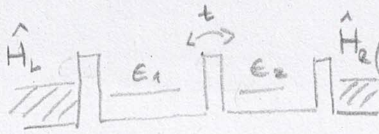
4.7 Conductance of QD in series



Consider the situation of QDs in series $\Rightarrow$ no proportional coupling and hence we have to resort to the general calculation of the conductance, $G = \lim_{\omega \to 0} \left(- \frac{\mathcal{I}m \tilde{\chi}^R_{II}}{\omega} \right)$.

Let us consider the system Hamiltonian cf. (4.68)

$$\hat{\mathcal{H}}^0_S = \sum_\sigma \left(\varepsilon_{1\sigma} d^+_{1\sigma} d_{1\sigma} + \varepsilon_{2\sigma} d^+_{2\sigma} d_{2\sigma} + t_{12} d^+_{1\sigma} d_{2\sigma} + t^*_{12} d^+_{2\sigma} d_{1\sigma} \right)$$

and $\hat{\mathcal{H}}_S = \hat{\mathcal{H}}^0_S + \hat{V}_{ee}$

where $\hat{V}_{ee} = \frac{1}{2} \sum_{i=1,2} \mathcal{U} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + \frac{1}{2} \sum_\sigma V_{12} \hat{n}_{1\sigma} \hat{n}_{2\sigma'}$

This problem is qualitative different from the SIAM due to the presence of orbital degrees of freedom

$\hookrightarrow$ interference effects (due to non proportional coupling)

In the following we shall set $\hat{V}_{ee} = 0$ and focus on these aspects.

Recall also $(\alpha = L, R)$ the tunneling and lead Hamiltonians

$$\begin{cases} \hat{H}_{T\alpha} = \sum_{\vec{k}\sigma} \left[t_\alpha \hat{c}^+_{\alpha\vec{k}\sigma} \hat{d}_{i_\alpha\sigma} + t^*_\alpha d^+_{i_\alpha\sigma} \hat{c}_{\alpha\vec{k}\sigma} \right] \\ \hat{H}_\alpha = \sum_{\vec{k}\sigma} c^+_{\alpha\vec{k}\sigma} c_{\alpha\vec{k}\sigma} \varepsilon_{\alpha\vec{k}} \end{cases} \quad d_{i_L} = d_1, \; d_{i_R} = d_2$$

step I : current operator

The current operator for this system is obtained from (4.70) 91b

$$\hat{I}_L = -\frac{ie}{\hbar}\left[\hat{H}_{TL}, \hat{H}_L\right] = -\frac{ie}{\hbar}\left(\hat{L} - \hat{L}^{+}\right)$$

where for the QD in series (cf. Eq. (4.71))

$$\hat{L} - \hat{L}^{+} = \sum_{\vec{k}\sigma}\left(t_L\, \hat{c}^{+}_{Lk\sigma}\hat{d}_{1\sigma} - t^{*}_L\, \hat{d}^{+}_{1\sigma}\hat{c}_{Lk\sigma}\right) \qquad (4.116)$$

step II : Current response

We need

$$\boxed{\begin{aligned}
\chi^{R}_{II}(t) &= -\frac{i}{\hbar}\theta(t)\left\langle\left[\hat{I}_L(t), \hat{I}_L(0)\right]\right\rangle_0 \\
&= -\frac{e^2}{\hbar^2}\Big\{ \underbrace{-\frac{i}{\hbar}\theta(t)\left\langle\left[\hat{L}(t), \hat{L}(0)\right]\right\rangle_0}_{(\mathrm{III})} \underbrace{-\frac{i}{\hbar}\theta(t)\left\langle\left[\hat{L}^{+}(t), \hat{L}^{+}(0)\right]\right\rangle_0}_{(\mathrm{IV})} \\
&\quad - \Big[\underbrace{-\frac{i}{\hbar}\theta(t)\left\langle\left[\hat{L}(t), \hat{L}^{+}(0)\right]\right\rangle_0}_{(\mathrm{I})} \underbrace{-\frac{i}{\hbar}\theta(t)\left\langle\left[\hat{L}^{+}(t), \hat{L}(0)\right]\right\rangle_0}_{(\mathrm{II})}\Big]\Big\}
\end{aligned}} \qquad (4.117)$$

note $[\hat{L}(t), \hat{L}(0)] = \hat{L}(t)\hat{L}(0) - \hat{L}(0)\hat{L}(t)$

and $[\hat{L}(t), \hat{L}(0)]^{+} = \hat{L}^{+}(0)\hat{L}^{+}(t) - \hat{L}^{+}(t)\hat{L}^{+}(0) = -[\hat{L}^{+}(t), \hat{L}(0)]$

similarly $[\hat{L}^{+}(t), \hat{L}(0)] = \hat{L}^{+}(t)\hat{L}(0) - \hat{L}(0)\hat{L}^{+}(t)$

and $[\hat{L}(t), \hat{L}^{+}(0)]^{+} = \hat{L}(0)\hat{L}^{+}(t) - \hat{L}^{+}(t)\hat{L}(0) = -[\hat{L}^{+}(t), \hat{L}(0)]$

Let us then focus on $\langle [\hat{L}(t), \hat{L}^{+}(0)] \rangle_0$

$\Rightarrow$ from (4.16)

$$B_I(t) \equiv + \frac{e^2}{\hbar^2} \langle [\hat{L}(t), \hat{L}^{+}(0)] \rangle_0 = \frac{e^2}{\hbar^2} \sum_{\vec{k}\vec{k}'\sigma\sigma'} |t_L|^2 \langle [\hat{c}^{+}_{L\vec{k}\sigma}(t) \hat{d}_{1\sigma}(t), \hat{d}^{+}_{1\sigma'} \hat{c}_{L\vec{k}'\sigma'}] \rangle_0 \tag{4.119}$$

develop the commutator

$$C = \langle \hat{c}^{+}_{L\vec{k}\sigma}(t) \hat{d}_{1\sigma}(t) \hat{d}^{+}_{1\sigma'} \hat{c}_{L\vec{k}'\sigma'} - \hat{d}^{+}_{1\sigma'} \hat{c}_{L\vec{k}'\sigma'} \hat{c}^{+}_{L\vec{k}\sigma}(t) \hat{d}_{1\sigma}(t) \rangle_0$$

Here we have the problem that Wick's theorem does not hold if $\hat{V}_{ee} \neq 0$. Also, a rotation to the even-odd basis does not help, since $H_T \sim (c_e, c_o)$, cf. page due to the local couplings.

We thus focus on the simple case $V_{ee}=0$ from now on.

<u>$V_{ee}=0$</u>

Wick's theorem applies to the commutator C. It becomes

$$\langle \dots \rangle_0 \underset{\text{wick}}{=} \underbrace{\langle \hat{c}^{+}_{L\vec{k}\sigma}(t) \hat{d}_{1\sigma}(t) \rangle_0}_{\times} \langle \hat{d}^{+}_{1\sigma'} \hat{c}_{L\vec{k}'\sigma'} \rangle_0 +$$

$$\langle \hat{c}^{+}_{L\vec{k}\sigma}(t) \hat{c}_{L\vec{k}'\sigma'} \rangle_0 \langle \hat{d}_{1\sigma}(t) \hat{d}^{+}_{1\sigma'} \rangle_0$$

$$- \underbrace{\langle \hat{d}^{+}_{1\sigma'} \hat{c}_{L\vec{k}'\sigma'} \rangle_0}_{\times\times} \langle \hat{c}^{+}_{L\vec{k}\sigma}(t) \hat{d}_{1\sigma}(t) \rangle_0$$

$$- \langle \hat{d}^{+(0)}_{1\sigma'} \hat{d}_{1\sigma}(t) \rangle_0 \langle \hat{c}^{(0)}_{L\vec{k}'\sigma'} \hat{c}^{+}_{L\vec{k}\sigma}(t) \rangle_0$$

