APPENDIX A.
SINGLE ELECTRON TUNNELING: SOME RESEARCH FINDINGS

1. PREFACE

This appendix contains analytical results referred to in the main text and a reference background for numeric computations. All formulas are intentionally presented in a complete form, to make them ready-to-use in programming implementation. Some recommendations concerning numeric algorithms are also given.

The reader of this chapter is supposed to be quite familiar with the derivation and the solution of the basic equations of the orthodox model. We will just list the results of Averin and Likharev[1] here. For an elementary introduction into the subject one can look in Ref. 2. Wherever possible, we follow the notations introduced in Ref. 1.

On first reading the book this chapter can be omitted.

2. ORTHODOX MODEL

The change of the kinetic energy of an electron during the jump through a tunnel junction $\Delta K = K_{\text{final}} - K_{\text{initial}}$ is

$$\begin{aligned}
\Delta \overrightarrow{K}_1 &= \frac{e}{C_\Sigma}\left[C_2 V - \left(n+\frac{1}{2}\right)e - C_g\left(V_g - \frac{V}{2}\right)\right], \\
\Delta \overleftarrow{K}_1 &= \frac{e}{C_\Sigma}\left[-C_2 V + \left(n-\frac{1}{2}\right)e + C_g\left(V_g - \frac{V}{2}\right)\right], \\
\Delta \overrightarrow{K}_2 &= \frac{e}{C_\Sigma}\left[C_1 V + \left(n-\frac{1}{2}\right)e + C_g\left(V_g + \frac{V}{2}\right)\right], \\
\Delta \overleftarrow{K}_2 &= \frac{e}{C_\Sigma}\left[-C_1 V - \left(n+\frac{1}{2}\right)e - C_g\left(V_g + \frac{V}{2}\right)\right]. \qquad (1)
\end{aligned}$$

Here $\Delta\overrightarrow{K}_\alpha$ is an energy decrement on tunneling through a contact α in left-to-right direction, $\Delta\overleftarrow{K}_\alpha$ is an energy decrement on tunneling through a contact α in right-to-left direction, n is the number of electrons on the island *before* the jump. Electrons are supposed to be *positive* with the charge $e = +1.6021 \times 10^{-19}$ C.

Note that for all ΔK in (1)

$$\Delta K(n \pm 1, V_g) = K(n, V_g \mp \frac{e}{C_g}), \tag{2}$$

and this is where the gate periodicity of a single grain SET transistor comes from.

Assuming continuos spectra in the leads we have tunneling rates:

$$\begin{aligned}
\overrightarrow{\Gamma}_1(n) &= \frac{\delta}{e^2} G_1 \sum_k n_{lead}(\xi_k - \Delta\overrightarrow{K}_1(n)) \Big[1 - n_{island}(\xi_k - \mu_n)\Big], \\
\overleftarrow{\Gamma}_1(n) &= \frac{\delta}{e^2} G_1 \sum_k n_{island}(\xi_k - \mu_n) \Big[1 - n_{lead}(\xi_k + \Delta\overleftarrow{K}_1(n))\Big], \\
\overrightarrow{\Gamma}_2(n) &= \frac{\delta}{e^2} G_2 \sum_k n_{island}(\xi_k - \mu_n) \Big[1 - n_{lead}(\xi_k + \Delta\overrightarrow{K}_2(n))\Big], \\
\overleftarrow{\Gamma}_2(n) &= \frac{\delta}{e^2} G_2 \sum_k n_{lead}(\xi_k - \Delta\overleftarrow{K}_2(n)) \Big[1 - n_{island}(\xi_k - \mu_n)\Big],
\end{aligned} \tag{3}$$

where G_1 and G_2 are the tunneling conductances, $n_{lead}(x)$ and $n_{island}(x)$ are the Fermi distribution functions for the lead and the island respectively, δ is an average interlevel spacing in the island, μ_n is the island's chemical potential in a grain charged with n electrons:

$$\mu_n = \frac{\xi_{n+1} + \xi_n}{2} \quad (\text{for } T \ll \delta), \tag{4}$$

n numerates energy levels so as ξ_0 is the highest occupied state and ξ_1 is the lowest empty state in the *neutral* island. For $T_{island} = T_{lead}$ and continuos spectra in the island (3) reduces to

$$\begin{aligned}
\overrightarrow{\Gamma}_{1,2} &= \frac{\frac{1}{e} I_{1,2}\left(\frac{\Delta\overrightarrow{K}_{1,2}}{e}\right)}{1 - \exp\left(-\frac{\Delta\overrightarrow{K}_{1,2}}{T}\right)}, \\
\overleftarrow{\Gamma}_{1,2} &= \frac{\frac{1}{e} I_{1,2}\left(\frac{\Delta\overleftarrow{K}_{1,2}}{e}\right)}{1 - \exp\left(-\frac{\Delta\overleftarrow{K}_{1,2}}{T}\right)},
\end{aligned} \tag{5}$$

where $I_1(U)$ and $I_2(U)$ are 'seed' $I(U)$ curves for the left and right barriers. If Ohm's law is applicable then $I_{1,2}(U) = G_{1,2}U$.

The master equation for evolution is

$$\begin{aligned}\dot{p}_n = &- (\overrightarrow{\Gamma}_1(n) + \overleftarrow{\Gamma}_1(n) + \overrightarrow{\Gamma}_2(n) + \overleftarrow{\Gamma}_2(n))p_n + \\ &+ (\overrightarrow{\Gamma}_1(n-1) + \overleftarrow{\Gamma}_2(n-1))p_{n-1} + \\ &+ (\overleftarrow{\Gamma}_1(n+1) + \overrightarrow{\Gamma}_2(n+1))p_{n+1},\end{aligned} \tag{6}$$

where p_n is the probability for the state with n additional electrons on the island to occur.

