## 4.4 Single time diagrammatics in Liouville space

In the Liouville space representation all operators acting on the RDM superoperatorial level. We introduce to this end the notion of L and R superoperators. Given an operator $\hat{O}$ in Hilbert space

$$\hat{O}_L \hat{X} = \hat{O}\hat{X} \qquad \hat{O}_R \hat{X} = \hat{X}\hat{O} \tag{4.72}$$

Using the definition of the tunnelling Hamiltonian in terms of $\hat{c}$ and $\hat{d}$ operators it is possible to write $\left( \hat{D}^p_b = \sum_i t^p_{i\ell\vec{k}\sigma} \hat{d}^p_{i\sigma} \right)$

$$\mathcal{L}_T = -\frac{i}{\hbar} \sum_{\substack{\alpha = L,R \\ b p}} \alpha p \left( \hat{c}^p_b \hat{D}^{\bar{p}}_b \right)_\alpha \qquad \begin{matrix} \alpha = L = 1 \\ \alpha = R = -1 \end{matrix} \tag{4.73}$$

where $b = \ell, \vec{k}, \sigma$ $\quad \ell$ = lead index.

Remembering now that the operators on the leads and on the system can be separated at no price, we can write immediately the fundamental component of the theory, the 2nd order Kernel in Schr. picture

$$\mathcal{P}\mathcal{L}_T \tilde{G}_0(0) \mathcal{L}_T \mathcal{P} = -\frac{1}{\hbar^2} \sum_{\{b_i, p_i, \alpha_i\}} \int_0^\infty d\tau \prod_i \alpha_i p_i \, \mathcal{P} \left( \hat{c}^{p_1}_{b_1} \hat{D}^{\bar{p}_1}_{b_1} \right)_{\alpha_1} G_0(\tau,0) \left( \hat{c}^{p_0}_{b_0} \hat{D}^{\bar{p}_0}_{b_0} \right)_{\alpha_0} \mathcal{P}$$

$$= -\frac{1}{\hbar^2} \int_0^\infty d\tau \sum_{b,p,\{\alpha_i\}} \prod_i \alpha_i \, \mathcal{P}\, \hat{c}^p_{b,\alpha_1} G_B(\tau,0)\, c^{\bar{p}}_{b,\alpha_0} \mathcal{P}\; \hat{D}^{\bar{p}}_{b,\alpha_1} G_S(\tau,0)\, D^p_{b,\alpha_0} \tag{4.74}$$

where $G_B(\tau,0) = e^{\mathcal{L}_B \tau}$ and $G_S(\tau,0) = e^{\mathcal{L}_S \tau}$. We can continue a step further by noticing

$$\mathcal{P}\, \hat{c}^p_{b,\alpha_1} G_B(\tau,0)\, \hat{c}^{\bar{p}}_{b,\alpha_2} \mathcal{P} = G_B(\tau,0)\, \mathcal{P}\, \hat{c}^p_{b,\alpha_1}(\tau)\, \hat{c}^{\bar{p}}_{b,\alpha_0} \mathcal{P} =$$

$$= \mathcal{P}\, \hat{c}^p_{b,\alpha_1}(\tau)\, \hat{c}^{\bar{p}}_{b,\alpha_0} \mathcal{P} = e^{ip\frac{\varepsilon_b \tau}{\hbar}} f^{(p\alpha_0)}_b(\varepsilon_b)\, \mathcal{P} . \tag{4.75}$$

The last equality is proven directly as follows: in general we can write:

$$\wp\, \hat{c}^{p_1}_{b_1,\alpha_1}\, \hat{c}^{p_0}_{b_0,\alpha_0}\, \wp = f^{(p_1\alpha_0)}_{b_1}(\varepsilon_{b_1})\, \delta_{b_1 b_0}\, \delta_{p_1 \bar{p}_0}\, \wp$$

$\boxed{1}$ $\delta_{b_1 b_2}$ and $\delta_{p_1 \bar{p}_2}$ are due to particle and energy conservation in each bath separately.