$\Rightarrow$ $\times$ and $\times\times$ contributions cancel

We recognize lesser and greater GFs

$$B_I(t) = \left(+\frac{e^2}{\hbar^2}\right)\langle [\hat{L}(t), \hat{L}^+(0)]\rangle_0 = \sum_{\vec{k}\vec{k}'} \sum_{\sigma\sigma'} (+e^2)|t_L|^2 \Big[G^<_{L\vec{k}'\sigma' L\vec{k}\sigma}(-t)\, G^>_{1\sigma 1\sigma'}(t)$$
$$- G^<_{1\sigma 1\sigma'}(t)\, G^>_{L\vec{k}'\sigma' L\vec{k}\sigma}(-t)\Big] \quad (4.118a)$$

with $\quad G^>_{xy} = -\frac{i}{\hbar}\langle \hat{x}(t)\hat{y}^+(0)\rangle$

$$G^<_{xy} = \frac{i}{\hbar}\langle \hat{y}^+(0)\,\hat{x}(t)\rangle$$

similarly

$$B_{II}(t) = \left(+\frac{e^2}{\hbar^2}\right)\langle [L^+(t), L(0)]\rangle_0 = \left(+\frac{e^2}{\hbar^2}\right)\sum_{\vec{k}\vec{k}'\sigma\sigma'} |t_L|^2 \langle [\hat{d}^+_{1\sigma}(t)\hat{c}_{L\vec{k}\sigma}(t), \hat{c}^+_{L\vec{k}'\sigma'}\hat{d}_{1\sigma'}]\rangle_0$$

$$= +\frac{e^2}{\hbar^2}\sum_{\vec{k}\vec{k}'\sigma\sigma'} |t_L|^2 \langle \hat{d}^+_{1\sigma}(t)\hat{c}_{L\vec{k}\sigma}(t)\hat{c}^+_{L\vec{k}'\sigma'}\hat{d}_{1\sigma'} - \hat{c}^+_{L\vec{k}'\sigma'}\hat{d}_{1\sigma'}\hat{d}^+_{1\sigma}(t)\hat{c}_{L\vec{k}\sigma}(t)\rangle_0$$

$$= +\frac{e^2}{\hbar^2}\sum_{\vec{k}\vec{k}'\sigma\sigma'} |t_L|^2 \Big\{\langle \hat{d}^+_{1\sigma}(t)\hat{d}_{1\sigma'}\rangle_0 \langle \hat{c}_{L\vec{k}\sigma}(t)\hat{c}^+_{L\vec{k}'\sigma'}\rangle_0 - \langle \hat{c}^+_{L\vec{k}'\sigma'}\hat{c}_{L\vec{k}\sigma}(t)\rangle_0 \langle \hat{d}_{1\sigma'}\hat{d}_{1\sigma}(t)\rangle_0\Big\}$$

$$= +e^2 \sum_{\vec{k}\vec{k}'\sigma\sigma'} |t_L|^2 \Big[G^<_{1\sigma' 1\sigma}(-t)\, G^>_{L\vec{k}\sigma L\vec{k}'\sigma'}(t) - G^<_{L\vec{k}\sigma L\vec{k}'\sigma'}(t)\, G^>_{1\sigma' 1\sigma}(-t)\Big] \quad (4.118b)$$

and

$$B_{III} = \left(-\frac{e^2}{\hbar^2}\right)\langle [\hat{L}(t), \hat{L}(0)]\rangle_0 = \left(-\frac{e^2}{\hbar^2}\right)\sum_{\vec{k}\vec{k}'}\sum_{\sigma\sigma'} (t_L)^2 \langle [c^+_{L\vec{k}\sigma}(t)\, d_{1\sigma}(t), c^+_{L\vec{k}'\sigma'}\, d_{1\sigma'}]\rangle_0$$

$$= -\frac{e^2}{\hbar^2}\sum_{\vec{k}\vec{k}'}\sum_{\sigma\sigma'} (t_L)^2 \langle c^+_{L\vec{k}\sigma}(t)\, d_{1\sigma}(t)\, c^+_{L\vec{k}'\sigma'}(0)\, d_{1\sigma'}(0) - c^+_{L\vec{k}'\sigma'}\, d_{1\sigma'}\, c^+_{L\vec{k}\sigma}(t)\, d_{1\sigma}(t)\rangle_0$$

$$= -\frac{e^2}{\hbar}\sum_{\vec{k}\vec{k}'}\sum_{\sigma\sigma'} (t_L)^2 (+)\Big[\langle c^+_{L\vec{k}\sigma}(t)\, d_{1\sigma'}\rangle_0 \langle d_{1\sigma}(t)\, c^+_{L\vec{k}'\sigma'}\rangle_0 - \langle c^+_{L\vec{k}'\sigma'}\, d_{1\sigma}(t)\rangle_0 \langle d_{1\sigma'}\, c^+_{L\vec{k}\sigma}(t)\rangle$$

$$= -e^2 \sum_{\vec{k}\vec{k}'} \sum_{\sigma\sigma'} (t_L)^2 \left[g^<_{1\sigma' L\vec{k}\sigma}(-t)\, g^>_{1\sigma L\vec{k}'\sigma'}(t) - g^<_{1\sigma L\vec{k}'\sigma'}(t)\, g^>_{1\sigma' L\vec{k}\sigma}(-t) \right] \quad (4.118_c)$$

Finally

$B_{IV} =$

$$-\frac{e^2}{\hbar^2} \langle [L^+(t), L^+(0)] \rangle_0 = -\frac{e^2}{\hbar} \sum_{\vec{k}\vec{k}'} \sum_{\sigma\sigma'} (t_L^*)^2 \langle [\hat{d}^+_{1\sigma}(t)\, \hat{c}_{L\vec{k}\sigma}(t), d^+_{1\sigma'} \hat{c}_{L\vec{k}'\sigma'}] \rangle_0$$

$$= -\frac{e^2}{\hbar} \sum_{\vec{k}\vec{k}'} \sum_{\sigma\sigma'} (t_L^*)^2 \{ \langle \hat{d}^+_{1\sigma}(t)\, \hat{c}_{L\vec{k}'\sigma'} \rangle_0 \langle \hat{c}_{L\vec{k}\sigma}(t)\, \hat{d}^+_{1\sigma'} \rangle_0 -$$

$$- \langle \hat{d}^+_{1\sigma'}\, \hat{c}_{L\vec{k}\sigma}(t) \rangle \langle \hat{c}_{L\vec{k}'\sigma'}\, \hat{d}^+_{1\sigma}(t) \rangle_0]$$

$$= -e^2 \sum_{\vec{k}\vec{k}'} \sum_{\sigma\sigma'} (t_L^*)^2 \left[g^<_{L\vec{k}'\sigma' 1\sigma}(-t)\, g^>_{L\vec{k}\sigma 1\sigma'}(t) - g^<_{L\vec{k}\sigma 1\sigma'}(t)\, g^>_{L\vec{k}'\sigma' 1\sigma}(-t) \right]$$

(4.118d

Summorizing

$$B_I(t) = +\frac{e^2}{\hbar^2} \langle [\hat{L}(t), \hat{L}^+(0)] \rangle_0 = +e^2 \sum_{\vec{k}\vec{k}'} \sum_{\sigma\sigma'} |t_L|^2 \left[G^<_{L\vec{k}'\sigma' L\vec{k}\sigma}(-t)\, G^>_{1\sigma 1\sigma'}(t) - G^<_{1\sigma 1\sigma'}(t)\, G^>_{L\vec{k}\sigma' L\vec{k}\sigma}(-t) \right]$$

(I)

$$B_{II} = +\frac{e^2}{\hbar^2} \langle [\hat{L}^+(t), \hat{L}(0)] \rangle_0 = +e^2 \sum_{\vec{k}\vec{k}'} \sum_{\sigma\sigma'} |t_L|^2 \left[G^<_{1\sigma' 1\sigma}(-t)\, G^>_{L\vec{k}\sigma L\vec{k}'\sigma'}(t) - G^<_{L\vec{k}\sigma L\vec{k}'\sigma'}(t)\, G^>_{1\sigma' 1\sigma}(-t) \right]$$

(II)

$$B_{III} = -\frac{e^2}{\hbar^2} \langle [\hat{L}(t), \hat{L}(0) \rangle_0 = -e^2 \sum_{\vec{k}\vec{k}'} \sum_{\sigma\sigma'} (t_L)^2 \left[g^<_{1\sigma' L\vec{k}\sigma}(-t)\, g^>_{1\sigma L\vec{k}'\sigma'}(t) - g^<_{1\sigma L\vec{k}'\sigma'}(t)\, g^>_{1\sigma' L\vec{k}\sigma}(-t) \right]$$

III

$$B_{IV} = -\frac{e^2}{\hbar^2} \langle [L^+(t), L^+(0)] \rangle_0 = -e^2 \sum_{\vec{k}\vec{k}'} \sum_{\sigma\sigma'} (t_L^*)^2 \left[g^<_{L\vec{k}'\sigma' 1\sigma}(-t)\, g^>_{L\vec{k}\sigma 1\sigma'}(t) - g^<_{L\vec{k}\sigma 1\sigma'}(t)\, g^>_{L\vec{k}'\sigma' 1\sigma}(-t) \right]$$