At equilibrium $\dot{p}_n \equiv 0$ and we have simple recurrent formulas for p_n:

$$\begin{aligned}p_n &= p_{n-1}\frac{\overrightarrow{\Gamma}_1(n-1) + \overleftarrow{\Gamma}_2(n-1)}{\overleftarrow{\Gamma}_1(n) + \overrightarrow{\Gamma}_2(n)}, \quad \text{for positive } n, \\ p_n &= p_{n+1}\frac{\overleftarrow{\Gamma}_1(n+1) + \overrightarrow{\Gamma}_2(n+1)}{\overrightarrow{\Gamma}_1(n) + \overleftarrow{\Gamma}_2(n)}, \quad \text{for negative } n.\end{aligned} \tag{7}$$

If we put, say, $p_0 = 1$, we can immediately calculate all p_n using (7) and finally find a current

$$I = \frac{e}{\Sigma}\sum_{-\infty}^{+\infty}\left(\overrightarrow{\Gamma}_1(n) - \overleftarrow{\Gamma}_1(n)\right)p_n, \tag{8}$$

where normalization factor Σ is given by the following sum:

$$\Sigma = \sum_{-\infty}^{+\infty} p_n.$$

To reduce numerical errors in a real program it's *much* better to find the most probable $n = n_{max}$, which can be determined from the condition

$$\begin{cases}\overrightarrow{\Gamma}_1(n_{max}-1) + \overleftarrow{\Gamma}_2(n_{max}-1) > \overleftarrow{\Gamma}_1(n_{max}) + \overrightarrow{\Gamma}_2(n_{max}) \\ \overleftarrow{\Gamma}_1(n_{max}+1) + \overrightarrow{\Gamma}_2(n_{max}+1) > \overrightarrow{\Gamma}_1(n_{max}) + \overleftarrow{\Gamma}_2(n_{max}),\end{cases}$$

and to apply recurrent formulas (7) starting from $n = n_{max}$ rather than from $n = 0$.

3. SINGLE GRAIN: NO RELAXATION

If we consider an extreme case of no relaxation in a grain then the Fermi distribution assumed in (3) will not take place anymore, and we have to find

a non-equilibrium distribution function, or, which is in fact easier, to operate with probabilities of different electron configurations directly.

Let

$$\{n\} = \{...01011...\} \tag{9}$$

be some electronic configuration (for any discrete energy level ξ_k in a grain 1 at position k marks an occupied level and 0 an empty one). Then $P_{\{n\}}$ will be a probability for the corresponding configuration to occur.

We will also introduce the following notations:

a. for any configuration $\{n\}$ with the level j non occupied, $\{n+j\}$ will denote a configuration with one additional electron placed on level j (this configuration has an additional charge $+e$) and

b. for any configuration $\{n\}$ with the level j occupied, $\{n-j\}$ will denote the configuration with one electron removed from level j (this configuration has an additional charge $-e$).

A master equation for evolution is

$$\begin{aligned}\dot{P}_{\{n\}} = &-\left(\sum_{all\ empty\ j}\gamma_{in}^{N}(j) + \sum_{all\ occupied\ j}\gamma_{out}^{N}(j)\right)P_{\{n\}} + \\ &+\sum_{all\ empty\ j}\gamma_{out}^{N+1}(j)P_{\{n+j\}} + \sum_{all\ occupied\ j}\gamma_{in}^{N-1}(j)P_{\{n-j\}},\end{aligned} \tag{10}$$

where j indexes energy levels, N is the number of additional electrons in configuration $\{n\}$, so that the grain charge $q = eN$, and

$$\begin{aligned}\gamma_{in}^{N}(j) &= \frac{\delta}{e^2}\left[G_1 n_{lead}(\xi_j - \Delta\overrightarrow{K}_1(N)) + G_2 n_{lead}(\xi_j - \Delta\overleftarrow{K}_2(N))\right], \\ \gamma_{out}^{N}(j) &= \frac{\delta}{e^2}\Big[G_1(1 - n_{lead}(\xi_j + \Delta\overleftarrow{K}_1(N))) + \\ &\quad + G_2(1 - n_{lead}(\xi_j + \Delta\overrightarrow{K}_2(N)))\Big].\end{aligned} \tag{11}$$

The current is given by

$$I = e\sum_{all\ \{n\}}\left(\sum_{all\ empty\ j}\overrightarrow{\gamma}_1^N(j) - \sum_{all\ occupied\ j}\overleftarrow{\gamma}_1^N(j)\right)P_{\{n\}}, \tag{12}$$

where

$$\begin{aligned}\overrightarrow{\gamma}_1^N(j) &= \frac{\delta}{e^2}G_1 n_{lead}(\xi_j - \Delta\overrightarrow{K}_1(N)), \\ \overleftarrow{\gamma}_1^N(j) &= \frac{\delta}{e^2}G_1\left[1 - n_{lead}(\xi_j + \Delta\overleftarrow{K}_1(N))\right].\end{aligned} \tag{13}$$

There is no more simple recurrent equations for $P_{\{n\}}$ like (7), so the only way is to solve the master equation (10) numerically.

