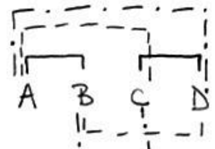
For example, for the 2^{nd} order contributions one counts:

$$
\begin{array}{ccccccccc}
2 & \times & 2 & \times & 2 & \times & 2 & = & 16 \\
\uparrow & & \uparrow & & \uparrow & & \uparrow & & \\
\sum_{p_0} & & \sum_{p_3} & & \underset{\text{inner}}{[\,,\,]} & & \underset{\text{outer}}{[\,,\,]} & &
\end{array}
$$

Wick's theorem imposes, though $p_0 = -p_3$ => the number of contribution reduces to 8.

For the 4^{th} order contributions:

$$
\begin{array}{ccccccc}
2^4 & \times & 2^4 & \times (3-1) & = & 512 \\
\uparrow & & \uparrow & \uparrow & & \\
\sum_{p_i} & & [\,,\,] & \text{"all"} - \text{"reducible"} = \text{irreducible} & &
\end{array}
$$



3 possibilities of double pairing

Wick's theorem imposes, though $p_0 = -p_3 \wedge p_1 = -p_2$ or => the number must

$p_0 = -p_2 \wedge p_1 = -p_3$ or

$p_0 = -p_1 \wedge p_2 = -p_3$

be divided by 4 since only two p_i are independent.

In general, a $2n$-th contribution to the Kernel $K^{aa'}_{bb'}$ in int. picture (odd contribution vanish identically) reads:

$$\prod_{\alpha=1}^{n} \langle \hat{C}^I_\alpha \rangle \langle b | \hat{\mathcal{D}}^I | a \rangle \langle a | \hat{\rho}^I_{red}(\tau) | a' \rangle \langle a' | \hat{\mathcal{D}}'^I | b' \rangle \quad (4.40)$$

where $\hat{C}^I_\alpha$ is formed by the product of <u>two</u> lead operators. Hence $\prod_\alpha \langle \hat{C}^I_\alpha \rangle$ is the product of n Wick's contractions while $\hat{\mathcal{D}}^I$ and $\hat{\mathcal{D}}'^I$ contain <u>together</u> the associated an dot operators.

Moreover one has to count over the sum over the orbital and spin index of the system $l\sigma$. For the $2n$-th order case there are $2n$ sums over l and σ. Wick's theorem reduces though the sums over σ to n. For what concerns the sums over l, in general no constriction reduces them unless for special geometrical configuration of the contact.

For each contribution (4.40) a DIAGRAM can be associated.
From the diagrams, the Laplace transform $K_{bb'}^{aa'}$ can be extracted.

4.1.1 Diagram rules in time domain

i) Each diagram consists of an upper and lower contour taking $a \to b$ and $b' \to a'$, respectively

$$|b\rangle \longleftarrow |a\rangle$$

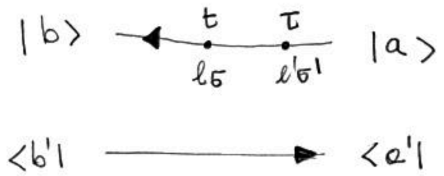
$$\langle b'| \longrightarrow \langle a'|$$

ii) Through all diagrams times grow from right to left
=> a, a' are "initial" states, b and b' are "final" states

$$|b\rangle \longleftarrow |a\rangle$$
$$t > \tau_2 > \tau_1 > \tau \qquad t = \tau_3\,,\ \tau = \tau_0$$
$$\langle b'| \longrightarrow \langle a'|$$

iii) Every system operator standing on the <u>left</u> of the RDM (belonging to $\mathcal{D}^I$) is associated to a vertex at a given time on the <u>upper</u> contour. Every operator on the <u>right</u> belonging to $\mathcal{D}'^{I}$) is associated to a vertex in the lower contour.

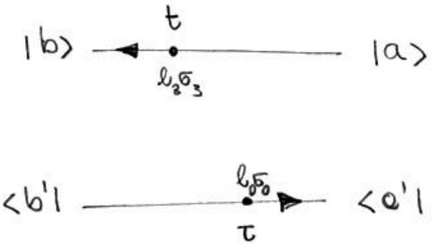
2^{nd} order



$$\Delta^{p_3}_{3,l_3\sigma_3}\,\Delta^{p_0}_{0,l_0\sigma_0}\,\rho^{I}_{red}(\tau)$$

or

or



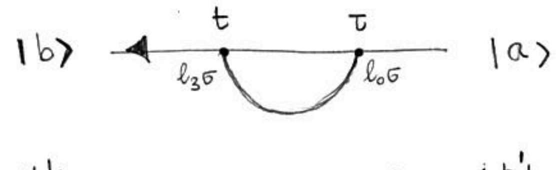
$$\Delta^{p_3}_{3,l_3\sigma_3}\,\rho^{I}_{red}(\tau)\,\Delta^{p_0}_{0,l_0\sigma_0}$$

or

At each vertex the charge of the state changes by ±1 depending by the sign of p_i.