IV

Notice:

a) $B_{I}(-t) = -B_{II}(t)$, $B_{III}(-t) = -B_{III}(t)$

$B_{IV}(-t) = -B_{IV}(t)$

$$\Rightarrow B_{I} + B_{II} + B_{III} + B_{IV} = \underline{\underline{B(t) = -B(-t)}}$$

b) Further, due to $\left(G^{>}_{xy}(t)\right)^{*} = \left(-\frac{i}{\hbar}\langle \hat{x}(t)\,\hat{y}^{+}(0)\rangle\right)^{*} = \frac{i}{\hbar}\langle \hat{y}(0)\,\hat{x}^{+}(t)\rangle$

Lehmann (check)

$$= \frac{i}{\hbar} G^{>}_{yx}(-t)$$

$$G^{>}_{xy}(t) = -\frac{i}{Z}\sum_{mm'} \langle m|e^{-\beta\hat{H}}\hat{x}|m'\rangle\langle m'|\hat{y}^{+}|m\rangle e^{i(E_m - E_{m'})\frac{t}{\hbar}}$$

$$\hookrightarrow G^{>}_{xy}(t)^{*} = \frac{i}{Z}\sum_{mm'} e^{-\beta E_m} x^{*}_{mm'} (y^{*}_{mm'})^{*} e^{-i(E_m - E_{m'})\frac{t}{\hbar}}$$

$$= \frac{i}{Z}\sum_{mm'} e^{-\beta E_m} (x^{+})_{m'm}\, y_{mm'}\, e^{-i(E_m - E_{m'})\frac{t}{\hbar}}$$

$$\Rightarrow \begin{cases} (B_{I})^{*} = -B_{II} \\ (B_{III})^{*} = -B_{IV} \end{cases}$$ also for $t_\alpha \in \mathbb{C}$

and hence $\underline{\underline{B^{*}(t) = -B(t)}}$ $\Rightarrow$ $B(t)$ pure imaginary

c)

(a) + (b) $\Rightarrow$ $B(t)$ pure imaginary and odd

Step III: Imaginary part of the response function

According to (4.117) is

$$\tilde{\chi}^{R}_{II}(\omega) = -\frac{i}{\hbar}\int_0^{\infty} dt\, e^{i\omega t} B(t) \qquad (4.119)$$

hence due to (c)

$$\mathrm{Im}\,\tilde{\chi}^{R}_{II}(\omega) = -\frac{1}{\hbar}\frac{1}{2}\int_{-\infty}^{+\infty} dt\, e^{i\omega t} B(t) \qquad (4.119b)$$

$B(t)$ purely imaginary and odd

$$\mathrm{Im}\,\tilde{\chi}^{R} = \mathrm{Im}\Big(\underbrace{-\frac{i}{\hbar}\frac{1}{2}\int_{-\infty}^{+\infty} dt\, e^{i\omega t} B(t)}_{\text{purely imaginary}}\Big)$$

$$= \frac{1}{i}\left(-\frac{i}{\hbar}\frac{1}{2}\int_{-\infty}^{+\infty} dt\, e^{i\omega t} B(t)\right)$$

Use

$$\int dt\, e^{i\omega t} f(t) g(-t) = \int \frac{d\omega'}{2\pi} \tilde{f}(\omega+\omega') \tilde{g}(\omega')$$

to get

$$\mathrm{Im}\, \tilde{\chi}^R_{II}(\omega) = (+e^2)\left(-\frac{1}{2\hbar}\right) \int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi} \sum_{\vec{k}\vec{k}'} \sum_{\sigma\sigma'} \cdot$$

$$(-)\Big[\Big(\underset{(\mathrm{II}\,b)}{G^>_{1\sigma'1\sigma}(\omega')\, G^<_{L\vec{k}\sigma L\vec{k}'\sigma'}(\omega'+\omega)} - \underset{(\mathrm{II}\,a)}{G^<_{1\sigma'1\sigma}(\omega')\, G^>_{L\vec{k}\sigma L\vec{k}'\sigma'}(\omega'+\omega)} \Big) |t_L|^2$$

$$+ \Big(\underset{(\mathrm{I}\,b)}{G^<_{1\sigma 1\sigma'}(\omega')\, G^>_{L\vec{k}'\sigma' L\vec{k}\sigma}(\omega'-\omega)} - \underset{\mathrm{I}\,a)}{G^>_{1\sigma 1\sigma'}(\omega')\, G^<_{L\vec{k}'\sigma' L\vec{k}\sigma}(\omega'-\omega)} \Big) |t_L|^2$$

$$- t_L^2 \Big(+ \underset{(\mathrm{III}\,b)}{g^>_{1\sigma' L\vec{k}\sigma}(\omega')\, g^<_{1\sigma L\vec{k}'\sigma'}(\omega'+\omega)} - \underset{(\mathrm{III}\,a)}{g^<_{1\sigma' L\vec{k}\sigma}(\omega')\, g^>_{1\sigma L\vec{k}'\sigma'}(\omega'+\omega)} \Big)$$

or $g^>_{1\sigma L\vec{k}'\sigma'}(\omega')\, g^<_{1\sigma' L\vec{k}\sigma}(\omega'-\omega)$

or $g^<_{L\vec{k}'\sigma' 1\sigma}(\omega')\quad g^>_{L\vec{k}\sigma 1\sigma'}(\omega'+\omega)$

$$- (t^*_L)^2 \Big(\underset{(\mathrm{IV}\,b)}{g^<_{L\vec{k}\sigma 1\sigma'}(\omega')\, g^>_{L\vec{k}'\sigma' 1\sigma}(\omega'-\omega)} - \underset{\mathrm{IV}\,a}{g^>_{L\vec{k}\sigma 1\sigma'}(\omega')\, g^<_{L\vec{k}'\sigma' 1\sigma}(\omega'-\omega)} \Big) \Big]$$

$\vec{k}, \vec{k}'$ as well as σ, σ' are dummy variables

$\Rightarrow$ change $\vec{k} \to \vec{k}'$ and $\sigma \to \sigma'$ in terms with "$-$" in front in I and II

$$\mathrm{Im}\, \tilde{\chi}^R_{II}(\omega) = e^2\left(-\frac{1}{2\hbar}\right) \int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi} \sum_{\vec{k}\vec{k}'} \sum_{\sigma\sigma'} \tag{4.119a}$$

$$\Big[|t_L|^2 \tilde{G}^>_{1\sigma'1\sigma}(\omega') \Big(\tilde{G}^<_{L\vec{k}\sigma L\vec{k}'\sigma'}(\omega'+\omega) - \tilde{G}^<_{L\vec{k}\sigma L\vec{k}'\sigma'}(\omega'-\omega) \Big) - |t_L|^2 \tilde{G}^<_{1\sigma'1\sigma}(\omega') \Big(\tilde{G}^>_{L\vec{k}\sigma \vec{k}'\sigma'}(\omega'+\omega) - \tilde{G}^>_{L\vec{k}'\sigma L\vec{k}\sigma'}(\omega'-\omega) \Big)$$

$$+ \Big(\tilde{g}^>_{1\sigma' L\vec{k}\sigma}(\omega')\, t_L^2 \big(\tilde{g}^<_{1\sigma L\vec{k}'\sigma'}(\omega'+\omega) - \tilde{g}^<_{1\sigma L\vec{k}'\sigma'}(\omega'-\omega) \big) - \tilde{g}^<_{L\vec{k}'\sigma' 1\sigma}(\omega')\, t_L^{*2} \big(\tilde{g}^>_{L\vec{k}\sigma 1\sigma'}(\omega'+\omega) - \tilde{g}^>_{L\vec{k}\sigma 1\sigma'}(\omega'-\omega) \big) \Big) \Big]$$

i) Notice that (4.119) has more terms, coming from the mixed GF $g^>, g^<$, than the expression (4.83) for the single dot case.

ii) The relations
$$\begin{cases} \tilde{G}^<_{xy}(\omega) = -\tilde{G}^>_{yx}(\omega)\, e^{-\beta(\hbar\omega-\mu_0)} & (4.120a) \\ \tilde{G}^A_{xy}(\omega) = \left(\tilde{G}^R_{yx}(\omega)\right)^* & (4.120b) \end{cases}$$

hold true for the equilibrium GFs, as well as
$$G^R - G^A = G^> - G^< \qquad (4.120c)$$

