5.8.8 Fourth order processes

Starting point is the form of the term $\tilde{K}^{(4)}\rho^{\infty}$ given by Eq. (5.58), i.e.

$$\tilde{K}^{(4)}\rho^{\infty} = -\frac{i}{\hbar}\sum_{\{\gamma_i\}}\ \sum_{p_1 p_2}\ \sum_{\substack{\alpha_1\sigma_1\\ \alpha_2\sigma_2}} \Big[$$  $$+$$  $$\Big]$$

Noticeably to these two diagrams in Liouville space it correspond

$$2\cdot 2^{8} = 256 \qquad \text{diagrams in Fock space!}^{(*)}$$

Recall that in second order we had $\underline{2\cdot 2^{2} = 8}$ different contributions in Fock space

In general which diagram class is relevant depends on the considered gate and bias voltages.

We distinguish them by the the difference

$$\Delta N = N_b - N_a$$

(*) Specifically,

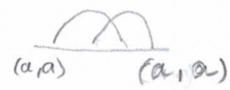
$\Delta N = 0$ cotunneling processes

$\Delta N = \pm 1$ cotunneling assisted sequential tunneling

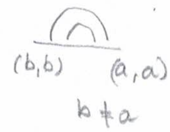
$\Delta N = \pm 2$ pair tunneling

Specifically :

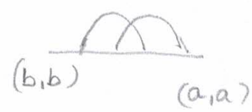
$\Delta N = 0$ cotunneling (COT) processes



$\Delta N = \pm 1$ cotunneling assisted sequential tunneling (CO-ST)

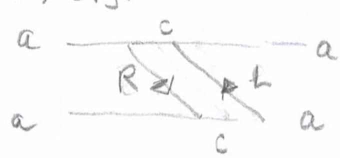


$\Delta N = \pm 2$ pair tunneling (PT)



a) $\underline{\Delta N = 0}$

In particular, COT processes are relevant in the situation in which second order processes are blocked due to Coulomb blockade ⇒ the charge in the system is fixed and only processes which do not change the final particle number are relevant, E.g.



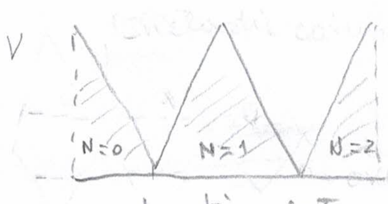
One distinguishes between

$\begin{cases} \text{elastic cotunneling if } E_b = E_a \\ \text{inelastic " if } E_b \neq E_a \end{cases}$ (e.g. $E_\uparrow \neq E_\downarrow$ for SIAM)

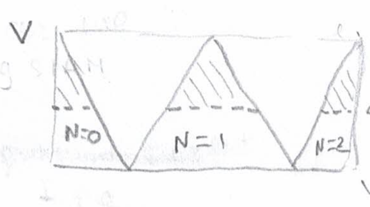
⇒ the latter processes are relevant only at finite bias above the threshold $eV = E_b - E_a$;

elastic cotunneling yields an overall background

e.g. SIAM



elastic COT



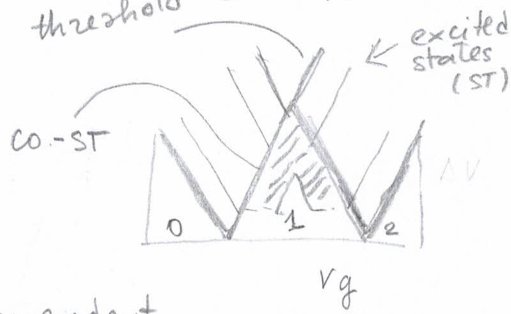
← inelastic cotunneling (gate independent)

5

b) $\Delta N=1$

Such processes, like the second order rates $\Gamma^{\pm}_{\alpha, ba}$ change the final number in the dot by ± 1

E.g.

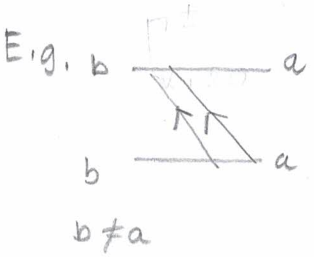


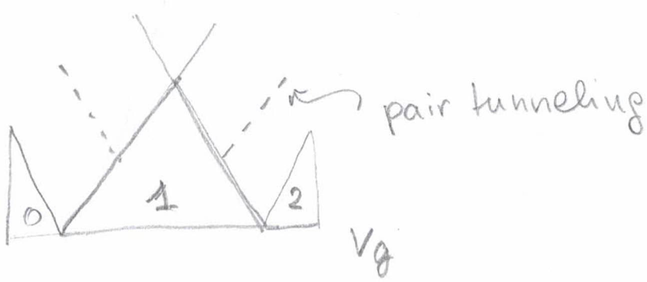
Such processes are gate voltage dependent and can contribute also in the Coulomb blockade region

c) $\Delta N=2$

Pair tunneling transfers simultaneously two electrons, and as such give finite contributions to the rates $\Gamma^{\pm}_{\alpha, 20}$

E.g.



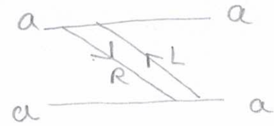


Similar to the CO-ST, also pair tunneling transitions depend on the gate voltage

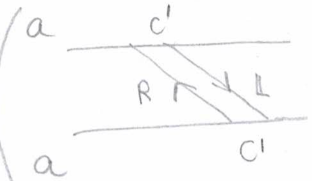
The cotunneling kernel

We focus explicitly on the forward cotunneling process $L \to R$ for elastic cotunneling

$\sum_{c \neq a}$ ()

$\Rightarrow \Gamma^{+}_{coT,el} = 2\,\mathrm{Re} \sum_{c \neq a}$  forward cotunneling rate

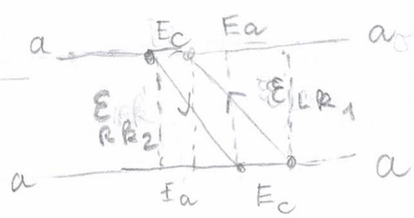
similarly for the backward rate

$\Gamma^{-}_{coT,el} = 2\,\mathrm{Re} \sum_{c' \neq a}$ ()

$\Rightarrow I_{coT,el} = e\left(\Gamma^{+}_{coT,el} - \Gamma^{-}_{coT,el}\right)$ for a fixed particle nr. N_a

