The tunnelling rate can for example be influenced by a bias voltage at the nanoparticle.

The tunnelling will now be discussed in more detail. Lets first assume that the island has the same amount of electrons as it has protons, such that the island is electroneutral as can been seen in figure 1. A weak external force may add an extra electron from the outside to the island. Now the island is negatively charged and will repel electrons from the outside by its electric field *E*.

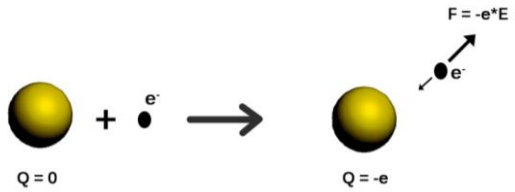

figure 1: At the left of the arrow an electroneutral island is depicted. One single electron is added to this island, due to a weak external force from outside. The result is shown on the right: a negatively charged island, which generates an electric field which repels other electrons.

However, in general the energy that is needed to add an electron to the island is not expressed as the strength of the electric field but as the charging energy as can be seen in equation (1). When one electron is added, the electrostatic potential changes by the charging energy. This charging energy is inversely proportional to the capacitance of the island, which is again related to the size of the island by C = εS/(4πd) [9]. So, the smaller the nanoparticle, the higher the charging energy.

$$E_c = e^2/C \quad (1)$$

$$E_a = E_C + E_k \quad (2)$$

$$E_a \geq 10\, k_B T \quad (3)$$

The charging energy is not the only energy contribution in this system. The electron addition energy E_a is a combination of the charging energy and the thermal energy as is given in (2). For high temperatures the thermal energy contribution will neglect single-electron effects which are due to the charging energy. In order to suppress the influence of thermal energy two precautions can be taken: lower the temperature and/or decrease the islands size, such that the condition in equation (3) is met [2]. In this relation k_B is the Boltzmann constant, which relates the energy of a individual particle to the temperature. In this paper simulations are for convenience based on a temperature of 0K.

2.1.2 Orthodox theory

Single-electron tunnelling can be described by different theories with each there pro's and con's. In this paper the 'Orthodox theory' [10] will be explained, since the CNN model will be based on this model. The Orthodox theory is a simple but very effective method in describing the physical behaviour of single electrons. It translates the quantization of charge into the quantization of a continuous spectrum of energy states.

The Orthodox theory makes the following major assumptions [2]:

1. The electron energy spectrum is considered continuous. This will give an adequate observation as long as $E_k << E_C$.
2. The tunnel time of an electron is negligibly small in comparison with other time scales, which is valid for tunnel barriers in single-electron devices.
3. Multiple tunnelling processes at the same time by a single electron called "cotunnelling" are neglected. This assumptions holds if the resistance R of all the tunnel barriers is much higher than the quantum resistance R_Q. R_Q is typically 6.5 kΩ [2].

The Orthodox theory manages to be in quantitative agreement with nearly all experimental data for systems with metal conductors. For semiconductor structures the theory gives qualitatively description of most obtained results. The networks in this research are based on metal conductors and will therefore give quantitative results based on the Orthodox theory.

Now the tunnel rate Γ will be introduced. The tunnel rate is the number of electrons that tunnel through a barrier per second. It depends on the reduction ΔW of the free (electrostatic) energy in the total system due to the tunnelling event as is shown in equation (4). One can observe from this equation that the tunnel rate is linear dependent on the change of free energy at 0K. The free energy depends on voltage drop across the barrier before V_i and after V_f a tunnel event as stated by equation (5).

$$\Gamma(\Delta W) = \frac{I\left(\frac{\Delta W}{e}\right)}{e} \frac{1}{1 - e^{-\frac{\Delta W}{k_B T}}} \qquad (4)$$

$$\Delta W = \frac{e(V_i + V_f)}{2} \qquad (5)$$

The calculations seems to be straight forward, but problems can already occur in basic circuits when multiple tunnelling events are possible on the same time. All possible states of the network have to be integrated into a system of master equations (6), which describes the change of probability p_i in time for each state. The master equation will blow up when a multidimensional space is considered with all its possible states. A way to solve these complex systems is with the Monte Carlo Method which will be discussed in section *2.2 SIMON: a Monte Carlo SET simulator* on page 9. [11] In this report the master equations will be mapped to a CNN to check if it can solve complex systems as will be explained in Chapter 3: Adaptation to a cellular neural network (CNN).

$$\frac{dp_i}{dt} = \sum_j (\Gamma_{j \to i} p_j - \Gamma_{i \to j} p_i) \qquad (6)$$

The most significant effects that are neglected by the Orthodoxy theory are cotunnelling and discrete energy levels. Cotunnelling is negligible if the resistance R of the barriers is much higher than the quantum resistance R_Q. The discrete energy levels start to play a role for very small islands. At that moment the quantum splitting E_k between electron energy levels may become larger than E_C and k_BT as a result the energy dependence of the tunnelling rate changes. For large differences in energy the tunnel rate will reach a constant rate.

2.1.3 Coulomb blockade and stability plots

At low temperatures for small structures and under the right conditions the tunnelling behaviour of electrons at nanoparticles can be described by the Orthodox theory as mentioned before. In this section a look is taken at the special behaviour of SET. Due to the charging energy a single nanoparticle can be in two states as is shown in the double tunnel junction in figure 2. Once the potential outside a nanoparticle has overcome the charging energy an electron can tunnel to the nanoparticle. However, to establish a current it should also leave the nanoparticle through another barrier. If the electron cannot leave the nanoparticle and its trapped it is called a Coulomb blockade.

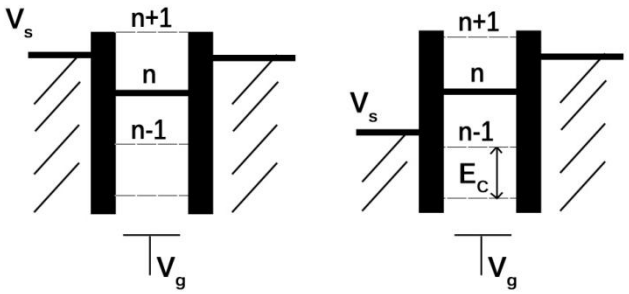

figure 2: Different states of conduction of a nanoparticle with energy level *n*. In the right network electrons can tunnel from and to the nanoparticle via energy level *n*, such that there is a current. At the left nanoparticle there is a so called Coulomb blockade and no current will flow.

The effect of the Coulomb blockade in double tunnel junctions can be seen from the Coulomb staircase and Coulomb oscillations in figure 3. In the top figure V_b is the bias or source voltage. The so called Coulomb blockade is clearly visible at V_b = 0V, because the charging energy must first be overcome before a current can start to flow. The step like behaviour is due to new energy levels that are able to conduct with an increasing bias voltage.

The spiky behaviour of the Coulomb oscillations in the bottom figure of figure 3 can be explained by the fact that this time the gate voltage V_g is changed and V_s is kept constant. An increasing gate voltage V_g shifts the energy levels up. Every time an energy level is in between two neighbouring potentials a small current will be the result. Every time it is not in this window there will be no current. By changing the gate voltage new energy levels will enter and leave the conducting regime, which causes the spikes. The Coulomb oscillations will only occur if the double tunnel junction is asymmetric, meaning that the potential at the source and the drain differ.

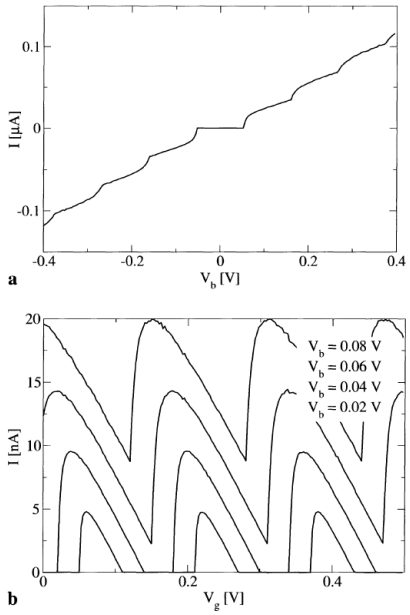

figure 3: The top figure, a I-Vb curve, shows the Coulomb staircase. The bottom figure, a I-Vg curve, shows the Coulomb oscillations. The simulation is done at 0K and the capacitances of the barriers are 1aF. (Source [3])

Now it is time to analyse the behaviour of the complete double tunnel junction. This can be done by looking at the current of the nanoparticle while adjusting both the bias and the gate voltage. This results in a stability plot as is shown in figure 4. The diamond structures are well known as Coulomb diamonds. The grey areas indicate the stable areas and the white areas are instable. So, instable means that there is a current and the stable areas are the result of the Coulomb blockade without a current.

