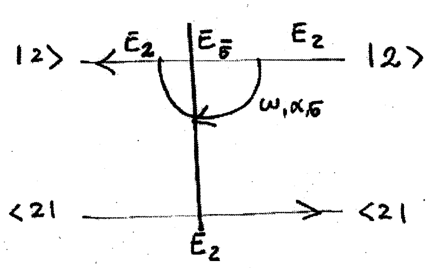
Back mapping in energy domain

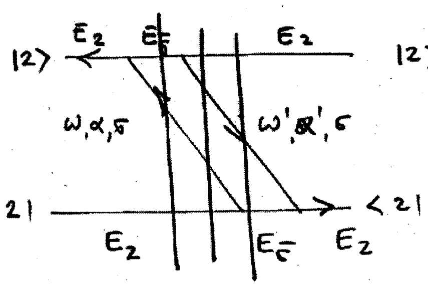
For a given $2n$-th order diagram as obtained in the time domain one can write a set of simple rules which allow to obtain at once the multiple energy integral associated to the Laplace transform of the Kernel.

$\boxed{1}$ To each of the fermion lines, assign an energy ω_i, as well as the lead and spin indices α_i, σ_i respectively $(1 \leq i \leq n)$.
To each section on the contours, assign the energy of the corresponding state

2nd order



4th order



$\boxed{2}$ Between two consecutive times τ_j and τ_{j+1} perform a vertical cut. You will obtain $2n-1$ cuts. From each cut obtain a denominator A_j: for each intersection of the cut with a fermion line or a contour, one adds up with a specific sign the energy assigned to the fermion line, respectively to the contour at the intersection. Thereby, the sign is determined by the directions of the fermion line, respectively the contour: If they hit the cut from the right, their energy has to be counted negative, if they come from the left, the sign is positive.

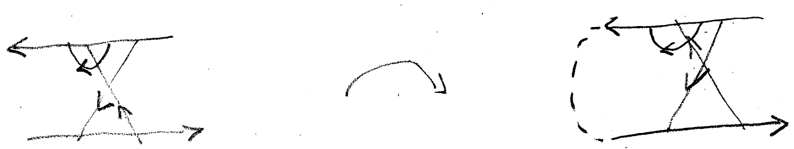
2^{nd} order $\Rightarrow$ $A_0 = E_2 - \omega - E_{\bar{\sigma}}$

4^{th} order $\Rightarrow$ $A_0 = E_{\bar{\sigma}} + \omega' - E_2$

$A_1 = E_2 - \omega + \omega' - E_2 = -\omega + \omega'$

$A_2 = E_2 - \omega + E_{\bar{\sigma}}$

$\boxed{3}$ For each fermionic line, determine a sign p_i which tells whether it belongs to an in-tunnelling ($p_i = +$) or an out-tunnelling process ($p_i = -$). Connect to this purpose the two contours at time t, thus obtaining a single oriented contour:



If the fermionic line runs forward with respect to the combined contour $\Rightarrow$ $p_i = -$, if it runs backwards $\Rightarrow$ $p_i = +$.

$\boxed{4}$ Determine q, which is the number of vertices on the lower contour plus the number of crossings of fermionic lines

2^{nd} $q = 0 + 0 = 0$

4^{th} $q = 2 + 0 = 2$

$\boxed{5}$ Write the final integral

$$-(-1)^q \frac{i}{\hbar} \lim_{\eta\to 0} \prod_{i=1}^{n} \int d\omega_i \, f_{\alpha_i}^{p_i}(\omega_i) \prod_{j=0}^{2n-2} \frac{1}{A_j + i\eta} \qquad (4.48)$$

2^{nd} order $\Rightarrow$ $$-\frac{i}{\hbar}\lim_{\eta\to 0}\int d\omega \frac{f_\alpha^-(\omega)}{-\omega + E_2 - E_{\bar{\sigma}} + i\eta}$$

4^{th} order $\Rightarrow$ $$-\frac{i}{\hbar}\lim_{\eta\to 0}\int d\omega \int d\omega' \frac{1}{-\omega+\omega'+i\eta} \, \frac{f_\alpha^+(\omega')}{-\omega + E_2 - E_{\bar{\sigma}} + i\eta} \, \frac{f_\alpha^-(\omega)}{\omega' - E_2 + E_{\bar{\sigma}} + i\eta}$$

[6] The tunnelling matrix elements associated to a vertex, $T^{p}_{\alpha\sigma}(b,a)$ has a superscript $p = \pm$ depending on the creation/annihilation character of the vertex. The subscript $\alpha\sigma$ indicate the lead and the spin quantum number of the electron in the tunnelling event. The arguments a and b represent the state - with respect of the contour alignment - before and after the vertex respectively.