According to the diagrammatic rules

$$\Gamma^{+}_{coT,el} = 2\,\mathrm{Re} \sum_{\substack{c \neq a \\ N_c = N_a + 1}} \left(-\frac{i}{\hbar}\right) |t_L|^2 |t_R|^2 \int d\varepsilon_1\, \omega_L \int d\varepsilon_2\, \omega_R \frac{f^{+}_{L}(\varepsilon_1)}{i0^{+} + (E_c - E_a) - \varepsilon_1} \, \frac{1}{i0^{+} + \varepsilon_2 - \varepsilon_1} \, \frac{f^{-}_{R}(\varepsilon_2)}{i0^{+} + (E_a - E_c) \ldots}$$



$\left(i0^{+} + (E_a - E_c) + \varepsilon_2\right)$

$$\Gamma^{-}_{coT,el} = 2\,\mathrm{Re} \sum_{\substack{c' \neq a \\ N_{c'} = N_a - 1}} \left(-\frac{i}{\hbar}\right) |t_L|^2 |t_R|^2 \int d\varepsilon_1\, \omega_L \int d\varepsilon_2\, \omega_R \frac{f^{-}_{L}(\varepsilon_1)\, f^{+}_{R}(\varepsilon_2)}{(i0^{+} + E_{c'} - E_a + \varepsilon_1)(i0^{+} + \varepsilon_1 - \varepsilon_2)(\;,\;)}$$

i.e,

$$\Gamma^{+}_{COT,ee} = 2Re\,(-i\hbar)\ \frac{\Gamma_L \Gamma_R}{(2\pi)^2} \int d\varepsilon_1 \int d\varepsilon_2\ \frac{f_L^{+}(\varepsilon_1)\, f_R^{-}(\varepsilon_2)}{(i0^+ + E_c - E_a - \varepsilon_1)(\varepsilon_2 - \varepsilon_1 + i0^+)(E_a - E_c + \varepsilon_2 + i0^+)} \quad (5.79)$$

Hence

i) $\Gamma^{+}_{COT,ee} \neq 0$ if $f_L^{+}(\varepsilon_1) f_R^{-}(\varepsilon_2) \neq 0$

$$\Leftrightarrow \quad \varepsilon_1 < \mu_L \quad \text{and} \quad \varepsilon_2 > \mu_R$$

ii) If we are in the CB region is

$$\begin{cases} \mu_{N+1} \gg \mu_L, \mu_R & \text{if } a \text{ is a state with } N+1 \text{ particles} \\ \mu_{N-1} \gg \mu_L, \mu_R \end{cases}$$

$E^g_{N-1}(V_g)$ —— —— $E^g_{N+1}(V_g)$

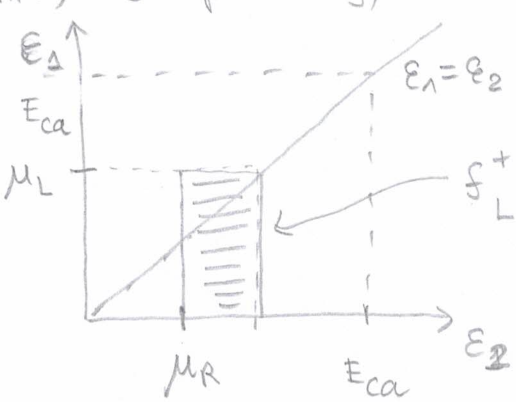
——

$E^g_N(V_g)$

$\Rightarrow \quad E_c - E_a = \mu_{N+1} \gg \mu_L, \mu_R$

$E_{c'} - E_a = \mu_{N-1} \gg \mu_L, \mu_R$

iii) Graphically, we can represent the integrand for Γ^{+}_{COT} as



$\mu_L = \mu_R + eV$

$\Rightarrow$ The contribution is maximized along the $\varepsilon_1 = \varepsilon_2$ line.
When $V=0$, the rectangle meets the line $\varepsilon_1 = \varepsilon_2$ in one point only.

iv) Thus, approximately,

$$\Gamma^{+}_{\mathrm{cot},el} \approx 2\,\mathrm{Re}\left(-i\hbar\frac{\Gamma_L\Gamma_R}{(2\pi)^2}\right)(-i\pi)\int d\varepsilon\,\frac{f_L^{+}(\varepsilon)\,f_R^{-}(\varepsilon)}{(E_{ca}-\varepsilon)(+\varepsilon-E_{ca})}$$

neglect $i0^+$ in outer ( ) and use again the Sokhotski-Plemely theorem

$$= \hbar\,\Gamma_L\Gamma_R\int\frac{d\varepsilon}{2\pi}\,\frac{f_L^{+}(\varepsilon)\,f_R^{-}(\varepsilon)}{(E_{ca}-\varepsilon)^2}$$

$$\Rightarrow\ \boxed{\Gamma^{+}_{\mathrm{cot},el} \sim \hbar\,\frac{\Gamma_L\Gamma_R}{(E_{ca})^2}\int\frac{d\varepsilon}{2\pi}\,f_L^{+}(\varepsilon)\,f_R^{-}(\varepsilon)} \qquad (5.80)$$

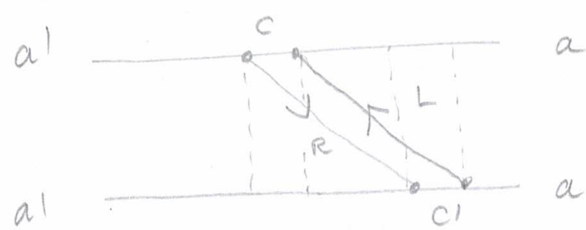
elastic cotunneling

which depends on the bias voltage through the Fermi functions but not on V_g

v) Similar considerations hold true for the inelastic cotunneling rates.

E.g.

$$\Gamma^{+}_{\mathrm{cot},in} = 2\,\mathrm{Re}\sum_{c,c'}$$



$a \neq a'$

$$\Rightarrow\ \Gamma^{+}_{\mathrm{cot},in} = 2\,\mathrm{Re}\left(-i\hbar\frac{\Gamma_L\Gamma_R}{(2\pi)^2}\right)\int d\varepsilon_1\int d\varepsilon_2\,\frac{f_L^{+}(\varepsilon_1)\,f_R^{-}(\varepsilon_2)}{(i0^+ + E_{c'}-E_a-\varepsilon_1)(i0^+ + E_{a'}-E_a-\varepsilon_1+\varepsilon_2)(i0^+ + E_{a'}-E_c+\varepsilon_2)} \qquad (5.81)$$

$\Rightarrow$ resonance for $\varepsilon_2-\varepsilon_1 = E_a - E_{a'}$

Finally

$$\Gamma^{+}_{cot,in} \approx -\hbar\,\Gamma_L\Gamma_R \int d\varepsilon \,\frac{f_L^{+}(\varepsilon)\, f_R^{-}(\varepsilon + E_{aa'})}{(E_{c'} - E_a - \varepsilon)(E_a - E_c + \varepsilon)} \qquad (5.82)$$

2) $\Gamma^{+}_{cot,in} \neq 0$ if $\varepsilon > \mu_R + E_{a'a}$ & $\varepsilon < \mu_L$ $\Leftarrow$ threshold at $eV = E_{a'a}$

$$\Gamma^{+}_{cot,in} \approx \frac{\hbar\Gamma_L\Gamma_R}{(E_{c'} - E_a)(E_c - E_a)} \int f_L^{+}(\varepsilon)\, f_R^{-}(\varepsilon + E_{aa'})\, d\varepsilon$$

Similar considerations apply to $\Gamma^{-}_{cot\,el}$, $\Gamma^{-}_{cot\,in}$

Our result are very general. Exemplarily we apply them to the single impurity Anderson model (SIAM), already discussed in Ch. 4.6 using the equation of motion method (EOM).

