5.7 n^{th} order kernels and diagrammatics in Liouville space

5.7.1 2nd order RDM kernel

We first look for the RDM kernel $\tilde{K}^{(2)}\rho^{\infty}$;

$$\tilde{K}^{(2)}\rho^{\infty} = \mathrm{Tr}_B\{\mathcal{L}_T\tilde{G}(0)\mathcal{L}_T\,\rho^{\infty}\otimes\hat{\rho}_B\}$$

with, according to eq. (5.44), $\mathcal{L}_T\hat{X} = -\frac{i}{\hbar}\sum_{\nu\alpha p}\sum_{\vec{k}\sigma} p\, C^{p\nu}_{\alpha\vec{k}\sigma}\, D^{\bar{p}\nu}_{\alpha\vec{k}\sigma}\,\hat{X}$

i) Action of $\tilde{G}(0)$

We observe that the right most Liouvillian $\mathcal{L}_T$ in the kernel $\tilde{K}^{(2)}\rho^{\infty}$ contains a bath operator $C^{p'\nu'}_{\alpha'\vec{k}'\sigma'}$.

this operator therefore defines the action of the bath Liouvillian in $\tilde{G}(0) = \dfrac{1}{0^+ - \mathcal{L}_S - \mathcal{L}_B}$.

Explicitly, using $\mathcal{L}_B C^p_{\alpha\vec{k}\sigma} = -\frac{i}{\hbar}[\hat{H}_B, \hat{C}^p_{\alpha\vec{k}\sigma}] = -\frac{i}{\hbar}p\varepsilon_{\alpha\vec{k}}\hat{C}^p_{\alpha\vec{k}\sigma}$

$$\boxed{\tilde{K}^{(2)}\rho^{\infty} = \left(-\frac{i}{\hbar}\right)^2 \sum_{\nu\alpha p}\sum_{\nu'\alpha' p'}\sum_{\vec{k}\sigma}\sum_{\vec{k}'\sigma'} pp'\,\mathrm{Tr}_B\left\{ C^{p\nu}_{\alpha\vec{k}\sigma} D^{\bar{p}\nu}_{\alpha\vec{k}\sigma}\frac{1}{0^+ - \mathcal{L}_S + \frac{i}{\hbar}p'\varepsilon_{\alpha'\vec{k}'}} C^{p'\nu'}_{\alpha'\vec{k}'\sigma'} D^{\bar{p}'\nu'}_{\alpha'\vec{k}'\sigma'}\hat{\rho}_B \otimes \right.} \quad (5.46)$$

ii) Wick contraction

using now $\{C^p, D^{\bar{p}}\} = 0$ and $X^{\nu}Y^{\nu'} = -\nu\nu' Y^{\nu'}X^{\nu}$

$$\tilde{\mathcal{K}}^{(2)}\rho^{\infty} = +\frac{i}{\hbar} \sum_{\nu\alpha p} \sum_{\nu'\alpha' p'} \sum_{\vec{k}\sigma} \sum_{\vec{k}'\sigma'} p p' \, \nu\nu' \,.$$

$$\cdot \; D^{\bar{p}\nu}_{\alpha\vec{k}\sigma} \frac{1}{i0^{+} - i\hbar \mathcal{L}_S - p'\varepsilon_{\alpha\vec{k}}} D^{\bar{p}'\nu'}_{\alpha'\vec{k}'\sigma'} \rho^{\infty} \, \mathrm{Tr}_B \left\{ C^{p\nu}_{\alpha\vec{k}\sigma} C^{p'\nu'}_{\alpha\vec{k}'\sigma'} \hat{\rho}_B \right\}$$

We can perform the partial trace using the bath correlators of the Fermi-Dirac statistics

$$\langle C^{p\nu}_{\alpha\vec{k}\sigma} \, C^{p'\nu'}_{\alpha\vec{k}'\sigma'} \rangle = \mathrm{Tr}_B \left\{ C^{p\nu}_{\alpha\vec{k}\sigma} C^{\bar{p}'\nu'}_{\alpha\vec{k}'\sigma'} \rho_B \right\} = \delta_{p\bar{p}'} \delta_{\alpha\alpha'} \delta_{\sigma\sigma'} \delta_{\vec{k}\vec{k}'} f^{p\nu'}_{\alpha}(\varepsilon_{\alpha\vec{k}})$$

notice that the index ν' is here only a number where

$$f^{+}_{\alpha}(\varepsilon) = \frac{1}{e^{\beta(\varepsilon - \mu_\alpha)} + 1} \,, \qquad f^{-}_{\alpha}(\varepsilon) = f_{\alpha}(-\varepsilon) = 1 - f^{+}_{\alpha}(\varepsilon)$$

i.e. $f^{+}(\varepsilon)$ is the Fermi function.

We thus find the (still general) 2nd order expression

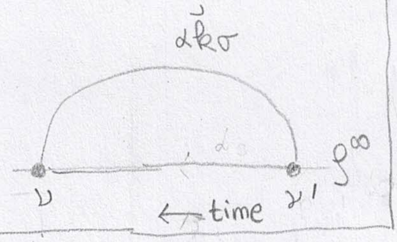
$$\boxed{\tilde{\mathcal{K}}^{(2)}\rho^{\infty} = -\frac{i}{\hbar} \sum_{\nu\nu'} \sum_{p} \sum_{\alpha\vec{k}\sigma} \nu\nu' D^{\bar{p}\nu}_{\alpha\vec{k}\sigma} \frac{f^{p\nu'}_{\alpha}(\varepsilon_{\alpha\vec{k}})}{i0^{+} - i\hbar\mathcal{L}_S + p\,\varepsilon_{\alpha\vec{k}\sigma}} D^{p\nu'}_{\alpha\vec{k}\sigma} \rho^{\infty}_{\infty}} \quad (5.47)$$

iii) Diagrammatics in Liouville space

We thus see that in second order the kernel $\tilde{K}^{(2)}$ consists of $\underline{2}$ system operators $D^{\bar{p}\nu}_{\alpha k\sigma}$, $D^{p\nu'}_{\alpha k\sigma}$ connected, due to the Wick's contraction, through a fermi function $f^{p\nu'}_{\alpha}$.
At a vertex the charge in the dot changes by one unit.

We represent this diagrammatically as

$$\boxed{\tilde{K}^{(2)}\rho^{\infty} = \sum_{\nu\nu'}\sum_{p}\sum_{\alpha\sigma}} \quad (5.48)$$



time grows from right to left.

where the two points $\bar{p}\nu$, $p\nu'$ correspond to the two "vertices" $D^{\bar{p}\nu}_{\alpha\vec{k}\sigma}$, $D^{p\nu'}_{\alpha\vec{k}\sigma}$ connected by the fermionic line $f^{p\nu'}_{\alpha}(\varepsilon_{\alpha\vec{k}\sigma})$;

Notice that the summation $\sum_{k}$ is implicit, ; product $\nu\nu'$ is in diagram

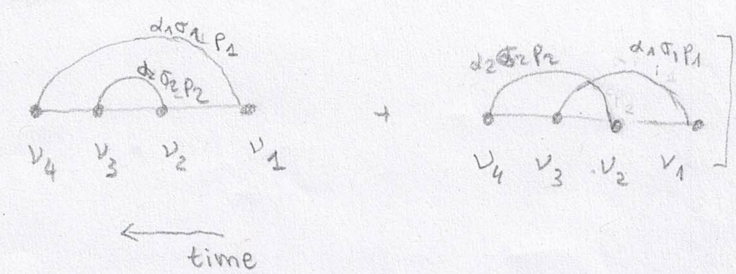
Note: It is easy to appreciate that this kind of representation in terms of fermionic lines and vertices also holds for the higher order of the perturbation theory.

Remember: $\boxed{\tilde{K}^{(2n)}_{(0)}\rho^{\infty} = \mathrm{Tr}_B\{ \mathcal{L}_T\, \tilde{G}_0\, (\Sigma_Q \tilde{G}_0)^{2n} \mathcal{L}_T\, \rho_B \otimes \rho_{\infty}\}}$ (5.49)

↳ $2n^{th}$ order : $2n$ vertices, n fermionic lines

e.g. fourth order (see later for details)

$$\tilde{K}^{(4)}\rho^{\infty} = \sum_{\nu_4\nu_3\nu_2\nu_1}(\ldots)\sum_{p_1p_2}\sum_{\substack{\alpha_1\alpha_2\\ \sigma_1\sigma_2}}\Big[\quad + \quad\Big]$$



etc.

Remember that each fermionic line contains a sum $\sum_{\vec{k}}$ and a sign.

In particular:

I) the sign is given by $(\nu_{2n}\nu_1)(-1)^q$

check! (I am not sure)

where q is the number of crossing of lead fermion line.

II) at each order only <u>irreducible</u> diagrams contribute.

Irreducible diagrams are those diagrams that cannot be cut in two disconnected pieces by a vertical line

e.g.

is a reducible diagram

5.7.2 2nd order current kernel

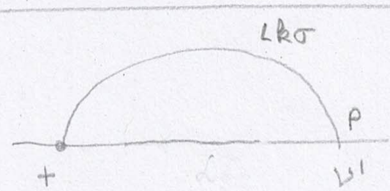
We can proceed analogously for the current kernel noticing that, due to the above mentioned distinctions between $d_T \hat{X}$ and $\hat{I}_L \hat{X}$, it holds

$$\boxed{\tilde{\mathcal{K}}^{(2)+}_{I_L} \rho^\infty = + \frac{ie}{\hbar} \sum_{\nu' p} \sum_{\vec{k}\sigma} p\nu' D^{\bar{p}+}_{L\vec{k}\sigma} \frac{f_L^{p\nu'}(\varepsilon_{L\vec{k}})}{i0^+ - i\hbar\mathcal{L}_S + p\varepsilon_{L\vec{k}\sigma}} D^{p\nu'}_{L\vec{k}\sigma} \rho^\infty} \quad (5.50)$$

i.e. compared to $\tilde{\mathcal{K}}\rho^\infty$ there is no sum over α and over ν. Furthermore, there is a difference in sign which depends on p.