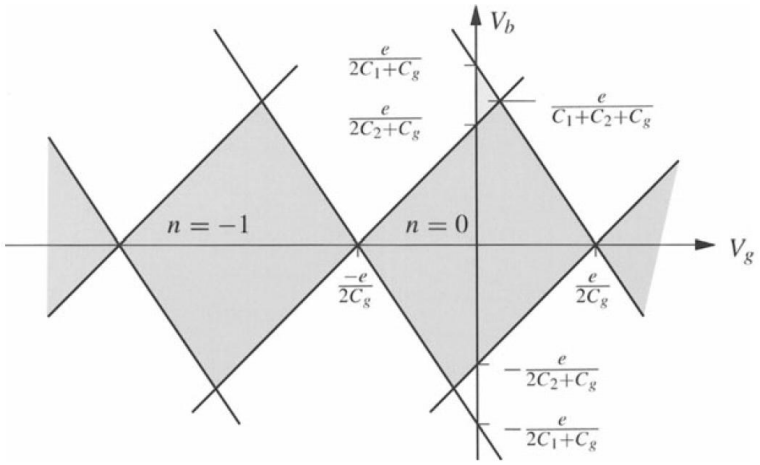

figure 4: Stability plot of a single nanoparticle with a source, gate and ground, which behaves as a single-electron transistor. The grey areas are stable. (Source [3])

2.1.4 Capacitance and voltage matrices

In order to find an expression for the tunnelling rate defined by the Orthodox theory the change in free energy ΔW of each tunnelling event must be calculated. To do this all the potentials and capacitances in the network must be known. The nanoparticles are interconnected by tunnel barriers which can be represented by a capacitance and resistance. Each individual nanoparticles can have a source, drain, bias and multiple neighbouring nanoparticles as is shown in figure 5. The potential $V(n,r)$ of nanoparticle *r* is expressed in equation (7). The voltage and capacitance matrices for a large network can be expressed as in equation (8). This equation is based on the circuit in figure 5 and the assumption that the charging energy is constant.

$$V(n,r) = \frac{C_{sr}V_{sr} + C_{gr}V_{gr} + C_m V(n_*, r') + C_{dn}V_{dn} - ne}{C_{sr} + C_{gr} + C_{mr} + C_{dn}} \quad (7)$$

$$\begin{pmatrix} V_1 \\ \vdots \\ V_r \end{pmatrix} = \begin{pmatrix} C_{\Sigma 1} & \cdots & -C_m \\ \vdots & \ddots & \vdots \\ -C_m & \cdots & C_{\Sigma r} \end{pmatrix}^{-1} \left[\begin{pmatrix} C_{s1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & C_{sr} \end{pmatrix} \begin{pmatrix} V_{s1} \\ \vdots \\ V_{sr} \end{pmatrix} + \begin{pmatrix} C_{d1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & C_{dr} \end{pmatrix} \begin{pmatrix} V_{d1} \\ \vdots \\ V_{dr} \end{pmatrix} + \begin{pmatrix} C_{g1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & C_{gr} \end{pmatrix} \begin{pmatrix} V_{g1} \\ \vdots \\ V_r \end{pmatrix} - \begin{pmatrix} n_1 \\ \vdots \\ n_r \end{pmatrix} e \right] \quad (8)$$

$$with\ C_{\Sigma r} = C_m + C_{sr} + C_{dr} + C_{gr}$$

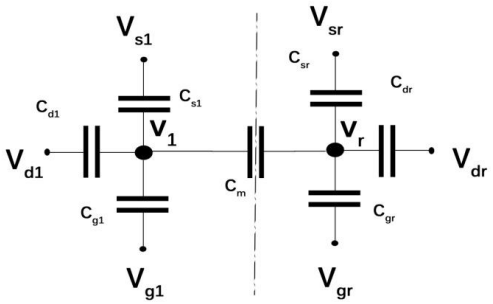

figure 5: This network shows all the voltages and capacitances within a nanoparticle network. V_r is the potential of nanoparticle *r*, V_{sr} is the source voltage, V_{gr} is the gate voltage and V_{dr} is the drain voltage of nanoparticle *r*.

2.1.5 Energy levels

The voltage relations in equation (7) and (8) depend on the energy level *n* of the nanoparticle. In figure 6 the energy levels are depicted for a single nanoparticle with the source and gate voltage set at 0V. The distance between succeeding energy levels is equal to the charging energy E_c. However, the energy levels are not defined correctly using the expression of the potential in equation (7). If the nanoparticle would be neutral the jump to the closest level is only half the charging energy. Therefore, the expression for the voltage in equation must be compensated by an offset of half the charging energy as is shown in figure 6.

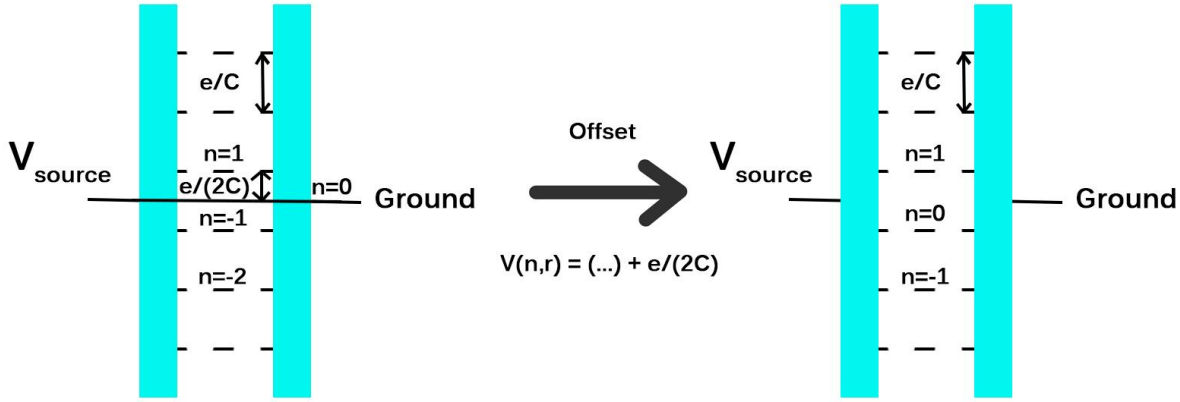

figure 6: At the left the energy levels of a nanoparticle without an offset. The source and gate voltage are 0V. In the right figure the offset is introduced.

In order the find out which highest occupied energy level n_* is applicable for a certain nanoparticle a rule of thumb can be used. If $V(n,r) = 0$ and the network is considered as a simple RC network without a charging energy, n can be calculated as is shown in equation (9). Considering the discrete energy levels near n will give a good estimation of the relevant energy levels.

$$n = \frac{1}{e}(C_{sr}V_{sr} + C_{gr}V_{gr} + C_m V(n_*, r') + C_{dn}V_{dn}) \quad (9)$$

2.2 SIMON: a Monte Carlo SET simulator

A proven simulator for single-electrons tunnel devices is SIMON [4],[5]. SIMON is capable of simulating the random dynamics of complex systems. The working principle of SIMON will now be discussed.

The basic working principle of the Monte Carlo method can be seen in the flowchart of figure 7. At first all the tunnel rates, free energy changes and the duration to the next tunnel events of all the possible tunnelling events are calculated. This is done using the capacitance matrix of the network. When all the calculations are done, one single event with the smallest duration will take place and this process is then started over and over. One can imagine that this takes a lot of computations time for large networks, so the computation time mainly depends on the number of tunnel junctions and nodes in the network.

Despite the long computation time the Monte Carlo method has the following advantages [5]:

1. It takes underlying microscopic physics into account for a better transient and dynamic characteristics of SET circuits.
2. It is not needed to know the relevant states before the simulation can start. Simulations can be done without knowing the previous state in contrast to the master equation approach.
3. It is possible to trade accuracy with simulation time. This is done by considering less states.

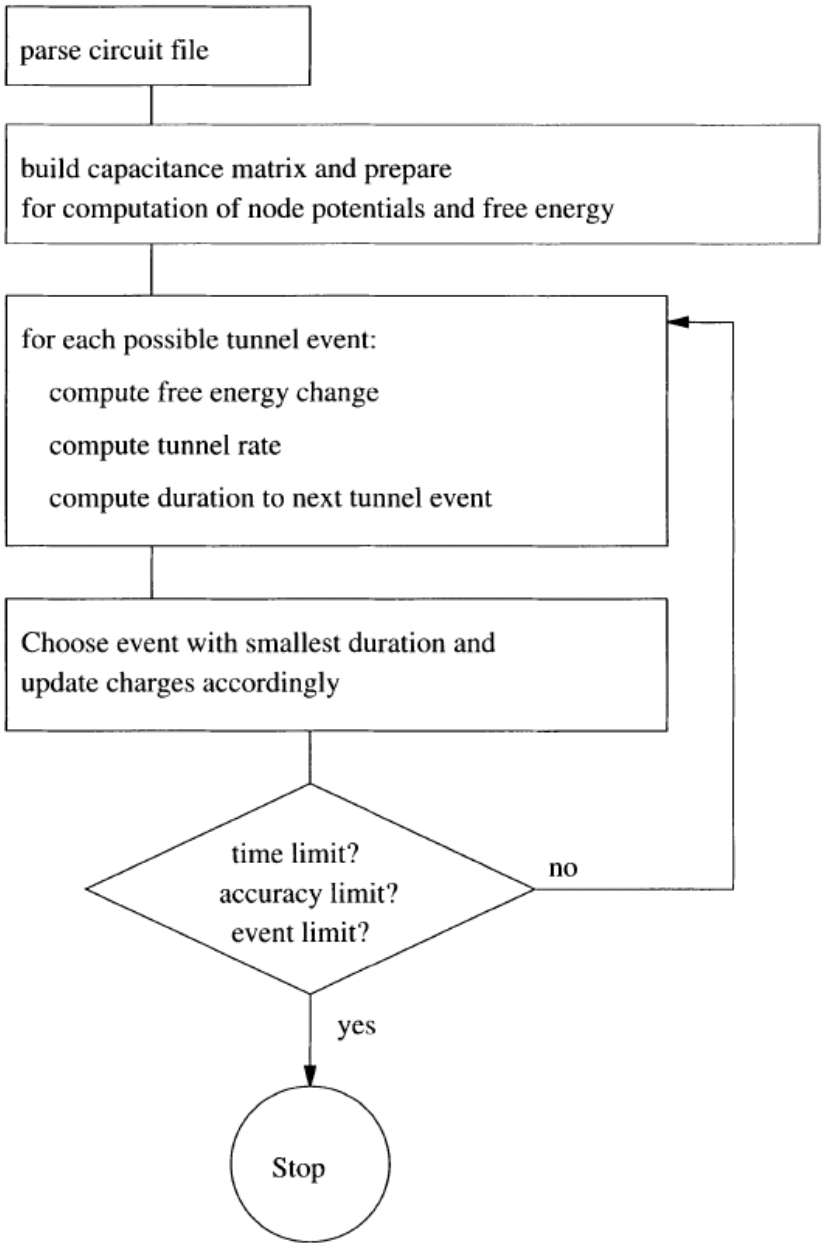

figure 7: Flowchart of the Monte Carlo method. (Source [3])

Chapter 3: Adaptation to a cellular neural network (CNN)

In this chapter the adaptation to a cellular neural network will be discussed by first looking at the characteristics of CNNs. Secondly the equivalence between single-electron tunnelling and CNN dynamics is explained. After this the current in the network is expressed. Finally the adaptation to SIMON and the CNN model in Mathematica is explained for an one and two nanoparticle network.