iv) The vertices of the system operators which are related via two contracted lead operators are connected by a <u>fermionic line</u>

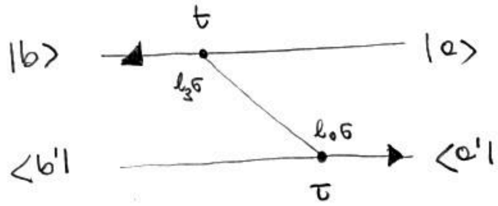
2^{nd} order



$$-\langle \hat{C}^{\bar{p}}_{3,l_3\sigma}\,\hat{C}^{p}_{0,l_0\sigma}\rangle\left(\hat{\Delta}^{p}_{3,l_3\sigma}\,\Delta^{\bar{p}}_{0,l_0\sigma}\,\rho^{I}_{red}(\tau)\right) \tag{4.41}$$

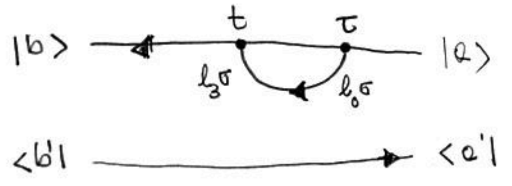
notice that Wick's contraction has imposed the constriction $p_0=\bar{p}_3$ and $\sigma_0=\sigma_3$.

2^{nd} order



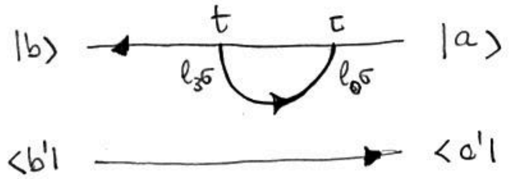
$$\langle \hat{C}^{p}_{0,l_0\sigma}\,\hat{C}^{\bar{p}}_{3,l_3\sigma}\rangle\left(\hat{\Delta}^{p}_{3,l_3\sigma}\,\rho^{I}_{red}(\tau)\,\hat{\Delta}^{\bar{p}}_{0,l_0\sigma}\right) \tag{4.42}$$

V) The fermion line <u>points</u> to the creation operator vertex specified by the index $p=+$ in the system operator.



$$- \langle \hat{C}^{+}_{0,l_0\sigma} \hat{C}^{-}_{3,l_3\sigma} \rangle \left(D^{+}_{3,l_3\sigma} D^{-}_{0,l_0\sigma} \rho^{I}_{red}(\tau) \right) \qquad (4.43)$$

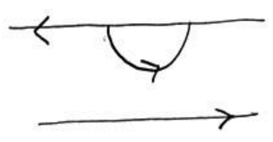
creation of an electron at τ_3 on the system



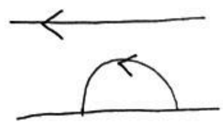
$$- \langle \hat{C}^{-}_{0,l_0\sigma} \hat{C}^{+}_{3,l_3\sigma} \rangle \left(D^{-}_{3,l_3\sigma} D^{+}_{0,l_0\sigma} \rho^{I}_{red}(\tau) \right) \qquad (4.44)$$

creation of an electron at τ_0 on the system

<u>Note</u>: the hermitian conjugate of a diagram corresponds to a <u>horizontal mirroring</u>: all vertices in the upper contour go to the lower contour and viceversa. Moreover, an incoming vertex becomes an outgoing one.

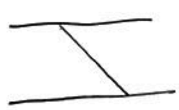


h.c



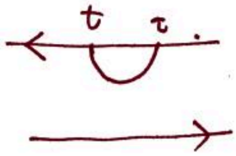
<u>Note</u>: if we do not specify $p=\pm$ and do not explicitly draw the h.c., the 8 2^{nd} order diagrams reduce to the two fundamental diagrams:

and



Sign associated to the different diagrams

The sign associated to the different diagrams depends on the number of anticommutation relation necessary to obtain the standard form:



comes from the contributions

$$- \mathrm{Tr}_{res}\{\hat{A}_3^+ \hat{A}_0^- \hat{\rho}_{red}^I(\tau) \hat{\rho}_{res}\} \quad \text{or}$$

$$- \mathrm{Tr}_{res}\{\hat{A}_3^- \hat{A}_0^+ \hat{\rho}_{red}^I(\tau) \hat{\rho}_{res}\}$$

more explicitly (for the first contribution)

$$- \sum_{l_3 l_0 \sigma} \mathrm{Tr}_{res}\{\hat{D}^+_{3,l_3\sigma} \hat{C}^-_{3,l_3\sigma} \hat{C}^+_{0,l_0\sigma} \hat{D}^-_{0,l_0\sigma} \hat{\rho}^I_{red}(\tau) \hat{\rho}_{res}\}$$

which is brought into the form of (4.41) by 2 anticommutations and leads

$$- \sum_{l_3 l_0 \sigma} \langle \hat{C}^-_{3,l_3\sigma} \hat{C}^+_{0,l_0\sigma} \rangle \left(\hat{D}^+_{3,l_3\sigma} \hat{D}^-_{0,l_0\sigma} \hat{\rho}^I_{red}(\tau) \right)$$