$\boxed{2}$ We calculate the 8 cases:

| | | | $p_1$ | $\alpha_0$ |
|---|---|---|---|---|
| $\wp\, c^+_L c_L \wp =$ | $\rho\, \mathrm{Tr}(c^+ c \rho) =$ | $\rho f^+$ | + | + |
| $\wp\, c^+_L c_R \wp =$ | $\rho\, \mathrm{Tr}(c^+ \rho c) =$ | $\rho f^-$ | + | − |
| $\wp\, c^+_R c_L \wp =$ | $\rho\, \mathrm{Tr}(c \rho c^+) =$ | $\rho f^+$ | + | + |
| $\wp\, c^+_R c_R \wp =$ | $\rho\, \mathrm{Tr}(\rho c c^+) =$ | $\rho f^-$ | + | − |
| $\wp\, c_L c^+_L \wp =$ | $\rho\, \mathrm{Tr}(c c^+ \rho) =$ | $\rho f^-$ | − | + |
| $\wp\, c_L c^+_R \wp =$ | $\rho\, \mathrm{Tr}(c \rho c^+) =$ | $\rho f^+$ | − | − |
| $\wp\, c_R c^+_L \wp =$ | $\rho\, \mathrm{Tr}(c^+ \rho c) =$ | $\rho f^-$ | − | + |
| $\wp\, c_R c^+_R \wp =$ | $\rho\, \mathrm{Tr}(\rho\, c^+_R c_R) =$ | $\rho f^+$ | − | − |

Eventually we obtain:

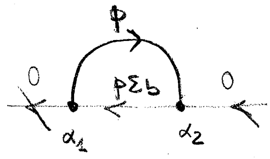
$$\wp \mathcal{L}_T \tilde{G}_0(0) \mathcal{L}_T \wp = -\frac{1}{\hbar^2} \int_0^\infty d\tau \sum_{\{\alpha_i\} p, b} \prod_i \alpha_i \; e^{i p \varepsilon_b \tau / \hbar} f_b^{(p\alpha_2)} D^{\bar{p}}_{b,\alpha_1}\, G_S(\tau,0)\, D^{p}_{b,\alpha_0}\, \wp$$

$$= +\frac{1}{\hbar^2} \sum_{\{\alpha_i\}, p, b} D^{\bar{p}}_{b\alpha_1} \frac{f_b^{(p\alpha_2)}}{+\frac{i p \varepsilon_b}{\hbar} + \mathcal{L}_S + \eta} D^{p}_{b,\alpha_0}\, \wp = -\frac{i}{\hbar} \sum_{\{\alpha_i\} b, b} \hat{D}^{\bar{p}}_{b\alpha_1} \frac{f_b^{(p\alpha_2)}}{p\varepsilon_b - i\hbar \mathcal{L}_S + i\eta} \hat{D}^{p}_{b\alpha_0}$$

$\eta \to 0^+$

Tentatively (the diagrammatic rules will be given below in a more precise form).

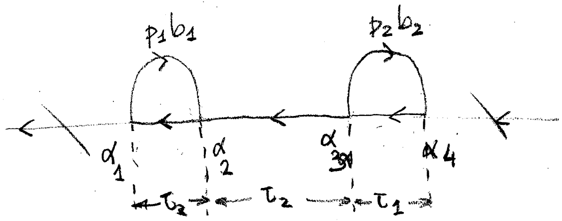
$$\mathcal{P} \mathcal{L}_T \tilde{G}_0(0) \mathcal{L}_T \mathcal{P} = \qquad (4.76)$$




We can now turn to the 4th order contribution

$$\tilde{K}^{(4)}(0) = \mathcal{P} \mathcal{L}_T \tilde{G}_0(0) \mathcal{L}_T \tilde{G}_0(0) \mathcal{L}_T \tilde{G}_0(0) \mathcal{L}_T \mathcal{P} - \mathcal{P} \mathcal{L}_T \tilde{G}_0(0) \mathcal{L}_T \mathcal{P} \tilde{G}_0(0) \mathcal{P} \mathcal{L}_T \tilde{G}_0(0) \mathcal{L}_T \mathcal{P}$$

The second contribution can be readily interpreted as:




where the propagation between the vertex 3 and 2 is given by $G_s$

$$\mathcal{P} \mathcal{L}_T \tilde{G}_0(0) \mathcal{L}_T \mathcal{P} \tilde{G}_0(0) \mathcal{P} \mathcal{L}_T \tilde{G}_0(0) \mathcal{L}_T \mathcal{P} =$$

$$= -\frac{1}{\hbar^2} \int_0^\infty d\tau_3 \sum_{\substack{b_1 p_1 \\ \{\alpha_1, \alpha_2\}}} \alpha_1 \alpha_2 \, e^{+i p_1 \varepsilon_{b_1} \tau_3} f_{b_1}^{(p_1 \alpha_2)}(\varepsilon_{b_1}) D^{\bar{p}_1}_{b_1, \alpha_1} G_s(\tau_1, 0) D^{p_1}_{b_1, \alpha_2}$$