In a grain with 8 energy levels, which is well enough to realise what will happen if we will turn the relaxation off, there will be 256 possible electronic configurations to sum over in (7). One practical trick to reduce the number of iterations is to start from $P_{\{n\}}$ found for the previous set of V, V_g. Fortunately, the convergence is surprisingly fast, and even the trivial Eiler's method works well.

4. DOUBLE DOT SYSTEM

Look: this is very simple!
Dima Golubev.

4.1. Energy decrements on tunneling.

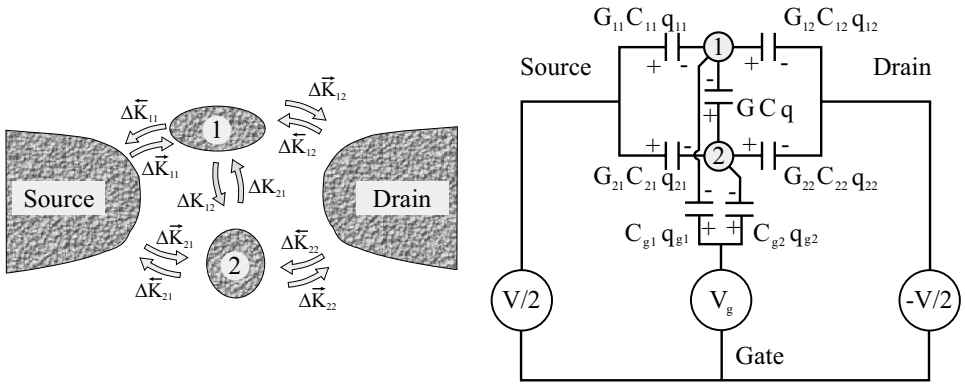

Fig. 1. Left: system topology and energy decrements on tunnelling jumps; Right: equivalent schematics.

If the number of electrons on the first grain is n_1 and on the second grain n_2, then an equilibrium charge configuration is (D. Golubev, 1999):

$$q_{11} = -\frac{CC_{11}}{C_\Delta^2}\Bigg[\quad \frac{C_{\Sigma 2}}{C}en_1 + en_2 - \\ - \left(C_{22} + \frac{C_{g2}}{2} + \frac{C_{\Sigma 2}}{C}\left(C_{12} + \frac{C_{g1}}{2}\right)\right)V + \left(C_{g2} + \frac{C_{\Sigma 2}}{C}C_{g1}\right)V_g\Bigg],$$

$$q_{22} = \frac{CC_{22}}{C_\Delta^2}\Bigg[\quad en_1 + \frac{C_{\Sigma 1}}{C} en_2 + \\ + \left(C_{11} + \frac{C_{g1}}{2} + \frac{C_{\Sigma 1}}{C}\left(C_{21} + \frac{C_{g2}}{2}\right)\right) V + \left(C_{g1} + \frac{C_{\Sigma 1}}{C} C_{g2}\right) V_g\Bigg],$$

$$q_{12} = \frac{CC_{12}}{C_\Delta^2}\Bigg[\quad \frac{C_{\Sigma 2}}{C} en_1 + en_2 + \\ + \left(C_{21} + \frac{C_{g2}}{2} + \frac{C_{\Sigma 2}}{C}\left(C_{11} + \frac{C_{g1}}{2}\right)\right) V + \left(C_{g2} + \frac{C_{\Sigma 2}}{C} C_{g1}\right) V_g\Bigg],$$

$$q_{21} = -\frac{CC_{21}}{C_\Delta^2}\Bigg[\quad en_1 + \frac{C_{\Sigma 1}}{C} en_2 - \\ - \left(C_{12} + \frac{C_{g1}}{2} + \frac{C_{\Sigma 1}}{C}\left(C_{22} + \frac{C_{g2}}{2}\right)\right) V + \left(C_{g1} + \frac{C_{\Sigma 1}}{C} C_{g2}\right) V_g\Bigg],$$

$$q_{g1} = -\frac{CC_{g1}}{C_\Delta^2}\Bigg[\frac{C_{\Sigma 2}}{C} en_1 + en_2 - \\ - \left(\frac{C_{\Sigma 2}}{C}\frac{C_{12} - C_{11}}{2} + \frac{C_{22} - C_{21}}{2}\right) V - \left(C_{21} + C_{22} + \frac{C_{\Sigma 2}}{C}\left(C_{11} + C_{12}\right)\right) V_g\Bigg],$$

$$q_{g2} = -\frac{CC_{g2}}{C_\Delta^2}\Bigg[en_1 + \frac{C_{\Sigma 1}}{C} en_2 + \\ + \left(\frac{C_{\Sigma 1}}{C}\frac{C_{21} - C_{22}}{2} + \frac{C_{11} - C_{12}}{2}\right) V - \left(C_{11} + C_{12} + \frac{C_{\Sigma 1}}{C}\left(C_{22} + C_{21}\right)\right) V_g\Bigg],$$

$$q = -\frac{C(C_{\Sigma 2} - C)}{C_\Delta^2}\left[en_1 - \left(C_{12} + \frac{C_{g1}}{2}\right) V + C_{g1} V_g\right] + \\ + \frac{C(C_{\Sigma 1} - C)}{C_\Delta^2}\left[en_2 - \left(C_{22} + \frac{C_{g2}}{2}\right) V + C_{g2} V_g\right]. \qquad (14)$$

Here we have defined $C_{\Sigma 1} = C_{11} + C_{12} + C_{g1} + C$, $C_{\Sigma 2} = C_{21} + C_{22} + C_{g2} + C$, and $C_\Delta^2 = C_{\Sigma 1} C_{\Sigma 2} - C^2$. For charge sign convention see Fig. 1.