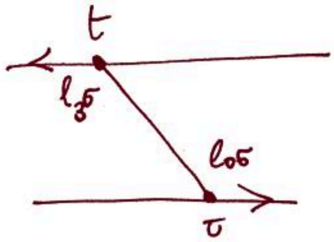
For the second contribution:

$$- \sum_{l_3 l_0 \sigma} \mathrm{Tr}_{res}\{\hat{C}^+_{3,l_3\sigma} \hat{D}^-_{3,l_3\sigma} \hat{D}^+_{0,l_0\sigma} \hat{C}^-_{0,l_0\sigma} \hat{\rho}^I_{red} \hat{\rho}_{res}\},$$

$$= - \sum_{l_3 l_0 \sigma} \langle \hat{C}^+_{3,l_3\sigma} \hat{C}^-_{0,l_0\sigma} \rangle \left(\hat{D}^-_{3,l_3\sigma} \hat{D}^+_{0,l_0\sigma} \hat{\rho}^I_{red}(\tau) \right)$$

or, with a common notation and omitting Σ, (4.41)

(4.42) instead is associated to



and comes from

$$+\ \mathrm{Tr}_{res}\left\{ \hat{A}_3^+ \, \hat{\rho}^I_{red}(\tau)\, \hat{\rho}_{res}\, \hat{A}_0^- \right\} \quad \text{or}$$

$$+\ \mathrm{Tr}_{res}\left\{ \hat{A}_3^- \, \hat{\rho}^I_{red}(\tau)\, \hat{\rho}_{res}\, \hat{A}_0^+ \right\}$$

where the inner commutation has been performed.

for the first case

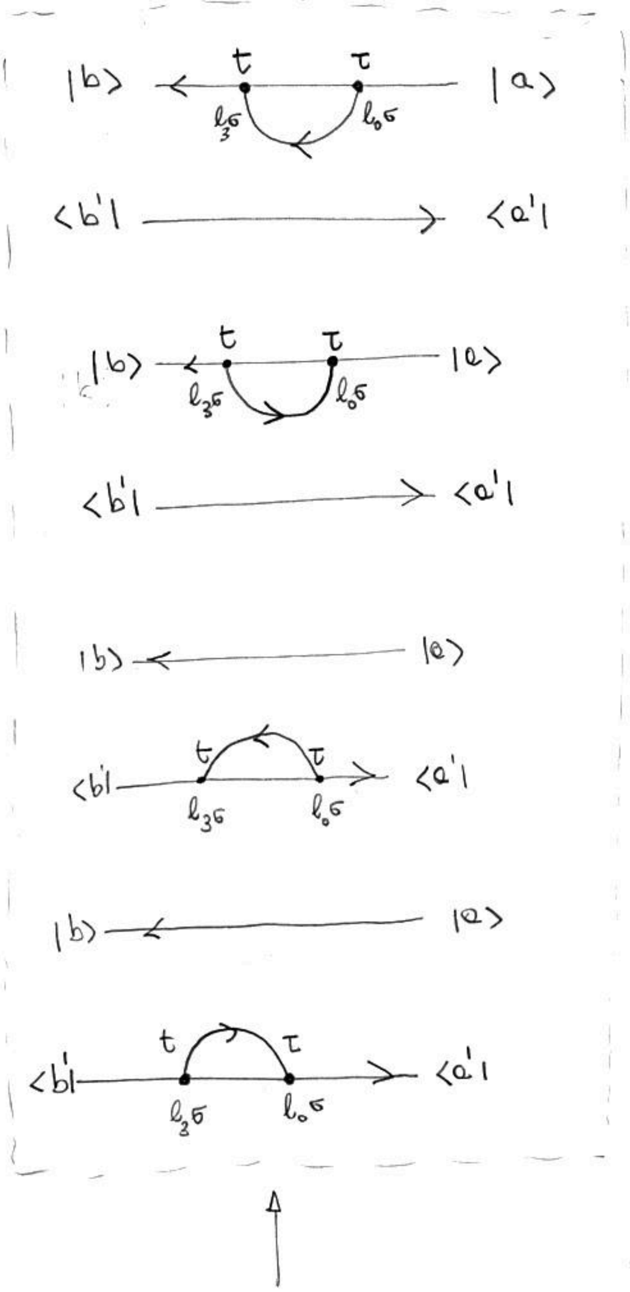
$$+\sum_{l_3 l_0 \sigma} \mathrm{Tr}_{res}\left\{ \hat{D}^+_{3,l_3\sigma}\, \hat{C}^-_{3,l_3\sigma}\, \hat{\rho}^I_{red}(\tau)\, \hat{\rho}_{res}\, \hat{C}^+_{0,l_0\sigma}\, \hat{D}^-_{0,l_0\sigma} \right\}$$

2 anticom $\{C, D\}$ and 1 comm D, ρ_{res} or C, ρ_{red}.