$$\cdot \int_0^\infty d\tau_2 \, G_s(\tau_2, 0) \cdot$$

$$-\frac{1}{\hbar^2} \int_0^\infty d\tau_1 \sum_{\substack{b_2 p_2 \\ \{\alpha_3, \alpha_4\}}} \alpha_3 \alpha_4 \, e^{i p_2 \varepsilon_{b_2} \tau_1} f_{b_2}^{(p_2 \alpha_4)}(\varepsilon_{b_2}) D^{\bar{p}_2}_{b_2, \alpha_3} G_s(\tau_3, 0) D^{p_2}_{b_2, \alpha_4} \mathcal{P}$$

(4.77)

The first contribution can be brought immediately into the form

$$\mathcal{P}\mathcal{L}_T \tilde{G}_0(0)\mathcal{L}_T \tilde{G}_0(0)\mathcal{L}_T \tilde{G}_0(0)\mathcal{L}_T \mathcal{P} =$$

$$= \frac{1}{\hbar^4}\int_0^\infty d\tau_1 \int_0^\infty d\tau_2 \int_0^\infty d\tau_3 \sum_{\{b_i,p_i,\alpha_i\}} \prod_i \alpha_i \,\mathcal{P}\, c^{p_3}_{b_3,\alpha_3} G_B(\tau_3,0)\, c^{p_2}_{b_2,\alpha_2} G_B(\tau_2,0)\, c^{p_1}_{b_1,\alpha_1} G_B(\tau_1,0)\, c^{p_0}_{b_0,\alpha_0}\mathcal{P}$$

$$D^{\bar{p}_3}_{b_3,\alpha_3} G_S(\tau_3,0)\, D^{\bar{p}_2}_{b_2,\alpha_2} G_S(\tau_2,0)\, D^{\bar{p}_1}_{b_1,\alpha_1} G_S(\tau_1,0)\, D^{\bar{p}_0}_{b_0,\alpha_0}\mathcal{P}$$

$$= \frac{1}{\hbar^4}\int_0^\infty dt_1 \int_{t_1}^\infty dt_2 \int_{t_2}^\infty dt_3 \sum_{\{b_i,p_i,\alpha_i\}} \prod_i \alpha_i \,\mathcal{P}\, c^{p_3}_{b_3,\alpha_3}(t_3)\, c^{p_2}_{b_2,\alpha_2}(t_2)\, c^{p_1}_{b_1,\alpha_1}(t_1)\, c^{p_0}_{b_0,\alpha_0}\mathcal{P}$$

$$G_S(t_3,0)\, D^{\bar{p}_3}_{b_3,\alpha_3}(t_3)\, D^{\bar{p}_2}_{b_2,\alpha_2}(t_2)\, D^{\bar{p}_1}_{b_1,\alpha_1}(t_1)\, D^{\bar{p}_0}_{b_0,\alpha_0}\mathcal{P}$$

$$\tau_1 = t_1 \qquad \tau_1+\tau_2 = t_2 \qquad \tau_1+\tau_2+\tau_3 = t_3 \tag{4.78}$$

Now we can apply Wick's theorem to the bath operators in Liouville spa[ce]. The result is the same as with operators but the sign obtaining by crossed contraction only apply to superoperators of the same type.
One should use the rule $X_\alpha Y_{\alpha'} = -\alpha\alpha' Y_{\alpha'} X_\alpha$ if $\{X,Y\}=0$.

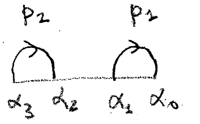
$$\mathcal{P}\, c^{p_3}_{b_3,\alpha_3} c^{p_2}_{b_2,\alpha_2} c^{p_1}_{b_1,\alpha_1} c^{p_0}_{b_0,\alpha_0}\mathcal{P} =$$