The drawback of the EOM was that it is restricted to weak interaction: $U \lesssim \Gamma$. The advantage is that it becomes exact when $U \to 0$.

Refresh

- $\hat{H}_T = \sum_\alpha \sum_{\vec{k}\sigma} \left(t_\alpha c^+_{\alpha\vec{k}\sigma} d_\sigma + t^*_\alpha \hat{d}^+_\sigma \hat{c}_{\alpha k\sigma} \right) = \hat{H}_{TL} + \hat{H}_{TR}$

Further

$$\hat{H}_{TL} = \hat{L} + \hat{L}^+ , \qquad \hat{H}_{TR} = \hat{R} + \hat{R}^+$$

where $\hat{L} = t_L c^+_{L\vec{k}\sigma} d_\sigma$, $\hat{R} = t_R c^+_{R\vec{k}\sigma} d_\sigma$

account for outgoing processes from the quantum dot

- $\hat{H}_S = \sum_\sigma \tilde{\varepsilon}_\sigma d^+_\sigma d_\sigma + U \hat{n}_\uparrow \hat{n}_\downarrow$

and $\tilde{\varepsilon}_\sigma(V_g) = \varepsilon_\sigma - \alpha e V_g$ (α is not a lead index!)

The eigenstates are thus
$|0\rangle \Rightarrow E_0 = 0$
$|\uparrow\rangle, |\downarrow\rangle \Rightarrow \tilde{\varepsilon}_\uparrow, \tilde{\varepsilon}_\downarrow$
$|\uparrow\downarrow\rangle = |2\rangle \Rightarrow \tilde{\varepsilon}_\uparrow + \tilde{\varepsilon}_\downarrow + U$

Without external magnetic field $\varepsilon_\uparrow = \varepsilon_\downarrow = \varepsilon_d$.

Current

According to (5.34) the current follows from

$$I = Tr_s \{ \tilde{\mathcal{K}}^{+}_{I_L} \rho^{\infty} \} = \sum_b \left(\sum_{aa'} (\tilde{\mathcal{K}}^{+}_{I_L})^{ba}_{ba'} \rho_{aa'} \right)$$

From the superselection rule for the elements of $\rho_{aa'}$

↳ $\rho_{aa'} = \delta_{aa'} \rho_{aa}$ for SIAM

i.e. $\rho_{aa'} = \rho_{00} |0\rangle\langle 0| + \rho_{\uparrow\uparrow} |\uparrow\rangle\langle\uparrow| + \rho_{\downarrow\downarrow} |\downarrow\rangle\langle\downarrow| + \rho_{22} |2\rangle\langle 2|$

Hence

$$\boxed{I = \sum_b \sum_a (\tilde{\mathcal{K}}^{+}_{I_L})^{ba}_{ba} \rho_{aa}} \qquad (5.83)$$

↳ We need: I) diagonal elements ρ_{aa}

↓

in turn

II) tensor elements $(\tilde{\mathcal{K}})^{ba}_{ba}$

and

III) the subclass of elements $(\tilde{\mathcal{K}}^{+}_{I_L})^{ba}_{ba}$

STEP I : STATIONARY RDM FOR THE SIAM

Start from the set of coupled equations (5.28). Using the superselection rule they become

$$0_{bb} = \sum_a \mathcal{K}^{ba}_{ba}\, \rho_{aa} \qquad (5.84)$$

Using further the sum rule (5.) with $a = a'$

$$0 = \sum_b \mathcal{K}^{ba}_{ba} \;\Rightarrow\; \mathcal{K}^{aa}_{aa} = -\sum_{b\neq a} \mathcal{K}^{ba}_{ba} \qquad (5.85b)$$

We thus find with $\sigma = \uparrow,\downarrow$ and $P_\alpha = \rho_{\alpha\alpha}$

$$\begin{cases} 0 = -\left(\sum_\sigma \mathcal{K}^{\sigma 0}_{\sigma 0} + \mathcal{K}^{20}_{20}\right) P_0 + \sum_\sigma \mathcal{K}^{0\sigma}_{0\sigma} P_\sigma + \mathcal{K}^{02}_{02} P_2 \\ 0_{\sigma\sigma} = \mathcal{K}^{\sigma 0}_{\sigma 0} P_0 - \left(\mathcal{K}^{0\sigma}_{0\sigma} + \mathcal{K}^{2\sigma}_{2\sigma}\right) P_\sigma + \mathcal{K}^{\sigma 2}_{\sigma 2} P_2 \\ 0_{22} = \mathcal{K}^{20}_{20} P_0 + \sum_\sigma \mathcal{K}^{2\sigma}_{2\sigma} P_\sigma - \left(\mathcal{K}^{02}_{02} + \sum_\sigma \mathcal{K}^{\sigma 2}_{\sigma 2}\right) P_2 \end{cases} \qquad (5.86)$$

Notice that due to the sum rule the sum of the columns is zero.