The Coulomb energy of the system is

$$E_{\text{Coulomb}} = \frac{q_{11}^2}{2C_{11}} + \frac{q_{12}^2}{2C_{12}} + \frac{q_{21}^2}{2C_{21}} + \frac{q_{22}^2}{2C_{22}} + \frac{q_{g1}^2}{2C_{g1}} + \frac{q_{g2}^2}{2C_{g2}} + \frac{q^2}{2C} \\ = \frac{e^2}{2}\frac{C_{\Sigma 2} n_1^2 + C_{\Sigma 1} n_2^2 + 2C n_1 n_2}{C_\Delta^2} + AV^2 + BV_g^2 + DVV_g. \qquad (15)$$

The last three terms do not depend on n_1, n_2 and, therefore, will not change after tunneling jump.

The work done by the voltage sources to charge the network capacitancies equals:

$$\begin{aligned} A &= \frac{V}{2}(q_{11}+q_{22}+q_{21}+q_{12}) + V_g(q_{g1}+q_{g2}) \\ &= -\frac{V}{2}\frac{[C_{\Sigma 2}(C_{11}-C_{12})+C(C_{21}-C_{22})]en_1}{C_\Delta^2} - \\ &\quad -\frac{V}{2}\frac{[C_{\Sigma 1}(C_{21}-C_{22})+C(C_{11}-C_{12})]en_2}{C_\Delta^2} - \\ &\quad -V_g\frac{[C_{\Sigma 2}C_{g1}+CC_{g2}]en_1+[C_{\Sigma 1}C_{g2}+CC_{g1}]en_2}{C_\Delta^2} + \\ &\quad +\widetilde{A}V^2+\widetilde{B}V_g^2+\widetilde{D}VV_g. \end{aligned} \tag{16}$$

So the total energy of the environment

$$E_{\rm total} = E_{\rm Coulomb} + A. \tag{17}$$

If an electron tunnels through, say, contact 11 from grain to lead, then before tunnelling the environment energy is $E_{\rm total}(n1,n2) = \frac{V}{2}(q_{11}(n1,n2)+\ldots)$. If all other charges in a system were frozen, then after tunneling the environment energy would be $\frac{V}{2}(q_{11}(n1,n2)+e+\ldots) = E_{\rm total}(n1,n2)+\frac{eV}{2}$. After charge redistribution, it will reduce to $E_{\rm total}(n1-1,n2)$. As a result, the change of the eletron kinetic energy is given by

$$\Delta K = -\Delta E_{\rm total} \pm \frac{eV}{2}. \tag{18}$$

The last term enters with + if immediatly after the tunneling, the value of any charge q_{11}, q_{12}, q_{21} or q_{22} increases by e, and it enters with the $-$ sign if it decreases.

Substituting (14) into (18) we have (see Fig. 1 for ΔK definitions):

$$\begin{aligned} \Delta\overrightarrow{K}_{11} &= \frac{1}{C_\Delta^2}\Bigg[-e^2\left(C_{\Sigma 2}\left(n_1+\frac{1}{2}\right)+Cn_2\right) + \\ &\qquad + eV(C_{\Sigma 2}C_{12}+CC_{22}) - e\left(V_g-\frac{V}{2}\right)(C_{\Sigma 2}C_{g1}+CC_{g2})\Bigg], \\ \Delta\overleftarrow{K}_{11} &= \frac{1}{C_\Delta^2}\Bigg[\quad e^2\left(C_{\Sigma 2}\left(n_1-\frac{1}{2}\right)+Cn_2\right) - \\ &\qquad - eV(C_{\Sigma 2}C_{12}+CC_{22}) + e\left(V_g-\frac{V}{2}\right)(C_{\Sigma 2}C_{g1}+CC_{g2})\Bigg], \\ \Delta\overrightarrow{K}_{12} &= \frac{1}{C_\Delta^2}\Bigg[\quad e^2\left(C_{\Sigma 2}\left(n_1-\frac{1}{2}\right)+Cn_2\right) + \end{aligned}$$

$$
\begin{aligned}
&+ eV(C_{\Sigma 2}C_{11} + CC_{21}) + e\left(V_g + \frac{V}{2}\right)(C_{\Sigma 2}C_{g1} + CC_{g2})\Big], \\
\Delta\overleftarrow{K}_{12} = \frac{1}{C_\Delta^2}\Big[&- e^2\left(C_{\Sigma 2}\left(n_1 + \frac{1}{2}\right) + Cn_2\right) - \\
&- eV(C_{\Sigma 2}C_{11} + CC_{21}) - e\left(V_g + \frac{V}{2}\right)(C_{\Sigma 2}C_{g1} + CC_{g2})\Big], \\
\Delta\overrightarrow{K}_{21} = \frac{1}{C_\Delta^2}\Big[&- e^2\left(Cn_1 + C_{\Sigma 1}\left(n_2 + \frac{1}{2}\right)\right) + \\
&+ eV(C_{\Sigma 1}C_{22} + CC_{12}) - e\left(V_g - \frac{V}{2}\right)(CC_{g1} + C_{\Sigma 1}C_{g2})\Big], \\
\Delta\overleftarrow{K}_{21} = \frac{1}{C_\Delta^2}\Big[&\quad e^2\left(Cn_1 + C_{\Sigma 1}\left(n_2 - \frac{1}{2}\right)\right) - \\
&- eV(C_{\Sigma 1}C_{22} + CC_{12}) + e\left(V_g - \frac{V}{2}\right)(CC_{g1} + C_{\Sigma 1}C_{g2})\Big], \\
\Delta\overrightarrow{K}_{22} = \frac{1}{C_\Delta^2}\Big[&\quad e^2\left(Cn_1 + C_{\Sigma 1}\left(n_2 - \frac{1}{2}\right)\right) + \\
&+ eV(C_{\Sigma 1}C_{21} + CC_{11}) + e\left(V_g + \frac{V}{2}\right)(CC_{g1} + C_{\Sigma 1}C_{g2})\Big], \\
\Delta\overleftarrow{K}_{22} = \frac{1}{C_\Delta^2}\Big[&- e^2\left(Cn_1 + C_{\Sigma 1}\left(n_2 + \frac{1}{2}\right)\right) - \\
&- eV(C_{\Sigma 1}C_{21} + CC_{11}) - e\left(V_g + \frac{V}{2}\right)(CC_{g1} + C_{\Sigma 1}C_{g2})\Big].
\end{aligned}
\tag{19}
$$