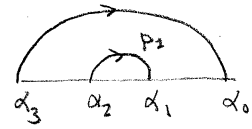
$$\delta_{b_2 b_3}\delta_{p_2\bar{p}_3}\delta_{b_1 b_0}\delta_{p_1\bar{p}_0}\,\mathcal{P}\, c^{p_3}_{b_3\alpha_3} c^{p_2}_{b_2\alpha_2}\mathcal{P}\,\mathcal{P}\, c^{p_1}_{b_1\alpha_1} c^{p_0}_{b_0\alpha_0}\mathcal{P}$$

$$-\alpha_1\alpha_2\,\delta_{b_3 b_1}\delta_{p_3\bar{p}_1}\delta_{b_2 b_0}\delta_{p_2\bar{p}_0}\,\mathcal{P}\, c^{p_3}_{b_3\alpha_3} c^{p_1}_{b_1\alpha_1}\mathcal{P}\,\mathcal{P}\, c^{p_2}_{b_2\alpha_2} c^{p_0}_{b_0\alpha_0}\mathcal{P}$$

$$+\cancel{\alpha_0^2}\alpha_1\alpha_2\,\delta_{b_3 b_0}\delta_{p_3\bar{p}_0}\delta_{b_2 b_1}\delta_{p_2\bar{p}_1}\,\mathcal{P}\, c^{p_3}_{b_3\alpha_3} c^{p_0}_{b_0\alpha_0}\mathcal{P}\,\mathcal{P}\, c^{p_2}_{b_2\alpha_2} c^{p_1}_{b_1\alpha_1}\mathcal{P} \tag{4.79}$$

Diagrammatically one thus obtains

$$\mathcal{P} L_T \tilde{G}_0(0) L_T \tilde{G}_0(0) L_T G_0 L_T \mathcal{P} =$$ 

$+$ 

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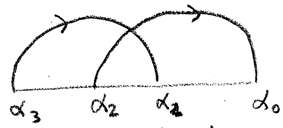
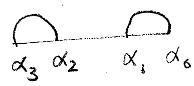
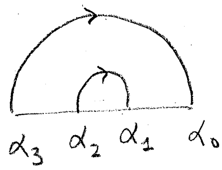
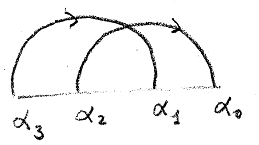
$+$ 


But the first diagram is exactly cancelled by the one associated to $\mathcal{P} L_T \hat{G}_0 L_T \mathcal{P} \tilde{G}_0(0) \mathcal{P} L_T \hat{G}_0(0) L_T \mathcal{P} =$ 

. Diagrammatically we can thus write

$$\tilde{K}^4(0) =$$ 

$+$ 

(4.80)

thus reducing to 2 the 128 diagrams generated in the Hilbert space with the double contour diagrammatics. The time integral in (4.78) can be performed easily and one obtains:

$$\tilde{K}(\lambda)^{(4)} = \frac{1}{\hbar^4} \sum_{\{b_i, p_i, \alpha_i\}} \prod_i \alpha_i$$

$$\alpha_1\alpha_2 \, f_{b_2}^{(p_2\alpha_0)}(\varepsilon_{b_2}) \, f_{b_1}^{(p_1\alpha_1)}(\varepsilon_{b_1}) \, \hat{D}^{\bar{p}_2}_{b_2\alpha_3} \frac{1}{\lambda - L_S - i\frac{p_2\varepsilon_{b_2}}{\hbar}} \hat{D}^{\bar{p}_1}_{b_1\alpha_2} \frac{1}{\lambda - L_S - i\frac{p_1\varepsilon_{b_1}}{\hbar} - i\frac{p_2\varepsilon_{b_2}}{\hbar}}$$

$$\hat{D}^{p_1}_{b_1,\alpha_1} \frac{1}{\lambda - L_S - i p_2 \varepsilon_{b_2}} \hat{D}^{p_2}_{b_2,\alpha_0} +$$

$$- \alpha_1\alpha_2 \, f_{b_2}^{(p_2\alpha_1)}(\varepsilon_{b_2}) \, f_{b_1}^{(p_1\alpha_0)}(\varepsilon_{b_1}) \, \hat{D}^{\bar{p}_2}_{b_2,\alpha_3} \frac{1}{\lambda - L_S - i\frac{p_2\varepsilon_{b_2}}{\hbar}} \hat{D}^{\bar{p}_1}_{b_1\alpha_2} \frac{1}{\lambda - L_S - i\frac{p_1\varepsilon_{b_1}}{\hbar} - i\frac{p_2\varepsilon_{b_2}}{\hbar}}$$

$$\left. \hat{D}^{p_2}_{b_2,\alpha_1} \frac{1}{\lambda - L_S - i p_1 \varepsilon_{b_1}} \hat{D}^{p_1}_{b_1,\alpha_0} \right] \tag{4.81}$$

## 4.4.1 Diagrammatic rules in the superoperator formalism

Ultimately one arrives to the following set of diagrammatic rules for a generic diagram of order $2n$.

i) Draw a propagation line oriented right to left. On it fix <u>$2n$ vertices</u>, each associated to an index $\alpha$ $(= \underset{+}{L}, \underset{-}{R})$

ii) Draw <u>$n$ fermionic lines</u> all oriented from left to right, each labelled with an index $p_i$ and an energy $\varepsilon_i$ $(i = 1 \dots n)$ connecting the $2n$ vertices in such a way that the diagram cannot be cut into 2 parts by cutting a single propagator line.

