4.2 Diagrammatic analysis in the time and energy domain

In the following we discuss a graphical (= diagrammatic) language which enables to visualize all contributions to the kernels $K^{(2)}$, $K^{(4)}$, K_c and K_{I_α}. Moreover we will derive rules to map the diagrams into the corresponding analytical expressions.

To start, we separate the tunnelling operator into a in- and out-tunnelling components:

$$\frac{1}{\hbar}\hat{H}_{T,I}(\tau_i) = \hat{A}_i^+ + \hat{A}_i^- \qquad (4.33)$$

with

$$\hat{A}_i^+ := \sum_{l\sigma} \hat{D}^+_{i,l\sigma}\,\hat{C}^-_{i,l\sigma} =: \sum_{l\sigma}\left(\hbar^{-1}\hat{d}^+_{l\sigma}(\tau_i)\right)\left(\sum_{b\vec{k}} t_{b\vec{k}l\sigma}\,\hat{c}_{b\vec{k}\sigma}(\tau_i)\right)$$

and

$$\hat{A}_i^- := \sum_{l\sigma} \hat{C}^+_{i,l\sigma}\,\hat{D}^-_{i,l\sigma} =: \sum_{l\sigma}\left(\sum_{b\vec{k}} t^*_{b\vec{k}l\sigma}\,\hat{c}^+_{b\vec{k}\sigma}(\tau_i)\right)\left(\hbar^{-1} d_{l\sigma}(\tau_i)\right) \qquad (4.33b)$$

where l labels a single particle basis for the system, $b = L, R$. Notice that via the tunnelling amplitude $t_{b\vec{k}l\sigma}$ some information on the system state $l\sigma$ propagates into the effective lead operator $\hat{C}^\pm_{i,l\sigma}$. The latter is the relevant lead operator with decaying correlator, contrary to $c_{\vec{k}\sigma}$. Since fermionic operators of leads and system anticommute:

$$\hat{C}^\pm_{i,l\sigma}\,\hat{D}^\mp_{i,l\sigma} = -\,\hat{D}^\mp_{i,l\sigma}\,\hat{C}^\pm_{i,l\sigma} \qquad (4.34).$$

Starting from the eq. (4.18) one obtains:

$$K_I^{(2)}(t,\tau)\,\hat{\rho}_{red,I}(\tau) = -\sum_{p_0 p_3 \in (+,-)} \mathrm{Tr}_B\left\{\left[\hat{A}_3^{p_3},\left[\hat{A}_0^{p_0},\, \rho_{red,I}(\tau)\otimes\hat{\rho}_B\right]\right]\right\} \qquad (4.35)$$

and

$$K_I^{(4)}(t,\tau)\,\hat{\rho}_{red,I}(\tau) = + \sum_{p_0 p_1 p_2 p_3 \in \{+,-\}} \int_{\tau}^{t} d\tau_1 \int_{\tau_1}^{t} d\tau_2$$

$$\Big(Tr_B\{[\hat{A}_3^{p_3},[\hat{A}_2^{p_2},[\hat{A}_1^{p_1},[\hat{A}_0^{p_0}, \rho_{red,I}(\tau)\otimes\hat{\rho}_B]]]]\}$$

$$- Tr_B\{[\hat{A}_3^{p_3},[\hat{A}_2^{p_2}, Tr_B\{[\hat{A}_1^{p_1},[\hat{A}_0^{p_0}, \hat{\rho}_{red,I}(\tau)\otimes\hat{\rho}_B]]\}\otimes\hat{\rho}_B]]\}\Big) \qquad (4.36)$$

where $\tau_0 = \tau$ and $\tau_3 = t$.

The evaluation of the commutators is a lengthy but straightforward task which is achieved invoking Wick's theorem and the cyclic invariance of the trace.