Again one can introduce the spectral function
$$A_{xy}(\omega) = -2\,\mathrm{Im}\,\tilde{G}^R_{xy}(\omega) \qquad (4.121)$$

Using the relations above
$$\begin{cases} A_{xy}(\omega) = i\left(1+e^{-\beta(\hbar\omega-\mu_0)}\right)\tilde{G}^>_{xy}(\omega) & (4.122a) \\ \tilde{G}^>_{xy}(\omega) = -i\left(1-f(\omega)\right)A_{xy}(\omega) & (4.122b) \end{cases}$$

and also
$$\begin{cases} \tilde{G}^>_{xy}(\omega) = [1-f(\omega)]\left(\tilde{G}^R_{xy}(\omega) - \tilde{G}^A_{xy}(\omega)\right) & (4.123a) \\ \tilde{G}^<_{xy}(\omega) = -f(\omega)\underbrace{\left(\tilde{G}^R_{xy}(\omega) - \tilde{G}^A_{xy}(\omega)\right)}_{2i\,\mathrm{Im}\,\tilde{G}^R} & (4.123b) \end{cases}$$

$$\Rightarrow \begin{cases} \tilde{G}^>_{xy} = -i A_{xy}\left(1-f(\omega)\right) \\ \tilde{G}^<_{xy} = i A_{xy} f(\omega) \end{cases}$$

Hence

$$\mathrm{Im}\,\tilde{\chi}^R_{II}(\omega) = -\frac{e^2}{2\hbar}\int_{-\infty}^{+\infty}\frac{d\omega'}{2\pi}\sum_{\vec{k}\vec{k}'}\sum_{\sigma\sigma'}\Big\{$$

$$|t_L|^2\Big[(1-f(\omega'))A_{1\sigma'1\sigma}(\omega')\big(-A_{Lk\sigma Lk'\sigma'}(\omega'+\omega)f(\omega'+\omega) + f(\omega'-\omega)A_{Lk\sigma Lk'\sigma'}(\omega'-\omega)\big) +$$

$$+ f(\omega')A_{1\sigma'1\sigma}(\omega')\big((1-f(\omega'+\omega))A_{Lk\sigma Lk'\sigma'}(\omega'+\omega) - (1-f(\omega'-\omega))A_{Lk\sigma Lk'\sigma'}(\omega'-\omega)\big)\Big]$$

$$-t_L^2(1-f(\omega'))\,a_{1\sigma' Lk\sigma}(\omega')\big(-f(\omega'+\omega)\,a_{1\sigma Lk'\sigma'}(\omega'+\omega) + f(\omega'-\omega)\,a_{1\sigma Lk'\sigma'}(\omega'-\omega)\big)$$

$$-(t_L^*)^2 f(\omega')\,a_{Lk'\sigma'1\sigma}(\omega')\big((1-f(\omega'+\omega))\,a_{Lk\sigma 1\sigma'}(\omega'+\omega) - (1-f(\omega'-\omega))\,a_{Lk\sigma 1\sigma'}(\omega'-\omega)\big)\Big\}$$

$\Rightarrow$ terms with products of Fermi functions cancel in A-terms

Thus

$$\mathrm{Im}\,\tilde{\chi}^R_{II}(\omega) = -\frac{e^2}{2\hbar}\int_{-\infty}^{+\infty}\frac{d\omega'}{2\pi}\sum_{\vec{k}\vec{k}'}\sum_{\sigma\sigma'}$$

$$\Big\{\Big[A_{1\sigma'1\sigma}(\omega')A_{Lk\sigma Lk'\sigma'}(\omega'+\omega)\underbrace{\big(-f(\omega'+\omega)+f(\omega')\big)}_{-\frac{\partial f}{\partial\omega'}\hbar\omega} +$$

$$+A_{1\sigma'1\sigma}(\omega')A_{Lk\sigma Lk'\sigma'}(\omega'-\omega)\underbrace{\big(f(\omega'-\omega)-f(\omega')\big)}_{\frac{\partial f}{\partial\omega'}(-\omega)}\Big]|t_L|^2$$

$$+\Big[-f(\omega')f(\omega'+\omega)\big(a_{1\sigma'Lk\sigma}(\omega')\,a_{1\sigma Lk'\sigma'}(\omega'+\omega)\,t_L^2 - a_{Lk'\sigma'1\sigma}(\omega')\,a_{Lk\sigma 1\sigma'}(\omega'+\omega)(t_L^*)^2\big)$$

$$+f(\omega')f(\omega'-\omega)\big(a_{1\sigma'Lk\sigma}(\omega')\,a_{1\sigma Lk'\sigma'}(\omega'-\omega)\,t_L^2 - a_{Lk'\sigma'1\sigma}(\omega')\,a_{Lk\sigma 1\sigma'}(\omega'-\omega)\,t_L^*$$

$$+f(\omega'+\omega)\,a_{1\sigma'Lk\sigma}(\omega')\,a_{1\sigma Lk'\sigma'}(\omega'+\omega)\,t_L^2 - f(\omega'-\omega)\,a_{1\sigma'Lk\sigma}(\omega')\,a_{1\sigma Lk'\sigma'}(\omega'-\omega)\,t_L^2 +$$

$$- f(\omega')\, a_{Lk'\sigma' 1\sigma}(\omega')\, a_{Lk\sigma 1\sigma'}(\omega'+\omega)\, t_L^{*2} + f(\omega')\, a_{Lk'\sigma' 1\sigma}(\omega')\, a_{Lk\sigma 1\sigma'}(\omega'-\omega)\, t_L^{*2}]\}$$

Consider [...]

by making a variable transformation

$$f(\omega')\, f(\omega'-\omega) \Big(a_{1\sigma' Lk\sigma}(\omega')\, a_{1\sigma L k'\sigma'}(\omega'-\omega)\, t_L^2 - a_{Lk'\sigma' 1\sigma'}(\omega')\, a_{Lk\sigma 1\sigma'}(\omega'-\omega)\, t_L^{*2}$$

$$\to f(\omega'+\omega)\, f(\omega') \Big(a_{1\sigma' Lk\sigma}(\omega'+\omega)\, a_{1\sigma L k'\sigma'}(\omega')\, t_L^2 - a_{Lk'\sigma' 1\sigma'}(\omega'+\omega)\, a_{Lk\sigma 1\sigma'}(\omega')\, t_L^{*2} \Big)$$

which cancels with first line upon $\begin{matrix} k \to k' \\ \sigma \to \sigma' \end{matrix}$

Similarly, the third and fourth line become

$$a_{1\sigma' Lk\sigma}(\omega')\, a_{1\sigma L k'\sigma'}(\omega'+\omega) \big(f(\omega'+\omega) - f(\omega') \big)\, t_L^2$$

$$+ a_{Lk'\sigma' 1\sigma}(\omega')\, a_{Lk\sigma 1\sigma'}(\omega'-\omega) \big(f(\omega') - f(\omega'-\omega) \big) \big(t_L^* \big)^2$$

We thus find for $\underline{\omega \to 0}$

$$\boxed{\begin{aligned} \operatorname{Im} \tilde{\chi}^R_{II}(\omega) = -\frac{e^2}{\hbar}\, \omega \int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi} \sum_{\vec{k}\vec{k}'} \sum_{\sigma\sigma'} (t_L)^2 \left(-\frac{\partial f}{\partial \omega'} \right) \qquad (4.124) \\ \Big[A_{1\sigma' 1\sigma}(\omega')\, A_{Lk\sigma Lk'\sigma'}(\omega') - \frac{1}{2} \Big(t_L^2\, a_{1\sigma' Lk\sigma}(\omega')\, a_{1\sigma Lk'\sigma'}(\omega') + t_L^{*2}\, a_{Lk'\sigma' 1\sigma}(\omega')\, a_{Lk\sigma 1\sigma'}(\omega') \Big) \Big] \end{aligned}}$$

Remember

$$a_{xy} = -2\,\mathrm{Im}\,\tilde{g}^R_{xy} = i\left(\tilde{g}^R_{xy} - \tilde{g}^A_{xy}\right)$$

and

$$\tilde{g}^R_{xy} = \left(\tilde{g}^A_{yx}\right)^*$$

$$\Rightarrow a_{yx}(\omega) = -2\,\mathrm{Im}\,\tilde{g}^R_{yx}(\omega) = i\left[\left(\tilde{g}^A_{xy}\right)^* - \left(\tilde{g}^R_{xy}\right)^*\right]$$

$$= -i\left[\left(\tilde{g}^R_{xy}\right)^* - \left(\tilde{g}^A_{xy}\right)^*\right] = a^*_{xy}(\omega) \underset{\uparrow}{=} a_{xy}$$

a_{xy} is real

The conductance formula thus simplifies to

$$\left(G = -\lim_{\omega \to 0} \omega\,\mathrm{Im}\,\chi^R_{IJ}(\omega)\right)$$

$$\boxed{G = \frac{e^2}{\hbar} \int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi} \sum_{\vec{k}\vec{k}'} \sum_{\sigma\sigma'} |t_L|^2 \left(-\frac{\partial f}{\partial \omega'}\right) \Big[\underbrace{A_{1\sigma' 1\sigma}(\omega')\, A_{Lk\sigma\, Lk'\sigma'}(\omega')}_{(a)} - \underbrace{\mathrm{Re}\left(a_{1\sigma' Lk\sigma}(\omega')\, a_{1\sigma Lk'\sigma'}(\omega')\right)}_{(b)} \Big]}$$

(4.124b)

4.90 (lecture)

<u>Note</u>: The first term of (4.124b) resembles the SIAM.