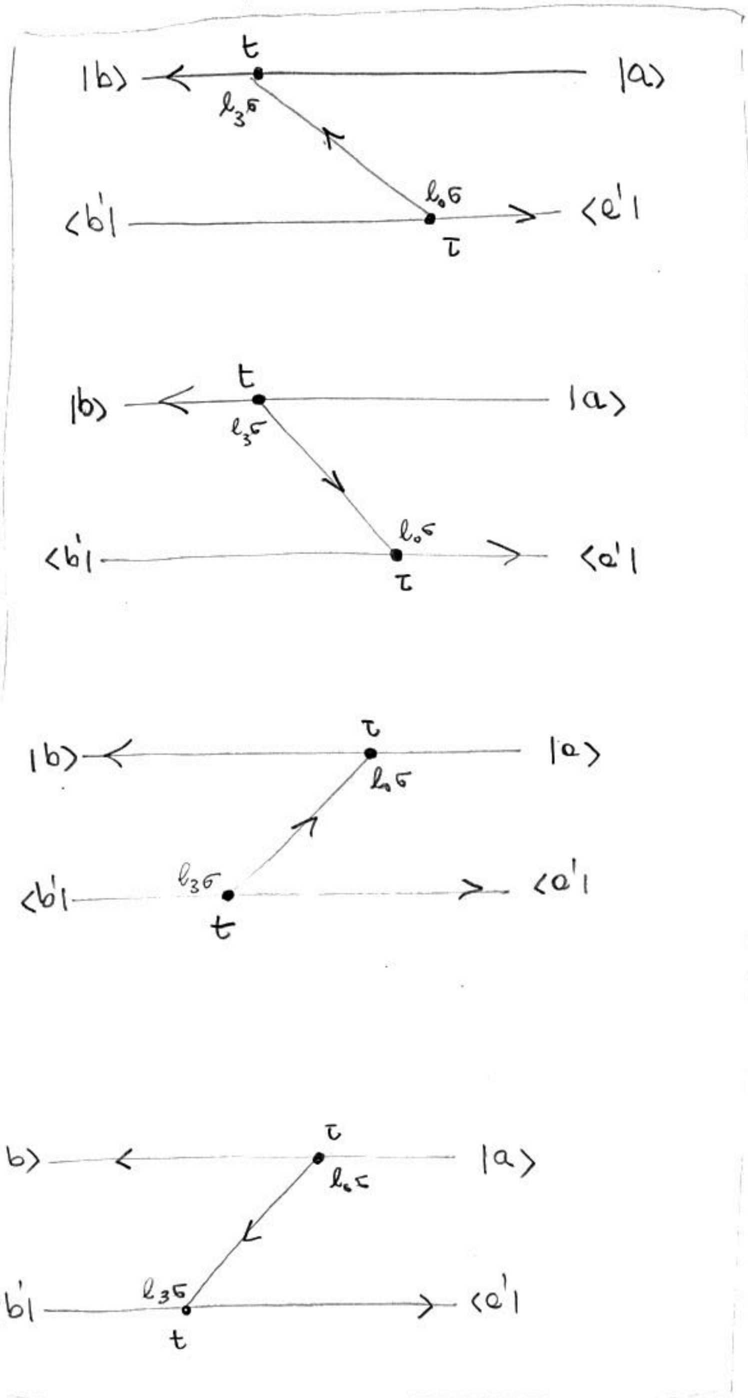
$$= \sum_{l_3 l_0 \sigma} \mathrm{Tr}_{res}\left\{ \hat{C}^-_{3,l_3\sigma}\, \hat{\rho}_{res}\, \hat{C}^+_{0,l_0\sigma} \right\} \hat{D}^+_{3,l_3\sigma}\, \hat{\rho}^I_{red}(\tau)\, \hat{D}^-_{0,l_0\sigma}$$

$$= \sum_{l_3 l_0 \sigma} \langle \hat{C}^+_{0,l_0\sigma}\, C^-_{3,l_3\sigma} \rangle \; D^+_{3,l_3\sigma}\, \hat{\rho}^I_{red}(\tau)\, D^-_{0,l_0\sigma}$$

Each of them stands in reality for 4 distinct contributions:



sum over l_0, l_3 and σ is assumed. All variables associated to a vertex are summed over.