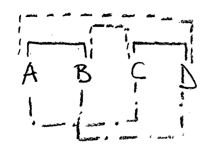
One obtains { 8 contributions in 2^{nd} order
| 128 contributions in 4^{th} order

Notice: the number of contributions given above takes into account the constraints on $\{p_i\}$ given by the Wick's theorem.
For example, for the 2^{nd} order contributions one counts:

$$\underset{\sum_{p_0}}{2} \times \underset{\sum_{p_3}}{2} \times \underset{\text{inner } [\,,\,]}{2} \times \underset{\text{outer } [\,,\,]}{2} = 16$$

Wick's theorem, though, imposes $p_0 = -p_3$ => the number of contributions reduces to 8.
For the 4^{th} order contributions

$$\underset{\sum_{\{p_i\}}}{2^4} \times \underset{[\,,\,]}{2^4} \times \underset{\text{contractions}}{(3-1)} = 512$$



the solid line contraction is cancelling out.

Wick's theorem imposes through $p_0 = -p_3 \wedge p_1 = -p_2$ or $\Rightarrow$ the number of
$p_0 = -p_2 \wedge p_1 = -p_3$ or
$p_0 = -p_1 \wedge p_2 = -p_3$

diagrams must be divided by 4 since only two p_i's are independent.

In general, a $2n$-th contribution $K^{(2n)aa'}_{I\,bb'}$ (odd contribution vanish identically) reads:

$$\prod_{q=1}^{n} \langle \hat{C}_{q,I} \rangle \langle b | \hat{\mathcal{D}}_I | a \rangle \langle a | \hat{\rho}_{red,I}(\tau) | a' \rangle \langle a' | \hat{\mathcal{D}}'_I | b' \rangle \qquad (4.37)$$

where $\hat{C}_{q,I}$ is formed by the product of <u>two</u> lead operators, being $\prod_q \langle \hat{C}_{q,I} \rangle$ the product of Wick's contractions, while $\hat{\mathcal{D}}_I$ and $\hat{\mathcal{D}}'_\alpha$ contain <u>together</u> the corresponding $2n$ dot operators.
Moreover one has to count over the sum over the system degrees of freedom l, σ. In case of unpolarized or parallel polarized leads σ is conserved and n sums survive. For l there are in general no conservation rules and $2n$ sums should be performed.

4.2.1 Diagrammatic rules in the time domain

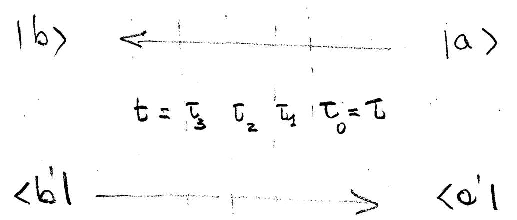
To each contribution (4.37) a DIAGRAM can be associated. The Laplace transform $\tilde{K}^{bb'}_{aa'}$.

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

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

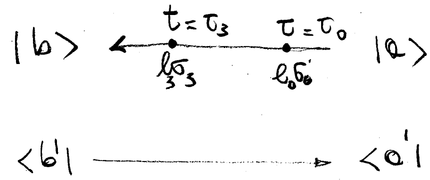
$\langle b'| \longrightarrow \langle a'|$

ii) Through the entire diagram time grows from <u>right</u> to <u>left</u>
$\Rightarrow$ $|a\rangle, \langle a'|$ are the "initial" states. $|b\rangle, \langle b'|$ the "final" ones.



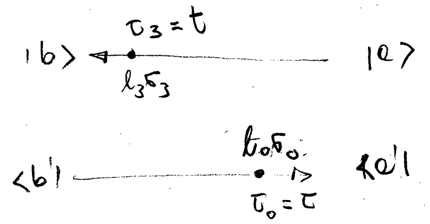
iii) Every system operator standing on the left of the RDM (belonging to $\hat{\mathcal{D}}_I$) is associated to a vertex at a given time on the upper contour. Each operator on the right (belonging to $\hat{\mathcal{D}}'_I$) is associated to a vertex in the lower contour.

Examples in 2nd order:



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

or

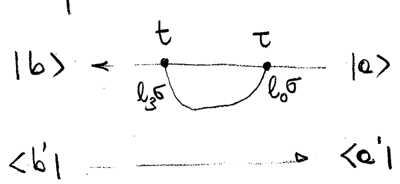


$$\hat{D}^{p_3}_{3\,l_3\sigma_3}\,\hat{\rho}_{red,I}(\tau)\,\hat{D}^{p_0}_{0,l_0\sigma_0}$$

At each vertex the charge of the state changes by ± 1 (from right to left) depending on the sign of p_i.