However, with the notable difference that there we had

$$A_{1\sigma' 1\sigma}(\omega')\, A_{0k\sigma\, 0k'\sigma'}(\omega')$$

i.e. the lead spectral function of the <u>odd</u> electrons!

Evaluation of retarded GF and then of A_{xy} , a_{xy}

We use again the EOM. Start with $G^R_{1\sigma' 1\sigma'}$ $\rightsquigarrow$ see also exercise 1 sheet 12

a) $$G^R_{1\sigma' 1\sigma}(t) = -\frac{i}{\hbar}\,\theta(t)\,\langle \{ \hat{d}_{1\sigma'}(t) , \hat{d}^+_{1\sigma}(0) \} \rangle_0$$

$\hookrightarrow$ $$i\hbar\,\partial_t G^R_{1\sigma' 1\sigma}(t) = \delta(t)\,\langle \{ \hat{d}_{1\sigma'}(t), \hat{d}^+_{1\sigma}(0) \}\rangle_0 - \frac{i}{\hbar}\,\theta(t)\,\langle \{ i\hbar\,\dot{\hat{d}}_{1\sigma'}(t), \hat{d}^+_{1\sigma}(0) \}\rangle$$

$$= \delta(t)\,\langle \underbrace{\{ \hat{d}_{1\sigma'} , \hat{d}^+_{1\sigma} \}}_{\delta_{\sigma\sigma'}} \rangle_0 - \frac{i}{\hbar}\,\theta(t)\,\langle - \{ [\hat{H}, \hat{d}_{1\sigma'}](t) , \hat{d}^+_{1\sigma} \} \rangle_0$$

with the total Hamiltonian

$$\Big(\hat{H} = \sum_{i\sigma} \varepsilon_{i\sigma}\, \hat{d}^+_{i\sigma} \hat{d}_{i\sigma} + \sum_{\sigma} \big(t_{12}\, \hat{d}^+_{1\sigma} \hat{d}_{2\sigma} + t^*_{12}\, \hat{d}^+_{2\sigma} \hat{d}_{1\sigma} \big) + \sum_{k\sigma i} \big(t_\alpha\, \hat{c}^+_{\alpha k\sigma} \hat{d}_{i\alpha\sigma} + h.c. \big) \Big)$$

$+ \hat{H}_{leads}$

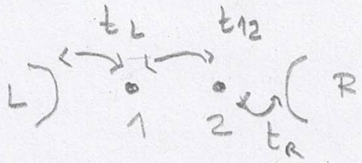
$\hookrightarrow$ $$[\hat{H} , \hat{d}_{1\sigma'}] = -\varepsilon_1 \hat{d}_{1\sigma'} - t_{12}\, \hat{d}_{2\sigma'} - \sum_{\vec{k}} t^*_L\, \hat{c}_{Lk\sigma'}$$

check t_L or t^*_L

$\hookrightarrow$ $$i\hbar\, G^R_{1\sigma' 1\sigma} = \delta(t)\,\delta_{\sigma\sigma'} - \varepsilon_1 G^R_{1\sigma' 1\sigma} - t_{12}\, G^R_{2\sigma' 1\sigma}(t) - \sum_{\vec{k}} t^*_L\, g^R_{Lk\sigma' 1\sigma}(t)$$

$\hookrightarrow$ $$\boxed{(\hbar\omega - \varepsilon_1 + i\eta)\, \tilde{G}^R_{1\sigma' 1\sigma} = \delta_{\sigma\sigma'} + t_{12}\, \tilde{G}^R_{2\sigma' 1\sigma}(\omega) + \sum_{\vec{k}} t^*_L\, \tilde{g}^R_{Lk\sigma' 1\sigma}(\omega)} \qquad (4.125)$$

new GF



Similarly

$$\delta(t)\,\langle\{d_{2\sigma},\,d^{+}_{1\sigma}\}\rangle$$

$$\begin{cases} (\hbar\omega-\varepsilon_2+i\eta)\,\tilde{G}^R_{2\sigma'1\sigma}(\omega) = 0 + t^*_{12}\,\tilde{G}^R_{1\sigma'1\sigma}(\omega) + \sum_{\vec{k}} t^*_R\,\tilde{g}^R_{R\vec{k}\sigma'1\sigma}(\omega) \\ (\hbar\omega-\varepsilon_{Lk\sigma'}+i\eta)\,\tilde{g}^R_{Lk\sigma'1\sigma}(\omega) = 0 + t_L\,\tilde{G}^R_{1\sigma'1\sigma}(\omega) \\ (\hbar\omega-\varepsilon_{Rk\sigma'}+i\eta)\,\tilde{g}^R_{Rk\sigma'1\sigma}(\omega) = 0 + t_R\,\tilde{G}^R_{2\sigma'1\sigma}(\omega) \end{cases} \qquad (4.126)$$

solving for the mixed GF

$$\tilde{g}^R_{Lk\sigma'1\sigma}(\omega) = \frac{t_L}{\hbar\omega-\varepsilon_{Lk\sigma'}+i\eta}\,\tilde{G}^R_{1\sigma'1\sigma} \qquad (4.127a)$$

$$\tilde{g}^R_{Rk\sigma'1\sigma}(\omega) = \frac{t_R}{\hbar\omega-\varepsilon_{Rk\sigma'}+i\eta}\,\tilde{G}^R_{2\sigma'1\sigma}(\omega) \qquad (4.127b)$$

and substituting in the expressions for $\tilde{G}^R_{1\sigma'1\sigma}$, $\tilde{G}^R_{2\sigma'1\sigma}$

$$\begin{cases} (\hbar\omega-\varepsilon_1+i\eta)\,\tilde{G}^R_{1\sigma'1\sigma} = \delta_{\sigma\sigma'} + t_{12}\,\tilde{G}^R_{2\sigma'1\sigma}(\omega) + \underbrace{\left(\sum_{\vec{k}} \frac{|t_L|^2}{\hbar\omega-\varepsilon_{Lk\sigma'}+i\eta}\right)}_{\equiv \Sigma^{\sigma'}_L(\omega)}\tilde{G}^R_{1\sigma'1\sigma} \\ (\hbar\omega-\varepsilon_2+i\eta)\,\tilde{G}^R_{2\sigma'1\sigma}(\omega) = t^*_{12}\,\tilde{G}^R_{1\sigma'1\sigma}(\omega) + \underbrace{\sum_{\vec{k}} \frac{|t_R|^2}{\hbar\omega-\varepsilon_{Rk\sigma'}+i\eta}}_{\equiv \Sigma^{\sigma'}_R(\omega)}\,\tilde{G}^R_{2\sigma'1\sigma}(\omega) \end{cases}$$