Diagrammatically in Liouville space

$$\tilde{\mathcal{K}}^{(2)+}_{I_L} \rho^\infty = e \sum_{\sigma} \sum_{\nu'} \sum_{p} (-p)$$



(5.51)

5.7.3 Fourth order kernel $\tilde{\mathcal{K}}^{(4)}\rho^\infty$

We derive now the above mentioned rules, valid at any order 2n, for the fourth order kernel.
According our Dyson expansion

$$\tilde{\mathcal{K}}^{(4)}\rho^\infty = \mathrm{Tr}_B\{\mathcal{L}_T \tilde{G}_0 \Sigma_Q \tilde{G}_0 \Sigma_Q \tilde{G}_0 \mathcal{L}_T \hat{\rho}_B \otimes \hat{\rho}^\infty\} \quad (5.52)$$

where $\Sigma_Q = Q\mathcal{L}_T Q$, $Q = 1-P$

Importantly, is the presence of the Q projector that ensures that only irreducible contributions enter in $\tilde{\mathcal{K}}^{(4)}\rho^\infty$. Explicitely

$$\tilde{\mathcal{K}}^{(4)}\rho^\infty = \mathrm{Tr}_B\{\mathcal{L}_T \tilde{G}_0 \underbrace{Q\mathcal{L}_T Q}_{\Sigma_Q} \tilde{G}_0 \underbrace{Q\mathcal{L}_T Q}_{\Sigma_Q} \tilde{G}_0 \mathcal{L}_T \hat{\rho}_B \otimes \hat{\rho}^\infty\}$$

notice that $P\mathcal{L}_T^{2n+1}P = 0$

and $[\tilde{G}_0, P] = [\tilde{G}_0, Q] = 0$, $QP = PQ = 0$

$\Rightarrow$ only the central Q survives (see proof next page)

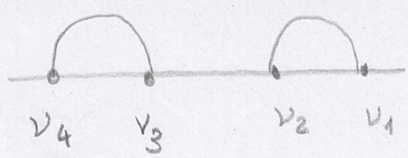
$$\boxed{\tilde{\mathcal{K}}^{(4)}\rho^\infty = \mathrm{Tr}_B\{\mathcal{L}_T \tilde{G}_0 \mathcal{L}_T \tilde{G}_0 Q \mathcal{L}_T \tilde{G}_0 \mathcal{L}_T \hat{\rho}_B \otimes \hat{\rho}^\infty\}} \quad (5.53)$$

$\Rightarrow$ the projector Q splits the kernel in the difference of the full and of a reducible part.

Explicitly

$$\boxed{\begin{aligned}\tilde{K}^{(4)}\rho^{\infty} &= \mathrm{Tr}_B\{\mathcal{L}_T\tilde{G}_0\mathcal{L}_T\tilde{G}_0\mathcal{L}_T\tilde{G}_0\mathcal{L}_T\hat{\rho}_B\otimes\hat{\rho}^{\infty}\} \\ &- \mathrm{Tr}_B\{\mathcal{L}_T\tilde{G}_0\mathcal{L}_T\tilde{G}_0 P\mathcal{L}_T\tilde{G}_0\mathcal{L}_T\hat{\rho}_B\otimes\rho^{\infty}\}\end{aligned}} \quad (5.54)$$

where the second contribution is interpreted as



Proof of (5.53)

$$\tilde{K}^{(4)}\rho^{\infty} = \mathrm{Tr}_B\{\mathcal{L}_T\tilde{G}_0 (Q)\mathcal{L}_T Q\tilde{G}_0 Q\mathcal{L}_T \underbrace{(1-P)}\tilde{G}_0\mathcal{L}_T\hat{\rho}_B\otimes\rho^{\infty}\}$$

due to $P\mathcal{L}_T P = 0$ is $P\tilde{G}_0\mathcal{L}_T P = 0$

$$= \mathrm{Tr}_B\{\mathcal{L}_T\tilde{G}_0 Q\mathcal{L}_T Q\tilde{G}_0(1-P)\mathcal{L}_T\tilde{G}_0\mathcal{L}_T\hat{\rho}_B\otimes\rho^{\infty}\}$$

$$= \mathrm{Tr}_B\{\mathcal{L}_T\tilde{G}_0 Q\mathcal{L}_T Q\tilde{G}_0\mathcal{L}_T\tilde{G}_0\mathcal{L}_T\hat{\rho}_B\otimes\hat{\rho}^{\infty}\}$$

$$- \mathrm{Tr}_B\{\mathcal{L}_T\tilde{G}_0 Q\mathcal{L}_T \underbrace{Q\tilde{G}_0 P}_{=\tilde{G}_0 Q P = 0}\mathcal{L}_T\tilde{G}_0\mathcal{L}_T\hat{\rho}_B\otimes\rho^{\infty}\}$$

$$= \mathrm{Tr}_B\{\mathcal{L}_T\tilde{G}_0(1-P)\mathcal{L}_T Q\tilde{G}_0\mathcal{L}_T\tilde{G}_0\mathcal{L}_T\hat{\rho}_B\otimes\rho^{\infty}\}$$

$$\underset{P\mathcal{L}_T^3 P = 0}{=} \mathrm{Tr}_B\{\mathcal{L}_T\tilde{G}_0\mathcal{L}_T Q\tilde{G}_0\mathcal{L}_T\tilde{G}_0\mathcal{L}_T\hat{\rho}_B\otimes\rho^{\infty}\}$$

From (5.54) we thus find

$$\tilde{K}^{(4)}\hat{\rho}^{\infty} = \left(-\frac{i}{\hbar}\right)^4 \sum_{\{l_i\}} \sum_{\{\nu_i\}} \sum_{\{p_i\}} \left(\prod_i p_i\right) \cdot$$

$l_i = (\alpha_i \sigma_i k_i)$ index for bath d.o.f., $i = 1,2,3,4$

$$\cdot \operatorname{Tr}_B \Big\{ C^{p_4\nu_4}_{l_4} D^{\bar{p}_4\nu_4}_{l_4} \frac{1}{0^+ - \mathcal{L}_S - \mathcal{L}_B} C^{p_3\nu_3}_{l_3} D^{\bar{p}_3\nu_3}_{l_3} \cdot$$

$$\cdot \frac{1}{0^+ - \mathcal{L}_S - \mathcal{L}_B} \mathcal{Q}\, C^{p_2\nu_2}_{l_2} D^{\bar{p}_2\nu_2}_{l_2} \frac{1}{0^+ - \mathcal{L}_S - \mathcal{L}_B} C^{p_1\nu_1}_{l_1} D^{\bar{p}_1\nu_1}_{l_1} \hat{\rho}^{\infty} \otimes \hat{\rho}_B \Big\} \qquad (5.55)$$

Using now $\mathcal{Q} = 1 - \mathcal{P}$, we can recast $\tilde{\mathcal{K}}^{(4)}\rho^{\infty}$ in the difference of the full and of the reducible part. Moving all C_i operators together yields, using $\overset{\nu}{x}\overset{\nu'}{y} = -\overset{\nu'}{y}\overset{\nu}{x}\,\nu\nu'$,

$$\tilde{K}^{(4)}\hat{\rho}^{\infty} = -\frac{i}{\hbar} \sum_{\{l_i\}} \sum_{\{\nu_i\}} \sum_{\{p_i\}} \left(\prod_i p_i\right)\left(\prod_i \nu_i\right) \cdot$$

$$\Big[D^{\bar{p}_4\nu_4}_{l_4} \frac{1}{i0^+ - i\hbar\mathcal{L}_S - \sum_{j=1}^{3} p_i \varepsilon_{l_i}} D^{\bar{p}_3\nu_3} \frac{1}{i0^+ - i\hbar\mathcal{L}_S \sum_{j=1}^{2} p_i \varepsilon_{l_i}} \cdot$$

$$\cdot D^{\bar{p}_2\nu_2}_{l_2} \frac{1}{i0^+ - \mathcal{L}_S - p_1\varepsilon_{l_1}} D^{\bar{p}_1\nu}_{l_1} \rho_{\infty} \operatorname{Tr}_B \Big\{ C^{p_4\nu_4}_{l_4} C^{p_3\nu_3}_{l_3} C^{p_2\nu_2}_{l_2} C^{p_1\nu_1}_{l_1} \Big\}$$

$$- D^{\bar{p}_4\nu_4}_{l_4} \frac{1}{i0^+ - i\hbar\mathcal{L}_S - p_3\varepsilon_{l_3}} D^{\bar{p}_3\nu_3}_{l_3} \frac{1}{i0^+ - i\hbar\mathcal{L}_S} \cdot$$

$$\cdot D^{\bar{p}\nu_2}_{p_2} \frac{1}{i0^+ - i\hbar\mathcal{L}_S - p_1\varepsilon_{l_1}} D^{\bar{p}_1\nu_1}_{l_1} \rho^{\infty} \langle C^{p_4\nu_4}_{l_4} C^{p_3\nu_3}_{l_3} \rangle \langle C^{p_2\nu_2}_{l_2} C^{p_1\nu_1}_{l_1} \rangle \Big] \qquad (5.56)$$

Extended Wick's theorem for noninteracting particles to superoperators

$$\langle C_4^{\nu_4} C_3^{\nu_3} C_2^{\nu_2} C_1^{\nu_1} \rangle = \langle C_4^{\nu_4} C_3^{\nu_3} \rangle \underset{(\mathrm{I})}{\langle C_2^{\nu_2} C_1^{\nu_1} \rangle} +$$

$$- \nu_3 \nu_2 \underset{(\mathrm{II})}{\langle C_4^{\nu_4} C_2^{\nu_2} \rangle \langle C_3^{\nu_3} C_1^{\nu_1} \rangle} + \nu_3 \nu_2 \underset{(\mathrm{III})}{\langle C_4^{\nu_4} C_1^{\nu_1} \rangle \langle C_3^{\nu_3} C_2^{\nu_2} \rangle} \tag{5.57}$$

We see that the term (I) exactly cancels the reducible part in (5.54). The sign of each diagram is $\prod_i \nu_i \, (-1)^{P\{\nu_i\}}$ where $P\{\nu_i\}$ is the nr. of permutations from the initial ordering.