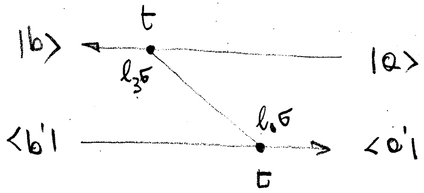
iv) The vertices of the system operators which are related by two contracted lead operators are connected by a fermionic line

Examples in 2nd order



$$-\langle \hat{C}^{\bar{p}}_{3,l_3\sigma}\,\hat{C}^{p}_{0,l_0\sigma}\rangle\,\left(\hat{D}^{p}_{3,l_3\sigma}\,\hat{D}^{\bar{p}}_{0,l_0\sigma}\,\hat{\rho}_{red,I}(\tau)\right) \quad (4.38)$$

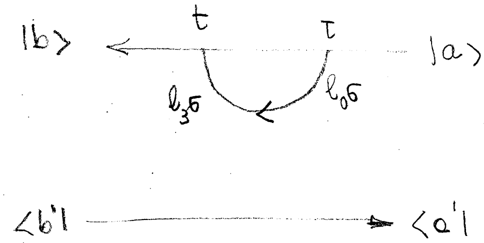
notice that Wick's contraction imposes $p_0 = \bar{p}_3$ and $\sigma_0 = \sigma_3$



$$\langle \hat{C}^{p}_{0,l_0\sigma}\, \hat{C}^{\bar{p}}_{3\, l_3\sigma} \rangle \left(\hat{D}^{p}_{3,l_3\sigma}\, \hat{\rho}_{red,I}(\tau)\, \hat{D}^{\bar{p}}_{0,l_0\sigma} \right) \tag{4.39}$$

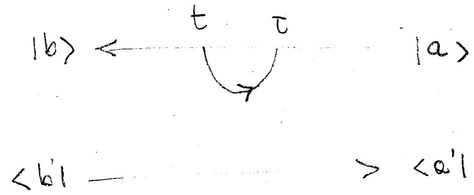
↑ cyclic prop. of the trace.

v) The fermionic line <u>points</u> towards the system creation operator vertex (specified by the index $p=+$ in the system operator



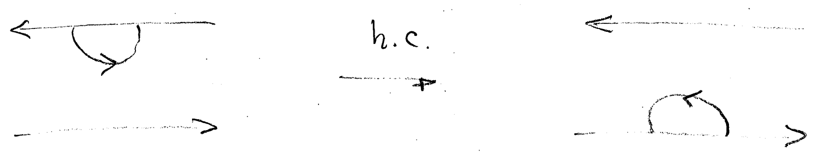
$$-\langle \hat{C}^{-}_{3 l_3\sigma}\, \hat{C}^{+}_{0 l_0\sigma} \rangle \left(\hat{D}^{+}_{3 l_0\sigma}\, \hat{D}^{-}_{0,l_0\sigma}\, \hat{\rho}_{red,I}(\tau) \right) \tag{4.40}$$

↑ creation of an electron on the system at τ_3

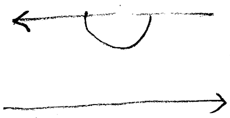


$$-\langle \hat{C}^{+}_{3 l_3\sigma}\, \hat{C}^{-}_{0 l_0\sigma} \rangle \left(\hat{D}^{-}_{3,l_3\sigma}\, \hat{D}^{+}_{0 l_0\sigma}\, \hat{\rho}_{red,I}(\tau) \right) \tag{4.41}$$

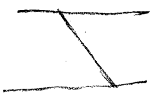
<u>Note</u>: the hermitian conjugate of a diagram correspond to an horizontal mirroring with all vertices on the upper contour going to the lower one and reversing of the direction of the fermionic lines



<u>Note</u>: By living implicit the direction of the Fermionic lines and h.c. we can reduce the 8 2nd order diagrams to 2