Again we see that the coupling to the left/right leads induces a finite self-energy Σ_L / Σ_R to the GF $\tilde{G}^R_{1\sigma'1\sigma}$ and $\tilde{G}^R_{2\sigma'1\sigma}$

$$\begin{cases} \left(\hbar\omega - \varepsilon_1 + i\eta - \Sigma_L(\omega)\right) \tilde{G}^R_{1\sigma'1\sigma} = \delta_{\sigma\sigma'} + t_{12}\, \tilde{G}^R_{2\sigma'1\sigma}(\omega) \\ \left(\hbar\omega - \varepsilon_2 + i\eta - \Sigma_R(\omega)\right) \tilde{G}^R_{2\sigma'1\sigma}(\omega) = t^*_{12}\, \tilde{G}^R_{1\sigma'1\sigma}(\omega) \end{cases} \qquad (4.129)$$

further, in the wide-band limit $\begin{cases} \Sigma_\alpha(\omega) = -i\frac{\hbar}{2}\Gamma_\alpha \\ \Gamma_\alpha = \frac{2\pi}{\hbar} |t_\alpha|^2 \varrho_\alpha(\mu_0) \end{cases}$

Solving for $\tilde{G}^R_{2\sigma'1\sigma}$

$$\tilde{G}^R_{2\sigma'1\sigma}(\omega) = \frac{t^*_{12}}{\hbar\omega - \varepsilon_2 - \Sigma_R}\, \tilde{G}^R_{1\sigma'1\sigma}$$

and hence

$$\tilde{G}^R_{1\sigma'1\sigma} = \frac{\delta_{\sigma\sigma'}}{\hbar\omega - \varepsilon_1 - \Sigma_L(\omega) - \dfrac{|t_{12}|^2}{\hbar\omega - \varepsilon_2 - \Sigma_R}}$$

i.e.

$$\boxed{\tilde{G}^R_{1\sigma'1\sigma} = \frac{\delta_{\sigma\sigma'}\left(\hbar\omega - \varepsilon_2 - \Sigma_R\right)}{\left(\hbar\omega - \varepsilon_1 - \Sigma_L(\omega)\right)\left(\hbar\omega - \varepsilon_2 - \Sigma_R\right) - |t_{12}|^2}} \qquad (4.129)$$

Note: We can look at (4.127) in matrix form

$$\underbrace{\begin{pmatrix} \hbar\omega - \varepsilon_1 + i\eta - \Sigma_L & -t_{12} \\ -t^*_{12} & \hbar\omega - \varepsilon_2 + i\eta - \Sigma_R \end{pmatrix}}_{\hbar\omega \mathbb{1}_2 - \mathcal{H}_S} \begin{pmatrix} \tilde{G}^R_{1\sigma' 1\sigma} \\ \tilde{G}^R_{2\sigma' 1\sigma} \end{pmatrix} = \begin{pmatrix} \delta_{\sigma\sigma'} \\ 0 \end{pmatrix}$$

similarly, we can look at the eqs. for $\tilde{G}^R_{1\sigma' 2\sigma}$ and $\tilde{G}^R_{2\sigma' 2\sigma}$

$$\boxed{\underbrace{\begin{pmatrix} \hbar\omega - \varepsilon_1 + i\eta - \Sigma_L & -t_{12} \\ -t^*_{12} & \hbar\omega - \varepsilon_2 + i\eta - \Sigma_R \end{pmatrix}}_{\hbar\omega\mathbb{1}_2 - h_S - \bar{\Sigma}} \underbrace{\begin{pmatrix} \tilde{G}^R_{1\sigma' 1\sigma} & \tilde{G}^R_{1\sigma' 2\sigma} \\ \tilde{G}^R_{2\sigma' 1\sigma} & \tilde{G}^R_{2\sigma' 2\sigma} \end{pmatrix}}_{\tilde{G}^R} = \delta_{\sigma\sigma'} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}} \quad (4.130)$$

i.e. for an N-site system one can introduce a matrix $\tilde{G}^R(E)$ such that $E\mathbb{1}_N - h_S - \bar{\Sigma}$ multiplied by $\tilde{G}^R(E)$ yields the unity matrix $\mathbb{1}_N$.

Here we work in the localized basis, and the matrix h_S represents the one-body system hamiltonian. The matrix $\bar{\Sigma}$ stems from the leads, whose effects are fully encapsulated in the self-energies $\Sigma_L, \Sigma_R \rightsquigarrow \bar{\Sigma} = \begin{pmatrix} \Sigma_L & 0 \\ 0 & \Sigma_R \end{pmatrix}$

By inverting (4.129) and setting $\sigma=\sigma'$ $\Rightarrow$ $\tilde{G}^R_{1\sigma 1\sigma} = \tilde{G}^R_{11}$ etc.

$$\begin{pmatrix} \tilde{G}^R_{11}(\omega) & \tilde{G}^R_{12}(\omega) \\ \tilde{G}^R_{21}(\omega) & \tilde{G}^R_{22}(\omega) \end{pmatrix} \underset{(*)}{\overset{\uparrow}{=}} \frac{\begin{pmatrix} \hbar\omega - \varepsilon_2 - \Sigma_R & + t_{12} \\ + t^*_{12} & \hbar\omega - \varepsilon_1 - \Sigma_L \end{pmatrix}}{(\hbar\omega - \varepsilon_1 - \Sigma_L)(\hbar\omega - \varepsilon_2 - \Sigma_R) - |t_{12}|^2} \tag{4.130b}$$

Finally, introducing the matrices

$$\boxed{\bar{\Sigma}_L = \Sigma_L \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \bar{\Sigma}_R = \Sigma_R \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad \mathcal{H}_0 = \begin{pmatrix} \varepsilon_1 & t_{12} \\ t^*_{12} & \varepsilon_2 \end{pmatrix}} \tag{4.131}$$

$$\Rightarrow \boxed{(E - \varepsilon_1 - \Sigma_L)(\hbar\omega - \varepsilon_2 - \Sigma_R) - |t_{12}|^2 = \det\left[E\mathbb{1}_2 - h_S - \bar{\Sigma}_L - \bar{\Sigma}_R\right]} \tag{4.132}$$

And hence

$$\tilde{G}^R = \frac{\begin{pmatrix} \hbar\omega - \varepsilon_2 - \Sigma_R & t_{12} \\ t^*_{12} & \hbar\omega - \varepsilon_1 - \Sigma_L \end{pmatrix}}{\det\left[\hbar\omega\mathbb{1}_2 - h_S - \bar{\Sigma}_L - \bar{\Sigma}_R\right]}$$

(*) We need $(h_S)^{-1}$, where $h_S = \begin{pmatrix} h_{11} & h_{12} \\ h_{21} & h_{22} \end{pmatrix}$

$$\Rightarrow h_S^{-1} = \frac{1}{\det h_S} \begin{pmatrix} h_{22} & -h_{12} \\ -h_{21} & h_{11} \end{pmatrix}$$

To calculate the conductance G we also need the mixed GF

$\underline{\tilde{g}^R_{1\sigma\,Lk'\sigma'}(\omega)}$ as well as the lead GF $\underline{\tilde{G}^R_{Lk\sigma\,Lk'\sigma'}}$.

Again they can be found using the EOM. Start with the lead GF.

$$G^R_{Lk\sigma\,Lk'\sigma'}(t) = -\frac{i}{\hbar}\theta(t)\langle\{\hat{c}_{Lk\sigma}(t), \hat{c}^+_{Lk'\sigma'}(0)\}\rangle_0$$

$$i\hbar\,\partial_t G^R_{Lk\sigma\,Lk'\sigma'}(t) = \delta(t)\underbrace{\langle\{\hat{c}_{Lk\sigma}, \hat{c}^+_{Lk'\sigma'}\}\rangle_0}_{\delta_{kk'}\delta_{\sigma\sigma'}}$$

$$-\frac{i}{\hbar}\theta(t)\langle\{-[\hat{H}, \hat{c}_{Lk\sigma}](t), \hat{c}^+_{Lk'\sigma'}\}\rangle_0$$

$$= \delta(t)\delta_{kk'}\delta_{\sigma\sigma'} + \varepsilon_{Lk\sigma}G^R_{Lk\sigma\,Lk'\sigma'} + t_L\, g^R_{1\sigma\,Lk'\sigma'}$$

$$\hookrightarrow \boxed{(\hbar\omega - \varepsilon_{Lk\sigma} + i\eta)\,\tilde{G}^R_{Lk\sigma\,Lk'\sigma'}(\omega) = \delta_{kk'}\delta_{\sigma\sigma'} + t_L\,\tilde{g}^R_{1\sigma\,Lk'\sigma'}(\omega)} \quad (4.133)$$

On the other hand

$$\tilde{g}^R_{xy}(\omega) = \left(\tilde{g}^A_{yx}(\omega)\right)^*$$

hence

$$\tilde{g}^R_{1\sigma\,Lk'\sigma'}(\omega) = \left(\tilde{g}^A_{Lk'\sigma'\,1\sigma}(\omega)\right)^*$$