Finally, for the tunneling between grains we find

$$
\begin{aligned}
\Delta K_{12} = \frac{1}{C_\Delta^2}\Big[&- e^2\left(-C_{\Sigma 2}\left(n_1 - \frac{1}{2}\right) + C_{\Sigma 1}\left(n_2 + \frac{1}{2}\right) + C(n_1 - n_2 - 1)\right) + \\
&+eV\left(C_{11}C_{22} - C_{12}C_{21} + C_{g1}\frac{C_{22} - C_{21}}{2} + C_{g2}\frac{C_{11} - C_{12}}{2}\right) + \\
&+eV_g\Big(C_{g1}(C_{22} + C_{21}) - C_{g2}(C_{11} + C_{12})\Big)\Big], \text{ for } 1 \to 2 \text{ jump}, \\
\Delta K_{21} = \frac{1}{C_\Delta^2}\Big[&- e^2\left(C_{\Sigma 2}\left(n_1 + \frac{1}{2}\right) - C_{\Sigma 1}\left(n_2 - \frac{1}{2}\right) + C(-n_1 + n_2 - 1)\right) - \\
&-eV\left(C_{11}C_{22} - C_{12}C_{21} + C_{g1}\frac{C_{22} - C_{21}}{2} + C_{g2}\frac{C_{11} - C_{12}}{2}\right) - \\
&-eV_g\Big(C_{g1}(C_{22} + C_{21}) - C_{g2}(C_{11} + C_{12})\Big)\Big], \text{ for } 2 \to 1 \text{ jump}.
\end{aligned}
\tag{20}
$$

4.2. Symmetry considerations.

Equations (19) and (20) are invariant with respect to some symmetry transformations.

a. We can swap indexes marking the grain numbers, i. e. we can redeclare grain no 1 as 2 and vice versa. So as a result of simultaneous replacement

$n_1 \leftrightarrows n_2$, $C_{11} \leftrightarrows C_{21}$, $C_{12} \leftrightarrows C_{22}$, $C_{g1} \leftrightarrows C_{g2}$, and $\mathrm{C}_{\Sigma 1} \leftrightarrows \mathrm{C}_{\Sigma 2}$

we will have the following transformations:

$\Delta\overrightarrow{K}_{1\alpha}(n_1, n_2) \leftrightarrows \Delta\overrightarrow{K}_{2\alpha}(n_2, n_1)$, $\Delta\overleftarrow{K}_{1\alpha}(n_1, n_2) \leftrightarrows \Delta\overleftarrow{K}_{2\alpha}(n_2, n_1)$, and $\Delta\mathrm{K}_{12}(\mathrm{n}_1, \mathrm{n}_2) \leftrightarrows \Delta\mathrm{K}_{21}(\mathrm{n}_2, \mathrm{n}_1)$.

b. Left/right symmetry: we can flip the whole network horizontally with simultaneous inversion of the bias voltage, which is equivalent to the following substitution:

$C_{11} \leftrightarrows C_{12}$, $C_{21} \leftrightarrows C_{22}$, $V \leftrightarrows -V$.

As a result, the tunneling jump from, say, the left tunneling barrier will be transformed into a jump through a right barrier in an *opposite* direction, so as

$$\Delta\overrightarrow{K}_{\alpha 1}(V, V_g) \leftrightarrows \Delta\overleftarrow{K}_{\alpha 2}(-V, V_g),\ \Delta\overleftarrow{K}_{\alpha 1}(V, V_g) \leftrightarrows \Delta\overrightarrow{K}_{\alpha 2}(-V, V_g).$$

Energy decrements for intergrain tunneling ΔK_{12} and ΔK_{21} are not affected by this transformation and they will convert to themselves.

c. Time inversion symmetry: if for any tunneling event from state n_1, n_2 to state n_1', n_2' the energy decrement is ΔK, then an inverse tunneling process from n_1', n_2' to n_1, n_2 must have an opposite energy decrement $-\Delta K$, and so

$\Delta\overrightarrow{K}_{11}(n_1, n_2) = -\Delta\overleftarrow{K}_{11}(n_1 + 1, n_2)$, $\Delta\overrightarrow{K}_{12}(n_1, n_2) = -\Delta\overleftarrow{K}_{12}(n_1 - 1, n_2)$,
$\Delta\overrightarrow{K}_{21}(n_1, n_2) = -\Delta\overleftarrow{K}_{21}(n_1, n_2 + 1)$, $\Delta\overrightarrow{K}_{22}(n_1, n_2) = -\Delta\overleftarrow{K}_{22}(n_1, n_2 - 1)$,
and $\Delta K_{12}(n_1, n_2) = -\Delta K_{21}(n_1 - 1, n_2 + 1)$.