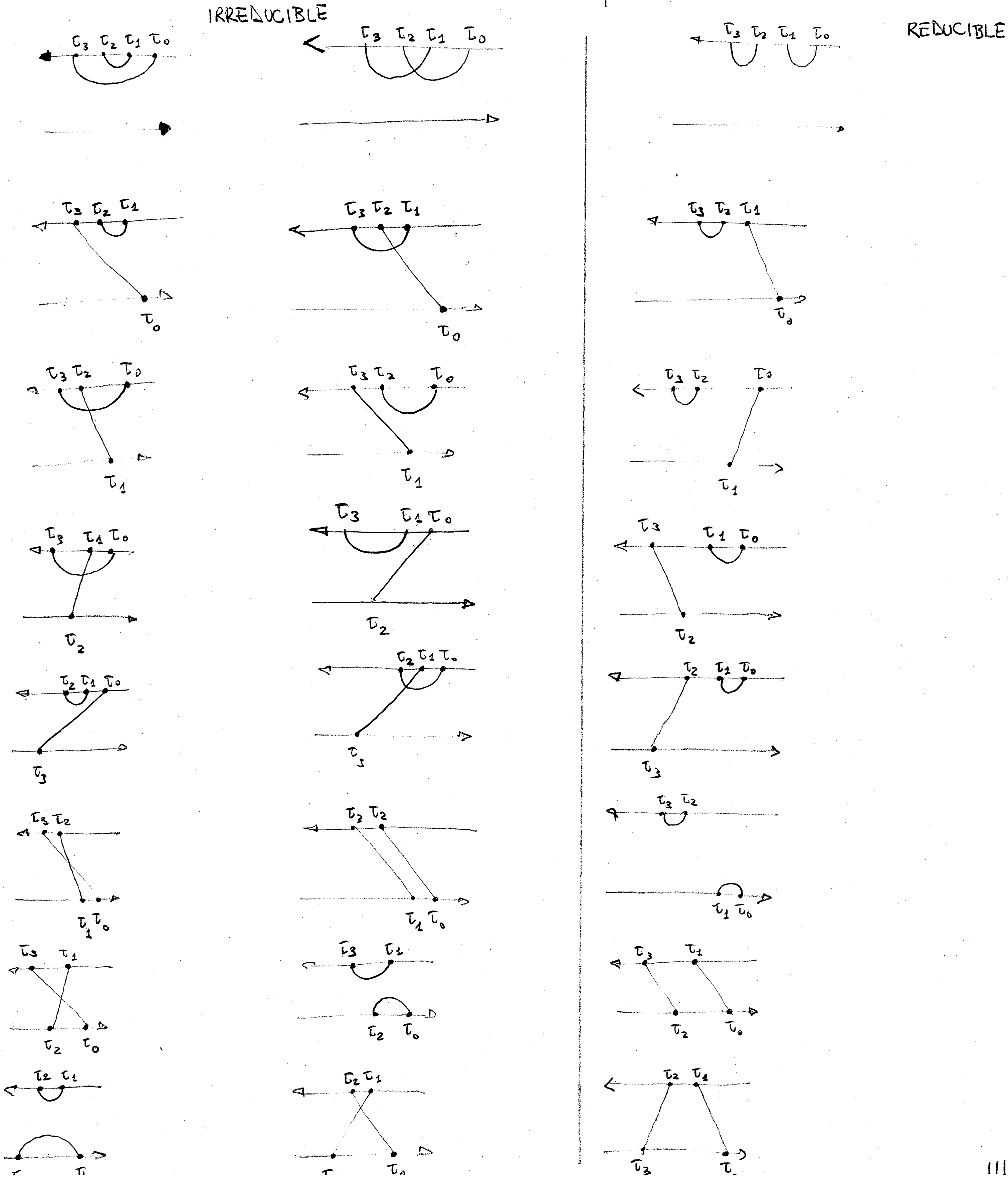


and



<u>Note</u> the sign of each diagram depends on the number of anticommutations necessary to obtain the standard form.

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

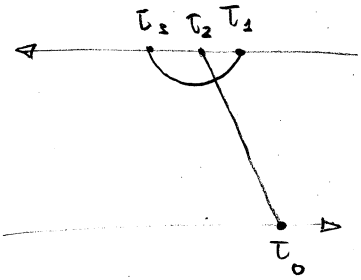


Note: a reducible diagram can be cutted in 2 parts by a vertical cut that does not cross a fermionic line.