↳ At the end only irreducible contributions survive.

Explicitly we end up with

$$\tilde{K}^{(4)} \rho^\infty = -\frac{i}{\hbar} \sum_{l_1 l_2} \sum_{p_1 p_2} \sum_{\{\nu_i\}} (\nu_4 \nu_1) \cdot$$

$$\left[- D_{l_2}^{\bar{p}_2 \nu_4} \frac{f_{l_2}^{+p_2 \nu_2}(\varepsilon_{l_2})}{i0^+ - i\hbar \alpha_s + p_2 \varepsilon_{l_2}} D_{l_2}^{\bar{p}_1 \nu_3} \frac{1}{i0^+ - i\hbar \alpha_s + (p_2 \varepsilon_2 + p_1 \varepsilon_1)} \cdot \right.$$

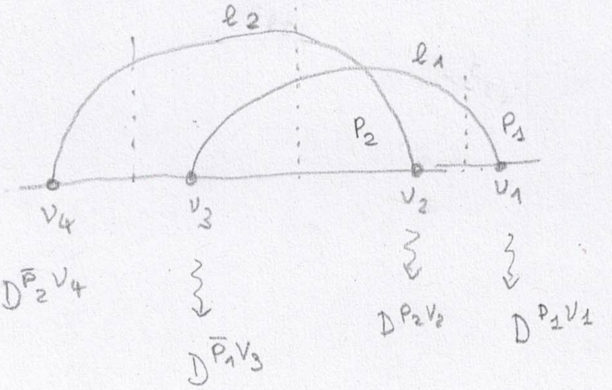
$$D_{l_2}^{p_2 \nu_2} \frac{f_{l_1}^{-p_1 \nu_1}(\varepsilon_{l_1})}{i0^+ - i\hbar \alpha_s + p_1 \varepsilon_{l_1}} D_{l_1}^{p_1 \nu_1} \rho^\infty +$$

$$+ D_{l_1}^{\bar{p}_1 \nu_4} \frac{f^{+p_2 \alpha_2}(\varepsilon_{l_2})}{i0^+ - i\hbar \alpha_s + p_1 \varepsilon_{l_1}} D_{l_2}^{\bar{p}_2 \nu_3} \frac{1}{i0^+ - i\hbar \alpha_s + (p_2 \varepsilon_{l_1} + p_1 \varepsilon_{l_1})} \cdot \tag{5.58}$$

$$\left. \cdot D_{l_2}^{p_2 \nu_2} \frac{f_{l_1}^{+p_1 \alpha_1}(\varepsilon_{l_1})}{i0^+ - i\hbar \alpha_s + p_1 \varepsilon_{l_1}} D_{l_1}^{p_1 \nu_1} \rho^\infty \right] = \sum_{\substack{\alpha_1 \sigma_1 \\ \alpha_2 \sigma_2}} \sum_{p_1 p_2} \sum_{\{\nu_i\}} \Big[$$  $+$  $\Big]$

The expression (5.49) starts to be complicated. However, we can use the diagrammatic rules to read out the contributions:

Example



I) to each fermioni line corresponds a Fermi function

↳ $f^{p_1 \nu_1}(\varepsilon_{\ell_1})\, f^{p_2 \nu_2}(\varepsilon_{\ell_2})$

II) the number of lead lines between two vertices determines the denominators

↳ $\dfrac{1}{i0^+ - i\hbar\lambda_s + p_2 \varepsilon_{\ell_2}}, \quad \dfrac{1}{i0^+ - i\hbar\lambda_s + (p_1\varepsilon_{\ell_1} + p_2 \varepsilon_{\ell_2})}, \quad \dfrac{1}{i0^+ - i\hbar\lambda_s + p_1 \varepsilon_{\ell_1}}$

$\longleftarrow$

III) To each vertex it corresponds a D-operator connected to a second D-operator throug a Fermi line

↳ $D^{\bar{p}_2 \nu_4} \dfrac{f}{(\ )} D^{\bar{p}_1 \nu_3} \dfrac{f^{p_2 \nu_2}}{(\ )} D^{p_2 \nu_2} \dfrac{f^{p_1 \nu_1}}{(\ )} D^{p_1 \nu_1}$

IV) The overall prefactor is given by (cf. Eq. (5.57))

$$-\frac{i}{\hbar} \cdot \prod_{\nu_i} (\nu_i)\, (-1)^{P(\{\nu_i\})} \overset{\text{fourth order}}{=} -\frac{i}{\hbar}\, \nu_4 \nu_1\, (-1)^q$$

where q is the number of crossing of fermionic lines

V) Take the sum $\sum_{k_1} \sum_{k_2}$

Note: The 4-th order diagrams  become relevant in Coulomb blockaded QD as they allow to transfer charge accross the dot by virtual processes (cotunneling)

The diagrams  lead to normalization of  through so called "charge fluctuations".

5.7.4 All order resummations : non perturbative effects

The dressed second order (DSO)

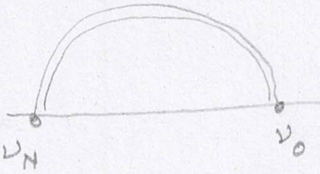
Important to account for finite lifetime effects : $i0^+ \rightarrow \Sigma_\alpha \sim \Gamma_\alpha$

but also for correlation effects like the Kondo resonance.

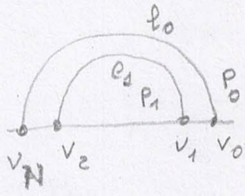
Importantly, to account for Kondo physics, an infinite subclass of diagrams has to be included.

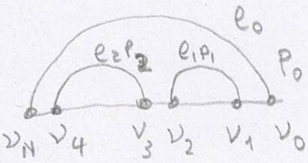
For this reason, we consider an example of a non perturbative resummation of diagrams known as the dressed second order (DSO) approximation

Specifically

$$\tilde{K}^{DSO} \equiv \sum_{\nu_0 \nu_N}' \sum_{p_0} \sum_{\alpha_0 \sigma_0}$$ 

$$= \sum_{\nu_0 \nu_N} \sum_{p_0 \alpha_0 \sigma_0} \Bigg[$$ 

$$+ \sum_{\nu_1 \nu_2, p_1} \sum_{\alpha_1 \sigma_1}$$ 

$$+ \sum_{\nu_1 \cdots \nu_4, p_1 p_2} \sum_{\alpha_1 \sigma_1, \alpha_2 \sigma_2}$$ 

$$+ \cdots \Bigg] \qquad (5.59)$$

I.e. in the DSO approximation charge fluctuations to all orders are summed up. Further the diagrams were chosen such that a vertical line cuts at most two fermion lines.

From the diagrammatic rules we thus immediately obtain

$$\tilde{K}^{DSO}\rho^\infty = -\frac{i}{\hbar}\sum_{\nu_0\nu_N}' \sum_{p_0}' \sum_{l_0} \nu_0\nu_N D_{l_0}^{\bar{p}_0\nu_N} \cdot$$

$$\cdot\Big[1 + \sum_{\substack{\nu_1\nu_2\\p_1}} \sum_{l_1}' \frac{1}{i0^+ - i\hbar\alpha_s + p_0\varepsilon_{l_0}} D_{l_1}^{\bar{p}_1\nu_2} \frac{f^{p_1\nu_1}(\varepsilon_{l_1})}{i0^+ - i\hbar\alpha_s + p_0\varepsilon_{l_0} + p_1\varepsilon_{l_1}} D_{l_1}^{p_1\nu_1} +$$

$$+ \Big(\sum_{\substack{\nu_3\nu_4\\p_2}}' \sum_{l_2} \frac{1}{i0^+ - i\hbar\alpha_s + p_0\varepsilon_{l_0}} D_{l_2}^{\bar{p}_2\nu_4} \frac{f^{p_2\nu_3}(\varepsilon_{l_2})}{i0^+ - i\hbar\alpha_s + p_0\varepsilon_{l_0} + p_2\varepsilon_{l_2}} D_{l_2}^{p_2\nu_3}\Big) \cdot$$

$$\Big(\frac{1}{i0^+ - i\hbar\alpha_s + p_0\varepsilon_{l_0}} \cdot \sum_{\substack{\nu_2\nu_1\\p_1}}' \sum_{l_1} D_{l_1}^{\bar{p}_1\nu_2} \frac{f^{p_1\nu_1}(\varepsilon_{l_1}) D_{l_1}^{p_1\nu_1}}{i0^+ - i\hbar\alpha_s + p_1\varepsilon_{l_1}} \Big)$$

$$+ \dots \Big] \frac{f^{p_0 l_0}(\varepsilon_{l_0})}{i0^+ - i\hbar\alpha_s + p_0\varepsilon_{l_0}} D_{l_0}^{p_0\nu_0} \rho^\infty \qquad (5.60)$$