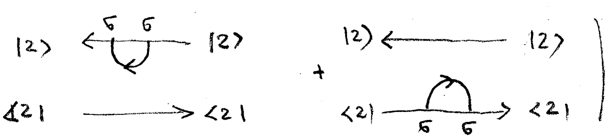
As an example we calculate one element of the Laplace transform of the Kernel for the Anderson impurity model, both in the 2^{nd} and 4^{th} order contribution in the tunnelling Hamiltonian.

The system Hamiltonian reads:

$$\hat{H}_{sys} = \sum_{\sigma=\uparrow,\downarrow} \varepsilon_\sigma \hat{n}_\sigma + U \hat{n}_\uparrow \hat{n}_\downarrow \qquad (4.49)$$

with the corresponding eigenvectors/eigenvalues: $|0\rangle, 0$; $|\sigma\rangle$ ε_σ; $|2\rangle$, $\varepsilon_\uparrow + \varepsilon_\downarrow + U = E_2$. The matrix elements that we calculate are $(\tilde{K}^{(2)})^{22}_{22}$ and $(\tilde{K}^{(4)})^{22}_{22}$. Let's start with the 2^{nd} order:

$$\left(\tilde{K}^{(2)}\right)^{22}_{22} = \sum_\sigma \Bigg(\qquad + \qquad \Bigg) \qquad (4.50)$$



Only 2 of the 8 diagrams composing the Kernel $K^{(2)}$ give a finite contribution, due to the particular choice of the initial and final state. Following the prescription of the diagrams in the time domain

$$\left(\tilde{K}^{(2)}\right)^{22}_{22} = -\lim_{\lambda\to 0} \sum_\sigma \int_0^\infty d\tau' \, e^{-\lambda\tau'} \langle \hat{C}^-_{3\sigma} \hat{C}^+_{0\sigma} \rangle \langle 2 | \hat{D}^+_{3\sigma} \hat{D}^-_{0\sigma} | 2 \rangle \langle 2 | 2 \rangle + \text{c.c.}$$

$$= -\sum_{\sigma\sigma'} \lim_{\lambda\to 0} \int_0^\infty d\tau' \, e^{-\lambda\tau'} \langle \hat{C}^-_{3\sigma} C^+_{0\sigma} \rangle \langle 2 | \hat{D}^+_{3\sigma} | \sigma' \rangle \langle \sigma' | \hat{D}^+_{0\sigma} | 2 \rangle + \text{c.c.}$$

$$(4.45) = -\frac{1}{\hbar^2}\sum_{\sigma\sigma'}\lim_{\lambda\to 0}\int_0^\infty d\tau'\, e^{-\lambda\tau'}\sum_{\alpha\vec{k}} f_\alpha^-(\omega_{\vec{k}})\, e^{-i\omega_{\vec{k}}/\hbar\,\tau'} \cdot$$

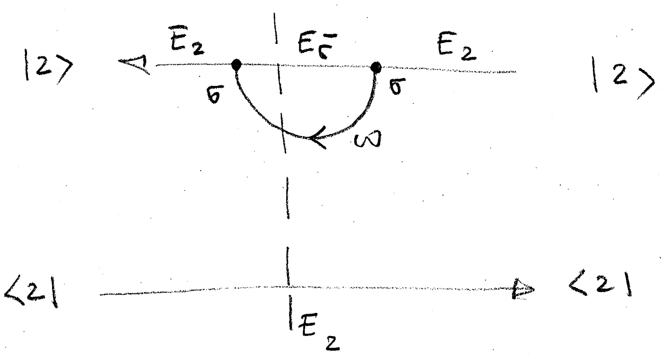
$$\langle 2|\, t_{\alpha\vec{k}\sigma}\, t^*_{\alpha\vec{k}'\sigma}\, e^{iE_2 t/\hbar}\, d_\sigma^+ |\sigma'\rangle\langle\sigma'|\, e^{-iE_{\sigma'}t/\hbar}\, e^{iE_{\sigma'}(t-\tau')/\hbar}\, d_\sigma\, e^{-\frac{i}{\hbar}E_2(t-\tau')}|2\rangle$$

$$+ \text{c.c.}$$

$$= -\frac{1}{\hbar^2}\sum_{\alpha\sigma}\lim_{\lambda\to 0}\int d\omega\, f_\alpha^-(\omega)\int_0^\infty d\tau'\, e^{-\lambda\tau'}\, e^{-\frac{i}{\hbar}(\omega+E_{\bar\sigma}-E_2)\tau'}\, T^+_{\alpha\sigma}(2,\bar\sigma)\, T^-_{\alpha\sigma}(\bar\sigma,2) + \text{c.c.}$$

$$= -\frac{1}{\hbar^2}\frac{1}{i/\hbar}\lim_{\lambda\to 0}\sum_{\alpha\sigma}\int d\omega\, f_\alpha^-(\omega)\,\frac{1}{\omega+E_{\bar\sigma}-E_2-i\lambda}\,\left|T^+_{\alpha\sigma}(2,\bar\sigma)\right|^2 + \text{c.c.}$$

$$= -\frac{i}{\hbar}\sum_{\alpha\sigma}\left|T^+_{\alpha\sigma}(2,\bar\sigma)\right|^2\lim_{\lambda\to 0}\int d\omega\,\frac{f_\alpha^-(\omega)}{-\omega+E_2-E_{\bar\sigma}+i\lambda} + \text{c.c.} \qquad (4.51)$$