Any of **a-c** symmetries reduces the number of independent formulas in (19) by a factor of 2, so there is really just one independent equation in (19).

Surprisingly, there is one more symmetry in (19) and (20):

d. All energy decrements change the sign and the tunneling direction on simultaneous inversion of all voltages and charges, i. e.

$\Delta\overrightarrow{K}_{\alpha\beta}(n_1, n_2, V, V_g) = -\Delta\overleftarrow{K}_{\alpha\beta}(-n_1, -n_2, -V, -V_g)$, and
$\Delta\overleftarrow{K}_{\alpha\beta}(n_1, n_2, V, V_g) = -\Delta\overrightarrow{K}_{\alpha\beta}(-n_1, -n_2, -V, -V_g)$,

If we apply this transformation to the current formula (27) then the current will change sign:

$$I(V, V_g) = -I(-V, -V_g), \text{ and } \frac{\mathrm{d}I}{\mathrm{d}V}(V, V_g) = \frac{\mathrm{d}I}{\mathrm{d}V} I(-V, -V_g). \qquad (21)$$

So an $I(V, V_g)$ plot is antisymmetric, and a $\frac{\mathrm{d}I}{\mathrm{d}V}(V, V_g)$ plot is symmetric. In the presence of a background charge, the centre of symmetry will be shifted along the gate axis.

If we complete transformation **d** with the inversion of electron charge $e \to -e$ then the current will not change. This could be reformulated as follows: the current through a system does not depend on the sign of charge carriers, i. e. whether the current transport is carried by electrons or holes.

4.3. Quasiperiodicity.

The position of Coulomb staircases in a $\frac{\mathrm{d}I}{\mathrm{d}V}(V, V_g)$ plot is determined by the condition that the energy decrement on tunnelling through some barrier crosses zero:

$\Delta\overrightarrow{K}_{\alpha\beta}(n_1, n_2, V, V_g) = 0$.

From (19) and (20) we have:

$$
\begin{aligned}
V\left(C_{12} + \frac{C}{C_{\Sigma 2}}C_{22}\right) - \left(V_g - \frac{V}{2}\right)\left(C_{g1} + \frac{C}{C_{\Sigma 2}}C_{g2}\right) &= e\left(n_1 + \frac{C}{C_{\Sigma 2}}n_2 \pm \frac{1}{2}\right), \\
-V\left(C_{11} + \frac{C}{C_{\Sigma 2}}C_{21}\right) - \left(V_g + \frac{V}{2}\right)\left(C_{g1} + \frac{C}{C_{\Sigma 2}}C_{g2}\right) &= e\left(n_1 + \frac{C}{C_{\Sigma 2}}n_2 \pm \frac{1}{2}\right), \\
V\left(\frac{C}{C_{\Sigma 1}}C_{12} + C_{22}\right) - \left(V_g - \frac{V}{2}\right)\left(\frac{C}{C_{\Sigma 1}}C_{g1} + C_{g2}\right) &= e\left(\frac{C}{C_{\Sigma 1}}n_1 + n_2 \pm \frac{1}{2}\right), \\
-V\left(\frac{C}{C_{\Sigma 1}}C_{11} + C_{21}\right) - \left(V_g + \frac{V}{2}\right)\left(\frac{C}{C_{\Sigma 1}}C_{g1} + C_{g2}\right) &= e\left(\frac{C}{C_{\Sigma 1}}n_1 + n_2 \pm \frac{1}{2}\right), \\
V\left(C_{11}C_{22} - C_{12}C_{21} + C_{g1}\frac{C_{22} - C_{21}}{2} + C_{g2}\frac{C_{11} - C_{12}}{2}\right) + & \\
+V_g C_{g1}(C_{22} + C_{21}) - C_{g2}(C_{11} + C_{12})) = & \\
= e\left(-(C_{\Sigma 2} - C)n_1 + (C_{\Sigma 1} - C)n_2 \pm (\frac{1}{2}C_{\Sigma 1} + \frac{1}{2}C_{\Sigma 2} - 1)\right). & \qquad (22)
\end{aligned}
$$

Because of time-reversal symmetry between tunneling jumps $\alpha \to \beta$ and $\beta \to \alpha$, the conditions $\Delta\overrightarrow{K}_{\alpha\beta}(n_\alpha) = 0$ and $\Delta\overleftarrow{K}_{\alpha\beta}(n_\alpha + 1) = 0$ impose the same relationship on V, V_g, and only 5 distinct sets of pecularities are defined by (22).