Already at this stage one recognizes a geometrical series $\sum_k r^k = \frac{1}{1-r}$. This yields

$$\tilde{K}^{DSO}\rho^\infty = -\frac{i}{\hbar}\sum_{\nu_0\nu_N} \sum_{p_0 l_0}\sum \nu_0\nu_N D_{l_0}^{\bar{p}_0\nu_N} \cdot$$

$$\cdot\Big[1 - \frac{1}{i0^+ - i\hbar\alpha_s + p_0\varepsilon_{l_0}} \sum_{\substack{\nu_1\nu_2\\p_1}} \sum_{l_1} D_{l_1}^{\bar{p}_1\nu_2} \frac{f^{p_1\nu_1}(\varepsilon_{l_1})}{i0^+ - i\hbar\alpha_s + p_0\varepsilon_{l_0} + p_1\varepsilon_{l_1}} D_{l_1}^{p_1\nu_1}\Big]^{-1}$$

$$\cdot \frac{f_0^{p_0 l_0}(\varepsilon_{l_0})}{i0^+ - i\hbar\alpha_s + p_0\varepsilon_{l_0}} D_{l_0}^{p_0\nu_0} \rho^\infty \qquad (5.61)$$

The bracket has the form

$$\underbrace{\frac{1}{i0^+ - i\hbar\delta_s + p_0\varepsilon_{\ell_0}}}_{\hat{x}} \underbrace{\left[i0^+ - i\hbar\alpha_s + p_0\varepsilon_{\ell_0} - \sum_{\substack{\nu_1\nu_2\\ p_1}} \sum_{e_1} D^{\bar{p}_1\nu_2} \frac{f^{p_1\nu_1}(\varepsilon_{e_1})}{i0^+ - i\hbar\alpha_s + p_0\varepsilon_{\ell_0} + p_1\varepsilon_{e_1}} D^{p_1\nu_1}_{e_1} \right]}_{\hat{y}}$$

We can use the property

$$(\hat{x}\hat{y})^{-1} = \hat{y}^{-1}\hat{x}^{-1} \qquad (5.62)$$

to get

$$\boxed{\tilde{K}^{DSO}\rho^\infty = -\frac{i}{\hbar} \sum_{\nu_0\nu_2} \sum_{p_0} \sum_{\ell_0} \bar{D}^{\bar{p}_0\nu_N}_{\ell_0} \frac{f^{p_0\ell_0}_{\ell_0}(\varepsilon_{\ell_0})}{i0^+ - i\hbar\alpha_s + p_0\varepsilon_{\ell_0} - \Sigma^{DSO}(\varepsilon_{\ell_0})} D^{p_0\nu_0}_{\ell_0}\rho^\infty}$$

(5.63)

with the DSO self-energy

$$\boxed{\Sigma^{DSO}(\varepsilon_{\ell_0}) = \sum_{\substack{\nu_1\nu_2\\ p_1}} \sum_{e_1} D^{\bar{p}_1\nu_2}_{e_1} \frac{f^{p_1\nu_1}(\varepsilon_{e_1})}{i0^+ - i\hbar\alpha_s + p_0\varepsilon_{\ell_0} + p_1\varepsilon_{e_1}} D^{p_1\nu_1}_{\ell_1}} \qquad (5.63b)$$

2) By comparing with the expression for $\tilde{K}^{(2)}\rho^\infty$, Eq. (5.47), we see that the effect of the charge fluctuations is to give a finite lifetime $\Gamma^{DSO} \sim \Im m\,\Sigma^{DSO}$ as well as a frequency shift $\sim \mathrm{Re}\,\Sigma^{DSO}$.

Note;

1. Σ^{DSO} is a simple approx to the exact self-energy Σ_p (cf. Eq. 5.21b)

2. In general (unless $U=0$)

$$\mathrm{Re}\,\Sigma'^{DSO} = \mathrm{Re}\,\Sigma^{DSO}(T) \neq 0$$

finite + temperature dependent

This temperature dependence is at the origin of the Kondo anomaly which start to be relevant for $k_B T \lesssim \Gamma$

3. The DSO approximation neglects diagrams with intersections

etc

or with more than two fermion lines

etc

Such contributions become increasingly relevant for $\Gamma \gtrsim k_B T$, which sets the validity regime of the DSO,

4. To obtain the exact results for the current I that we found for the case $U=0$ we need to include all diagrams with up to four fermion lines. In fact diagrams with more than four lines vanish identically when $U=0$: $\tilde{\mathcal{K}}^{U=0}_{p\infty} =$

5.8 Diagrammatics in Fock space

The above diagrammatic representation is still operatorial. We are interested to evaluate the elements $\left(\tilde{\mathcal{K}}^{(2)}\right)^{ba}_{b'a'}$ of the RDM kernel (cf. Eq. (5.30))

5.8.1. Second order Kernel

Explicitly, with $\rho^{\infty} = \sum_{aa'} \rho_{aa'} |a\rangle\langle a'|$, is

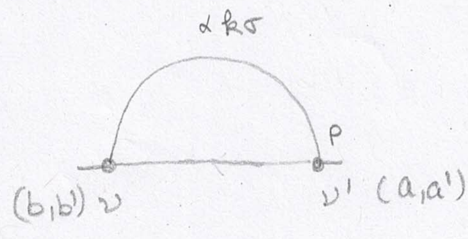
$$\left(\tilde{\mathcal{K}}^{(2)}\right)^{ba}_{b'a'} = \langle b| \left(\tilde{\mathcal{K}}^{(2)} |a\rangle\langle a'|\right) |b'\rangle \qquad (5.62)$$

Using the expression (5.47) we thus obtain

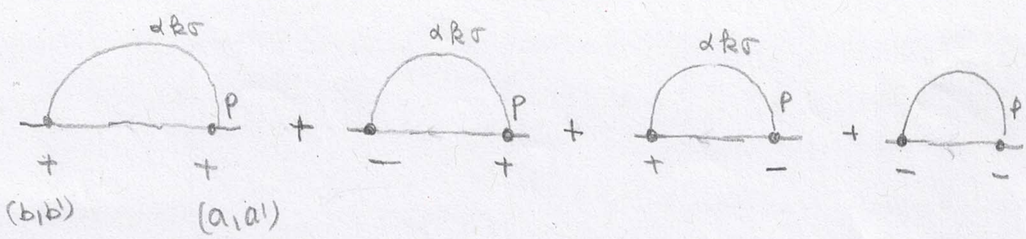
$$\left(\tilde{\mathcal{K}}^{(2)}\right)^{ba}_{b'a'} = -\frac{i}{\hbar} \sum_{\nu\nu'} \sum_{p} \sum_{\alpha \vec{k} \sigma} \nu\nu'$$

$$\langle b| \left(D^{\bar{p}\nu}_{\alpha k \sigma} \frac{f^{p\nu'}_{\alpha}(\varepsilon_{\alpha \vec{k}})}{i0^{+} - i\hbar \mathcal{L}_{s} + p\varepsilon_{\alpha \vec{k}}} D^{p\nu'}_{\alpha k \sigma} |a\rangle\langle a'| \right) |b'\rangle$$

$$\equiv \sum_{\alpha\sigma} \sum_{\nu\nu'} \sum_{p}{}'$$



$$= \sum_{\alpha\sigma} \sum_{p}{}' \Bigg[$$

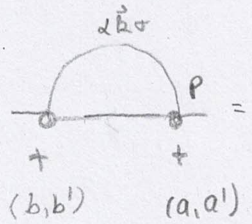


$$\Bigg]$$

where the sum over the Liouville index was performed.

Let us analyze the four contribution separately

a) $\boxed{++}$



$$= \left(-\frac{i}{\hbar}\right)\sum_{\vec k}\langle b|\Big(\underbrace{D^{\bar p +}_{\alpha\vec k\sigma}}_{D^{\bar p}_{\alpha\vec k\sigma}} \frac{f^p(\varepsilon_{\alpha\vec k\sigma})}{i0^+ - i\hbar\mathcal{L}_s + p\varepsilon_{\alpha k}} \underbrace{D^{p+}_{\alpha\vec k\sigma}}_{D^p_{\alpha k\sigma}}|a\rangle\langle a'|\Big)|b'\rangle$$

- Recall also that $D^p_{\alpha\vec k\sigma}|a\rangle = \sum_i t^p_{\alpha\vec k\sigma}\, d^p_{i\sigma}|a\rangle$.

I.e, $d^p_{i\sigma}|a\rangle$ are states with 1 particle $\begin{cases}\text{more} & \text{if } p=+\\ \text{less} & \text{if } p=-\end{cases}$

than the state $|a\rangle$. They do not need to be eigenstates of $\hat H_s$

- It is then convenient to insert $\mathbb{1} = \sum_c |c\rangle\langle c|$

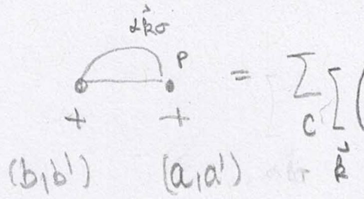
$$\hookrightarrow \quad = \left(-\frac{i}{\hbar}\right)\sum_c\sum_{\vec k}\langle b|\Big[\Big(D^{\bar p}_{\alpha\vec k\sigma}\frac{f^p(\varepsilon_{\alpha\vec k\sigma})}{i0^+ - i\hbar\mathcal{L}_s + p\varepsilon_{\alpha k}}|c\rangle\langle c|D^p_{\alpha\vec k\sigma}|a\rangle\langle a'|\Big)\Big]|b'\rangle$$

and use

$$\mathcal{L}_s|c\rangle\langle a'| = -\frac{i}{\hbar}\left(\hat H_s|c\rangle\langle a'| - |c\rangle\langle a'|\hat H_s\right) =$$

$$= -\frac{i}{\hbar}(E_c - E_{a'})|c\rangle\langle a'|$$

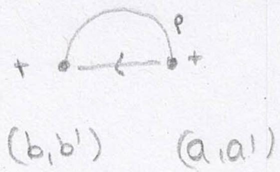
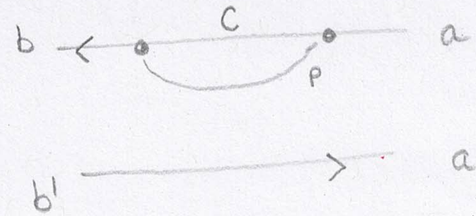
Hence



$$= \sum_c \left[\left(\frac{-i}{\hbar}\right) \langle b | D^{\bar{p}}_{\alpha \vec{k} \sigma} | c \rangle \frac{f^{p}(\varepsilon_{\alpha k \sigma})}{i0^{+} - (E_c - E_{a'}) + p\,\varepsilon_{\alpha k \sigma}} \langle c | D^{p}_{\alpha \vec{k} \sigma} | a \rangle \, \delta_{a'b'} \right.$$

Notice that since $|a'\rangle = |b'\rangle$ and due to the consecutive action of $D^{\bar{p}} D^{p}$ on $|a\rangle$ $\hookrightarrow$ $N_{a'} = N_{b'}$ & $N_b = N_a$ $\Rightarrow$ <u>no change in charge</u>

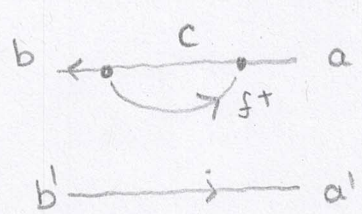
This is better visualized in a <u>two time-lines</u> <u>contour</u>, with the convention that all vertices with $\nu = +$ lie on the upper contour.