3.1 Characteristics of CNNs

To be able to adapt a network of nanoparticles to a CNN the characteristics of such a CNN must be determined. In this report the list below shows the characteristics of the CNN as described by T. Roska and L. Chua [12]. A CNN is,

1. a network of nonlinear cells
2. where each cell has an output corresponding to its state
3. which is determined by its own input bias plus...
4. local interactions by feedback and feedforward mechanisms
5. that is measured and controlled by global lines (which maybe sparse)

In figure 8 the mapping of a nanoparticle network to a CNN is visible. All the characteristics of the list above are taken into account. In table 1 the realization in a nanoparticle network is explained more elaborate.

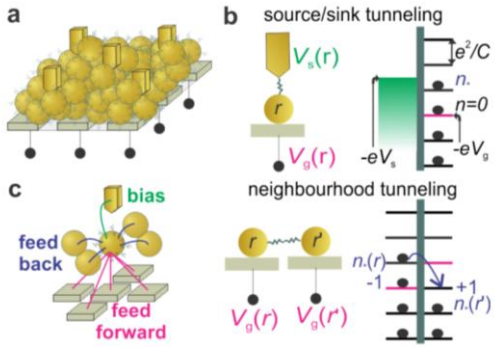

figure 8: a) A schematic of a nanoparticle network. b) In this network electrons tunnel between neighbouring nanoparticles and source/sink electrodes as described by the master equation (10) introduced in the next section. c) Simplifying the master equation satisfies the essential characteristics of a CNN as is explained in table 1. [13]

CNN characteristic	Realization in NP network
Network of cells	A network of NPs with source/sink electrodes at the top and gate electrodes at the bottom (fig **a**)
Output	n_*, the highest occupied energy level on each nanoparticle (fig **b**)
State(s)	$p(n)$, the probability of electron occupancy in level n. Ignoring higher order tunneling processes, the output is mostly dependent only on $n = n_*, n_* + 1$.
Input bias	For NP at position r (fig **b**), a source/sink voltage $V_s(r)$ with respect to a gate voltage $V_g(r)$
Local interaction • feedback • feedforward • bias	For a cell at position r with neighbours $r' \in N_r$, the state $p(n, r)$ is dependent on • neighbourhood outputs, $n_*(r')$ • neighbourhood inputs, $V_g(r')$ • local bias, $V_s(r) - V_g(r)$
Global programming	The set of control and gate voltages spread across the network, are used to steer the electrons. Current sensing electrodes are used to probe the output. The set of voltages are optimized using a GA to obtain desired output functionality.

table 1: A table with all CNN characteristics and how they are realised in the nanoparticle network. [13]

3.2 Equivalence between single-electron tunnelling and CNN dynamics

The following assumptions in this section are proposed by C.P. Lawrence.[13] The master equation for single-electron transport in general is

$$\frac{dp(n,r)}{dt} = \sum_{r\prime\in N}[\Gamma_{r\prime r}(n' \to n) * p(n',r') - \Gamma_{rr'}(n \to n')p(n,r)] + \int dn'[\Gamma_{sr}(n' \to n)p(n',s) - \Gamma_{rs}(n \to n')p(n,r) \quad (10)$$

where

- $p(n,r)$ is the probability of an electron to be in energy level *n* at a nanoparticle located in position *r*
- $\Gamma_{r\prime r}(\mathrm{n}' \to \mathrm{n})$ is the rate for the tunnelling process from position *r'* to *r*, energy level *n'* to *n*
- *n'* iterates over all possible energy levels Z, *r'* iterates over all nanoparticles in neighbourhood N_r

To estimate a lower-bound for the dynamical complexity of this system, the equations are simplified by introducing many working assumptions:

- Neighbourhood tunnelling: electrons only tunnel from the highest occupied energy level n_*
- Source/sink tunnelling: electrons tunnel from or to the energy level $-eV_s$ with a tunnel rate $\Gamma_{\mathrm{sr}}(\to \mathrm{n})$ or $\Gamma_{\mathrm{rs}}(\mathrm{n} \to)$
- $p(n_* + 1, r') = 0$
- $\Gamma(\mathrm{E}_1 - \mathrm{E}_2) = \mathrm{R}\left\{\frac{\mathrm{E}_1 - \mathrm{E}_2}{\mathrm{e}^2\mathrm{R}_0}\right\} = \mathrm{R}\left\{\frac{\mathrm{V}_2 - \mathrm{V}_1}{\mathrm{eR}_0}\right\}$, gives the tunnelling rate as a function of energy/voltage and a constant tunnel resistance. $\mathrm{R}\{\mathrm{x}\} = \begin{cases} \mathrm{x} & \mathrm{x} > 0 \\ 0 & \mathrm{x} \leq 0 \end{cases}$ is a ramp function
- $V(n,r) = \frac{\sum_k^\infty C_{k*}V_k - ne}{C_{\sum n}}$ gives the corresponding voltage potential by assuming a constant charging energy

The simplified master equation thus becomes,

$$\frac{dp(n,r)}{dt} = \sum_{r\prime\in N}[\Gamma_{r\prime r}(n_*(r') \to n) - \Gamma_{rr'}(n \to n_*(r'))p(n,r)] + \Gamma_{sr}(\to n) - \Gamma_{rs}(n \to)p(n,r) \quad (11)$$

$$\frac{dp(n,r)}{dt} = \sum_{r\prime\in N} R\left\{\frac{\mathrm{V_r} - \mathrm{V_{r\prime}}}{\mathrm{eR_0}}\right\} - p(n,r)\sum_{r\prime\in N} R\left\{\frac{\mathrm{V_{r\prime}} - \mathrm{V_r}}{\mathrm{eR_0}}\right\} + R\left\{\frac{\mathrm{V_r} - \mathrm{V_s}}{\mathrm{eR_0}}\right\} - p(n,r)R\left\{\frac{\mathrm{V_s} - \mathrm{V_r}}{\mathrm{eR_0}}\right\} \quad (12)$$

The master equation will be solved for stable systems, so $\frac{dp(n,r)}{dt} = 0$ such that the probability of an electron to be at nanoparticle *r* at energy level *n* is,

$$p(n,r) = \frac{\sum_{r\prime\in N}[\Gamma_{r\prime r}(n_*(r') \to n)] + \Gamma_{sr}(\to n)}{\sum_{r\prime\in N}[\Gamma_{rr'}(n \to n_*(r'))] + \Gamma_{rs}(n \to)} \quad (13)$$

3.3 Current relation

In order to give expression to the current in a network one can look at the tunnelling rates of electrons leaving and entering a nanoparticle and the probabilities of electrons to be at a certain energy level. The probability times the tunnel rate gives the number of electrons per second that tunnel, which is current. In general a current can be expressed as,

$$I_{r\to r'} = \sum_n p(n,r) * \Gamma_{\mathrm{rr'}}\left(\mathrm{n} \to \mathrm{n}_*(\mathrm{r}')\right) \qquad (14)$$

The current in the two nanoparticle system can be described as is shown in equation (15). In figure 9 a graphical representation of the two nanoparticle network is shown.

$$\begin{pmatrix} I_a \\ I_b \\ I_c \end{pmatrix} = \begin{pmatrix} \sum_n [\Gamma_{\mathrm{sr}_1}(\to \mathrm{n}) - p(n,r_1) * \Gamma_{\mathrm{r}_1\mathrm{s}}(\mathrm{n} \to)] \\ \sum_n [\Gamma_{\mathrm{r'r}}(\mathrm{n}_*(\mathrm{r}_2') \to \mathrm{n}) - p(n,r_1) * \Gamma_{\mathrm{rr'}}(\mathrm{n} \to \mathrm{n}_*(\mathrm{r}_2'))] - \sum_n [\Gamma_{\mathrm{rr'}}(\mathrm{n}_*(\mathrm{r}_1') \to \mathrm{n}) - p(n,r_2) * \Gamma_{\mathrm{rr'}}(\mathrm{n} \to \mathrm{n}_*(\mathrm{r}_1'))] \\ \sum_n [\Gamma_{\mathrm{sr}_2}(\to \mathrm{n}) - p(n,r_2) * \Gamma_{\mathrm{r}_2\mathrm{s}}(\mathrm{n} \to)] \end{pmatrix} \qquad (15)$$

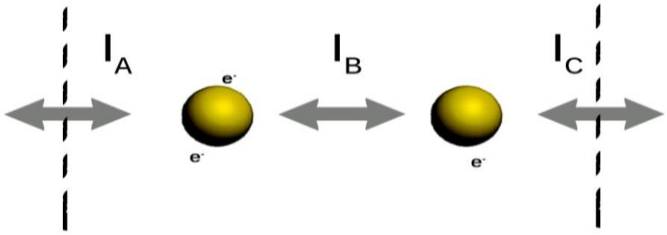

figure 9: In this schematic two nanoparticles are drawn which interact with each other and with the source and sink indicated by the dashed vertical lines. All the possible currents between the source, sink and nanoparticles are I_A, I_B and I_C.

3.4 Translation to Mathematica code

In table 2 the mathematical descriptions of the CNN model are translated to the code in Mathematica. In Mathematica the symbol *r'* cannot be used and is replaced by the *rr*.