The terms with "−" describe processes which diminish the population P_α, viceversa "+" processes increase it

↳ to solve for P_α we use three of the four eqs. and the normalization condition: $\boxed{\sum_\alpha P_\alpha = 1}$

Explicitly

$$\begin{cases} 0 = \mathcal{K}^{00}_{00} P_0 + \sum_\sigma \mathcal{K}^{0\sigma}_{0\sigma} P_\sigma + \mathcal{K}^{02}_{02} P_2 \\ 0 = \sum_\sigma \mathcal{K}^{\sigma 0}_{\sigma 0} P_0 + \mathcal{K}^{\sigma\sigma}_{\sigma\sigma} P_\sigma + \sum_\sigma \mathcal{K}^{\sigma 2}_{\sigma 2} P_2 \\ 0 = \mathcal{K}^{20}_{20} P_0 + \sum_\sigma \mathcal{K}^{2\sigma}_{2\sigma} P_\sigma + \mathcal{K}^{22}_{22} P_2 \end{cases}$$

and

$$1 = P_0 + \sum_\sigma P_\sigma + P_2$$

We define as $k_{\alpha\beta}$ the matrix elements of the kernel matrix, with $k_{\alpha\beta} \equiv \mathcal{K}^{\alpha\beta}_{\alpha\beta} = (K)_{\alpha\beta}$

Further, we take e.g. the first three rows of K

$$\Rightarrow \underbrace{\begin{pmatrix} k_{11} & k_{12} & k_{13} & k_{14} \\ k_{12} & k_{22} & k_{23} & k_{24} \\ k_{31} & k_{32} & k_{33} & k_{34} \\ 1 & 1 & 1 & 1 \end{pmatrix}}_{\equiv A} \begin{pmatrix} P_0 \\ P_\uparrow \\ P_\downarrow \\ P_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

and

$$\boxed{\begin{pmatrix} P_0 \\ P_\uparrow \\ P_\downarrow \\ P_2 \end{pmatrix} = A^{-1} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}} \qquad (5.87)$$

Further, we introduce the tunneling rates

$$\begin{cases} \Gamma^{+}_{ba} \equiv (\mathcal{K})^{ba}_{ba} & \text{if } N_b > N_a \\ \\ \Gamma^{-}_{ab} \equiv (\mathcal{K})^{ba}_{ba} & \text{if } N_b < N_a \end{cases} \qquad (5.88)$$

Thus eq. (5.86) becomes (cf. also for comparison sheet 14)

$$\begin{cases} 0 = -\left(\sum_\sigma \Gamma^{+}_{\sigma 0} + \Gamma^{+}_{20}\right) P_0 + \sum_\sigma \Gamma^{-}_{\sigma 0} P_\sigma + \Gamma^{-}_{20} P_2 \\ \\ 0 = \Gamma^{+}_{\sigma 0} P_0 - \left(\Gamma^{-}_{\sigma 0} + \Gamma^{+}_{2\sigma}\right) P_\sigma + \Gamma^{-}_{2\sigma} P_2 \\ \\ 0 = \Gamma^{+}_{20} P_0 + \sum_\sigma \Gamma^{+}_{2\sigma} P_\sigma - \left(\Gamma^{-}_{20} + \sum_\sigma \Gamma^{-}_{2\sigma}\right) P_2 \end{cases} \qquad (5.89b)$$

Together with $1 = \sum_\alpha P_\alpha$, P_α can be expressed uniquely in terms of the rates $\Gamma^{\pm}_{ab}$!

E.g. <u>2nd order approximation</u> $\Rightarrow$ $\boxed{\Gamma^{\pm}_{20} = 0}$ (see later).

$$\begin{pmatrix} P_0 \\ P_\uparrow \\ P_\downarrow \\ P_2 \end{pmatrix} = \frac{1}{w} \begin{pmatrix} \sum_\sigma \Gamma^{-}_{\bar\sigma 0} \Gamma^{-}_{2\bar\sigma} \left(\Gamma^{-}_{\sigma 0} + \Gamma^{+}_{2\sigma}\right) \\ \sum_\sigma \left(\Gamma^{+}_{\uparrow 0} \Gamma^{-}_{\downarrow 0} \Gamma^{-}_{2\sigma} + \Gamma^{+}_{2\downarrow} \Gamma^{-}_{2\uparrow} \Gamma^{+}_{\sigma 0}\right) \\ \sum_\sigma \left(\Gamma^{+}_{\downarrow 0} \Gamma^{-}_{\uparrow 0} \Gamma^{-}_{2\bar\sigma} + \Gamma^{+}_{2\uparrow} \Gamma^{-}_{2\downarrow} \Gamma^{+}_{\bar\sigma 0}\right) \\ \sum_\sigma \Gamma^{+}_{\bar\sigma 0} \Gamma^{+}_{2\bar\sigma} \left(\Gamma^{-}_{\sigma 0} + \Gamma^{+}_{2\sigma}\right) \end{pmatrix} \qquad (5.90)$$

With $\mathcal{N}$ a normalization constant ensuring $\sum_a P_a = 1$:

$$\mathcal{N} = \sum_\sigma \Big[\Gamma^-_{2\sigma} \left(\Gamma^-_{\uparrow 0} \Gamma^+_{\downarrow 0} + \Gamma^-_{\downarrow 0} \Gamma_{\uparrow 0} \right) + \Gamma^-_{\sigma 0} \left(\Gamma^-_{2\sigma} + \Gamma^+_{\bar\sigma 0} \right) \Gamma^+_{2\bar\sigma} + \Gamma^+_{\sigma 0} \left(\Gamma^-_{2\uparrow} \Gamma^+_{2\downarrow} + \Gamma_{2\downarrow} \Gamma^+_{2\uparrow} \right) \Big] \tag{5.91b}$$

where

$$\Gamma_{ab} \equiv \Gamma^+_{ab} + \Gamma^-_{ab}$$

Further, in 2nd order it holds, cf. later. (cf. exercise sheet 14)

$$\Gamma^{\pm}_{ab} = \frac{2\pi}{\hbar} \sum_{\alpha = L,R} |t_\alpha|^2 \mathcal{D}_a(\varepsilon_F) f^{\pm}_\alpha (E_{ab}) = \sum_\alpha \Gamma_\alpha f^{\pm}_\alpha (E_{ab})$$

where

$$\Gamma_\alpha = \frac{2\pi}{\hbar} |t_\alpha|^2 \mathcal{D}_a(\varepsilon_F) \quad \text{and} \quad E_{ab} = E_a - E_b$$

I.e. E_{ab} is a difference of many-body energies.

$\Rightarrow$ Populations are fully expressed in terms of rates $\Gamma^{\pm}_{ab}$!

6.3. TRANSPORT REGIMES ~~FOR THE SIAM~~

Attention: numbering is different from previous pages

We are now in the position of being able to investigate various transport regimes in the SIAM, by making use of the general solution for the current (6.10), being expressed in terms of elements of the current kernel and of populations.