We can draw some important conclusions from (22):

a. All Coulomb pecularities form straight lines in $\frac{\mathrm{d}I}{\mathrm{d}V}(V, V_g)$ plot. Indeed, any equation in (22) has a linear form

$$A_{\alpha\beta}V + B_{\alpha\beta}V_g = C_{\alpha\beta}n_1 + D_{\alpha\beta}n_2 + const. \qquad (23)$$

b. Each tunneling barrier defines a set of pecularities which are parallel to each other, i. e. a double dot system has five distinct slopes in the $\frac{\mathrm{d}I}{\mathrm{d}V}$

pattern. This is because (for some mysterious reason) there are no cross-terms like $n_\alpha V$ and $n_\alpha V_g$ in (15) and, thus, in (22).

c. There is no more periodicity with respect to a gate voltage, like (2) in a single-dot system. Nevertheless, the whole $\frac{\mathrm{d}I}{\mathrm{d}V}$ pattern is quasiperiodic, because all staircases coming from the first grain have offsets $n_1+(C/C_{\Sigma 2})n_2+\cdots$, from the second one - $(C/C_{\Sigma 1})n_1+n_2+\ldots$, and from intergrain tunneling - $(C_{\Sigma 2}-C)n_1-(C_{\Sigma 1}-C)n_2+\cdots$.

Note that the condition $\Delta\overrightarrow{K}_{\alpha\beta}=0$ gives the same slope as the condition $q_{\alpha\beta}=const$. It means that the voltage applied to a specific tunneling barrier is constant if we cross a (V,V_g) plane in the direction of a staircase associated with this tunnelling gap. But to calculate proper offsets, one should use (22), not (14).

4.4. Master equation for evolution.

The most interesting question for us was: how will a spectroscopy measurement of discrete energy levels in the first grain be affected by the presence of a second grain nearby? Therefore, we will assume that the first grain has a discrete energy spectrum with energy levels ξ_n, while the second one has a continuos spectrum. Then

$$
\begin{aligned}
\overrightarrow{\Gamma}_{11}(n_1,n_2) &= \frac{\delta}{e^2}G_{11}\sum_k n_{\mathrm{lead}}(\xi_k-\Delta\overrightarrow{K}_{11})[1-n_{\mathrm{island1}}(\xi_k-\mu_{n1})],\\
\overleftarrow{\Gamma}_{11}(n_1,n_2) &= \frac{\delta}{e^2}G_{11}\sum_k [1-n_{\mathrm{lead}}(\xi_k+\Delta\overleftarrow{K}_{11L})]n_{\mathrm{island1}}(\xi_k-\mu_{n1})],\\
\overrightarrow{\Gamma}_{12}(n_1,n_2) &= \frac{\delta}{e^2}G_{12}\sum_k [1-n_{\mathrm{lead}}(\xi_k+\Delta\overrightarrow{K}_{12})]n_{\mathrm{island1}}(\xi_k-\mu_{n1})],\\
\overleftarrow{\Gamma}_{12}(n_1,n_2) &= \frac{\delta}{e^2}G_{12}\sum_k n_{\mathrm{lead}}(\xi_k-\Delta\overleftarrow{K}_{12})[1-n_{\mathrm{island1}}(\xi_k-\mu_{n1})],\\
\Gamma_{12}(n_1,n_2) &= \frac{\delta}{e^2}G\sum_k n_{\mathrm{island1}}(\xi_k-\mu_{n1})[1-n_{\mathrm{island2}}(\xi_k+\Delta K_{12})],\\
\Gamma_{21}(n_1,n_2) &= \frac{\delta}{e^2}G\sum_k [1-n_{\mathrm{island1}}(\xi_k-\mu_{n1})]n_{\mathrm{island2}}(\xi_k-\Delta K_{21}),
\end{aligned}
\tag{24}
$$

where Γ_{ij} is the tunneling rate through the gap ij, δ is an average level spacing in the first grain, μ is it's chemical potential given by (4), ξ_k are

discrete energy levels (ξ_0 is the highest occupied state), and $n(x)$ is the electron distribution function.

For tunneling between leads and the second grain we have:

$$\overrightarrow{\Gamma}_{2\alpha} = \frac{\frac{1}{2} I_{2\alpha}\left(\frac{\Delta \overrightarrow{K}_{2\alpha}}{e}\right)}{1 - \exp\left(-\frac{\Delta \overrightarrow{K}_{2\alpha}}{e}\right)},$$

$$\overleftarrow{\Gamma}_{2\alpha} = \frac{\frac{1}{2} I_{2\alpha}\left(\frac{\Delta \overleftarrow{K}_{2\alpha}}{e}\right)}{1 - \exp\left(-\frac{\Delta \overleftarrow{K}_{2\alpha}}{e}\right)}, \ \alpha = 1, 2. \tag{25}$$

The master equation for the double dot system is

$$\begin{aligned}
\dot{p}_{n1,n2} = -\Big(& \overrightarrow{\Gamma}_{11}(n_1, n_2) + \overleftarrow{\Gamma}_{11}(n_1, n_2) + \overrightarrow{\Gamma}_{12}(n_1, n_2) + \overleftarrow{\Gamma}_{12}(n_1, n_2) + \\
& \overrightarrow{\Gamma}_{21}(n_1, n_2) + \overleftarrow{\Gamma}_{21}(n_1, n_2) + \overrightarrow{\Gamma}_{22}(n_1, n_2) + \overleftarrow{\Gamma}_{22}(n_1, n_2) + \\
& + \Gamma_{12}(n_1, n_2) + \Gamma_{21}(n_1, n_2)\Big) p_{n_1,n_2} + \\
& + \Big(\overrightarrow{\Gamma}_{11}(n_1 - 1, n_2) + \overleftarrow{\Gamma}_{12}(n_1 - 1, n_2)\Big) p_{n_1-1,n_2} + \\
& + \Big(\overrightarrow{\Gamma}_{21}(n_1, n_2 - 1) + \overleftarrow{\Gamma}_{22}(n_1, n_2 - 1)\Big) p_{n_1,n_2-1} + \\
& + \Big(\overleftarrow{\Gamma}_{11}(n_1 + 1, n_2) + \overrightarrow{\Gamma}_{12}(n_1 + 1, n_2)\Big) p_{n_1+1,n_2} + \\
& + \Big(\overleftarrow{\Gamma}_{21}(n_1, n_2 + 1) + \overrightarrow{\Gamma}_{22}(n_1, n_2 + 1)\Big) p_{n_1,n_2+1} + \\
+ \Gamma_{21}(n_1 - 1, n_2 + 1) p_{n_1-1,n_2+1} & + \Gamma_{12}(n_1 + 1, n_2 + 1) p_{n_1+1,n_2-1}.
\end{aligned} \tag{26}$$