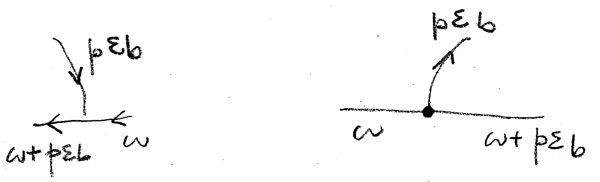
iii) Assign to each fermionic line the number $f_{b_i}^{(p_i \alpha)}(\varepsilon_i)$ where $\alpha$ is the side index of the arriving vertex.

iv) Assign to each vertex a "dressed" system operator $D^{p_i}_{b_i;\alpha}$ or $D^{\bar{p}_i}_{b_i;\alpha'}$ respectively for the vertex with ingoing $(\alpha)$ or outgoing $(\alpha')$ fermionic line. Notice that $\hat{D}$ has the dimensions of energy.

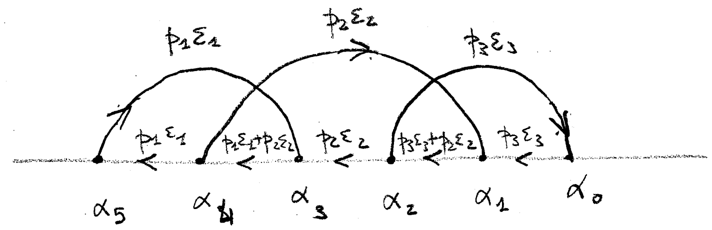
v) Assign to each propagator line between vertices the operator

$$G_{SB}(\omega) = \frac{1}{\omega - i\hbar \mathcal{L}_s + i\eta}$$

vi) The energy in each vertex should be conserved.



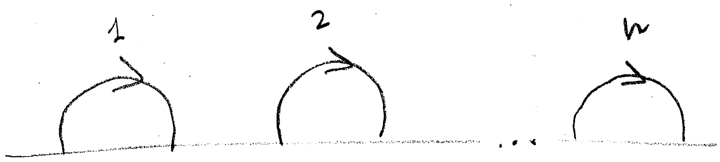
Example of labelled $6^{th}$ order diagram




Now we turn to the translation of the diagram into a formula

i) Write the product of the vertex operators and the propagators from left to right, respecting the order of the graph

ii) Multiply by a prefactor $\left(-\frac{i}{\hbar}\right)\prod_i \alpha_i \,(-1)^{P(\{\alpha_i\})}$ where $P(\{\alpha_i\})$ is the number of permutation of equal side vertices necessary to recast the graph into a completely reducible form

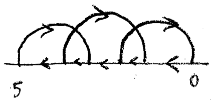



which respects the time ordering of the contraction (the direction of the fermionic lines)

iii) Sum over all internal degrees of freedom: i.e. $\sum_{\{\alpha_i\}}\sum_{\{p_i\}}\sum_{\{b_i\}}$. The last sum can be expressed as

$\sum_{l_i=L,R}\sum_{\sigma_i}\int d\varepsilon_i\, \mathcal{D}_{l_i\sigma_i}(\varepsilon_i)$ where $\mathcal{D}_{l_i\sigma_i}$ is the density of states for the electrons of spin $\sigma_i$ in the lead $l_i$.