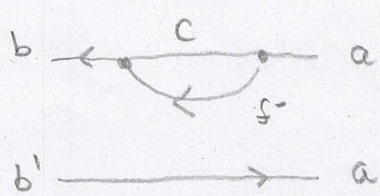
 $= \sum_c$  $\delta_{a'b'}$

i) Notice that in the numerator the difference $E_c - E_{a'}$ of the energies of the two states $|c\rangle$ and $|a'\rangle$ appear.

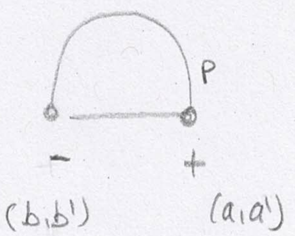
ii) We have assigned a forward/backward direction to the upper/lower contour

iii) Further specifying whether $p=+$ or $p=-$ one gets two distinct contributions

$p = +$  $\delta_{a'b'}$ $\qquad N_c = N_a + 1$

$p = -$  $\delta_{a'b'}$ $\qquad N_c = N_a - 1$

b) $\boxed{+-}$



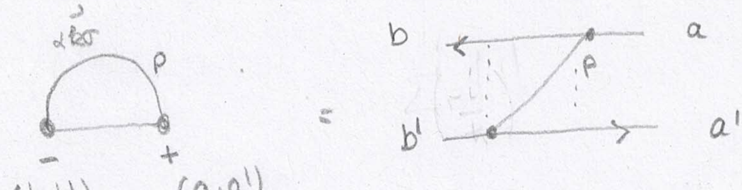
Let us consider $D^{\bar p -} \mathcal{L}_S D^{p+} |a\rangle\langle a'| = (\mathcal{L}_S D^p |a\rangle\langle a'|) D^{\bar p}$

$$= \sum_c (\mathcal{L}_S |c\rangle\langle c| D^p |a\rangle\langle a'|) D^{\bar p} = -\frac{i}{\hbar}\sum_c (E_c - E_{a'})|c\rangle\langle c|D^p|a\rangle\langle a'|D^{\bar p}$$

$$\Rightarrow \langle b| D^{\bar p -}\mathcal{L}_S D^{p+}|a\rangle\langle a'|b'\rangle = -\frac{i}{\hbar}\sum_c \delta_{b,c}(E_b-E_{a'})\langle b|D^p|a\rangle\langle a'|D^{\bar p}|$$

$$= -\frac{i}{\hbar}(E_b - E_{a'})\langle b|D^p|a\rangle\langle a'|D^{\bar p}|b'\rangle$$

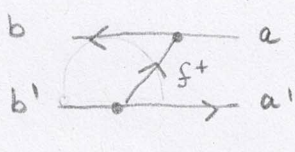
Putting this together we finally obtain



$$= -\left(\frac{-i}{\hbar}\right)\sum_{\alpha\vec k} \langle b|D^p_{\alpha\vec k\sigma}|a\rangle \frac{f^p_\alpha(\varepsilon_{\alpha\vec k\sigma})}{i0^+ - (E_b - E_{a'}) + p\,\varepsilon_{\alpha\vec k\sigma}} \langle a'|D^{\bar p}_{\alpha\vec k\sigma}|b'\rangle$$

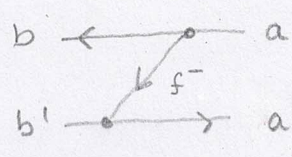
from $\nu_1\cdot\nu_2 = -1$

Further specifying $p=\pm$



$N_b = N_a + 1$
$N_{b'} = N_a + 1$,

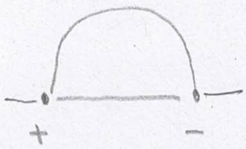
$p = +$



$N_b = N_a - 1$
$N_{b'} = N_{a'} - 1$

$p = -$

c) $\boxed{-\ +}$



We consider then $D^{\bar p +} \mathcal{L}_s D^{p-} |a\rangle\langle a'| =$

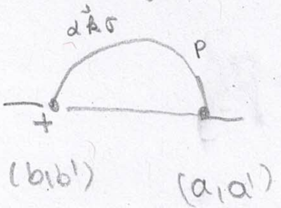
$$= D^{\bar p}\mathcal{L}_s |a\rangle\langle a'| D^p$$

$$= \sum_c D^{\bar p}\mathcal{L}_s|a\rangle\langle a'|D^p|c\rangle\langle c|$$

$$= -\frac{i}{\hbar}\sum_c D^{\bar p}\,(E_a - E_c)\,|a\rangle\langle a'|D^p|c\rangle\langle c|$$

$$\Rightarrow \quad \langle b| D^{\bar p +}\mathcal{L}_s|a\rangle\langle a'||b'\rangle = -\frac{i}{\hbar}(E_a-E_{b'})\,\langle b|D^{\bar p}|a\rangle\,\langle a'|D^p|b'\rangle$$

Finally



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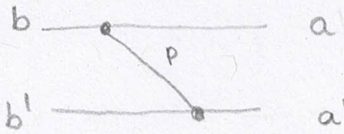
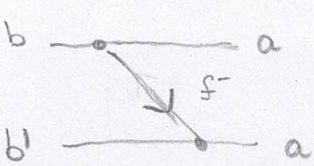


$$= -\left(-\frac{i}{\hbar}\right)\sum_{\vec k}\langle b|D^{\bar p}|a\rangle\,\frac{f^{-p}(\varepsilon_{\alpha\vec k\sigma})}{i0^+ - (E_a - E_{b'}) + p\,\varepsilon_{\alpha\vec k\sigma}}\,\langle a'|D^p|b'\rangle$$

from $\nu_1\cdot\nu_2 = -1$

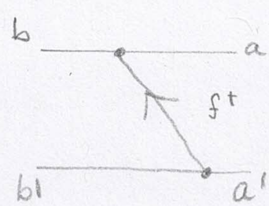
Further specifying $p=\pm$



$N_b = N_a - 1$

$N_{b'} = N_{a'} - 1$,

$p=+$

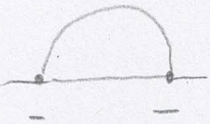


$N_b = N_a + 1$

$N_{b'} = N_{a'} + 1$

$p=-$

d) $\boxed{- \; -}$

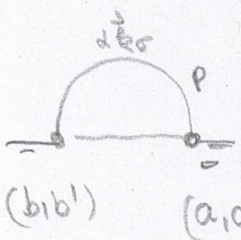


$$\Rightarrow \quad D^{\bar{p}-}\mathcal{L}_s D^{p-} |a\rangle\langle a'| = D^{\bar{p}-}\mathcal{L}_s \left(|a\rangle\langle a'| D^{p} \right)$$

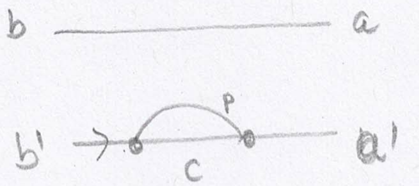
$$= \sum_c D^{\bar{p}-} \left(\mathcal{L}_s |a\rangle\langle a'| D^{p} |c\rangle\langle c| \right) = -\frac{i}{\hbar} \sum_c \left(E_a - E_c \right) D^{\bar{p}-} |a\rangle\langle a'| D^{p} |c\rangle\langle c|$$

$$\Rightarrow \quad \langle b| \left(D^{\bar{p}-}\mathcal{L}_s D^{p-} |a\rangle\langle a'| \right) |b'\rangle = -\frac{i}{\hbar} \sum_c \left(E_a - E_c \right) \delta_{ab} \langle a'| D^{p} |c\rangle \langle c| D^{\bar{p}} |b'\rangle$$

Finally



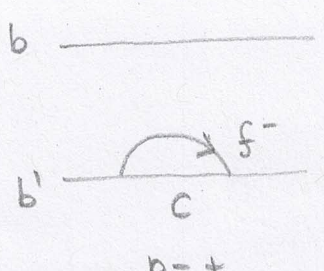
$= \sum_c$



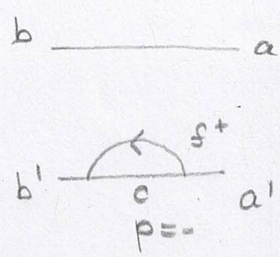
δ_{ab}

$$= -\left(\frac{i}{\hbar} \right) \sum_{\vec{k}} \langle a'| D^{p} |c\rangle \frac{f^{-p}(\varepsilon_{\alpha k \sigma})}{i0^{+} - (E_a - E_c) + p\,\varepsilon_{\alpha k \sigma}} \langle c| D^{\bar{p}} |b'\rangle$$

Moreover, again is $p = \pm$



$N_c = N_{a'} - 1$ $\quad \delta_{ab}$,

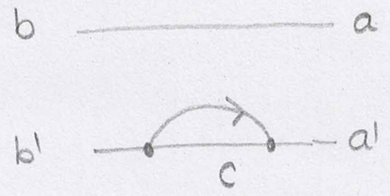


$N_c = N_{a'} + 1$

5.8.2 Diagrammatic rules (second order)

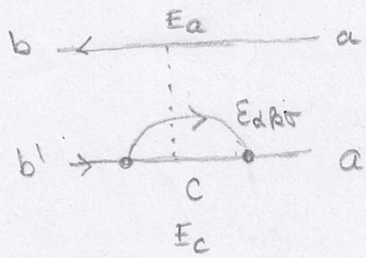
From this example we see that given a generic diagram, it is possible to write down its expression.