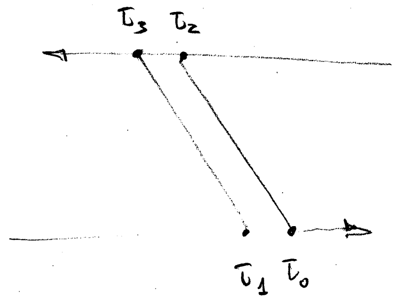
The 8 diagrams per each class are obtained by assigning a direction to each fermionic line (4 choices) and by hermitian conjugation.

Let us now consider for clarity two examples of 4^{th} order diagrams in the time domain and derive their explicit expression

(1)



(2)



First of all one should remember that every contribution stems from

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

(1) It has the earliest vertex on the lower contour which means that the diagram stem from the analytical contribution

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

Contractions (fermionic lines) come now into play due to the trace over the baths

$$- \mathrm{Tr}_B \left\{ \sum_{\{l\}\{\sigma\}\{p\}} p_3 \hat{C}_3{}^{p_3}_{l_3\sigma_3} \hat{D}_3{}^{\bar{p}_3}_{l_3\sigma_3} p_2 \hat{C}_2{}^{p_2}_{l_2\sigma_2} \hat{D}_2{}^{\bar{p}_2}_{l_2\sigma_2} p_1 \hat{C}_1{}^{p_1}_{l_1\sigma_1} \hat{D}_1{}^{\bar{p}_1}_{l_1\sigma_1} \hat{\rho}_{red,I}(\tau_0) \otimes \rho_B\, p_0 \hat{C}_0{}^{p_0}_{l_0\sigma_0} \hat{D}^{\bar{p}_0}_{l_0}$$

We factorize system and bath components. $\hat{D}$ operator to the left, $\hat{C}$ to the right.

Interestingly $[\hat{\rho}_{red,I}(\tau), \hat{C}^{p_i}_{i,l_i\sigma_i}] = 0$ and $[\hat{\rho}_B, \hat{D}^{p_i'}_{i l_i \sigma_i}] = 0$ due to particle number conservation of $\hat{\rho}_{red;I}$ and $\hat{\rho}_B$ in the system and bath respectively. This observation implies, in general for a contribution of order $2n$

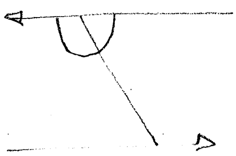
$$\prod_{i=1}^{2n} p_i\, \hat{C}^{p_i}_{i\, l_i\sigma_i} \hat{D}^{\bar{p}_i}_{i l_i \sigma_i} = \prod_{i'=1}^{2n} p_{i'} (-1)^{\sum_{j'=1}^{2n-1} j'} \prod_i \hat{C}^{p_i}_{i l_i \sigma_i} \prod_{j'} \hat{D}^{\bar{p}_{j'}}_{j' l_{j'} \sigma_{j'}}$$

$$= \prod_{i=1}^{2n} p_i \underbrace{(-1)^{(2n-1)2n/2}}_{(-1)^n} \prod_i \hat{C}^{p_i}_{i l_i \sigma_i} \prod_j \hat{D}^{\bar{p}_j}_{j\, l_j \sigma_j} \tag{4.42}$$

Now, the contractions of lead operators due to Wick's theorem imposes the p_i to match in pairs $\{p_i\, \bar{p}_i\}$ => we obtain

$$\cancel{(-1)^{2n}} \prod_i \hat{C}^{p_i}_{i l_i \sigma_i} \prod_j \hat{D}^{\bar{p}_j}_{j l_j \sigma_j}$$

To all orders one can separate $\hat{C}$ and $\hat{D}$ operators at no prize. Only the relative position of $\hat{C}$ with respect to $\hat{\rho}_B$ and $\hat{D}$ with respect to $\hat{\rho}_{red,I}$ must be maintained.