For the example above we obtain:




$$= -\frac{i}{\hbar}\sum_{\{\alpha_i\}}\sum_{\{p_i\}}\sum_{\{l_i\}}\sum_{\{\sigma_i\}}\int d\vec{\varepsilon}\,\prod_{j=1}^{3}\mathcal{D}_{l_j\sigma_j}(\varepsilon_j)\prod_{i=0}^{5}\alpha_i(-\alpha_4\alpha_3)(-\alpha_2\alpha_1)$$

$$f_{l_1}^{(p_1\alpha_3)}(\varepsilon_1)\, f_{l_2}^{(p_2\alpha_1)}(\varepsilon_2)\, f_{l_3}^{(p_3\alpha_0)}(\varepsilon_3)$$

$$\mathcal{D}^{\bar{p}_1}_{l_1\sigma_1,\alpha_5}\frac{1}{p_1\varepsilon_1 - i\hbar\Lambda_s + i\eta}\,\mathcal{D}^{\bar{p}_2}_{l_2\sigma_2,\alpha_4}\frac{1}{p_1\varepsilon_1 + p_2\varepsilon_2 - i\hbar\Lambda_s + i\eta}\,\mathcal{D}^{p_1}_{l_1\sigma_1,\alpha_3}\frac{1}{p_2\varepsilon_2 - i\hbar\Lambda_s + i\eta}$$

$$\mathcal{D}^{\bar{p}_3}_{l_3\sigma_3,\alpha_2}\frac{1}{p_3\varepsilon_3 + p_2\varepsilon_2 - i\hbar\Lambda_s + i\eta}\,\mathcal{D}^{p_2}_{l_2\sigma_2,\alpha_1}\frac{1}{p_3\varepsilon_3 - i\hbar\Lambda_s + i\eta}\,\mathcal{D}^{p_3}_{l_3\sigma_3,\alpha_0}\,\rho \qquad (4.82)$$

Notice that it can be convenient for the understanding of the different physical processes to introduce the concept of single particle rate matrices

$$\Gamma^{p}_{nm}(l\sigma_l;\varepsilon) = \frac{2\pi}{\hbar}\sum_{\vec{k}} t^{\bar{p}}_{l\vec{k}\sigma_l,n}\, t^{p}_{l\vec{k}\sigma_l,m}\, \delta(\varepsilon - \varepsilon_{l\vec{k}\sigma_l})$$

where $n = i,\sigma_0$ is a combined orbital and spin index for the system and $\sigma_l$ is a spin index for the (natural) quantisation axis of lead $l$. and $\Gamma$ the units of <u>rate</u>. Let's analyze his application to the II and IV order Kernels:

$$K^{(II)} = -\frac{i}{\hbar}\sum_{\{\alpha_i\}}\sum_{pb}\alpha_1\alpha_2\, \Delta^{\bar{p}}_{b\alpha_2}\frac{f_b^{(p\alpha_1)}(\varepsilon_b)}{p\varepsilon_b - i\hbar\lambda_s + i\eta}\Delta^{p}_{b\alpha_1}$$

with $b$ a collective bath index indicating $l\vec{k}\sigma_l$.

$$f^{\pm}_b(\varepsilon_b) = f^{\pm}_l(\varepsilon_{l\vec{k}\sigma_l}) = f^{\pm}(\varepsilon_{l\vec{k}\sigma_l} - \mu_l)$$

$$\Delta^{p}_{b\alpha} = \sum_n t^{p}_{l\vec{k}\sigma_l,n}\, d^{p}_{n,\alpha}$$

Now we recast the sum over the bath degrees of freedom:

$$\sum_b = \sum_{l\vec{k}\sigma} = \sum_{l\sigma}\int d\varepsilon \sum_{\vec{k}}\delta(\varepsilon - \varepsilon_{l\vec{k}\sigma_l})$$

Thus the second order Kernel can be written as

$$\tilde{K}^{(II)} = -\frac{i}{\hbar}\sum_{\{\alpha_i\}}\sum_{pl\sigma_l}\sum_{nm}\int d\varepsilon \sum_{\vec{k}}\delta(\varepsilon - \varepsilon_{l\vec{k}\sigma_l})\, \alpha_1\alpha_2\, t^{\bar{p}}_{l\vec{k}\sigma_l,n}\, t^{p}_{l\vec{k}\sigma_l,m}\, d^{\bar{p}}_{n,\alpha_2}\frac{f_l^{(p\alpha_1)}(\varepsilon)}{p\varepsilon - i\hbar\lambda_s + i\eta}\, d^{p}_{m,\alpha_1}$$

$$= -\frac{i}{2\pi}\sum_{\{\alpha_i\}}\sum_{pl\sigma_l}\sum_{nm}\int d\varepsilon\, \alpha_1\alpha_2\, \Gamma^{p}_{nm}(l\sigma_l;\varepsilon)\, d^{\bar{p}}_{n,\alpha_2}\frac{f_l^{(p\alpha_1)}(\varepsilon)}{p\varepsilon - i\hbar\lambda_s + i\eta}\, d^{p}_{m,\alpha_1}$$