We allow a bias and gate voltage: $\hat{H}_C \to \hat{H}_C - \alpha e V_g \hat{N} \Rightarrow \hat{H}_C = \sum_{\alpha} (\varepsilon_\alpha - \alpha e V_g) \hat{n}_\alpha = \sum_{\alpha} \varepsilon_\alpha (V_g)$

We shall consider various situations: I. Weak coupling, II. Intermediate coupling

6.3.1. Weak coupling (2nd order, 4th order in H_T $\Leftrightarrow$ first order, 2nd order in Γ)

This regime is characterized by

$$\Gamma < k_B T \ll U \qquad (6.23)$$

where $\Gamma = \sum_e \left(\Gamma^+_{e,ab} + \Gamma^-_{e,ab}\right) = \sum_e \frac{2\pi}{\hbar} \alpha_e (f^+_e + f^-_e) = \sum_e \frac{2\pi}{\hbar} \alpha_e = \sum_e \Gamma_e$ total linewidth indep of a, b

i) Second order current

This current we have already derived and is given by (6.12) or (6.13):

$$I^{(2)}_e = e \sum_\sigma \left[\Gamma^+_{e,\sigma 0} \rho_{00} + \Gamma^+_{e,2\sigma} \rho_{\sigma\sigma} - \Gamma^-_{e,\sigma 0} \rho_{\sigma\sigma} - \Gamma^-_{e,2\sigma} \rho_{22} \right].$$

moreover ($E_\uparrow = E_\downarrow$)

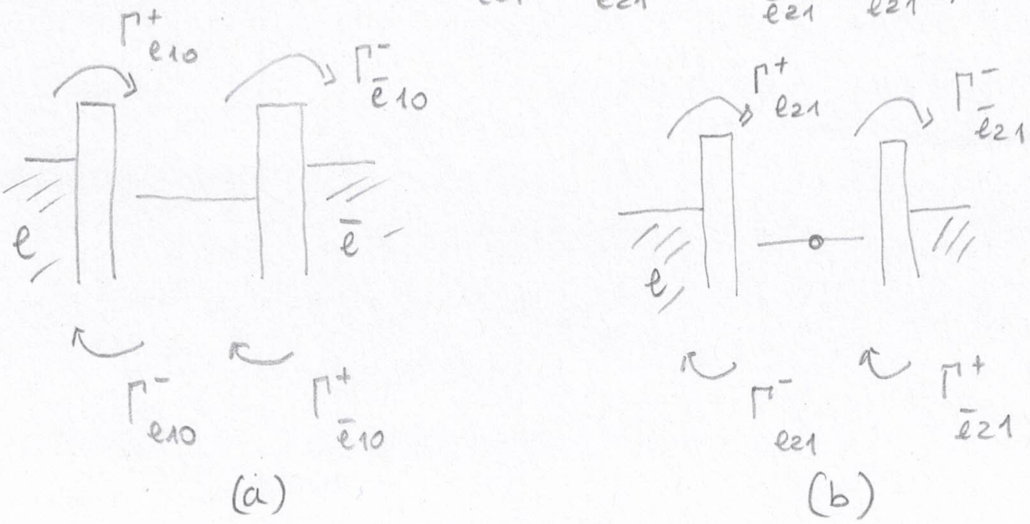
$$\begin{pmatrix} \rho_{00} \\ \rho_{\sigma\sigma} \\ \rho_{22} \end{pmatrix} = \frac{1}{\vartheta} \begin{pmatrix} \Gamma^-_{\sigma 0} \Gamma^-_{2\sigma} \\ \Gamma^+_{\sigma 0} \Gamma^-_{2\sigma} \\ \Gamma^+_{\sigma 0} \Gamma^+_{2\sigma} \end{pmatrix} \qquad (6.24) \qquad \text{where } \vartheta = \Gamma^-_{2\sigma} \Gamma_{\sigma 0} + \Gamma^+_{\sigma 0} \Gamma_{21} \qquad (6.24b)$$

and

$$\Gamma_{ab} = \Gamma^+_{ab} + \Gamma^-_{ab}, \qquad \Gamma^\pm_{ab} = \sum_e \Gamma^\pm_{e,ab} \qquad (6.25)$$

We thus find, with $\Gamma_{2\sigma} = \Gamma_{21}$ etc.

$$I_e^{(2)} = \frac{2e}{w} \left(\Gamma^-_{21}, \Gamma^+_{10} \right) \begin{pmatrix} \Gamma^+_{e10}\Gamma^-_{\bar{e}10} - \Gamma^-_{e10}\Gamma^+_{\bar{e}10} \\ \Gamma^+_{e21}\Gamma^-_{\bar{e}21} - \Gamma^+_{\bar{e}21}\Gamma^-_{e21} \end{pmatrix} \quad (6.26)$$



Two sequential tunneling processes are necessary to transfer charge in the forward or backward direction

example : process (a) forward

$\Gamma^+_{e10} \neq 0$ & $\Gamma^-_{\bar{e}10} \neq 0 \iff f^+_e(E_{10})$ & $f^-_{\bar{e}}(E_{10}) \neq 0$

$\underset{\lim T\to 0}{\iff}$ $E_{10}(V_g) - \mu_e \leq 0$ & $E_{10}(V_g) - \mu_{\bar{e}} \geq 0$

recall that $\mu_1(V_g) = E_1(V_g) - E_0(V_g) = (E_1 - \alpha e V_g) - E_0$

with a gate voltage which acts on Hsys as $H_{sys} \to H_{sys} + \hat{N}\alpha e V_g$

$\Rightarrow$ transport condition is (forward direction) $\mu_e \geq \mu_1(V_g) \geq \mu_{\bar{e}}$

In general $\boxed{\mu_e \geq \mu_N(V_g) \geq \mu_{\bar{e}}}$ forward transport (6.27)

Because $\mu_e = \mu_0 + eV_e = \mu_0 + e\varkappa_e V$, $\mu_{\bar{e}} = \mu_0 + eV_{\bar{e}} = \mu_0 - e\varkappa_{\bar{e}} V_e$, $\varkappa_e + \varkappa_{\bar{e}}$

$\Rightarrow$ (6.27) is also a condition on the bias voltage

Similarly for backward transport

$$\boxed{\mu_e \leq \mu_N(V_g) \leq \mu_{\bar{e}}} \quad \text{backward transport} \quad (6.27b)$$

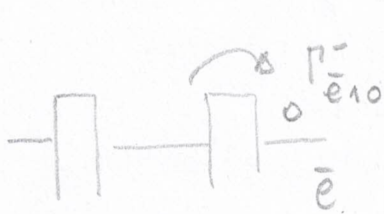
Such conditions can be obtained also simply from energy conservation arguments.