Consider for example



$\delta_{a,b}$

and draw a vertical line between two vertices



$\delta_{a,b}$

i) to all lines intersected by the vertical line assign energies.

In particular, if the ~~lines~~ point from

left $\to$ right + energy $\Rightarrow$ denominator

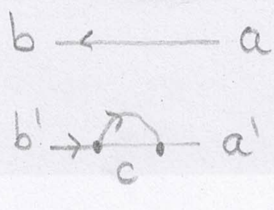
right $\to$ left − energy

$$\frac{1}{i0^+ + E_c - E_a + \varepsilon_{\alpha k\sigma}}$$

ii) Assign $f^+(\varepsilon_{\alpha k\sigma})$ for an incoming line

$f^-(\varepsilon_{\alpha k\sigma})$ " outgoing line

iii) Multiply by $(-\frac{i}{\hbar})(-1)^v$, where v is the nr. of vertices on lower contour, and include $\alpha)\sum_k$ for each fermionic line

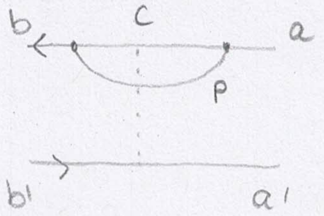
$\hookrightarrow$ δ_{ab} 

$$= \left(-\frac{i}{\hbar}\right)\sum_k \langle b'|D^-|c\rangle \frac{f^-(\varepsilon_{\alpha k\sigma})\ \langle c|D^+|a'\rangle}{i0^+ - (E_a - E_c) + \varepsilon_{\alpha k\sigma}}$$

5.8.3 complex conjugation

Consider

$\nu_1 = +, \ \nu_2 = +$



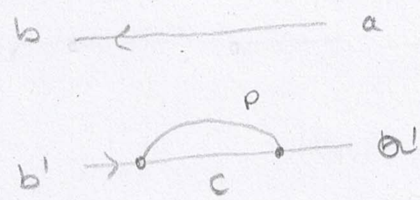
$\delta_{a'b'}$

$$= -\frac{i}{\hbar} \sum_k \langle b | D^{\bar{p}} | c \rangle \frac{f^p(\varepsilon_k)}{i0^+ + E_{a'} - E_c + p\varepsilon_k} \langle c | D^p | a \rangle \, \delta_{a'b'}$$

diagrammatic rules

and

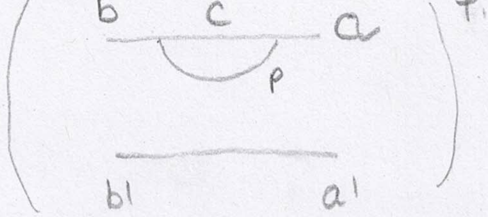
$\nu_1 = -, \ \nu_2 = -$



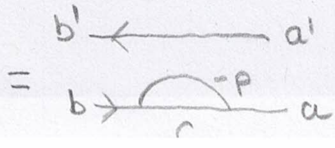
δ_{ab}

$$= -\frac{i}{\hbar} \sum_k \langle a' | D^p | c \rangle \frac{f^{-p}(\varepsilon_k)}{i0^+ + (E_c - E_a) + p\varepsilon_k} \langle c | D^{\bar{p}} | b' \rangle \, \delta_{ab}$$

↳ by comparison hermitian conjugation amounts to a mirroring of all vertices and indices

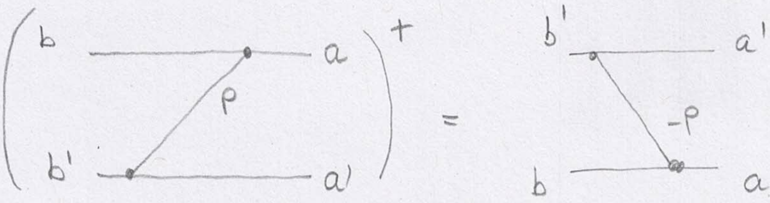


$$= \frac{i}{\hbar} \sum_k \langle b | D^p | c \rangle \frac{f^p(\varepsilon_k)}{-i0^+ + E_{a'} - E_c + p\varepsilon_k} \langle c | D^{\bar{p}} | a \rangle \, \delta_{a'b'}$$

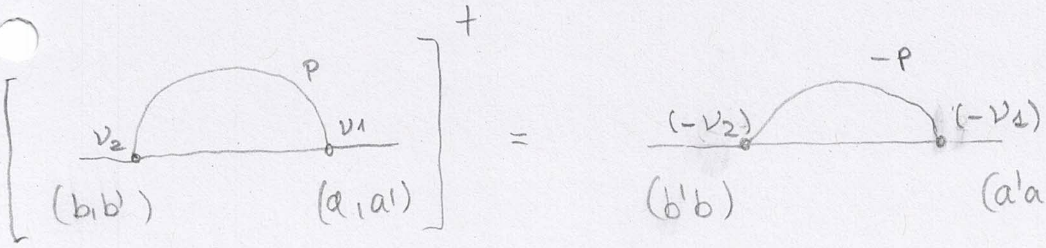


$\delta_{a'b'}$

Similarly



Complex conjugation in Liouville space



This rule can be generalized to any order

$$\{\nu_i\} \longrightarrow \{-\nu_i\}$$

$$\{p_i\} \longrightarrow \{-p_i\} \quad \leftarrow \text{check}$$

$$(b, b') \longrightarrow (b', b)$$

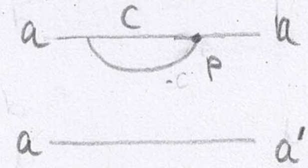
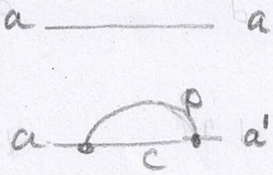
$$(a, a') \longrightarrow (a', a)$$

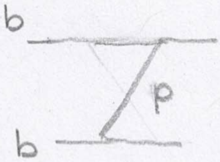
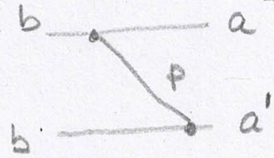
5.8.4 Sum rule for RDM kernel

$$\sum_b {}' \, K^{b\,a}_{b\,a'} = 0 \qquad \forall\, a, a'$$

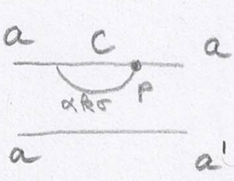
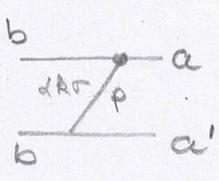
$$\hookrightarrow \; K^{aa}_{aa'} = - \sum_{b \neq a} K^{ba}_{ba'}$$

Diagrammatically, in 2nd order

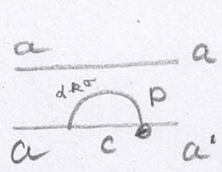
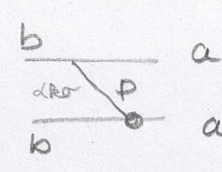
$$K^{aa}_{aa'} = \sum_{\alpha\sigma}{}' \sum_{p}{}' \sum_{c}{}' \Big[$$  $\delta_{aa'}$ +  $\Big]$

$$= - \sum_{\alpha\sigma}{}' \sum_{p}{}' \sum_{a \neq b}{}' \Big[$$  +  $\Big]$

This relation is valid at the level of individual diagrams sets which differ in the position of the last vertex

$$\sum_{\sigma}{}' \sum_{c}{}'$$  $$= - \sum_{\sigma}{}' \sum_{a \neq b}$$ 

similarly

$$\sum_{\sigma}{}' \sum_{c}{}'$$  $$= - \sum_{\sigma}{}' \sum_{a \neq b}$$ 

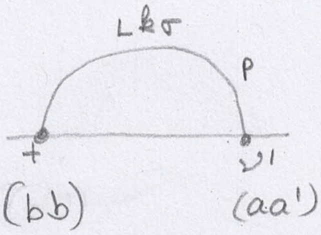
If we denote as $(\tilde{K}^{+})^{ba}_{ba'}$ and $(\tilde{K}^{-})^{ba}_{ba'}$ the diagrams with the last vertex ν on the upper / lower contour we get the general relation

$$\boxed{(\tilde{K}^{\nu})^{aa}_{aa'} = - \sum_{b \neq a} (\tilde{K}^{-\nu})^{ba}_{ba'}} \quad (5.6?)$$

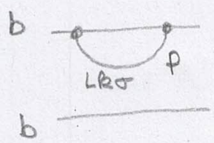
5.8.5 Current kernel $\left(\tilde{K}^{+}_{I_L}\right)^{ba}_{ba'}$ (second order)

According to (5.42b) the second order current kernel has the diagrammatic expression

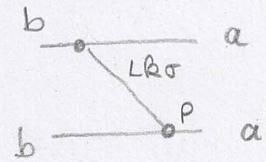
$$\left(\tilde{K}^{+(2)}_{L}\right)^{ba}_{ba'} \underset{(*)}{=} -e \sum_\sigma \sum_{\nu'} \sum_p p$$



$$= -e \sum_\sigma \sum_p p \Big[$$



$\delta_{a'b}$ +

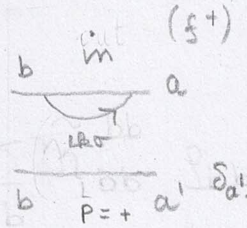


$\Big]$ (5.64)

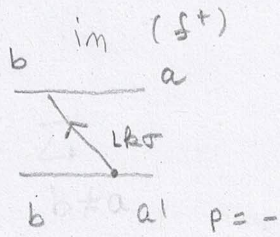
i.e., there is a difference in the sign of the outgoing line p=− with respect to the RDM kernel.