Since

$$g^A_{Lk'\sigma' 1\sigma}(t) = \frac{i}{\hbar}\theta(-t)\langle\{c_{Lk'\sigma'}(t), d^+_{1\sigma}\}\rangle_0$$

$$i\hbar\partial_t g^A_{Lk'\sigma' 1\sigma}(t) = -\delta(t)\frac{i}{\hbar}\langle\{c_{Lk'\sigma'}, d^+_{1\sigma}\}\rangle_0 + \frac{i}{\hbar}\theta(-t)\langle\{-[\hat{H}, c_{Lk'\sigma'}](t), d^+_{1\sigma}\}\rangle_0$$

$$\langle\{c_{Lk'\sigma'}, d^+_{1\sigma}\}\rangle_0 = 0$$

$$= \varepsilon_{Lk'} g^A_{Lk'\sigma' 1\sigma}(t) + t_L G^A_{1\sigma' 1\sigma}(t)$$

advanced

$$\hookrightarrow (\hbar\omega - \varepsilon_{Lk'} - i\eta)\tilde{g}^A_{Lk'\sigma 1\sigma}(\omega) = t_L \tilde{G}^A_{1\sigma' 1\sigma}(\omega)$$

$$\boxed{\tilde{g}^A_{Lk'\sigma 1\sigma}(\omega) = \frac{t_L}{\hbar\omega - \varepsilon_{Lk'} - i\eta}\tilde{G}^A_{1\sigma' 1\sigma}(\omega)}$$

check t_L or t_L^*

yielding

$$\boxed{\tilde{g}^R_{1\sigma Lk'\sigma}(\omega) = \frac{t_L^*}{\hbar\omega - \varepsilon_{Lk'} + i\eta}\tilde{G}^R_{1\sigma 1\sigma'}(\omega)} \quad (4.134)$$

We hence find

$$\boxed{\tilde{G}^R_{Lk\sigma Lk'\sigma'}(\omega) = \frac{\delta_{kk'}\delta_{\sigma\sigma'}}{\hbar\omega - \varepsilon_{Lk} + i\eta} + \frac{|t_L|^2}{\hbar\omega - \varepsilon_{Lk} + i\eta}\frac{\tilde{G}^R_{1\sigma 1\sigma'}}{\hbar\omega - \varepsilon_{Lk'} + i\eta}} \quad (4.135)$$

And by summing over the momenta

$$\sum_{\vec{k}\vec{k}'} \tilde{G}^R_{L\vec{k}\sigma\, L\vec{k}'\sigma'}(\omega) = \delta_{\sigma\sigma'} \frac{1}{|t_L|^2} \Sigma_L(\omega) + \frac{1}{|t_L|^2} (\Sigma_L(\omega))^2 \tilde{G}^R_{1\sigma\, 1\sigma'}(\omega)$$

wide band limit $\Sigma_L(\omega) = -i\frac{\hbar}{2}\Gamma_L$

$$\sum_{\vec{k}\vec{k}'} \tilde{G}^R_{L\vec{k}\sigma\, L\vec{k}'\sigma'}(\omega) = -i\frac{\hbar}{2}\frac{\Gamma_L}{|t_L|^2} - \left(\frac{\hbar\Gamma_L}{2}\right)^2 \frac{1}{|t_L|^2} \tilde{G}^R_{1\sigma\, 1\sigma'}(\omega)$$

Hence, cf. (4.124)

$$\boxed{\sum_{\vec{k}\vec{k}'} |t_L|^2 A_{L\vec{k}\sigma\, L\vec{k}'\sigma'}(\omega) = \hbar\Gamma_L - \left(\frac{\hbar\Gamma_L}{2}\right)^2 A_{1\sigma 1\sigma'}(\omega)} \quad (4.136)$$

$A = -2\,\mathrm{Im}\,\tilde{G}^R$

It follows that for the (a) term in (4.124b)

$$\boxed{\sum_{\sigma\sigma'} \sum_{\vec{k}\vec{k}'} |t_L|^2 A_{1\sigma' 1\sigma}(\omega) A_{L\vec{k}\sigma\, L\vec{k}'\sigma'}(\omega) = 2\left[\hbar\Gamma_L - \left(\frac{\hbar\Gamma_L}{2}\right)^2 A_{11}(\omega)\right] A_{11}(\omega)}$$

$$A_{1\sigma' 1\sigma}(\omega) = A_{11}\,\delta_{\sigma\sigma'} \quad (4.136b)$$

We now turn to the (b) term in (4.124b)

$$\sum_{\vec{k}\vec{k}'}\sum_{\sigma\sigma'} a_{1\sigma' Lk\sigma}(\omega')\, a_{1\sigma Lk'\sigma'}(\omega') \quad (t_L)^2$$

$$= \sum_{\vec{k}\vec{k}'}\sum_{\sigma\sigma'} (t_L)^2 \; 4\, \mathrm{Im}\, \tilde{g}^R_{1\sigma' Lk\sigma}\; \mathrm{Im}\, \tilde{g}^R_{1\sigma Lk'\sigma'}$$

$$= \sum_{\sigma\sigma'} (t_L)^2 \; 4 \left(\mathrm{Im} \sum_k \tilde{g}^R_{1\sigma' Lk\sigma}\right)\left(\mathrm{Im} \sum_{k'} \tilde{g}^R_{1\sigma Lk'\sigma'}\right)$$

$$= \sum_{\sigma\sigma'} 4\, \mathrm{Im}\left(e^{-i\varphi_L} \Sigma_L(\omega)\, \tilde{G}^R_{1\sigma 1\sigma'}\right)\left(\mathrm{Im}\, e^{-i\varphi_L} \Sigma_L(\omega)\, \tilde{G}^R_{1\sigma' 1\sigma}\right)$$

(4.134)

$$\tilde{g}^R_{1\sigma Lk'\sigma'}(\omega) = \frac{t_L^*}{\hbar\omega - \varepsilon_{Lk'} + i\eta}\, \tilde{G}^R_{1\sigma 1\sigma'}(\omega) = \frac{|t_L| e^{-i\varphi_L}}{\hbar\omega - \varepsilon_{Lk'} + i\eta}\, \tilde{G}^R_{1\sigma 1\sigma'}(\omega)$$

wide band limit $\quad \Sigma_L(\omega) = -\frac{i\hbar}{2}\Gamma_L$

$$= \sum_{\sigma\sigma'} (\hbar\Gamma_L)^2 \; \mathrm{Re}\left(e^{-i\varphi_L} \tilde{G}^R_{1\sigma 1\sigma'}\right) \mathrm{Re}\left(e^{-i\varphi_L} \tilde{G}^R_{1\sigma' 1\sigma}\right)$$

Remember that $\tilde{G}^R_{1\sigma 1\sigma'} = \delta_{\sigma\sigma'} \tilde{G}^R_{11}$

$$\Rightarrow \boxed{\sum_{kk'}\sum_{\sigma\sigma'} a_{1\sigma' Lk\sigma}(\omega')\, a_{1\sigma Lk'\sigma'}(\omega')\, (t_L)^2 = 2(\hbar\Gamma_L)^2 \left(\mathrm{Re}\, e^{-i\varphi_L} \tilde{G}^R_{11}\right)^2} \qquad (4.137)$$

Collecting (a) + (b)

$$\boxed{G = \frac{2e^2}{\hbar}\int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}\left(-\frac{\partial f}{\partial\omega}\right)\left\{ 2\hbar\Gamma_L A_{11}(\omega) - \left(\frac{\hbar\Gamma_L}{2}\right)^2\left[A_{11}^2(\omega) + \left(2\,\mathrm{Re}\,e^{-i\varphi_L}\tilde{G}^R_{11}\right)^2\right]\right\}} \quad (4.138)$$

if $t_L \in \mathbb{R} \Rightarrow \varphi_L = 0$

$$\boxed{G = \frac{2e^2}{\hbar}\int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}\left(-\frac{\partial f}{\partial\omega}\right)\left\{ \hbar\Gamma_L A_{11}(\omega) - (\hbar\Gamma_L)^2\left[\left(\mathrm{Im}\,\tilde{G}^R_{11}\right)^2 + \left(\mathrm{Re}\,\tilde{G}^R_{11}\right)^2\right]\right\}} \quad (4.138b)$$

The conductance of QD in series is thus not only given by an integral involving only the spectral function $A_{11}(\omega)$ & $\mathrm{Im}\, G^R_{11}$ but also to the real part $\mathrm{Re}\,\tilde{G}^R_{11}$.