Example: forward process a

$E^{tot}(i) = E^{tot}(f)$

$$E_e + E_0(V_g) = E_e - \varepsilon_k + E_1(V_g) \iff \varepsilon_k = E_1(V_g) - E_0(V_g) = \mu_1(V_g)$$

and because $\varepsilon_k \leq \mu_e \Rightarrow \boxed{\mu_1(V_g) \leq \mu_e = \mu_0 + eV_e}$

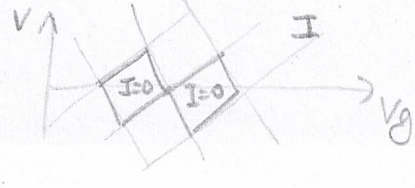


$E^{tot}(i) = E^{tot}(f)$

$$E_{\bar{e}} + E_1(V_g) = E_{\bar{e}} + \varepsilon_k + E_0(V_g) \iff \varepsilon_k = \mu_1(V_g)$$

because $\varepsilon_k \geq \mu_{\bar{e}} \Rightarrow \boxed{\mu_1(V_g) \geq \mu_{\bar{e}} = \mu_0 + eV_{\bar{e}}}$

By elaborating on conditions (6.27) e (6.27b) with
Coulomb diamonds are obtained



$\mu_e = \mu_0 + e\chi_e V$
$\mu_{\bar{e}} = \mu_0 - e\chi_{\bar{e}} V$
$\mu_N(V_g) = \mu_N(0) - \alpha e V_g$

This condition is general and valid $\forall$ second order process transferring charge in and out of the dot

$$\boxed{\mu_S \geq \mu(N, V_g) \geq \mu_D}$$ for processes $N-1 \to N \to N-1$

Note: Due to $\mu_{S,D} = \mu_0 \pm e\varkappa_{S,D} V$, $\mu(N,V_g) = E_N - E_{N-1} - \alpha e V_g$

this gives conditions on V_g and V

$$\begin{cases} \mu_0 + e\varkappa_D V \geq E_N - E_{N-1} - eV_g\alpha \\ E_N - E_{N-1} - \alpha eV_g \geq \mu_0 - e\varkappa_S V \end{cases}$$

Source transitions $N \to N+1$

$V > 0$

drain transitions $N+1 \to N$

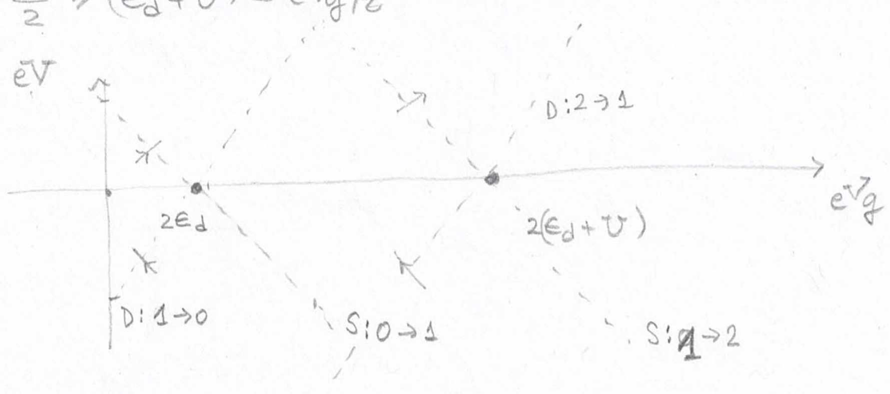
set for simplicity $\mu_0 = 0$, $\varkappa_S = +\varkappa_D = 1/2$ $\iff$ $V_S = \varkappa_S V = \frac{1}{2}V$

$\alpha = 1/2$ $\quad$ $V_D = -\varkappa_D V = -\frac{1}{2}V$

$$\frac{eV}{2} \geq E_1 - \frac{eV_g}{2} = \epsilon_d - eV_g/2 \qquad N=1$$

source

$$\frac{eV}{2} \geq (\epsilon_d + U) - eV_g/2 \qquad N=2$$



Adding the drain transitions

$$\epsilon_d - \frac{1}{2}eV_g \geq -\frac{e}{2}V \qquad N=1$$

drain

$$(\epsilon_d + U) - \frac{1}{2}eV_g \geq -\frac{e}{2}V \qquad N=2$$

Note at the crossing of source and drain lines on the eV_g axis is

i) $\frac{eV_g}{2} = \epsilon_d$ or ii) $\frac{eV_g}{2} = \epsilon_d + U$

case i) $\frac{eV_g}{2} = \epsilon_d \Rightarrow E_1 - \alpha eV_g = \epsilon_d - \frac{eV_g}{2} = 0 = E_0$ i.e. $\boxed{\tilde{E}_1 = \tilde{E}_0}$ 49

(and $E_2 - 2\alpha eV_g = \tilde{E}_2 = (2\epsilon_d + U) - 2\epsilon_d = U$ $\quad \tilde{E}_2 = U$

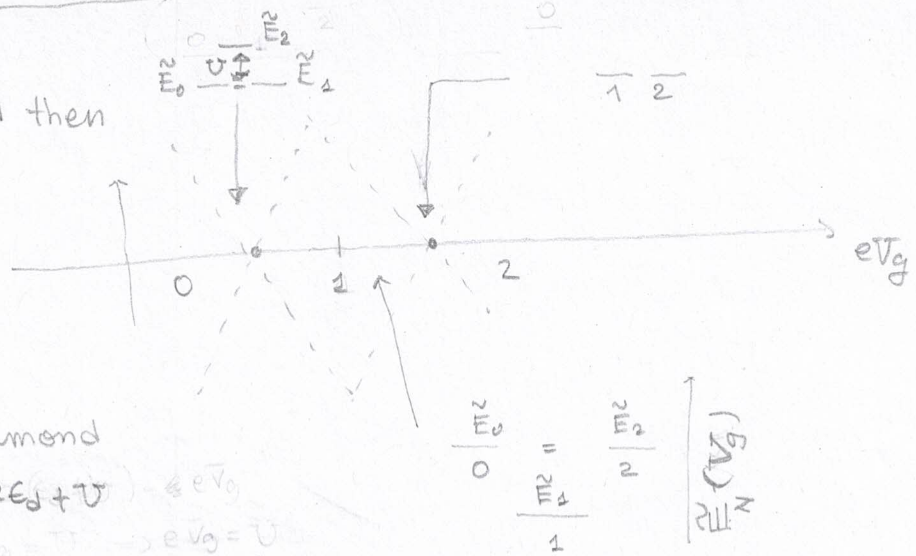
case ii) $\frac{eV_g}{2} = \epsilon_d + U \Rightarrow E_2 - \alpha eV_g = 2\epsilon_d + U - \frac{eV_g}{2} = \epsilon_d$

$\Leftrightarrow E_2 - 2(\alpha eV_g) = \tilde{E}_2 = \epsilon_d - (\alpha eV_g) = \tilde{E}_1$ i.e. $\boxed{\tilde{E}_2 = \tilde{E}_1}$