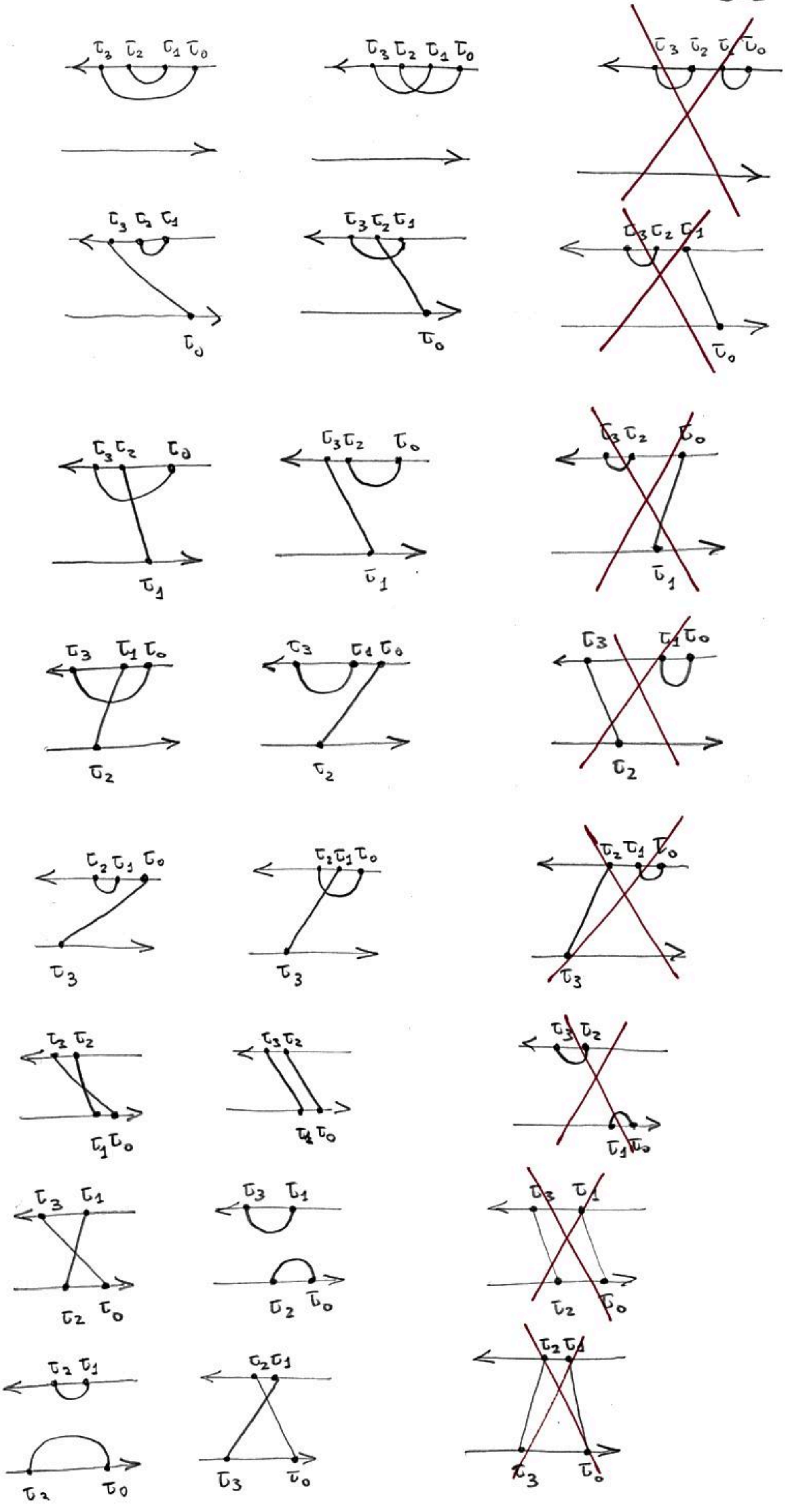


All the 2nd order diagrams grouped into 2 classes.

Note, in the specific case, the particular choice of the initial and final states (|a⟩, ⟨a'| ; |b⟩, ⟨b'| respectively) imposes severe selection rules on the vertices and l_0 and l_3 could result in being completely fixed. That is the case for example if the interaction is well described by the constant interaction approximation.

Analogously, for the 4^{th} order diagrams we can identify 16 classes with 8 elements each. Here are the schematic representation of the classes:

IRREDUCIBLE REDUCIBLE



<u>Note</u>: a reducible diagram can be cutted in 2 parts by a vertical cut that does not cross a fermionic line.

<u>Note</u>: The 8 diagrams per each class are obtained by assigning a direction to each fermionic line (4 choices) and by hermitian conjugation (ie vertical mirroring + direction reversal of the fermionic line, × 2).

Note: for the calculation of the stationary density matrix one needs the Laplace transform of the time evolution Kernel in the Schrödinger picture. Explicitly; from (4.25)

$$K^{aa'}_{bb'} = K^{(2)\,aa'}_{bb'} + K^{(4)\,aa'}_{bb'} + \dots$$

where

$$K^{(2)\,aa'}_{bb'} = \lim_{\lambda\to 0} \int_0^\infty d(t-\tau)\, e^{-\lambda(t-\tau)}\, e^{-i/\hbar(E_b-E_{b'})t}\, e^{i/\hbar(E_a-E_{a'})\tau}$$

$$\langle b|\, K^{I(2)}(t,\tau)\left[|a\rangle\langle a'|\right]|b'\rangle$$

with the substitution $\tau' = t-\tau \Rightarrow \tau = t-t'$

$$\Rightarrow K^{(2)\,aa'}_{bb'} = \lim_{\lambda\to 0} \int_0^\infty d\tau'\, e^{-\lambda\tau'}\, e^{-i/\hbar(E_b-E_{b'})t}\, e^{i/\hbar(E_a-E_{a'})(t-\tau')}$$

$$\langle b|\, K^{I(2)}(t,t-\tau')\left[|a\rangle\langle a'|\right]|b'\rangle \tag{4.45}$$