CNN model	Mathematica model
$\begin{pmatrix} V_1 \\ \vdots \\ V_r \end{pmatrix} = \begin{pmatrix} C_{\sum 1} & \cdots & -C_m \\ \vdots & \ddots & \vdots \\ -C_m & \cdots & C_{\sum r} \end{pmatrix}^{-1} \left[\begin{pmatrix} C_{s1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & C_{sr} \end{pmatrix} \begin{pmatrix} V_{s1} \\ \vdots \\ V_{sr} \end{pmatrix} + \begin{pmatrix} C_{d1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & C_{dr} \end{pmatrix} \begin{pmatrix} V_{d1} \\ \vdots \\ V_{dr} \end{pmatrix} + \begin{pmatrix} C_{g1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & C_{gr} \end{pmatrix} \begin{pmatrix} V_{g1} \\ \vdots \\ V_r \end{pmatrix} - \begin{pmatrix} n_1 \\ \vdots \\ n_r \end{pmatrix} e \right]$	$\mathrm{MatrixV} := \mathrm{Inverse[MatrixC].\,(MatrixCs.\,MatrixV + MatrixCg.\,MatrixVg + MatrixCd.\,MatrixVd - Matrixn * } e)$
$\begin{pmatrix} A & \cdots & B \\ \vdots & \ddots & \vdots \\ C & \cdots & D \end{pmatrix}$ $\to$ *general expression for all matrices*	$\mathrm{MatrixX} = \{\{\mathrm{A}, B\}, \{C, D\}\}$
$V(n,r) = \dfrac{C_{sr}V_{sr} + C_{gr}V_{gr} + C_m V(n_*, r') + C_{dn}V_{dn} - ne}{C_{sr} + C_{gr} + C_{mr} + C_{dn}}$	$v[[r]] = \mathrm{MatrixV}$
$\mathrm{R\{x\}} = \begin{cases} \mathrm{x} & \mathrm{x} > 0 \\ 0 & \mathrm{x} \leq 0 \end{cases}$	$\mathrm{tunneling[x\_]:= If}[x > 0, x, 0];$
$\dfrac{\mathrm{V(r')} - \mathrm{V(r)}}{\mathrm{eR}_0}$	$\mathrm{X[r\_,rr\_]=}\dfrac{v[[r]]-v[[\mathrm{rr}]]}{e*\mathrm{MatrixR}[[r,\mathrm{rr}]]}$

$\sum_{r\prime\in N} R\left\{\frac{\mathrm{V_r}-\mathrm{V_{r\prime}}}{\mathrm{eR_0}}\right\}$	$\mathrm{Ttoneighbour[r\_, rr\_]:} = \sum_{\mathrm{rr=1}}^{\mathrm{numneighb+1}} \mathrm{tunneling[Toneighbour}[r, \mathrm{rr}]]$
$\sum_{r\prime\in N} R\left\{\frac{\mathrm{V_{r\prime}}-\mathrm{V_r}}{\mathrm{eR_0}}\right\}$	$\mathrm{Tfromneighbour[r\_, rr\_]:} = \sum_{\mathrm{rr=1}}^{\mathrm{numneighb+1}} \mathrm{tunneling[Fromneighbour}[r, \mathrm{rr}]]$
$R\left\{\frac{\mathrm{V_r}-\mathrm{V_s}}{\mathrm{eR_0}}\right\}$	$\mathrm{Ttoss[r\_]:= tunneling[Tosource}[r]] + \mathrm{tunneling[Tosink}[r]]$
$R\left\{\frac{\mathrm{V_s}-\mathrm{V_r}}{\mathrm{eR_0}}\right\}$	$\mathrm{Tfromss[r\_]:= tunneling[Fromsource}[r]] + \mathrm{tunneling[Fromsink}[r]]$
$\sum_{r\prime\in N}[\Gamma_{r\prime r}(n_*(r')\to n)] + \Gamma_{sr}(\to n)$	$\mathrm{Tfrom[r\_]:= If[(n1 == 0 \vert\vert n2 = = 0), 0, Tfromneighbour}[r, \mathrm{rr}]] + \mathrm{Tfromss}[r]$
$\sum_{r\prime\in N}[\Gamma_{rr\prime}(n\to n_*(r'))] + \Gamma_{rs}(n\to)$	$\mathrm{Tto[r\_]:= If[(n1 == 0 \vert\vert n2 = = 0), 0, Ttoneighbour}[r, \mathrm{rr}]] + \mathrm{Ttoss}[r]$
$p(n,r) = \frac{\sum_{r\prime\in N}[\Gamma_{r\prime r}(n_*(r')\to n)] + \Gamma_{sr}(\to n)}{\sum_{r\prime\in N}[\Gamma_{rr\prime}(n\to n_*(r'))] + \Gamma_{rs}(n\to)}$	$\mathrm{pr[r\_]:= If[Tto}[r] == 0, 0, \frac{\mathrm{Tfrom}[r]}{\mathrm{Tto}[r]}]$

table 2: Mapping of the CNN model to the code in Mathematica.

3.4.1 Adaptation of the one nanoparticle network

The first model will only consists of one nanoparticle to check if the fundamental behaviour of the nanoparticle can be described by the CNN model. The circuit used in SIMON can be seen in figure 10.

All the tunnel barriers will have a resistance of 10kΩ, the bias capacitance will be kept at 20aF and the temperature is set to 0K for all simulations. The source capacitance C_s and mutual capacitance C_m can be changed depending on the goal of the simulation. Different capacitance values should give different shapes of Coulomb diamonds.

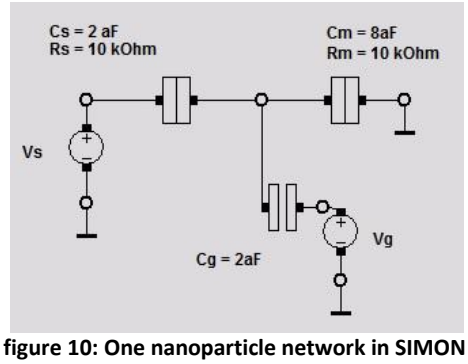

figure 10: One nanoparticle network in SIMON

The code used to describe a one nanoparticle network in Mathematica is shown in *Appendix A: Mathematica script of one nanoparticle network* on page 28. The model in Mathematica is quite

simple, because the only unknown variable, is the energy level *n* of this one nanoparticle. The probability expressed in equation (13) can easily be calculated for each energy level. First of all the potentials are calculated using equation (8).Then the tunnel rates are calculated and finally the probability is expressed.

To make the calculations more efficient not all the energy levels should be considered when calculating the probability. It should be enough to consider only the relevant energy levels as explained in section *2.1.5 Energy levels*. This is done by using the following line of code,

$$\text{MatrixN} := \frac{1}{e}(\text{MatrixCs}.\,\text{MatrixVs} + \text{MatrixCg}.\,\text{MatrixVg} + \text{MatrixCd}.\,\text{MatrixVd})$$

To define the relevant energy levels the energy levels close to the value in *MatrixN* should be found. This can be done using the following line of code to make a list of levels,

$$\{\text{n}, \text{Floor}[\text{MatrixN}[\text{r}]] - \text{NUMlevels}, \text{Ceiling}[\text{MatrixN}[\text{r}]] + \text{NUMlevels}\}$$

The probability gives information about the way an energy level is filled and this can be done in three states as mentioned below in table 3. The graphical representation of these states is shown in figure 11. Of course, only the occupied energy levels will have a current contribution in the network. Therefore, by checking for the relevant energy levels if one of them is sometimes occupied, one can determine if the network is stable or not. Only one occupied energy level is enough to have a current contribution and for the network to be instable.

State	**Probability**
Always **filled**	p(n,r) = 1
Sometimes **occupied**	0 < p(n,r) < 1
Always **empty**	p(n,r) = 0

table 3: Three different possible states of an energy level with its probability.

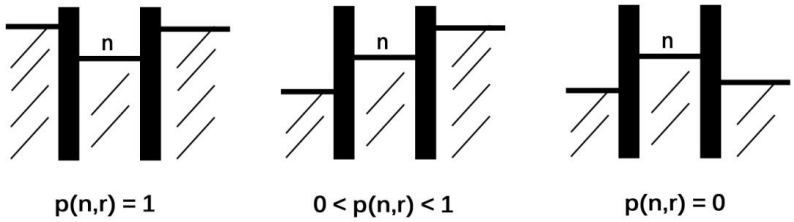

figure 11: Different states of the energy level n

The pseudo code of the Mathematica script can be considered as follows:

- Initialise capacitance and voltage matrices
- Calculate the potentials of all nodes
- Approximate the relevant energy levels
- Calculate tunnelling rates to and from the nanoparticle for these energy levels
- Calculate the probability of each energy level
- Evaluate the probabilities by checking if the configuration is stable or instable
    - An energy level is in the occupied state -> Instable
    - No energy level is in the occupied state -> Stable

3.4.2 Adaptation of the two nanoparticle network

The next step is to look at a more complicated two nanoparticle network. An interesting network to look at is the network in figure 12, because the nanoparticles are placed in parallel and coupled which gives an interesting stability. This network is thoroughly examined by K.S. Makarenko in her book *Charge Transport in Bottum-Up Inorganic-Organic and Quantum-Coherent Nanostructures* [14]. The two nanoparticles are placed in parallel to the source and the drain as can be seen in figure 12. All the tunnel barriers will have a fixed resistance of 10kΩ and the temperature is set to 0K.