$\Rightarrow$ these are called charge neutrality point as the ground states electrodem. energies for N and N+1 particles are degenerate

$$\boxed{\tilde{E}_N(V_g) = \tilde{E}_{N+1}(V_g)}$$

We find then



Middle of diamond

$eV_g = 2\epsilon_d + U$

$\Rightarrow \tilde{E}_2 = E_2 - 2\alpha eV_g = (2\epsilon_d + U) - eV_g = 0 = \tilde{E}_0$

$\tilde{E}_1 = E_1 - \alpha eV_g = \epsilon_d - \frac{eV_g}{2} = \epsilon_d - \epsilon_d - U = -U$

$\Rightarrow$ fazit: Transport condition in 2nd order

$eV > 0$ $\quad \boxed{\mu_S \geq \mu(N, V_g) \geq \mu_D}$ $\rightarrow$ • Coulomb diamonds

• transport spectroscopy

Proportional coupling

The expression (6.26) simplifies in the case where $\Gamma = \sum_\ell \Gamma_\ell = \Gamma_R + \Gamma_L$ can be rewritten as $\Gamma = u_R \Gamma + u_L \Gamma$ with $u_R + u_L = 1$, the case of proportional coupling

$$\Rightarrow \Gamma^+_{\ell,ab} = \underbrace{\frac{2\pi}{\hbar} \underbrace{\mathcal{D}_\ell |T_\ell|^2}_{\alpha_\ell}}_{\Gamma_\ell} f^+_\ell(E_{ab}) = \underbrace{u_\ell}_{\uparrow} \Gamma f^+_\ell(E_{ab}) \qquad (6.28)$$

no dependence on a,b but only on ℓ

where

$$u_\ell + u_{\bar\ell} = 1 \qquad \text{and} \qquad \Gamma \equiv \frac{2\pi}{\hbar} \sum_\ell \mathcal{D}_\ell |T_\ell|^2$$

$$\Rightarrow \Gamma_{\ell ab} = \Gamma^+_{\ell ab} + \Gamma^-_{\ell ab} = u_\ell \Gamma f^+_\ell + u_\ell \Gamma f^-_\ell = u_\ell \Gamma \quad \text{indep. of } ab!$$

Hence

$$\begin{cases} \Gamma^+_{\ell 10} \Gamma^-_{\bar\ell 10} - \Gamma^-_{\ell 10} \Gamma^+_{\bar\ell 10} \underset{\uparrow (*)}{=} \Gamma^+_{\ell 10} \Gamma_{\bar\ell 10} - \Gamma_{\ell 10} \Gamma^+_{\bar\ell 10} \overset{\text{prop. coup.}}{=} \Gamma \left(u_{\bar\ell} \Gamma^+_{\ell 10} - u_\ell \Gamma^+_{\bar\ell 10} \right) \\ \\ \Gamma^+_{\ell 21} \Gamma^-_{\bar\ell 21} - \Gamma^+_{\bar\ell 21} \Gamma^-_{\ell 21} = \Gamma_{\ell 21} \Gamma^-_{\bar\ell 21} - \Gamma_{\bar\ell 21} \Gamma^-_{\ell 21} \overset{\text{prop. coup}}{=} \Gamma \left(u_\ell \Gamma^-_{\bar\ell 21} - u_{\bar\ell} \Gamma^-_{\ell 21} \right) \end{cases}$$

(*) add $0 = \Gamma^+_{\ell 10} \Gamma^+_{\bar\ell 10} - \Gamma^+_{\ell 10} \Gamma^+_{\bar\ell 10}$

Using (6.26) one then obtains

$$I^{(2)}_e = eN_h\left(u_{\bar e}\Gamma^+_{e10} - u_e\Gamma^+_{\bar e 10}\right) + eN_e\left(u_e\Gamma^-_{\bar e 21} - u_{\bar e}\Gamma^-_{e21}\right) \qquad (6.29)$$

where

$$N_e = 2\,\frac{\Gamma_{21}\Gamma^+_{10}}{\Gamma_{21}\Gamma^+_{10} + \Gamma^-_{21}\Gamma_{10}} = \mathrm{Tr}_{sys}\{\hat N \hat\rho_{red}\} \qquad (6.30a)$$ average electron nr.

$$N_h = 2 - N_e \qquad (6.30b)$$ average hole nr.

recalling that

$$\Gamma^+_{eab} = u_e\Gamma f^+(E_{ab}) \quad , \quad \Gamma^-_{eab} = u_e\Gamma f^-(E_{ab})$$

we thus have

$$\boxed{\begin{aligned} I^{(2)}_e = {} & eN_h\Gamma\, u_e u_{\bar e}\left[f^+_e(E_{10}) - f^+_{\bar e}(E_{10})\right] + \\ & eN_e\Gamma\, u_e u_{\bar e}\left[f^-_{\bar e}(E_{21}) - f^-_e(E_{21})\right] \end{aligned}} \qquad (6.30)$$

and, due to $\Gamma_{ab} = \sum_e \Gamma^e_{eab} = \left(\sum_e u_e\right)\Gamma = \Gamma$, in proportional coupling

$$N_e = 2\,\frac{\Gamma^+_{10}}{\Gamma^+_{10} + \Gamma^-_{21}} \quad , \quad N_h = 2\,\frac{\Gamma^-_{21}}{\Gamma^+_{10} + \Gamma^-_{21}}$$

Recalling $f^-(x) = 1 - f^+(x)$

$$\boxed{I^{(2)}_e = eN_h\Gamma u_e u_{\bar e}\left[f^+_e(E_{10}) - f^+_{\bar e}(E_{10})\right] + eN_e\Gamma u_e u_{\bar e}\left[f^+_e(E_{21}) - f^-_{\bar e}(E_{21})\right]} \quad (6.31)$$