Likewise for the 4th order, shifting

$$\begin{aligned} t-\tau &= \tau' \\ t-\tau_1 &= \tau_1' \\ t-\tau_2 &= \tau_2' \end{aligned} \quad \Rightarrow \quad \tau_i - \tau_j = \tau_j' - \tau_i'$$

one gets

$$K^{(4)\,aa'}_{bb'} = \lim_{\lambda\to 0} \int_0^\infty d\tau'\, e^{-\lambda\tau'} \int_0^{\tau'} d\tau_1' \int_0^{\tau_1'} d\tau_2'\, e^{-i/\hbar(E_b-E_{b'})t}\, e^{i/\hbar(E_a-E_{a'})(t-\tau')}$$

$$\langle b|\, K^{I(4)}(t,t-\tau_2',t-\tau_1',t-\tau')\left[|a\rangle\langle a'|\right]|b'\rangle \tag{4.46}$$

The time dependence of the Kernels $K^{(2)}$ and $K^{(4)}$ is the one of the $\hat{C}_i^{p_i}$ and $\hat{D}_i^{p_i}$ operators.

For example, a term $\langle \hat{C}^{p_i}_{i,l_i\sigma} \hat{C}^{p_j}_{j,l_j\sigma} \rangle \hat{D}^{\bar{p}_i}_{i,l_i\sigma} \hat{D}^{\bar{p}_j}_{j,l_j\sigma}$ yields the contribution:

$$\langle \hat{C}^{p_i}_{i,l_i\sigma} \hat{C}^{p_j}_{j,l_j\sigma} \rangle \hat{D}^{\bar{p}_i}_{i,l_i\sigma} \hat{D}^{\bar{p}_j}_{j,l_j\sigma} = \delta_{p_i,-p_j} \frac{1}{\hbar^2} \sum_{\alpha\vec{k}} f_\alpha^{p_i}(\omega_{\vec{k}})\, e^{p_i \frac{i\omega_{\vec{k}}}{\hbar}(\tau_i-\tau_j)} \,.$$

$$t^{p_i}_{\alpha\vec{k}\sigma l_i}\, t^{p_j}_{\alpha\vec{k}\sigma l_j}\; e^{i \hat{H}_s/\hbar\, \tau_i}\, \hat{d}^{\bar{p}_i}_{l_i\sigma}\, e^{-iH_s/\hbar(\tau_i-\tau_j)}\, \hat{d}^{+\bar{p}_j}_{l_j\sigma}\, e^{-i/\hbar \hat{H}_s \tau_j} \qquad (4.47)$$

with the notation $t^{p_i} = \begin{cases} t^* & p_i = + \\ t & p_i = - \end{cases}$ $\quad d^{p_i} = \begin{cases} d^{+} & p_i = + \\ d & p_i = - \end{cases}$

where we have used the relations

$$\langle \hat{c}^{p_i}_{\alpha\vec{k}\sigma}\, \hat{c}^{p_j}_{\alpha'\vec{k}'\sigma'} \rangle = \delta_{\alpha\alpha'}\, \delta_{\sigma\sigma'}\, \delta_{\vec{k}\vec{k}'}\, \delta_{p_i,-p_j}\, f_\alpha^{p_i}(\omega_{\vec{k}}) \quad \text{and}$$

$$\hat{c}^{p_i}_{\alpha\vec{k}\sigma}(\tau_i) = e^{ip_i\omega_{\vec{k}}\tau_i/\hbar}\, \hat{c}^{p_i}_{\alpha\vec{k}\sigma}.$$

Moreover we have defined

$$f_\alpha^{+}(\omega_{\vec{k}}) := f(\beta\omega_{\vec{k}} - \beta\mu_\alpha) = \frac{1}{e^{\beta(\omega_{\vec{k}}-\mu_\alpha)}+1} \quad \text{and} \quad f_\alpha^{-}(\omega) = 1 - f_\alpha^{+}(\omega) \qquad (4.48)$$

Note: one can recast $\sum_{\vec{k}} \to \int d\omega\, \mathcal{D}(\omega)$ where $\mathcal{D}_\alpha(\omega)$ is the density of states of the lead α.