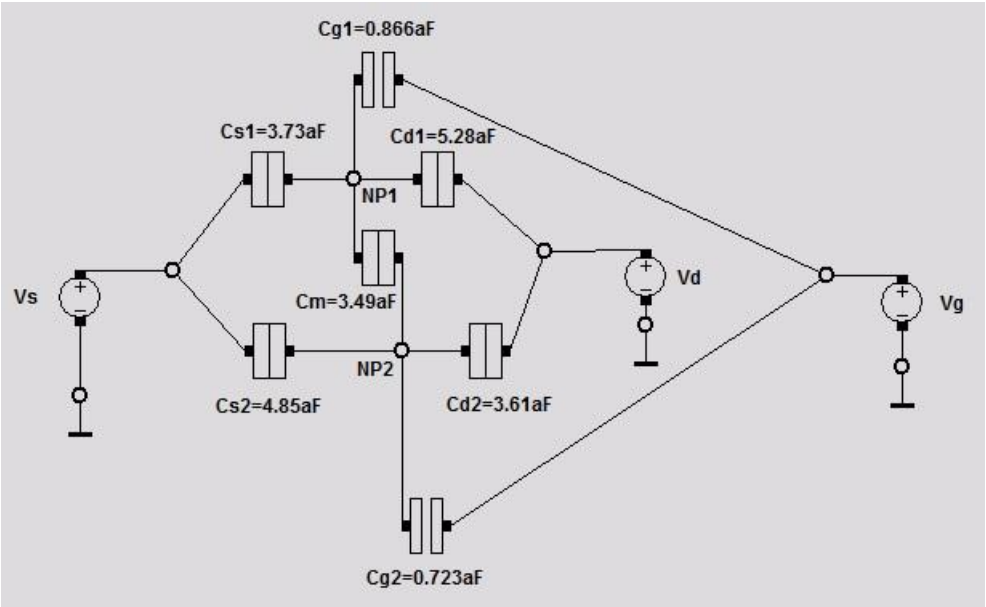

figure 12: Two particle network in SIMON inspired by the work of Ksenia S. Makarenko. [14]

The equivalent CNN model of the SIMON model introduced in the section above can be found in *Appendix B: Mathematica script of a two nanoparticle network* on page 31.

The first step is to calculate all the voltages in the circuit. This time nanoparticle 1 and 2 interact with each other and both potentials are dependent on each other. As explained in section *2.1.4 Capacitance and voltage matrices* the complete network can be described by capacitance and voltage matrices. By doing this matrix calculation all the potentials in the network for any given combination of energy levels can be calculated by equation (8).

After this the energy levels can be expressed by taking care of the offset. This is done using the following lines of code,

$$\mathrm{Ec} := \frac{e}{2 * \mathrm{Diagonal[MatrixC]}}$$

$$\mathrm{levels} = \mathrm{MatrixV} + \mathrm{Ec}$$

Finally the probability can again be expressed using the tunnel rates and taken the offset into account. In the two nanoparticle case the probability is 1 if the energy level is in the occupied state and 0 if the level is always full or empty. Therefore, only energy levels with a probability of 1 will conduct electrons.

Chapter 4: Implementation & Method

In this chapter the implementation and testing method of different networks is described. There will be started with a simple network of just one nanoparticle. A few basic examples from literature will be examined for this network like the well known Coulomb staircase and oscillations. After that a look is taken at the stability plot. Finally the current and stability of the two nanoparticle model will be considered.

4.1 A single nanoparticle simulation

4.1.1 Coulomb staircase and Coulomb oscillations

The first comparison between the CNN model and SIMON will be by comparing the Coulomb staircase and Coulomb oscillations of both models. The Coulomb staircase will be obtained by adjusting the voltage source from -1.0V to 1.0V and the bias voltage is fixed at 0V. In SIMON the current from the source to the nanoparticle is measured as can be seen in figure 13. In Mathematica the probability times the tunnel rate from and to the source will give the current. The source and mutual capacitance are set to 0aF in this simulation. The expected charging energy will be $E_c = e/C = 0.08V$. To compare the results of the CNN model in Mathematica and the results in SIMON the obtained data of both programs are converted to Excel and plot in one figure.

The next simulation will show the Coulomb oscillations by adjusting the gate voltage from -1.0V to 1.0V and fixing the source voltage at 0.05V. In SIMON the current from the source tot nanoparticle is measured as can be seen in figure 13. In Mathematica the probability times the tunnel rate from and to the source will give the current. The source and mutual capacitance are set to 0aF in this simulation. To compare the results of the CNN model in Mathematica and the results in SIMON the obtained data of both programs are converted to Excel and plot in one figure.

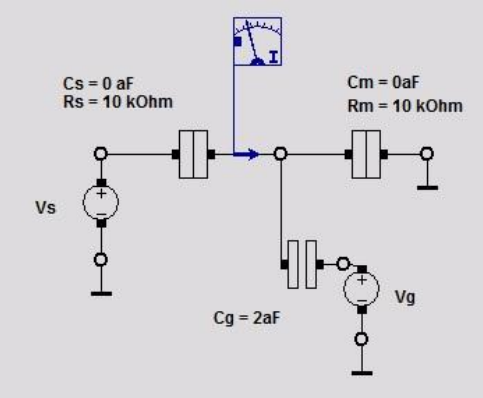

figure 13: Measuring circuit for Coulomb staircase and oscillations in SIMON.

4.1.2 Stability plot

Next the stability plot of the one nanoparticle circuit in figure 10 will be made. A stability plot shows normally the amount of activity for a certain configuration of the network. Activity means in that context the number of electrons per second that tunnel. However, later on in this report will be explained that the current cannot be calculated for multiple nanoparticle systems, therefore it is more convenient to check whether a system is stable (no current) or instable (any current).

The stability plot is obtained by varying V_g from -0.1V to 0.1V and V_s from -0.03V to 0.03V. To get a good comparison the data from SIMON is exported to Mathematica and plotted in the same way as

the CNN model in Mathematica. This means that the activity at no conduction is 0 and set to 1 for any current. The model is tested for multiple configurations of the capacitances to see if the shapes keep matching. The first test is based on Cs=2aF, Cg=2af and Cm=8aF. The second test is done for Cs=Cg=Cm=2aF.

As described before in section *2.1.4 Capacitance and voltage matrices* the algorithm estimates the appropriate energy levels for a combination of potentials. In this case a total range of four energy levels is considered. The estimation is correct if the diamonds will repeat themselves along the x-axis (gate voltage). The gate voltage will be changed from -3V to 3V, the source voltage is changed from -0.5V to 0.5V and the capacitances in this network are all 0.16aF.

4.2 Two nanoparticles simulation

4.2.1 Energy levels

To check if the energy levels are correctly calculated by the CNN model, the energy levels will be visually compared to the stability plot in SIMON. This stability plot is shown in figure 14. The energy levels will be compared by looking at the six different regimes indicated in the figure at Vs=3mV. Regime 1,3 and 5 should be stable and regime 2,4 and 6 should be instable.

After this the probability for each energy should be checked to see if this is implemented the right way.

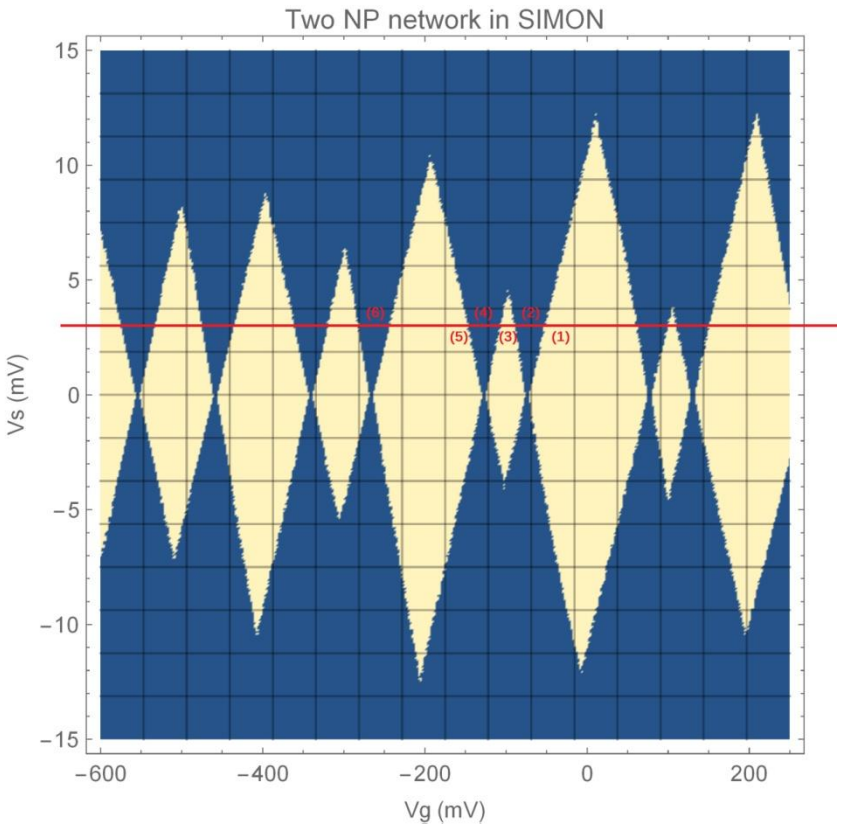

figure 14: The stability plot of the two nanoparticle network in figure 12 is shown. The red line indicates the six chosen regimes at Vs=3mV.

4.2.2 Current

By evaluating numerically a random network one can easily check whether the current relation discussed in section 3.3 Current relation on page 13 holds and satisfies the expected behaviour. In this case one expects that the source current equals the sink current. To check this the random network in figure 15 will be examined. If the relation holds for this network one should investigate more situations and check whether this holds for all possible networks.

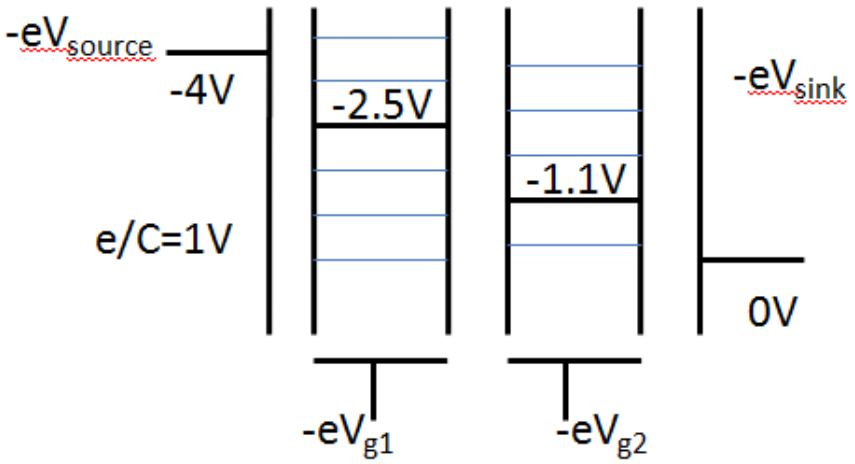

figure 15: A random network to check if the proposed current equations hold. From left to right are visible: the source, the first nanoparticle, the second nanoparticle and the sink. The source voltage is -4V, the sink voltage is 0V and the two nanoparticles are biased at -2.5V and -1.1V. The charging energy is 1V and this will give a highest occupied energy level for the first nanoparticle at n = 1 and for the second nanoparticle at n = 2.