(*) recall the diagrammatic rules in second order for which the sign of a diagram is $\left(\frac{-i}{\hbar}\right)\nu_1\nu_2$.

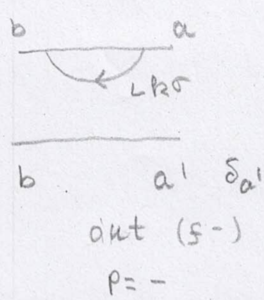
$$\hookrightarrow \left(\tilde{K}^{+(2)}_{L}\right)^{ba}_{ba'} = -e\sum_\sigma \Big[$$



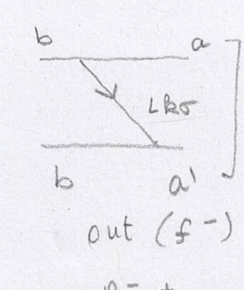
$\delta_{a'b}$ −



−



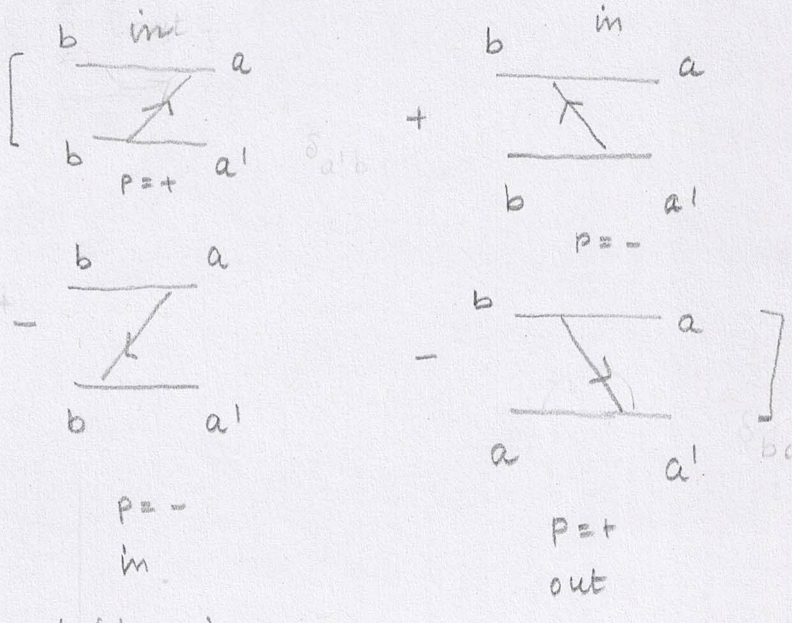
$\delta_{a'b}$ +



$\Big]$ (5.65)

Using now the sum rule (5.63) for the first and third diagram

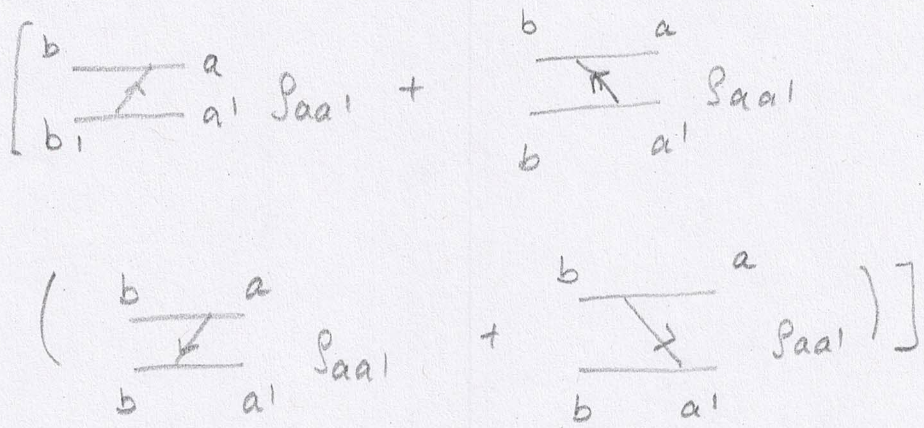
$$\left(\tilde{K}^{+(2)}_{I_L}\right)^{ba}_{ba'} = +e \sum_{\sigma} \Big[$$



The second order current thus is

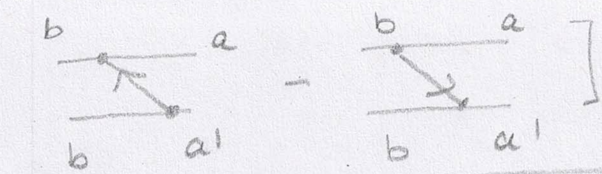
$$I^{(2)}_L = e \sum_{\substack{aa' \\ b \neq a}} \left(\tilde{\mathcal{K}}^{+(2)}_{I_L}\right)^{ba}_{ba'} \rho_{aa'} =$$

$$= e \sum_{\substack{b \neq a \\ a, a'}} \sum_{\sigma} \Big[$$



using the mirror rule for hermitian conjugation for the first and third diagram

$$\boxed{I^{(2)}_L = 2e \,\mathrm{Re} \sum_{b \neq a} \sum_{aa'} \Big[$$



$$\Big] \rho_{aa'}} \qquad (5.66)$$

5.8.6 Explicit evaluation of $(\tilde{\mathcal{K}}^{(2)})^{ba}_{ba'}$

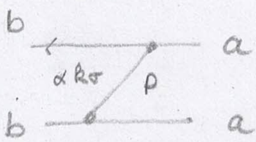
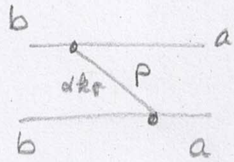
We are now in a position of evaluating all elements of the RDM kernel.

We exemplarily look at $(\tilde{\mathcal{K}}^{(2)})^{ba}_{ba}$

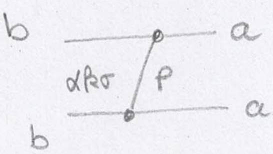
i) consider first $b \neq a$ with $N_b \neq N_a$

$$(\tilde{\mathcal{K}}^{(2)})^{ba}_{ba} = \begin{cases} \Gamma^{+}_{ba} & \text{if } N_b > N_a \\ \Gamma^{-}_{ab} & \text{if } N_b < N_a \end{cases}$$

$\rightarrow$ since the particle nr. changes the only diagrams which survive have $\nu_1\nu_2 = -$

$$(\tilde{\mathcal{K}}^{(2)})^{ba}_{ba} = \sum_{\substack{-\\ \nu_1\nu_2 = -}} \left(-\frac{i}{\hbar}\right) \sum_{\alpha\sigma} \sum_{p} \Big($$  $$+$$  $$\Big)$$

$$= \frac{i}{\hbar} \sum_{\alpha\sigma} \sum_{p} \sum_{k} \left[\frac{|\langle b | D^{p} | a \rangle|^2 \, f^{p}(\varepsilon_{\alpha k\sigma})}{i0^+ + E_a - E_b + p\varepsilon_{\alpha k\sigma}} + \frac{|\langle b | D^{\bar{p}} | a \rangle|^2 \, f^{-p}(\varepsilon_{\alpha k\sigma})}{i0^+ + E_b - E_a + p\,\varepsilon_{\alpha k\sigma}} \right]$$

$$= 2\,\mathrm{Re} \sum_{\alpha\sigma} \sum_{p}$$  $$(5.67)$$

recall hermitian conjugate obtained with mirror rule

ii) Recall the Sokhotski-Plemelj theorem

$$\int_{-\infty}^{+\infty} d\varepsilon \, \frac{h(\varepsilon)}{i0^+ + p(\varepsilon - \Delta)} = -i\pi h(\Delta) + p \fint d\varepsilon \, \frac{h(\varepsilon)}{\varepsilon - \Delta} \qquad (5.68)$$

where $\fint$ denotes the Cauchy principal value.

Hence

$$(\mathcal{K}^{(2)})^{ba}_{ba} = 2\,\mathrm{Re} \sum_{\alpha\sigma} \sum_{p} \left(\frac{i}{\hbar}\right) \int d\varepsilon \, \mathcal{D}_\alpha(\varepsilon) \, |D^p_{ab}|^2 \, \frac{f^p(\varepsilon)}{i0^+ + p(\varepsilon - E_{ba})}$$

$$\sum_{\vec{k}} \to \int d\varepsilon \, \mathcal{D}_\alpha(\varepsilon)$$

$$= \frac{2\pi}{\hbar} \sum_{\alpha\sigma} \sum_{p} \mathcal{D}_\alpha \, |D^p_{ab}|^2 \, f^p(E_{ba})$$

Depending on whether $N_b > N_a$ or $N_a > N_b$ only one matrix element D^p_{ab} is non vanishing.

2) According to the definition of $\Gamma^\pm_{ab}$

$$\boxed{\Gamma^\pm_{ab} = \frac{2\pi}{\hbar} \sum_{\alpha\sigma} \mathcal{D}_\alpha \, |D^\pm_{ab}|^2 \, f^\pm(E_{ba})} \qquad (5.69)$$

second order kernel

Notice that both $\mathcal{D}_\alpha$ and $D^{\pm}_{ab}$ are in general function of the energy.