Integral form

$\Gamma^{+}_{e\sigma 0} =$ 

$$= \lim_{\eta\to 0^+} 2\mathrm{Re}\left\{ \frac{i}{\hbar} \int d\varepsilon\, \overset{|T_e|^2}{\overset{\curlyvee}{\mathcal{D}_e}}\, \frac{f_e^+(\varepsilon)}{\varepsilon - E_{\sigma 0} + i\eta} \right\} = \frac{2\pi}{\hbar} \overset{|T_e|^2}{\overset{\curlyvee}{\mathcal{D}_e}}\, f_e^+(E_{\sigma 0}) = \mathfrak{u}_e \Gamma f_e^+(E_{\sigma 0})$$

diagrammatic rules

and similarly for $\Gamma^{-}_{e\sigma 0}$ or $\Gamma^{\pm}_{e,2\sigma}$

$$I^{(2)} = N_h \mathfrak{u}_e \mathfrak{u}_{\bar e} |T|^2 \lim_{\eta\to 0} 2\mathrm{Re}\left\{ \frac{i}{\hbar} \int d\varepsilon\, \frac{\mathcal{D}(\varepsilon_F)}{\varepsilon - E_{\sigma 0} + i\eta} \left[f_e(\varepsilon) - f_{\bar e}(\varepsilon) \right] \right\}$$

$$+ N_e \mathfrak{u}_e \mathfrak{u}_{\bar e} |T|^2 \lim_{\eta\to 0} 2\mathrm{Re}\left\{ \frac{i}{\hbar} \int d\varepsilon\, \frac{\mathcal{D}(\varepsilon_F)}{\varepsilon - E_{21} + i\eta} \left[f_e^+(\varepsilon) - f_{\bar e}(\varepsilon) \right] \right\}$$

$f^-(\varepsilon) = 1 - f^+(\varepsilon)$

Hence the final result reads:

$$\boxed{I^{(2)} = e\,\mathfrak{u}_e \mathfrak{u}_{\bar e} \frac{\Gamma}{(2\pi/\hbar)} \lim_{\eta\to 0} 2\mathrm{Re}\left\{ \frac{i}{\hbar} \int d\varepsilon \left[\frac{N_h}{\varepsilon - E_{\sigma 0} + i\eta} + \frac{N_e}{\varepsilon - E_{21} + i\eta} \right] \left(f_e(\varepsilon) - f_{\bar e}(\varepsilon) \right) \right\}} \tag{6.32}$$

This result clearly shows that the current in second order is proportional to Γ and to the difference of Fermi functions. The latter provide both bias voltage and temperature dependence; the gate voltage dependence is on the other hand in

$$E_{\sigma 0} = (E_\sigma - \alpha e V_g N) - (E_0 - \alpha e V_g (N-1)) = E_\sigma - E_0 - \alpha e V_g$$

Differential conductance and linear conductance

- differential conductance $\frac{dI}{dV}$ as obtained by differentiating (6.32) with respect to the bias voltage $V = V_S - V_D$

- linear conductance

$$G = \lim_{V \to 0} \frac{dI}{dV} \quad (6.33)$$

From (6.32) we notice that $f_e(\varepsilon) = \frac{1}{e^{\beta(\varepsilon - \mu_e)} + 1}$, $\begin{cases} \mu_e = \mu_0 + eV_e \\ \quad = \mu_0 + e\chi_e V \\ \mu_{\bar{e}} = \mu_0 + eV_{\bar{e}} = \\ \quad = \mu_0 - e\chi_{\bar{e}} V \end{cases}$

$$\Rightarrow \lim_{V \to 0} f_e(\varepsilon) = f(\varepsilon) \underbrace{- \beta e V \chi_e}_{= -\beta\mu_e} f'(\varepsilon) + O(V^2)$$

where $f(\varepsilon) = \frac{1}{e^{\beta(\varepsilon - \mu_0)} + 1}$ and $\chi_e + \chi_{\bar{e}} = 1$

such that it holds for the difference of Fermi functions

$$\lim_{V \to 0} f_e(\varepsilon) - f_{\bar{e}}(\varepsilon) = -\beta e V(\chi_e + \chi_{\bar{e}}) f'(\varepsilon) = -\beta e V f'(\varepsilon)$$

yielding

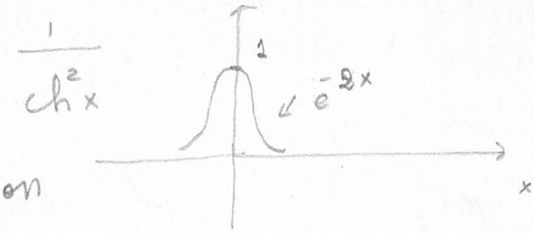
$$\begin{cases} G = -\beta e^2 \chi_e \chi_{\bar{e}} \frac{\Gamma}{(2\pi/\hbar)} \lim_{\eta \to 0} 2\,\mathrm{Re} \left\{ \frac{i}{\hbar} \int d\varepsilon \left[\frac{N_R}{\varepsilon - E_{\sigma 0} + i\eta} + \frac{N_e}{\varepsilon - E_{21} + i\eta} \right] f'(\varepsilon) \right\} \\ f'(\varepsilon) = -\frac{\beta}{4} \frac{1}{\mathrm{ch}^2 \frac{\beta(\varepsilon - \mu_0)}{2}} \end{cases}$$

We thus obtain the final form

$$G = e^2 \mathcal{U}_e \mathcal{U}_{\bar{e}} \frac{\Gamma}{2\pi/\hbar} (-\beta) \frac{2}{\hbar} \lim_{\eta\to 0} \int d\varepsilon \left\{ N_h \frac{\eta}{(\varepsilon - E_{\sigma 0})^2 + \eta^2} + N_e \frac{\eta}{(\varepsilon - E_{21})^2 + \eta^2} \right\} f'(\varepsilon)$$

or

$$\boxed{G = \frac{e^2 \mathcal{U}_e \mathcal{U}_{\bar{e}}}{4 k_B T} \frac{\Gamma}{\pi} \lim_{\eta\to 0} \int d\varepsilon \left[\underbrace{N_h \frac{\eta}{(\varepsilon - E_{\sigma 0})^2 + \eta^2} + N_e \frac{\eta}{(\varepsilon - E_{21})^2 + \eta^2}}_{\text{Lorentzian of width } \eta} \right] \underbrace{\frac{1}{ch^2 \beta \frac{(\varepsilon - \mu_0)}{2}}}_{\text{peaked function of width } k_B T}}$$



Because $\eta \to 0$ the Lorentzian is a δ-function yielding the analytical expression

$$\boxed{G = \frac{e^2 \mathcal{U}_e \mathcal{U}_{\bar{e}}}{4 k_B T} \frac{\Gamma}{\pi} \left[\frac{N_h}{ch^2 \beta \left(\frac{E_{\sigma 0}(V_g) - \mu_0}{2} \right)} + \frac{N_e}{ch^2 \beta \, \frac{E_{21}(V_g) - \mu_0}{2}} \right]} \tag{6.34}$$

$E_\sigma - E_0 - \alpha e V_g = \mu_0$

$\Leftrightarrow \quad \mu_1(V_g) = \mu_0$

$E_2 - E_1 - \alpha e V_g = \mu_0$

$\Leftrightarrow \quad \mu_2(V_g) = \mu_0$

Both the width and the height depend on T :

width $\sim T$

maximum $\sim \frac{1}{T}$