<u>Note</u>: Even if only $\Gamma_L \tilde{G}^R_{11}$ appears in (4.138b), as seen from the expression (4.130b) for $\tilde{G}^R_{11}$,

also the self-energy $\Sigma_R = -i\frac{\hbar}{2}\Gamma_R$ and the hopping t_{12} as well the energy ε_2 enter in $\tilde{G}^R_{11}$.

Indeed we find (<u>exercise</u>)

$$\boxed{\hbar\Gamma_L A_{11}(\omega) - (\hbar\Gamma_L)^2|G^R_{11}|^2 = \hbar^2\Gamma_L\Gamma_R \frac{|t_{12}|^2}{|\det(\hbar\omega \mathbb{1}_2 - \mathcal{H}_0 - \bar{\Sigma}_L - \bar{\Sigma}_R)|^2}} \quad (4.\ldots$$

which is perfectly symmetric upon exchange $L \leftrightarrow R$ & $1 \leftrightarrow 2$

By looking explicitly at the matrix $\tilde{G}^R(\omega)$ in (4.130), we see that in fact the result in (4.139) can be recast in terms of the diagonal elements $\tilde{G}^R_{12}$ and $\tilde{G}_{21}$:

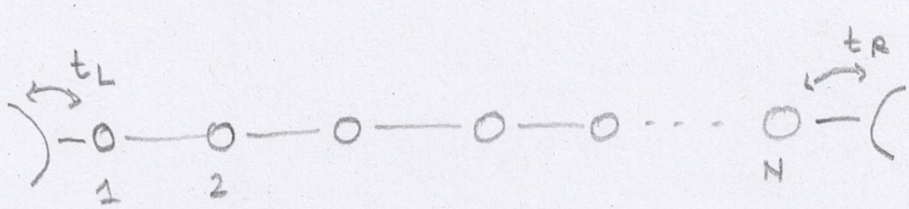
$$\hbar^2 \Gamma_L \Gamma_R \frac{|t_{12}|^2}{|\det(\hbar\omega \mathbb{1}_2 - \mathcal{H}_0 - \Sigma_L - \Sigma_R)|^2} = \hbar^2 \Gamma_L \Gamma_R |\tilde{G}^R_{12}|^2 \tag{4.140}$$

yielding the equivalent result

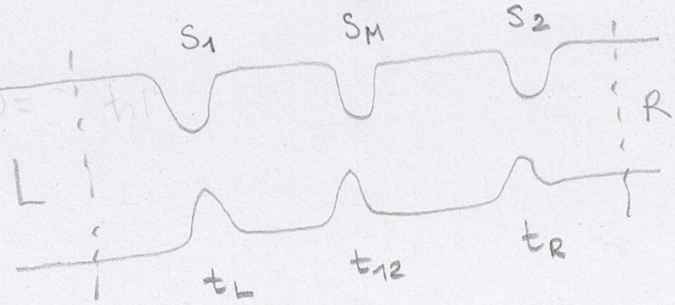
$$\boxed{G = \frac{2e^2}{\hbar} \int \frac{d\omega}{2\pi} \left(-\frac{\partial f}{\partial \omega}\right) \hbar^2 \Gamma_L \Gamma_R |\tilde{G}^R_{12}|^2} \tag{4.141}$$

Note: For N dots in series this result is generalized to

$$\boxed{G = \frac{2e^2}{\hbar} \int \frac{d\omega}{2\pi} \left(-\frac{\partial f}{\partial \omega}\right) \hbar^2 \Gamma_L \Gamma_R |\tilde{G}^R_{1N}|^2} \tag{4.142}$$



Note: By considering again the problem in terms of a scattering problem, we conclude from the Landauer formula that the transmission probability of two-dots in series is



$$G = \frac{2e^2}{h} \int dE \; T(E) \left(-\frac{\partial f}{\partial E}\right)$$

with $\boxed{T(E) = \hbar^2 \Gamma_L \Gamma_R \, |\tilde{G}^R_{12}|^2 = \mathrm{Tr}\{t^\dagger t\}^2}$

being the transmission probability associated to the total S-matrix $S = S_1 \otimes S_M \otimes S_2$

i.e.

$$\boxed{T(E) = \hbar^2 \Gamma_L \Gamma_R \frac{|t_{12}|^2}{|\det(E \mathbb{1}_2 - h_S - \overline{\Sigma}_L - \overline{\Sigma}_R)|^2}} \quad (4.140)$$

<u>Note</u> : Trace formula for the transmission matrix

We have already introduced the matrix forms of the GF $\tilde{G}^{R/A}$ as well as of the self-energies $\bar{\Sigma}_R$ and $\bar{\Sigma}_L$:

$$\tilde{G}^R = \begin{pmatrix} \tilde{G}^R_{11} & \tilde{G}^R_{12} \\ \tilde{G}^R_{21} & \tilde{G}^R_{22} \end{pmatrix}, \quad \tilde{G}^A = \begin{pmatrix} \tilde{G}^A_{11} & \tilde{G}^A_{12} \\ \tilde{G}^A_{21} & \tilde{G}^A_{22} \end{pmatrix}$$

$$\bar{\Sigma}_R = \begin{pmatrix} 0 & 0 \\ 0 & \Sigma_R \end{pmatrix}, \quad \bar{\Sigma}_L = \begin{pmatrix} \Sigma_L & 0 \\ 0 & 0 \end{pmatrix}$$

in wide-band limit
$$\Sigma_R = -i\frac{\hbar\Gamma_R}{2}, \quad \Sigma_L = -i\frac{\hbar}{2}\Gamma_L$$

$\Rightarrow$ By recalling that $(\tilde{G}^R)^\dagger = \tilde{G}^A$ it follows

$$\boxed{T(E) = \mathrm{Tr}\left\{\hbar^2 \bar{\Gamma}_L \tilde{G}^R \bar{\Gamma}_R \tilde{G}^A\right\}} \quad (4.141)$$

which recovers Eq. (4.73)

upon defining

$$\hbar\bar{\Gamma}_R = \begin{pmatrix} 0 & 0 \\ 0 & \hbar\Gamma_R \end{pmatrix}, \quad \hbar\bar{\Gamma}_L = \begin{pmatrix} \hbar\Gamma_L & 0 \\ 0 & 0 \end{pmatrix}$$

<u>Proof</u>

$$\bar{\Gamma}_L = \Gamma_L \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad , \quad \bar{\Gamma}_R = \hbar \Gamma_R \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\hookrightarrow \quad \bar{\Gamma}_R \tilde{G}^A = \Gamma_R \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \tilde{G}^A_{11} & \tilde{G}^A_{12} \\ \tilde{G}^A_{21} & \tilde{G}^A_{22} \end{pmatrix} = \Gamma_R \begin{pmatrix} 0 & 0 \\ \tilde{G}^A_{21} & \tilde{G}^A_{22} \end{pmatrix}$$

$$\hookrightarrow \quad \tilde{G}^R \left(\bar{\Gamma}_R \tilde{G}^A \right) = \Gamma_R \begin{pmatrix} \tilde{G}^R_{11} & \tilde{G}^R_{12} \\ \tilde{G}^R_{21} & \tilde{G}^R_{22} \end{pmatrix} \begin{pmatrix} 0 & 0 \\ \tilde{G}^A_{21} & \tilde{G}^A_{22} \end{pmatrix}$$

$$= \Gamma_R \begin{pmatrix} \tilde{G}^R_{12} \tilde{G}^A_{21} & \tilde{G}^R_{12} \tilde{G}^A_{22} \\ \tilde{G}^R_{22} \tilde{G}^A_{21} & \tilde{G}^R_{22} \tilde{G}^A_{22} \end{pmatrix}$$

$$\hookrightarrow \hbar^2 \bar{\Gamma}_L \tilde{G}^R \bar{\Gamma}_R \tilde{G}^A = \hbar^2 \Gamma_L \Gamma_R \begin{pmatrix} \tilde{G}^R_{12} \tilde{G}^A_{21} & \tilde{G}^R_{12} \tilde{G}^A_{22} \\ 0 & 0 \end{pmatrix}$$

$$\hookrightarrow \quad \mathrm{Tr} \left\{ \hbar \bar{\Gamma}_L \tilde{G}^R \bar{\Gamma}_R \tilde{G}^A \right\} = \hbar^2 \Gamma_L \Gamma_R \left| \tilde{G}^R_{12} \right|^2$$