Analogously one can proceed with the fourth order contribution, to obtain:

$$\tilde{K}^{(\mathrm{IV}\,D)} = -\frac{i\hbar}{(4\pi)^2} \sum_{\{\alpha_i\}} \sum_{\{p\}} \sum_{\{\ell\}} \sum_{\{\sigma\}} \sum_{\{n\}\{m\}} \int d\varepsilon\, d\varepsilon'\; \alpha_1 \alpha_4\, \Gamma^{p}_{nm}(\ell\sigma_\ell; \varepsilon)\, \Gamma^{p'}_{n'm'}(\ell\sigma_{\ell'}; \varepsilon')$$

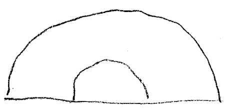
$$f_{\ell}^{(p\alpha_1)}(\varepsilon)\, f_{\ell'}^{p'(\alpha_2)}(\varepsilon')\; d^{\bar{p}}_{n\alpha_4} \frac{1}{\varepsilon p - i\hbar\Lambda_s + i\eta}\, d^{\bar{p}'}_{n'\alpha_3} \frac{1}{\varepsilon' p' + \varepsilon p - i\hbar\Lambda_s + i\eta}\, d^{p'}_{m'\alpha_2} \frac{1}{\varepsilon p - i\hbar\Lambda_s + i\eta}\, d^{p}_{m\alpha}$$

$$\tilde{K}^{(\mathrm{IV}\,x)} = -\frac{i\hbar}{(4\pi)^2} \sum_{\{\alpha_i\}} \sum_{\{p\}\{\ell\}\{\sigma\}} \sum_{\{n\}\{m\}} \int d\varepsilon\, d\varepsilon'\, (-\alpha_1\alpha_4)\, \Gamma^{p}_{nm}(\ell\sigma; \varepsilon)\, \Gamma^{p'}_{n'm'}(\ell'\sigma'; \varepsilon')\, f_{\ell}^{(p\alpha_1)}(\varepsilon)\, f^{(p'\alpha_2)}(\varepsilon')$$

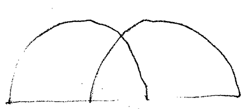
$$d^{\bar{p}}_{n\alpha_4} \frac{1}{\varepsilon p - i\hbar\Lambda_s + i\eta}\, d^{\bar{p}'}_{n'\alpha_3} \frac{1}{\varepsilon p + \varepsilon' p' - i\hbar\Lambda_s + i\eta}\, d^{p}_{m\alpha_2} \frac{1}{\varepsilon' p' - i\hbar\Lambda_s + i\eta}\, d^{p'}_{m'\alpha_1}$$

where we have assigned for convenience an index D and X to the diagrams

(IV D)



(IV x)

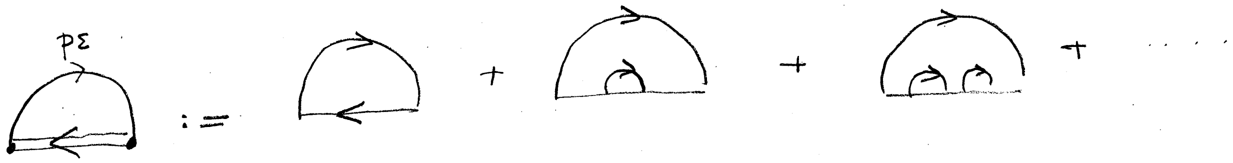


## 4.5 All order resummations: non perturbative effects

Some properties of the transport characteristics through a nanojunction cannot be understood within a perturbative scheme; e.g. the coupling broadened conductance peaks or the Kondo conductance peak for odd particle Coulomb diamonds. There are 2 cases in which the diagrammatic approach presented above allows for resummation to all orders. The dressed second order and the resonant tunnelling approximation.