Chapter 5: Results & discussion

In this chapter the results of the simulations will be presented and discussed.

5.1 Results single nanoparticle simulation

5.1.1 Coulomb staircase and Coulomb oscillations

The results of the Coulomb staircase and Coulomb oscillations are respectively shown in figure 16 and figure 17. In the figure of the Coulomb staircase one can clearly see that the Coulomb blockades of both models match. There is no current from 0.46V to 0.54V, therefore the charging energy is 0.08V for this nanoparticle as expected. The slope of the current for the CNN model does not match with the slope of the current in SIMON. However, the slope could be adjusted by changing the ramp function as it is given in section 3.2 Equivalence between single-electron tunnelling and CNN dynamics on page 12.

The Coulomb oscillations of the CNN model and SIMON have the same period, but the amount of current is again not equal. In this case the solution can be changing the ramp function as well. There is also a small mismatch in the width of each peak.

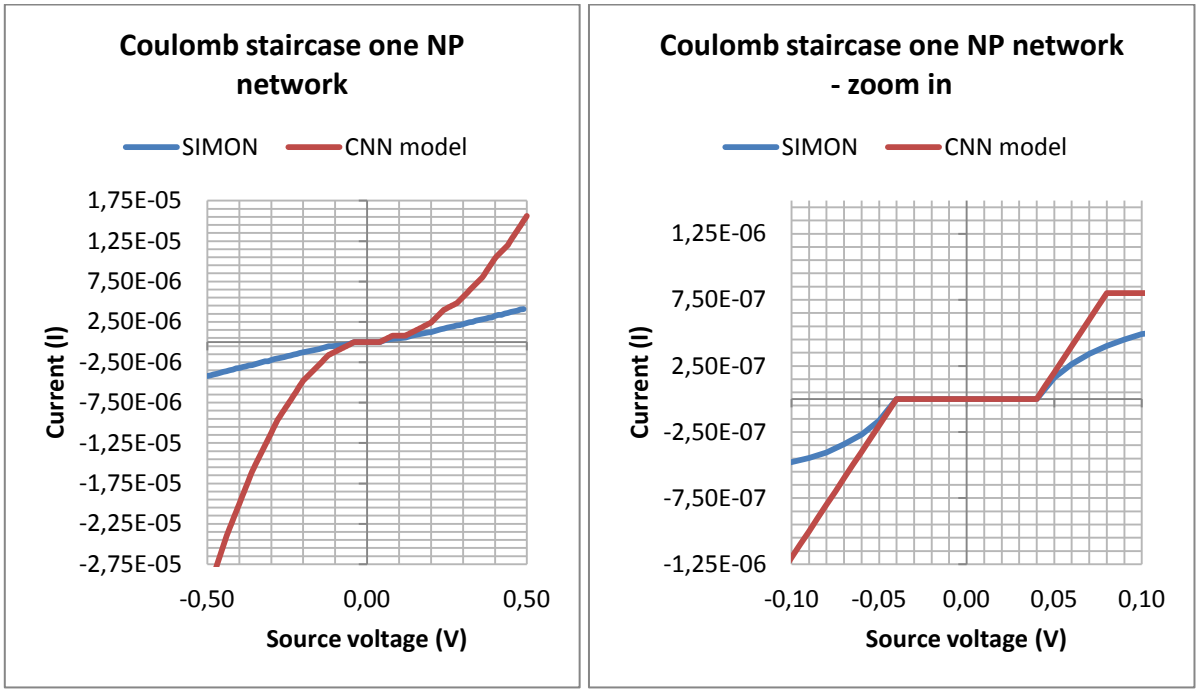

figure 16: The Coulomb staircase of the nanoparticle network for the CNN model and SIMON is shown by plotting the current versus the source voltage. In this network Vg=0V. The left figure shows the complete plot and the right figure shows a zoom in of the Coulomb blockade. The current for the CNN model is expressed as the probability times the tunnel rate from and to the source.

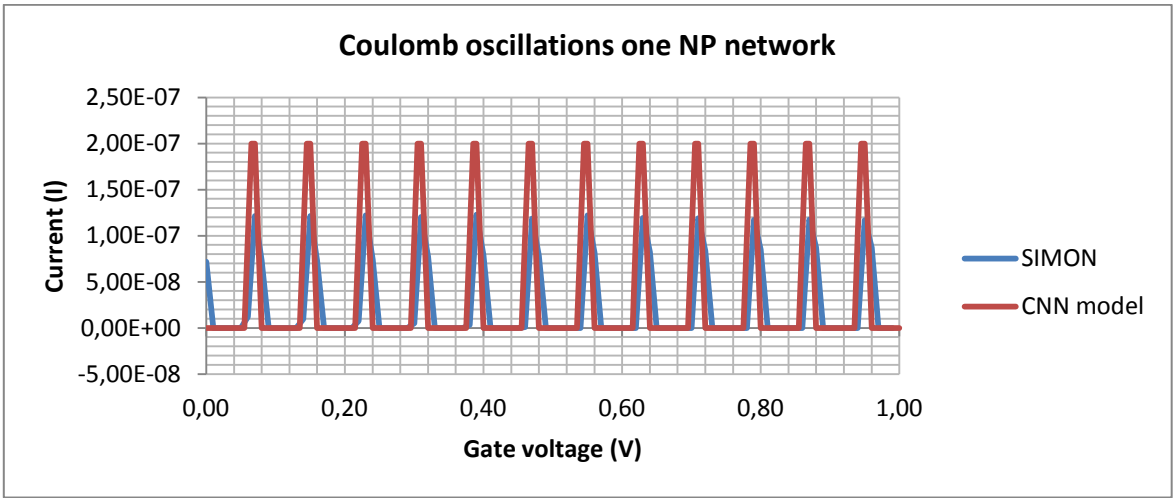

figure 17: The Coulomb oscillation of the one nanoparticle network for the CNN model and SIMON is shown by plotting the current versus the gate voltage. In this network Vs=0.05V. The current in Mathematica is expressed as the probability times the tunnel rate from and to the source.

5.1.2 Stability plot

The stability plots of the one nanoparticle network are shown in figure 18 and figure 19. There is an exact match between the stability plots of the CNN model and SIMON. The values do also match with the values from literature in figure 4.

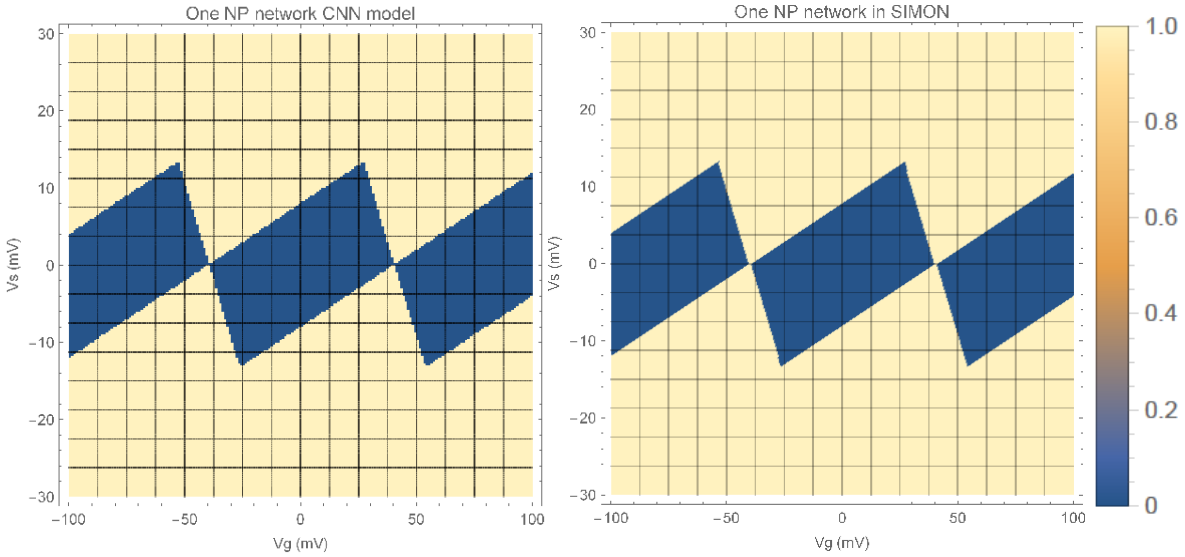

figure 18: The left figures correspond to the results of the CNN model and the results to the right correspond to results of SIMON. At the x-axis the gate voltage is shown and at the y-axis the source voltage. The capacitance values are Cs=20aF, Cg=20af and Cm=80aF.