And the current is given by

$$I = e \sum_{n1,n2=-\infty}^{+\infty} \Big(\overrightarrow{\Gamma}_{11}(n_1, n_2) - \overleftarrow{\Gamma}_{11}(n_1, n_2) + \overrightarrow{\Gamma}_{21}(n_1, n_2) - \overleftarrow{\Gamma}_{21}(n_1, n_2)\Big) p_{n_1,n_2}. \tag{27}$$

4.5. Numerical recipies.

One-zero, one-zero, zero-zero, zero-one ...
Karin Andersson.

Master equation (26) is a system of linear differential equations. If we present probability distribution p_{n_1,n_2} as a vector $\vec{p} = |p_j\rangle$ where j is some index

running over all (n_1, n_2) pairs, then we can rewrite (26) as

$$\dot{\vec{p}} = -\widehat{\Gamma}\vec{p}. \tag{28}$$

The formal solution of (28) is

$$\begin{aligned}\vec{p}(t) &= e^{-t\widehat{\Gamma}}\vec{p}(0) = (\widehat{\mathrm{E}} - t\widehat{\Gamma} + \frac{t^2}{2}\widehat{\Gamma}^2 - \frac{t^3}{6}\widehat{\Gamma}^3 + \frac{t^4}{24}\widehat{\Gamma}^4 + \cdots) \\ &= (\widehat{\mathrm{E}} - t\widehat{\Gamma})(\widehat{\mathrm{E}} - \frac{t}{2}\widehat{\Gamma})(\widehat{\mathrm{E}} - \frac{t}{3}\widehat{\Gamma})(\widehat{\mathrm{E}} - \frac{t}{4}\widehat{\Gamma})\vec{p}(0) + o(t^4),\end{aligned} \tag{29}$$

where $\widehat{\mathrm{E}}$ is a unity matrix.

As one can see from (29), for linear systems a standard fourth-order Runge-Kutta method reduces to four recursive calls to a first-order Eiler's extrapolation formula with steps $\frac{t}{4}$, $\frac{t}{3}$, $\frac{t}{2}$, t.

To minimise execution time, it is better to use an adaptive step t. Ideally, it should be inversely proportional to a maximum eigenvalue of evolution matrix $\widehat{\Gamma}$ λ_{max}. Practically, it's good enough to replace an unknown λ_{max} with a sum of all eigenvalues $\sum \lambda_j = tr(\widehat{\Gamma})$, where the trace of the evolution matrix can be found from (26) and equals

$$\begin{aligned}tr(\widehat{\Gamma}) = \sum_{n1,n2=-\infty}^{\infty} \Big(&\overrightarrow{\Gamma}_{11}(n_1,n_2) + \overleftarrow{\Gamma}_{11}(n_1,n_2) + \overrightarrow{\Gamma}_{12}(n_1,n_2) + \overleftarrow{\Gamma}_{12}(n_1,n_2) + \\ &+\overrightarrow{\Gamma}_{21}(n_1,n_2) + \overleftarrow{\Gamma}_{21}(n_1,n_2) + \overrightarrow{\Gamma}_{22}(n_1,n_2) + \overleftarrow{\Gamma}_{22}(n_1,n_2) + \\ &+\Gamma_{12}(n_1,n_2) + \Gamma_{21}(n_1,n_2)\Big).\end{aligned} \tag{30}$$

There is one hidden problem associated with the dynamic approach (28). To illustrate it, let's consider a system with all capacitancies C approximately equal to each other (which is normally the case) and tunnelling conductancies $G_{11} = G_{21} = 1000G_{21} = 1000G_{22} = 1000G$. For such a system, a second grain charge relaxation time $\tau_2 \approx C/G$ is about 1000 times higher than the charge relaxation time for the first grain $\tau_1 \approx C/G_{11} = 1000C/G$. To keep convergence in iteration procedure (29), a time step t should be less than τ_1, but to reach an equilibrium charge on the second grain, the total integration time Nt should be greater than τ_2. As a result, the minimum number of iterations, i. e. the execution time, increases proportionally to $N = \tau_2/\tau_1 = \max(G_{11}, G_{12}, G)/\max(G_{21}, G_{22}, G)$. This problem is specific to a multi-grain network, because in a single grain system a high-ohmic tunneling gap is always shunted by the low-resistive one.

It's worth to mention here that we've observed a tremendous increase of execution time also in Monte-Carlo simulations with Simon for systems with two strongly different relaxation times.

One way to escape this problem is to bypass the dynamic equation (28) and to search for a static solution directly:

$$\widehat{\Gamma}\vec{p} = 0. \tag{31}$$

Unfortunately, the standard Gauss elimination algorithm does not exploit the fact that almost all coefficients in evolution matrix $\widehat{\Gamma}$ are zeroes (see 26), and is very inefficient for this particular case.

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