Assumption: If we assume an energy independent tunnelling coupling $t_{\alpha\vec{k}l\sigma} = t_{\alpha\sigma}$ => it is convenient to introduce the many-body tunnelling amplitudes;

$$T^{+}_{\alpha\sigma}(a,b) := \sqrt{\mathcal{D}_\alpha} \sum_{l} t_{\alpha\sigma} \langle a|\, \hat{d}^{+}_{l\sigma}\, |b\rangle \qquad (4.49)$$

$$T^{-}_{\alpha\sigma}(a,b) := \left(T^{+}_{\alpha\sigma}(b,a)\right)^*$$

also known as tunnelling matrix elements (TME)

4.1.2 Current Kernel

Now that we have learned the convenience of the diagrammatic representation it would be advantageous to formulate also the current kernel in terms of diagrams. We know that the current kernel $K^{I}_{I_\alpha}(t,\bar{\tau})$ differs from the time evolution kernel $K^{I}(t,\tau)$ only by the replacement of the Liouville superoperator $\mathcal{L}^{\mp}(t)$ with the current operator $\hat{I}_\alpha(t)$. This fact has the following diagrammatic implications:

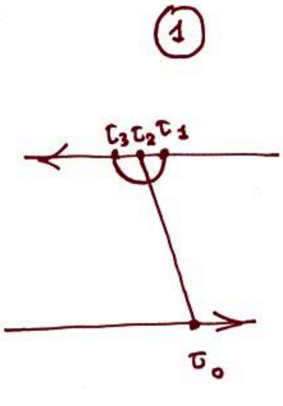
1- As $\hat{I}_\alpha$ contains only operators from lead α, there is no sum over the lead index of the fermion line connected to the latest vertex (at time t), the latter belongs exclusively to lead α.

2- As $\hat{I}_\alpha$ is a normal operator and not a superoperator involving a commutator, the vertex at time t lie on the upper contour

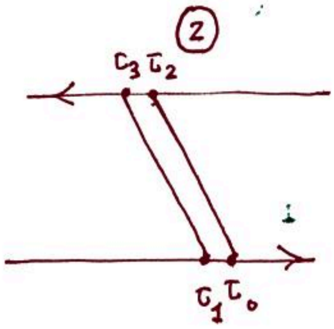
3- As $\hat{I}_\alpha$ differs from $\hat{H}_{T\alpha}$ by the sign of the out-tunnelling contribution, the sign of diagrams with the fermion line pointing away from the latest vertex must be inverted

<u>Note</u>: Due to the cyclic property of the full trace involved in the calculation of the average current, it is also possible to use diagrams with the last vertex on the lower contour.

Two examples of 4^{th} order diagram backmapping in the time domain



and



First of all one should remember that every contribution stems from:

$$\mathrm{Tr}_{res}\left\{\left[\hat{A}_3^{p_3},\left[\hat{A}_2^{p_2},\left[\hat{A}_1^{p_1},\left[\hat{A}_0^{p_0},\ \rho^I_{red}(\tau_0)\otimes\hat{\rho}_{res}\right]\right]\right]\right\}$$

1 Has the rearliest vertex on the lower contour which means that diagram comes from the analytical contribution (II term of the innest commentator)

$$-\mathrm{Tr}_{res}\left\{\hat{A}_3^{p_3}\hat{A}_2^{p_2}\hat{A}_1^{p_1}\,\hat{\rho}^I_{red}(\tau_0)\otimes\hat{\rho}_{res}\,\hat{A}_0^{p_0}\right\}$$

Contractions come now into play due to the trace over reservoirs

$$-\mathrm{Tr}_{res}\left\{\sum_{\{l\}\{\sigma\}\{p\}} p_3\hat{C}^{p_3}_{3,l_3\sigma_3}\hat{D}^{\bar{p}_3}_{3,l_3\sigma_3}\,p_2\hat{C}^{p_2}_{2,l_2\sigma_2}\hat{D}^{\bar{p}_2}_{2,l_2\sigma_2}\,p_1\hat{C}^{p_1}_{1,l_1\sigma_1}D^{\bar{p}_1}_{1,l_1\sigma_1}\,\hat{\rho}^I_{red}(\tau_0)\otimes\hat{\rho}_{res}\,p_0\hat{C}^{p_0}_{0,l_0\sigma_0}\hat{D}^{\bar{p}_0}_{0,l_0\sigma_0}\right.$$

Now we want to factorize the system and the reservoir components. We move all $\hat{D}$ operators to the left and all $\hat{C}$ operators to the right.

Interestingly $[\hat\rho^{I}_{red}(\tau), \hat C^{p_i}_{i,l_i\sigma_i}]=0$ and $[\hat\rho_{res}, \hat D^{p_i}_{i,l_i\sigma_i}]=0$ which implies that we can most generally consider the following case:

A contribution of order $2n$ reads:

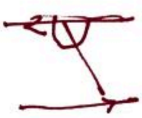
$$\prod_{i=1}^{2n} \phi_i\, \hat C^{p_i}_{i,l_i\sigma_i}\, \hat D^{\bar p_i}_{i,l_i\sigma_i} = \prod_{i=1}^{2n} \phi_i\, (-1)^{\sum_{i=1}^{2n-i} i} \prod_i \hat C^{p_i}_{i,l_i\sigma_i} \prod_j \hat D^{\bar p_j}_{j,l_j\sigma_j}$$

$$= \prod_{i=1}^{2n} \phi_i\, \underbrace{(-1)^{(2n-1)\cancel{2}n/\cancel{2}}}_{(-1)^n} \prod_i \hat C^{p_i}_{i,l_i\sigma_i} \prod_j \hat D^{\bar p_j}_{j,l_j\sigma_j}$$