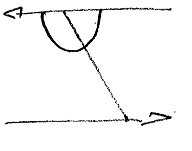


cyclic prop. of Tr_B

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

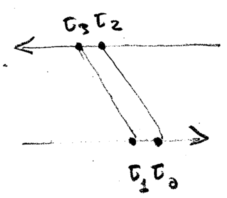
$$\cdot \hat{D}^{\bar{p}_3}_{3 l_3\sigma_3} \hat{D}^{\bar{p}_2}_{2 l_2\sigma_2} D^{\bar{p}_1}_{1 l_1\sigma_1} \hat{\rho}_{red,I}(\tau) D^{\bar{p}_0}_{0 l_0\sigma_0}$$

Finally, the graph prescribe the contraction (20), (31) to be performed



$$= \sum_{\substack{p p' \\ \sigma \sigma' \\ \{l\}}} \langle \hat{C}^{p}_{0 l_0\sigma} \hat{C}^{\bar{p}}_{2 l_2\sigma} \rangle \langle \hat{C}^{p'}_{3, l_3\sigma'} \hat{C}^{\bar{p}'}_{1, l_1\sigma'} \rangle \hat{D}^{\bar{p}'}_{3 l_3\sigma'} D^{p}_{2 l_2\sigma} D^{p'}_{1 l_1\sigma'} \hat{\rho}_{red,I}(\tau) \hat{D}^{\bar{p}}_{0, l_0}$$

The second diagram is analogously calculated



$$C\, Tr_B \left\{ \sum_{\{l\}\{\sigma\}\{p\}} \hat{C}^{p_3}_{3l_3\sigma_3}\, \hat{C}^{p_2}_{2l_2\sigma_2}\, \hat{\rho}_B\, \hat{C}^{p_0}_{0l_0\sigma_0}\, \hat{C}^{p_1}_{1l_1\sigma_1} \right\} \Delta^{\bar{p}_3}_{3l_3\sigma_3} \Delta^{\bar{p}_2}_{2l_2\sigma_2}\, \rho_{red}\, \Delta^{\bar{p}_0}_{0l_0\sigma_0} \Delta^{\bar{p}_1}_{1l_1\sigma_1}$$

$$= \sum_{\substack{pp' \\ \sigma\sigma' \\ \{l\}}} \langle \hat{C}^{p}_{0l_0\sigma}\, \hat{C}^{\bar{p}}_{2l_2\sigma} \rangle \langle \hat{C}^{p'}_{1l_1\sigma'}\, \hat{C}^{\bar{p}'}_{3l_3\sigma'} \rangle\, \Delta^{p'}_{3l_3\sigma'} \Delta^{p}_{2l_2\sigma}\, \rho_{red}(\tau_0)\, \Delta^{\bar{p}}_{0l_0\sigma} \Delta^{\bar{p}'}_{1l_1\sigma'}$$

The expression above should still be integrated $\int_{\tau_0}^{\tau} d\tau_1 \int_{\tau_1}^{\tau} d\tau_2$

4.2.2 Current Kernel

We know that the current kernel $K_{I_\alpha, I}(t,\tau)$ differs from the time evolution kernel $K_I(t,\tau)$ by the replacement of the Liouville superoperator $\mathcal{L}_{T,I}(t)$ 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 for the fermion line connected to the latest vertex. The latter belongs exclusively to the lead α.

2- As $\hat{I}_\alpha$ is a normal operator and not a superoperator the vertex at time t lies 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 fermionic line pointing away from the last vertex must be inverted.

Note: 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.

4.2.3 Diagrammatic rules in the energy domain

The diagrammatic rules in the energy domain are formulated for the Laplace transform of the Kernel in the Schrödinger picture. Explicitly, from (4.11)

$$K^{(2)\,aa'}_{bb'} = \lim_{\lambda\to 0}\int_0^\infty d(t-\tau)\, e^{-\lambda(t-\tau)}\, e^{-i/\hbar(E_b-E_{b'})t}\, e^{i/\hbar(E_a-E_{a'})\tau}$$
$$\langle b|\mathrm{Tr}_B\{\mathcal{L}_{T,I}(t)\,\mathcal{L}_{T,I}(\tau)\,|a\rangle\langle a'|\otimes\hat{\rho}_B\}|b'\rangle$$