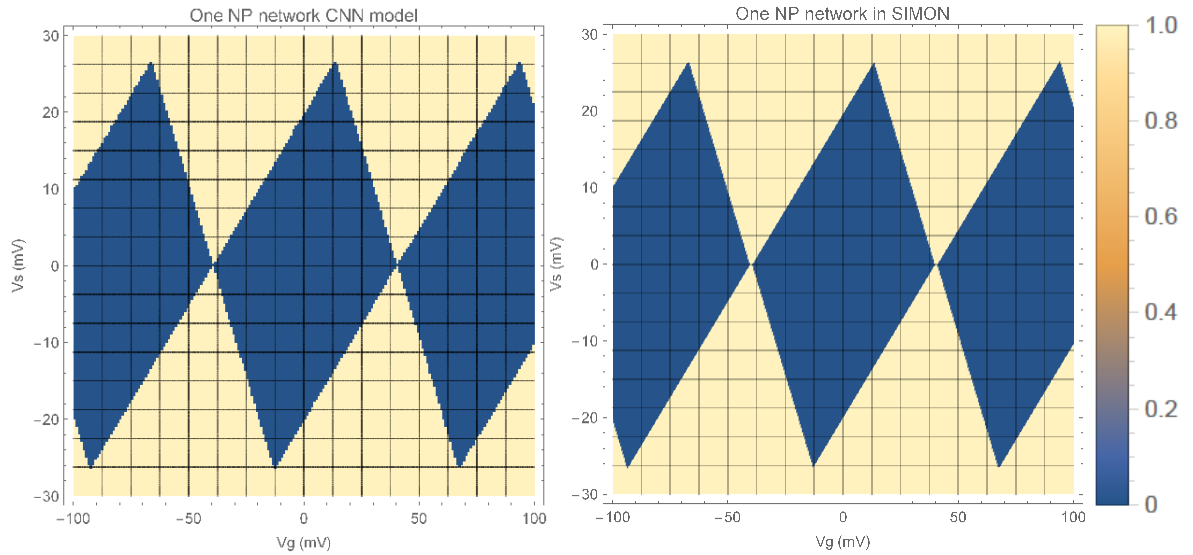

figure 19: The left figures correspond to the results of the CNN model and the results to the right correspond to results of SIMON. At the x-axis the gate voltage is shown and at the y-axis the source voltage. The capacitance values are Cs=Cg=Cm=20aF.

In figure 20 it is clear that the Coulomb diamonds will repeat themselves along the x-axis as expected. This means that the approximation of finding the highest occupied energy level works and four energy levels is enough to simulate the behaviour of a one nanoparticle network.

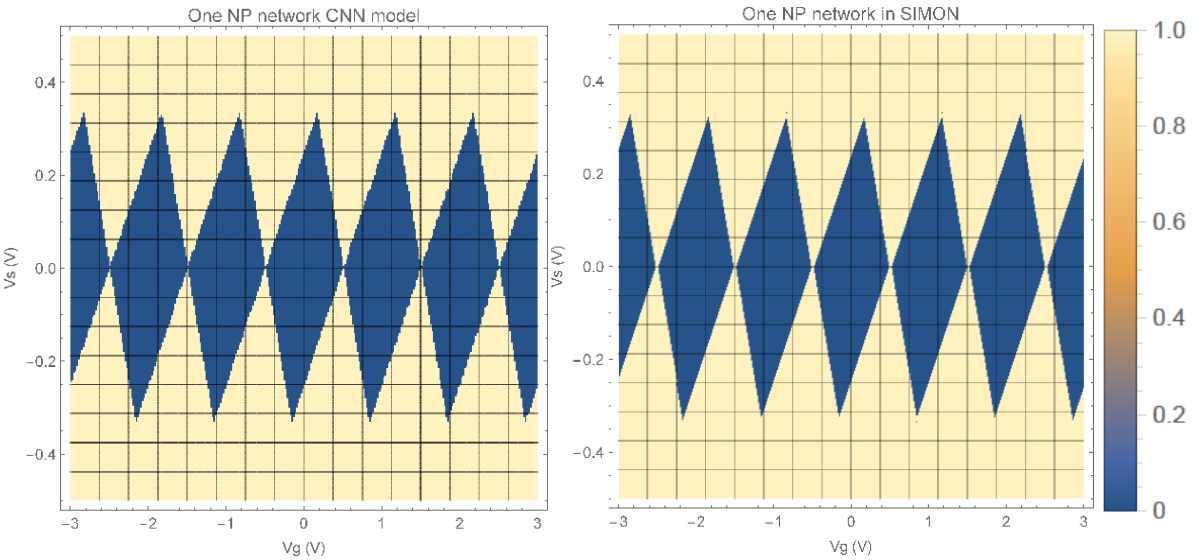

figure 20: In this stability plot the source voltage is again plot versus the gate voltage and all capacitances are 0.16aF. The left figure shows the result for the CNN model and the right figure is the result of SIMON.

5.2 Results multiple nanoparticles simulation

In this section the results of the two nanoparticle network will be presented and discussed.

5.2.1 Energy levels

The energy levels of the CNN model are plot in figure 21 for the six different regimes. One can visually check that regime 1,3 and 5 are indeed stable and regime 2,4 and 6 are instable. So, the energy levels are implemented the right way.

However, if a look is taken at the probabilities there is a mismatch. In figure 22 there is an example given of a wrong probability. If we look at the energy level (0,0) the number of electrons on both nanoparticles is 0. The second nanoparticle will give a probability of 1, because it is in between ground and the level (0,0) of nanoparticle 1. It does not know that level (0,0) of nanoparticle 1 will never be filled and gives therefore wrong information.

figure 21: The calculated energy levels for the CNN model.

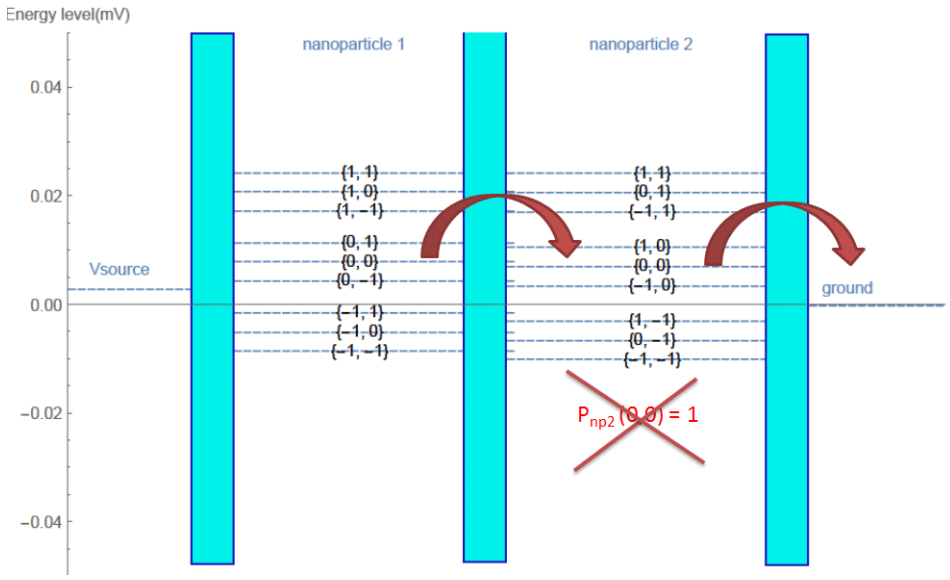

figure 22: Example of a wrongly expressed probability.

5.2.2 Current

The random network proposed in section *4.2.2 Current* is numerically evaluated to check if the proposed current equations holds. The results of the equations are in equation (16). Despitefully the current I_A does not equal the current in I_C as expected, therefore the current cannot be derived from this CNN model. One can see that the total amount of current in the network is in balance. This is because for each individual nanoparticle the same amount of current that enters the nanoparticle leaves the nanoparticle, but there is no communication between the neighbours, so there can be a difference in current between two neighbours.

Another problem is the fact that only the highest occupied energy level of the neighbour is taken into account when looking at the tunnelling rates. Even if lower energy levels of neighbouring particles conduct, their current contribution is not taken into account.

$$\begin{pmatrix} I_a \\ I_b \\ I_c \end{pmatrix} = \begin{pmatrix} 5 * 10^{-6} A \\ -71 * 10^{-6} A \\ -76 * 10^{-6} A \end{pmatrix} \qquad (16)$$

$$I_a + I_b + I_c = 0 \;\&\; I_a \neq I_c$$

Chapter 6: Conclusion & recommendations

6.1 Conclusion

To sum up, the goal of this research was to check if the adopted CNN model is valid by comparing it to simulations in SIMON. First of all one can conclude that the current in a nanoparticle network cannot be expressed using the CNN model. However, giving expression to the stability of a nanoparticle network seems more promising.

The stability of an one nanoparticle model can perfectly be simulated by the CNN model and matches with literature. A nice feature is that the simulation time is reduced by only calculating a minimum amount of relevant energy levels for a certain configuration of potentials.

So far, the stability of the two nanoparticle model cannot be simulated. The energy levels are in agreement with the expected levels, but the probability is wrong. The master equation is too much simplified and the tunnel rates of the neighbouring particles should be coupled.

The moment the two nanoparticle network shows accurate results the number of nanoparticles can easily be scaled up, since the two nanoparticle problem is written using only matrices, which are scalable to any size.

6.2 Recommendations

The tunnel rates of the neighbouring particles should be coupled, such that the probability can be expressed in the right way.

In the future it is good to integrate for multiple nanoparticle networks also the feature of calculating only the relevant energy levels instead of taking all levels into account. This will save a lot of computation time and it will be easier to simulate stability plots of a higher resolution.

Another interesting thing to look at is of course two nanoparticles placed in series and see what kind of results that gives. There was despitefully no time left to have a look at that.

Acknowledgement

This bachelor thesis could not have successfully been finished without the generous help of a few people. These people took a lot of their valuable time and helped me to gain insight into the wonderful world of nanoparticles and helped to overcome the obstacles that I found on my way.

I would like to thank Celestine Lawrence and Wilfred van der Wiel for their advice and help as supervisors during this project. They were of great support and gave me new insights and introduced me to the right people to help me further.

I would also like to thank Hajo Broersma and Ruud van Damme for their input during regular meetings. Finally I would like to thank Alexander Golubov and Peter Bobbert for having an useful discussion which gave me more insight.