Now, the contractions of Wick's theorem imposes the ϕ_i to match in $\underline{\underline{n}}$ pairs $\{\phi_i, \bar\phi_i\}$ => from the first product we obtain

$$(-1)^n \times (-1)^n \prod \hat C_i \prod \hat D_j = \prod_i \hat C_i \prod_j \hat D_j$$

To all orders one can extract $\hat C$ and $\hat D$ operators without prize. Returning to our 4th order diagram:



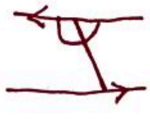
$$= -\sum_{\{l\}\{\sigma\}\{p\}} \mathrm{Tr}_{res}\left\{ \hat C^{p_3}_{3,l_3\sigma_3} \hat C^{p_2}_{2,l_2\sigma_2} \hat C^{p_1}_{1,l_1\sigma_1} \hat\rho_{res} \hat C^{p_0}_{0,l_0\sigma_0} \right\} \cdot$$

$$\cdot\, \hat D^{\bar p_3}_{3,l_3\sigma_3} \hat D^{\bar p_2}_{2,l_2\sigma_2} \hat D^{\bar p_1}_{1,l_1\sigma_1} \hat\rho^{I}_{red}(\tau_0) \hat D^{\bar p_0}_{0,l_0\sigma_0}$$

$$\overset{\text{cyclic}}{=} -\sum_{\{l\}\{\sigma\}\{p\}} \mathrm{Tr}_{res}\left\{ \hat C_0^{p_0} \hat C_3^{p_3} \hat C_2^{p_2} \hat C_1^{p_1} \hat\rho_{res} \right\} \cdot$$

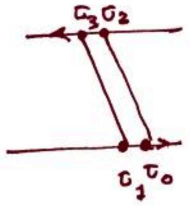
$$D_3^{\bar p_3} D_2^{\bar p_2} D_1^{\bar p_1} \hat\rho^{I}_{red}(\tau_0) \hat D_0^{\bar p_0}$$

Finally, from the graph we see the contraction (3 1) and (1 0)
This is not a direct contraction. For this reason an extra minus



$$= \sum_{\substack{p,p' \\ \sigma\sigma' \\ \{\ell\}}} \langle \hat{C}^{p}_{0,\ell_0\sigma} \hat{C}^{\bar{p}}_{2,\ell_2\sigma} \rangle \langle \hat{C}^{p'}_{3,\ell_3\sigma'} \hat{C}^{\bar{p}'}_{1,\ell_1\sigma'} \rangle \hat{D}^{\bar{p}'}_{3,\ell_3\sigma'} D^{p}_{2,\ell_2\sigma} D^{p'}_{1,\ell_1\sigma'} \rho_{red}(\tau_0) \hat{D}^{\bar{p}}_{0,\ell_0\sigma}$$

Now the second diagram as a further exercise.



$$= \mathrm{Tr}_{res} \Big\{ \sum_{\{\ell\}\{\sigma\}\{p\}} \hat{C}^{p_3}_3 \hat{C}^{p_2}_2 \hat{\rho}_{res} \hat{C}^{p_0}_0 \hat{C}^{p_1}_1 \Big\} \hat{D}^{\bar{p}_3}_3 \hat{D}^{\bar{p}_2}_2 \hat{\rho}^{I}_{red}(\tau_0) \hat{D}^{\bar{p}_0}_0 \hat{D}^{\bar{p}_1}_1$$

$$= \sum_{\{\ell\}\{\sigma\}\{p\}} \mathrm{Tr}_{res} \Big\{ \hat{C}^{p_0}_0 \hat{C}^{p_1}_1 \hat{C}^{p_3}_3 \hat{C}^{p_2}_2 \hat{\rho}_{res} \Big\} \hat{D}^{\bar{p}_3}_3 \hat{D}^{\bar{p}_2}_2 \hat{\rho}^{I}_{red}(\tau_0) \hat{D}^{\bar{p}_0}_0 \hat{D}^{\bar{p}_1}_1$$

$$= \sum_{\substack{p p' \\ \sigma\sigma' \\ \{\ell\}}} \langle \hat{C}^{p}_{0,\ell_0\sigma} \hat{C}^{\bar{p}}_{2,\ell_2\sigma} \rangle \langle \hat{C}^{p'}_{1,\ell_1\sigma'} \hat{C}^{\bar{p}'}_{3,\ell_3\sigma'} \rangle \hat{D}^{p'}_{3,\ell_3\sigma'} \hat{D}^{p}_{2,\ell_2\sigma} \hat{\rho}^{I}_{red}(\tau_0) D^{\bar{p}}_{0,\ell_0\sigma} D^{\bar{p}'}_{1,\ell_1\sigma'}$$