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

$$K^{(2)\,aa'}_{bb'} = \lim_{\lambda\to 0}\int_0^\infty d\tau'\, e^{-\lambda\tau'}\, e^{-i/\hbar(E_b-E_{b'})t}\, e^{i/\hbar(E_a-E_{a'})(t-\tau')}$$
$$\langle b|\mathrm{Tr}_B\{\mathcal{L}_{T,I}(t)\,\mathcal{L}_{T,I}(t-\tau')\,|a\rangle\langle a'|\otimes\hat{\rho}_B\}|b'\rangle \qquad (4.43)$$

likewise for the 4^{th} order one obtains with the shifts: $\tau' = t-\tau$, $\tau_1' = t-\tau_1$, $\tau_2' = t-\tau_2$

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

$$\langle b|\Big(\mathrm{Tr}_B\{\mathcal{L}_{T,I}(t)\,\mathcal{L}_{T,I}(t-\tau_2')\,\mathcal{L}_{T,I}(t-\tau_1')\,\mathcal{L}_{T,I}(t-\tau')\,|a\rangle\langle a'|\otimes\rho_B\}|b'\rangle \qquad (4.44)$$
$$-\mathrm{Tr}_B\{\mathcal{L}_{T,I}(t)\,\mathcal{L}_{T,I}(t-\tau_2')\,\mathrm{Tr}_B\{\mathcal{L}_{T,I}(t-\tau_1')\,\mathcal{L}_{T,I}(t-\tau')\,|a\rangle\langle a'|\otimes\hat{\rho}_B\}\otimes\rho_B\}\Big)|1$$

The explicit calculation of the contraction in the time domain yields:

$$\langle \hat{C}^{p_i}_{i l_i \sigma_i} \hat{C}^{p_j}_{j l_j \sigma_j} \rangle \hat{D}^{\bar{p}_i}_{i l_i \sigma_i} \hat{D}^{\bar{p}_j}_{j l_j \sigma_j} =$$

$$= \delta_{p_i, -p_j} \delta_{\sigma_i \sigma_j} \frac{1}{\hbar^2} \sum_{\alpha \vec{k}} f^{p_i}_{\alpha}(\omega_{\vec{k}}) e^{p_i \frac{i \omega_{\vec{k}}}{\hbar}(\tau_i - \tau_j)} \cdot$$

$$\cdot \, t^{p_i}_{\alpha \vec{k} \sigma l_i} t^{\bar{p}_i}_{\alpha \vec{k} \sigma l_j} e^{i \hat{H}_S/\hbar \, \tau_i} \hat{d}^{\bar{p}_i}_{l_i \sigma} e^{-i H_S/\hbar (\tau_i - \tau_j)} \hat{d}^{\bar{p}_i}_{l_j \sigma} e^{-i/\hbar \hat{H}_S \tau_j} \tag{4.45}$$

where we have used the relations

$$\langle \hat{c}^{p_i}_{\alpha \vec{k} \sigma} \hat{c}^{p_j}_{\alpha' \vec{k}' \sigma'} \rangle = \delta_{\alpha \alpha'} \delta_{\sigma \sigma'} \delta_{\vec{k} \vec{k}'} \delta_{p_i, -p_j} f^{p_i}_{\alpha}(\omega_{\vec{k}}) \text{ and} \tag{4.46}$$

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

Moreover we have defined

$$f^{+}_{\alpha}(\omega_{\vec{k}}) := f(\beta \omega_{\vec{k}} - \mu_\alpha) = \frac{1}{e^{\beta(\omega_{\vec{k}} - \mu_\alpha)} + 1} \quad \text{and} \quad f^{-}_{\alpha}(\omega) = 1 - f^{+}_{\alpha}(\omega) \tag{4.47}$$

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

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

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

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

also known as tunnelling matrix elements (TME).

By inserting (4.45) in the equations (4.43) and (4.44) one notices that

1. The exponentials disappear thank to the first and last time propagator associated to $\mathcal{L}_{T,I}(t)$ and $\mathcal{L}_{T,I}(t-\tau')$

2. The Kernels become independent of the final time t

3. $K^{(4)}$ is convolutive in the time τ_1' τ_2'.

4. Using the property of the Laplace transform that the Laplace transform of the convolution is the product of the Laplace transforms => all time integrals can be easily performed. (they are simply integrals of exponential functions)

We are thus ready to give the rules to transform a diagram into the corresponding analytical expression contributing to the Laplace transform of the Kernel.