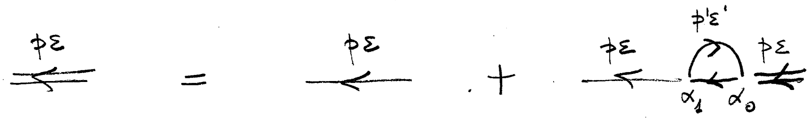
### 4.5.1 Dressed second order approximation (DSO)

The idea of the DSO is to construct an effective second order kernel containing renormalizations to every order. Diagrammatically




(4.83)

It is clear that the dressed propagator characterizing the DSO approximation can be evaluated by means of a Dyson-like equation




(4.84)

$$G^{DSO}(p\varepsilon) = \frac{1}{p\varepsilon - i\hbar L_s + i\eta} + \frac{1}{p\varepsilon - i\hbar L_s + i\eta} \sum_{\substack{\alpha_1 \alpha_0 \\ p'\ell'}} \int d\varepsilon' \, \mathcal{D}^{\bar{p}'}_{\ell\sigma',\alpha_1} \frac{f^{(p'\alpha_0)}_{\ell'}(\varepsilon')}{\varepsilon p + \varepsilon' p' - i\hbar L_s + i\eta} \mathcal{D}^{p'}_{\ell\sigma',\alpha_0} G^{DSO}$$

The equation above is easily solved in $G^{DSO}(p\varepsilon)$ (it is a linear equation!)

We can, in fact, introduce the DSO self-energy

$$\Sigma^{DSO}(p\varepsilon) = \sum_{\substack{\alpha_1\alpha_0 \\ p'l'}} \int d\varepsilon' \, \mathcal{D}_{l'\sigma'}(\varepsilon') \, \Delta^{\bar{p}'}_{l'\sigma',\alpha_1} \frac{f_{l'}^{(p'\alpha_0)}(\varepsilon')}{\varepsilon p + \varepsilon' p' - i\hbar \mathcal{L}_s + i\eta} \Delta^{p'}_{l\sigma',\alpha} \tag{4.85}$$

and express:

$$G^{DSO}(p\varepsilon) = \frac{1}{p\varepsilon - i\hbar\mathcal{L}_s - \Sigma^{DSO}(p\varepsilon)} \tag{4.86}$$

proof of (4.86)

$$G^{DSO}(p\varepsilon) = G^0_{SB}(p\varepsilon) + G^0_{SB}(p\varepsilon)\,\Sigma^{DSO}(p\varepsilon)\,G^{DSO}(p\varepsilon)$$

$$\left(1 - G_{SB}(p\varepsilon)\,\Sigma^{DSO}(p\varepsilon)\right) G^{DSO}(p\varepsilon) = G_{SB}(p\varepsilon)$$

$$G^{DSO}(p\varepsilon) = \left(1 - G_{SB}(p\varepsilon)\,\Sigma^{DSO}(p\varepsilon)\right)^{-1} G_{SB}(p\varepsilon) =$$

$$= \left[\left(G_{SB}(p\varepsilon)\right)^{-1}\left(1 - G_{SB}(p\varepsilon)\,\Sigma^{DSO}(p\varepsilon)\right)\right]^{-1}$$

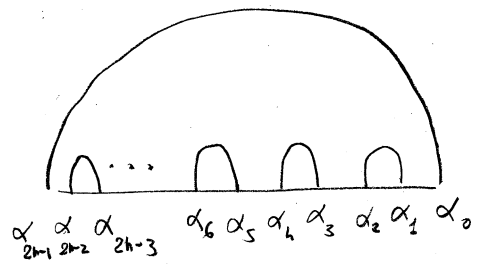
$$= \left[G_{SB}(p\varepsilon)^{-1} - \Sigma^{DSO}(p\varepsilon)\right]^{-1}.$$

■

The dressed second order Kernel reads:

$$\tilde{K}^{DSO} = -\frac{i}{\hbar} \sum_{\substack{\alpha_1\alpha_0 \\ pl\sigma}} \alpha_1\alpha_0 \int d\varepsilon \, \mathcal{D}_{l\sigma}(\varepsilon) \, \Delta^{\bar{p}}_{l\sigma,\alpha_1} \frac{f_l^{(p\alpha_0)}(\varepsilon)}{p\varepsilon - i\hbar\mathcal{L}_s - \Sigma^{DSO}(p\varepsilon)} \Delta^{p}_{l\sigma,\alpha_0} \tag{4.87}$$

Notice: $\Sigma^{DSO}$ has no $\alpha$ prefactors since $(-1)^{P(\alpha_i)} = \prod_{i=1}^{2n-2} \alpha_i$ for a diagram of the type:




The physical meaning of (4.87) rely on the presence of $\Sigma^{DSO}$ in the denominator of the propagator. In the calculation of the rates (i.e. the different components of $\tilde{K}^{DSO}$) the bias and gate dependence is not given only by the temperature (in $f$) and the system energy difference ($\Delta_s$) but also by the tunnelling coupling $\Gamma$ contained in the imaginary part of $\Sigma^{DSO}$.