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Appendix A: Mathematica script of one nanoparticle network

Constants

In[1]:=
```
e = 1.60 * 10^-19;
R0 = 1 * 10^5;
Cg1 = 20 * 10^-19;
Cs1 = 20 * 10^-19;
Cd1 = 80 * 10^-19;

NUMlevels = 1;
(* The total number of calculated energy levels is NUMlevels*2+2 *)
numneighb = 0;
(* Number of neighbours is equal to the number of particles -1 *)
```

Initialisation

In[8]:=
```
vd1 = 0;
vs1 = vs;
vg1 = vg;
```

In[11]:=
```
MatrixC = {Cs1 + Cg1 + Cd1};
MatrixCs = {Cs1};
MatrixCg = {Cg1};
MatrixCd = {Cd1};
(* Defines the capacitance matrices each row maps to a particle *)
MatrixVs := {vs1};
MatrixVg := {vg1};
MatrixVd := {vd1};
Matrixn := level[n1];
level[n_] := n - 1 / 2;
(* Defines the voltage matrices each row maps to a particle *)
MatrixV := 1 / MatrixC *
    (MatrixCs.MatrixVs + MatrixCg.MatrixVg + MatrixCd.MatrixVd - Matrixn * e);
MatrixN := 1/e (MatrixCs.MatrixVs + MatrixCg.MatrixVg + MatrixCd.MatrixVd);
(* Calculates all the node potentials and sets them in matrix v *)
MatrixR = {10^99};
MatrixRs = {R0};
MatrixRd = {R0};
(* Defines the resistance matrix,
not connected nodes have a very high resistance *)
```

In[25]:=
```
Toneighbour[r_, rr_] := (v[[r]] - v[[rr]]) / (e * MatrixR[[r]]);
(* All tunnelling electrons from node r to neighbours *)
Tosource[r_] := (v[[r]] - MatrixVs[[r]]) / (e * MatrixRs[[r]]);
Tosink[r_] := (v[[r]] - MatrixVd[[r]]) / (e * MatrixRd[[r]]);
(* All tunnelling electrons from node r to source or drain *)
Fromneighbour[r_, rr_] := (v[[rr]] - v[[r]]) / (e * MatrixR[r]);
(* All tunnelling electrons from neighbours to node r *)
Fromsource[r_] := (MatrixVs[[r]] - v[[r]]) / (e * MatrixRs[[r]]);
Fromsink[r_] := (MatrixVd[[r]] - v[[r]]) / (e * MatrixRd[[r]]);
(* All tunnelling electrons from source or drain to node r *)
```

In[31]:=
```
Ttoneighbour[r_] := Sum[tunneling[Toneighbour[r, rr]], {rr, 1, numneighb+1}];
Ttoss[r_] := tunneling[Tosource[r]] + tunneling[Tosink[r]];
Tfromneighbour[r_] := Sum[tunneling[Fromneighbour[r, rr]], {rr, 1, numneighb+1}];
Tfromss[r_] := tunneling[Fromsource[r]] + tunneling[Fromsink[r]];

Tfrom[r_] := Tfromneighbour[r] + Tfromss[r];
Tto[r_] := Ttoneighbour[r] + Ttoss[r];
(* Defines the tunneling rates of all surrounding neighbours,
sources and sinks *)
tunneling[x_] := If[x > 0, x, 0];
(* Determines if an electron can tunnel *)
```

In[38]:=
```
pr[r_] := If[Tto[r] == 0, 0, Tfrom[r] / Tto[r]];
(* Calculates the probability of an electron
 to be at an energy level on particle r. Energy levels
 which are always full or empty have a probability of 0 *)
```

Matrix calculations

In[39]:=
```
matrix[r_] := (Nrelev = MatrixN; Table[v = MatrixV;
   pr[r], {n1, Floor[Nrelev] - NUMlevels, Ceiling[Nrelev] + NUMlevels}])
(*creates matrix with probalities for each individual energy level*)
```

In[40]:=
```
DensTable = Table[If[Total@matrix[1] == 0, 0, 1],
   {vs, -0.03, 0.03, .0025}, {vg, -0.1, 0.1, 0.01}];
(* Checks if the system is stable or instable for a given vs and vg *)
```

Graphical representation

In[41]:=
```
ListDensityPlot[DensTable, PlotRange → All, Mesh → Automatic,
 PlotLegends → Automatic, FrameLabel → {"Vg (mV)", "Vs (mV)"},
 PlotLabel → "One NP network CNN model",
 InterpolationOrder → 0, DataRange → {{-100, 100}, {-30, 30}}]
```

```
NUMlevels = 1;
Nr = 2;
Ngsd = 3;

e = 1.60 * 10^-19;
R0 = 1 * 10^5;
Cg1 = 8.66 * 10^-19;
Cg2 = 7.23 * 10^-19;
Cm = 3.49 * 10^-18;
Cs1 = 3.73 * 10^-18;
Cs2 = 4.85 * 10^-18;
Cd1 = 5.28 * 10^-18;
Cd2 = 3.61 * 10^-18;
```

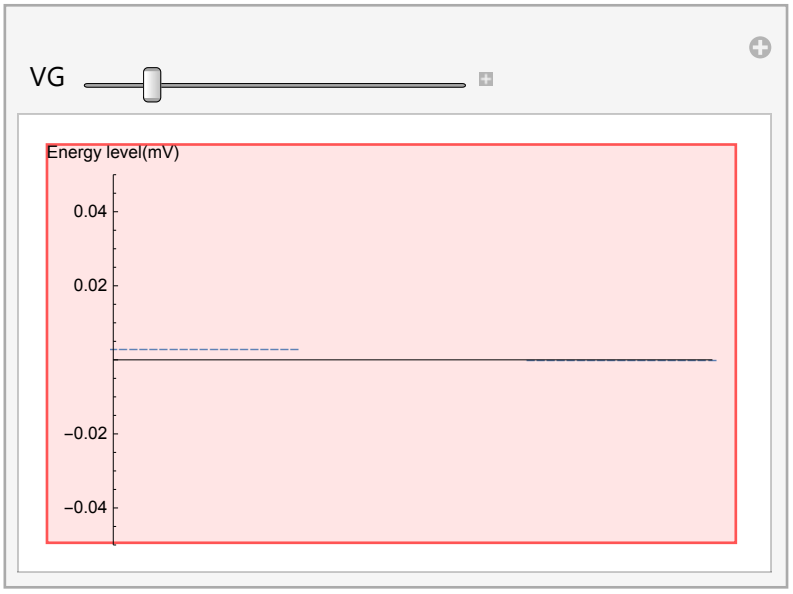
Initialisation

```
MatrixC = {{Cs1 + Cg1 + Cd1 + Cm, -Cm}, {-Cm, Cs2 + Cg2 + Cd2 + Cm}};
MatrixCgsd = {{Cg1, Cs1, Cd1}, {Cg2, Cs2, Cd2}};
MatrixVgsd := {vg, vs, 0};
Matrixn := {n1, n2};
Ec := e / (2 * Diagonal[MatrixC]);
MatrixV := Inverse[MatrixC].(MatrixCgsd.MatrixVgsd - Matrixn * e);
MatrixN := 1/e (MatrixCgsd.MatrixVgsd);
MatrixRgsd = {{∞, R0, R0}, {∞, R0, R0}};
MatrixR = {{∞, R0}, {R0, ∞}};
(* Defines the resistance matrix,
not connected nodes have a very high resistance *)


Fromrr[r_, rr_] := (v[[r]] - v[[rr]] + Ec[[r]] - Ec[[rr]]) / (e * MatrixR[[r, rr]]);
Fromgsd[r_, i_] := (v[[r]] - MatrixVgsd[[i]] + Ec[[r]]) / (e * MatrixRgsd[[r, i]]);

Torr[r_, rr_] := (v[[rr]] - v[[r]] - Ec[[r]] + Ec[[rr]]) / (e * MatrixR[[r, rr]]);
Togsd[r_, i_] := (MatrixVgsd[[i]] - v[[r]] - Ec[[r]]) / (e * MatrixRgsd[[r, i]]);
```

```
Ttoneighbour[r_] := ∑_{rr=1}^{Nr} tunneling@Torr[r, rr];
Ttoss[r_] := ∑_{i=1}^{Ngsd} tunneling@Togsd[r, i];
Tfromneighbour[r_] := ∑_{rr=1}^{Nr} tunneling@Fromrr[r, rr];
Tfromss[r_] := ∑_{i=1}^{Ngsd} tunneling@Fromgsd[r, i];

Tin[r_] := Tfromneighbour[r] + Tfromss[r];
Tout[r_] := Ttoneighbour[r] + Ttoss[r];
(* Defines the tunneling rates of all surrounding neighbours,
sources and sinks *)
tunneling[x_] := If[x > 0, x, 0];
(* Determines if an electron can tunnel *)
v = MatrixV; pr[r_] := If[Tto[r] == 0, 0, Tfrom[r]/Tto[r]];
```

Visualise energy levels

```
Manipulate[
 vs = -0.003;
 vg = VG;
 levels = Flatten[ Table[vv = MatrixV + Ec;
    {{1, -vv[[1]]}, {2, -vv[[2]]}}, {n1, -1, 1}, {n2, -1, 1}]];
 Nlevels = Flatten[ Table[vv = MatrixV + Ec;
    Text[{n1, n2}, #] & /@ {{1, -vv[[1]]}, {2, -vv[[2]]}},
    {n1, -1, 1}, {n2, -1, 1}]];
 Show[{ListPlot[val = Partition[Join[{0, -vs, 3, 0}, levels], 2],
    PlotMarkers → "-----------------------------------",
    AxesLabel → {, "Energy level(mV)"}, Ticks → {None, Automatic},
    PlotRange → {{0, 3}, {-.05, .05}}], Graphics@Nlevels}], {VG , -.25, 0}]
```



Appendix C: Mathematica script for importing text documents SIMON

```
data = Import["C:\\Users\\Laptop-Douwe\\Dropbox\\BSc
      Project\\SIMON2.0\\Single island.set.s1", "Table"];

activity = Table[data[[n + m, 3]], {m, 3, 159 600, 400}, {n, 0, 400}];

discrete = Table[If[activity[[m, n]] > 0, 1, 0], {m, 1, 399}, {n, 1, 399}];

ListDensityPlot[Reverse[discrete], Mesh → Automatic,
 PlotLegends → Automatic, FrameLabel → {"Vg (mV)", "Vs (mV)"},
 PlotLabel → "One NP network in SIMON", DataRange → {{-100, 100}, {-30, 30}}]
```