In the wide band limit $\mathcal{D}_\alpha(\varepsilon) \sim \mathcal{D}_\alpha(E_F)$.

Further usually $t_{\alpha\sigma k i} \sim t_\alpha$

$$\Rightarrow \begin{cases} \Gamma^{\pm}_{ab} = \sum_\alpha \Gamma_\alpha f^{\pm}(E_{ba}) \cdot \sum_{\sigma i}' |\langle b| \sum_i d^{\pm}_{i\sigma} |a\rangle|^2 & (5.70) \\ \Gamma_\alpha = \frac{2\pi}{\hbar} \mathcal{D}_\alpha |t_\alpha|^2 & (5.71) \end{cases}$$

wide band limit + $t_{\alpha\sigma k i} \sim t_\alpha$

iii) $(\tilde{\mathcal{K}})^{bb}_{bb}$ follows from the sum rule

$$(\tilde{\mathcal{K}})^{bb}_{bb} = - \sum_{a \neq b} (\tilde{\mathcal{K}}^{ba}_{ba})$$

iv) Finally notice that the sum over the leads is additive:

$$\begin{cases} \Gamma^{\pm}_{ab} = \sum_\alpha \Gamma^{\pm}_{\alpha, ab} & (5.72) \\ \Gamma^{\pm}_{\alpha, ab} = \Gamma_\alpha f^{\pm}(E_{ba}) \sum_{\sigma i} |\langle b| \sum_i d^{\pm}_{i\sigma} |a\rangle|^2 & (5.73) \end{cases}$$

5.8.7. Current formula

we can use the previous considerations to get a general current formula

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

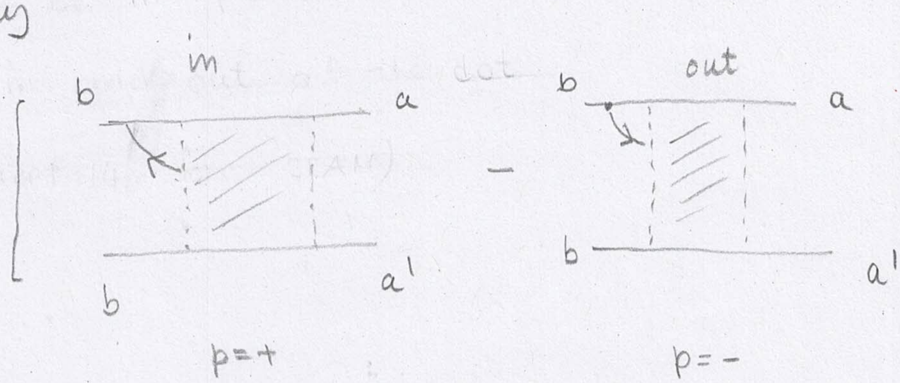
$$= \sum_{aa'} \left(\tilde{\mathcal{K}}^{+}_{I_L}\right)^{aa}_{aa'} \rho_{aa'} + \sum_{b\neq a} \sum_{aa'} \left(\tilde{\mathcal{K}}^{+}_{I_L}\right)^{ba}_{ba'} \rho_{aa'}$$

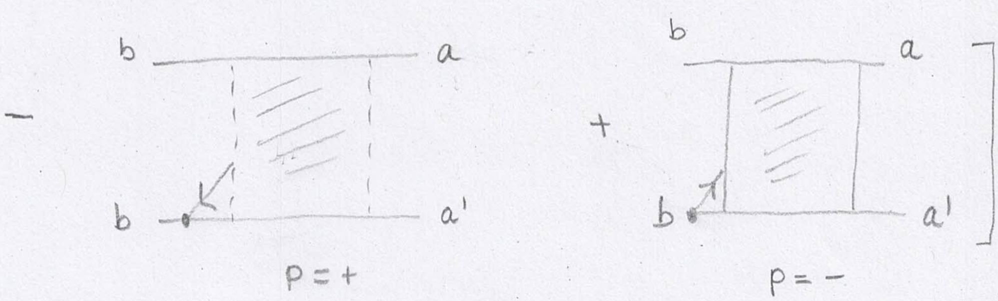
$$\Rightarrow \boxed{I_L = \sum_{b\neq a} \sum_{aa'} \left[\left(\tilde{\mathcal{K}}^{+}_{I_L}\right)^{ba}_{ba'} - \left(\tilde{\mathcal{K}}^{-}_{I_L}\right)^{ba}_{ba'}\right] \rho_{aa'}} \qquad (5.45)$$

sum rule (5.63) also applies to current kernel

Diagrammaticilly

$$I_L = e \sum_{b\neq a} \sum_{aa'}$$

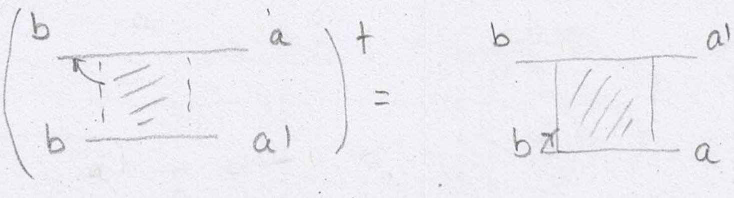


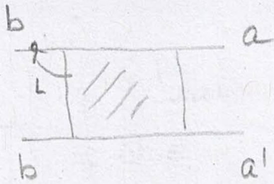


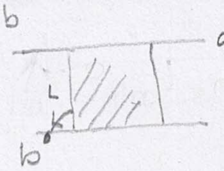
$\rho_{aa'}$

Remember mirror rule for hermitian conjugation

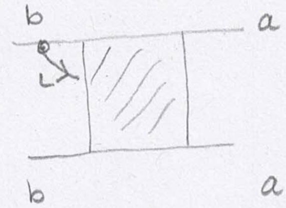
e.g.

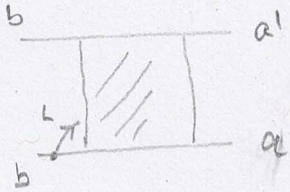


2) $I_L = e \sum_{b \neq a} {\sum_{aa'}}' \Big[$ 

$\rho_{aa'} \; + $ 

$\rho_{a'a}$

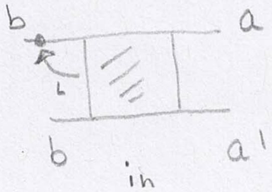
$-$ 

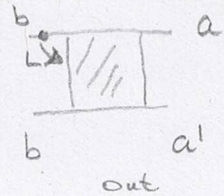
$\rho_{aa'} \; - $ 

$\rho_{a'a} \Big]$

Hence

$$\boxed{I_L = e\, 2\,\mathrm{Re} \sum_{b\neq a} \sum_{aa'} \Big[\quad - \quad \Big] \rho_{aa'}}$$



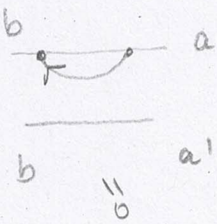


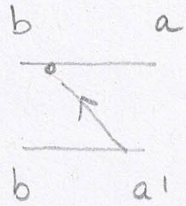
(5.76)

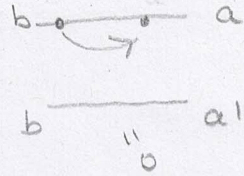
This formula is very general and applies to $\forall$ order in the perturbation theory.

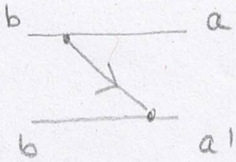
It tells us that the current is the difference of outcoming and outcoming processes!

<u>Example</u>: second order

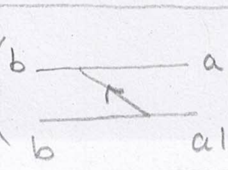
$I_L^{(2)} = e\,2\,\mathrm{Re} \sum_{b\neq a} \sum_{aa'} \Big[$ 

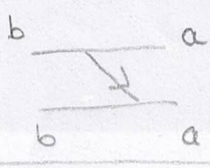
$+$ 

$-$ 

$-$ 

$\Big] \rho_{aa'}$

$\Rightarrow \boxed{I_L^{(2)} = e\,2\,\mathrm{Re} \sum_{b\neq a} \sum_{aa'} \Big($ 

$-$ 

$\Big) \rho_{aa'}}$ (5.77)

Example: SIAM

RDM is diagonal : $\rho_{aa'} = \rho_{aa}\, \delta_{aa'}$

↳ $$\boxed{I_L^{(2)} = \sum_{b} \sum_{a \neq a} \left(\Gamma^{+}_{L,ba} - \Gamma^{-}_{L,ba} \right) \rho_{aa}} \qquad (5.78)$$

where

$$\begin{cases} \Gamma^{+}_{L,ba} = \left(\tilde{\mathcal{K}}_L \right)^{ba}_{ba} & \text{if } N_b > N_a \\ \Gamma^{-}_{L,ba} = \left(\tilde{\mathcal{K}}_L \right)^{ab}_{ab} & \text{if } N_b < N_a \end{cases}$$

and given by Eqs. (5.69) and (5.72)

2) since the SIAM as only the spin as degree of freedom

$$\Gamma^{\pm}_{\alpha,ba} = \Gamma_\alpha f^{\pm}_\alpha (E_{ba}) \sum_\sigma | \langle b | d^{\pm}_\sigma | a \rangle |^2$$

As to be discussed later, cf. CH. 5.9, the Fermi function determine when the rates $\Gamma^{\pm}_{\alpha,ba} \neq 0$

This yields the known conditions for non vanishing second order current as already seen for the SIAM

$$\begin{cases} \mu_L \geq \mu(N+1) \geq \mu_R & \text{forward tunneling} \\ \mu_L \leq \mu(N+1) \leq \mu_R & \text{backward tunneling} \end{cases}$$

and in turn the occurrence of Coulomb diamonds