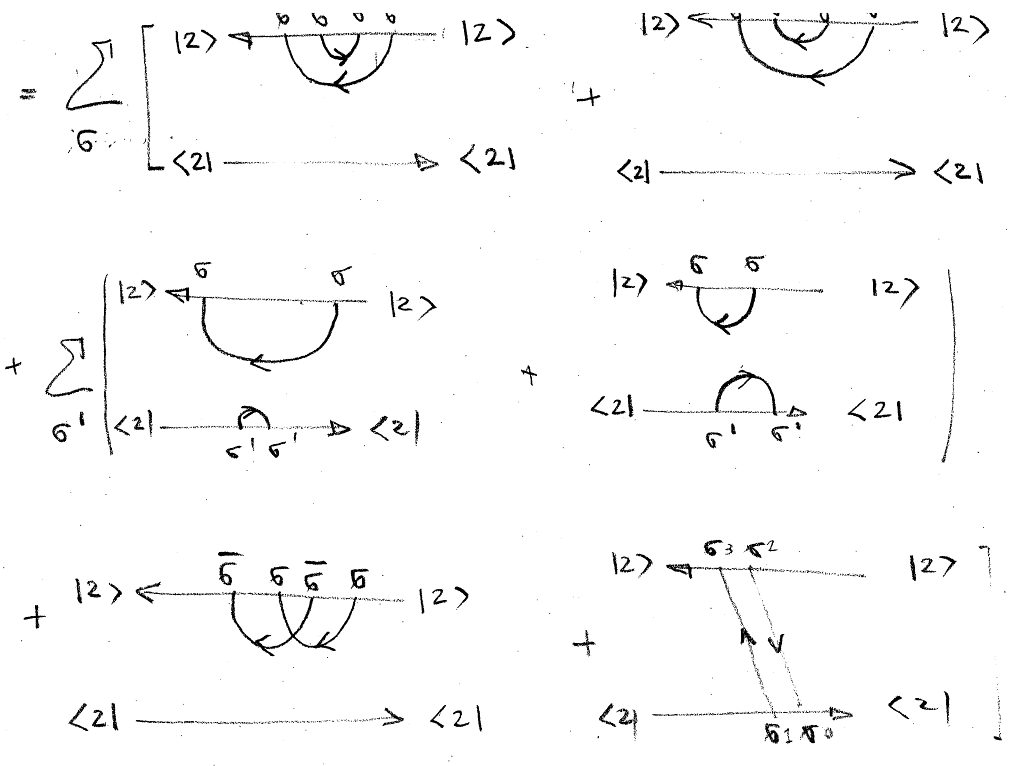


The integral in (4.66) can be calculated with the help of the residual theorem. It yields:

$$\left(K^{(2)}\right)^{22}_{22} = -\frac{2\pi}{\hbar}\sum_{\alpha\sigma}\left|T^+_{\alpha\sigma}(2,\bar\sigma)\right|^2 f^-(E_2-E_{\bar\sigma}-\mu_\alpha) \qquad (4.52)$$

Now we want to address the 4^{th} order contribution to the same element of the time-evolution kernel:

$$\left(\tilde{K}^{(4)}\right)^{22}_{22} = \sum_{\sigma}$$



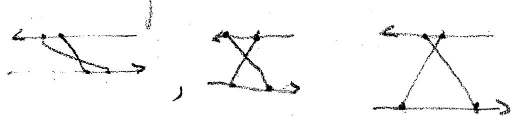
$$+\ h.c. \qquad (4.53)$$

The rules for extracting the "5 diagrams" above out of the 16 listed at page 111 are

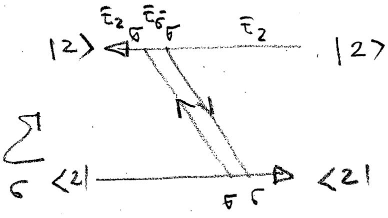
(i) - each contour should have an even number of vertices paired into in and out ones.

(ii) - the first vertex along the contour orientation must be an out-going one.

(iii) - if the second vertex is out-going (in-going) it must be of opposite (equal) spin with respect to the first one.

Rule (i) excludes half of the 4^{th} order diagrams. Rule (ii) excludes the three (classes of) crossed diagrams . Eventually rule (iii) fixes the orientation of the fermionic lines of the residual 5 classes and leaves "only" the diagrams listed above.

Exemplarily we calculate the last contribution



$$= \lim_{\lambda\to 0} \sum_\sigma \int_0^\infty d\tau' e^{-\lambda\tau'} \int_0^{\tau'} d\tau_1' \int_0^{\tau_1'} d\tau_2' \langle \hat c^+_{1\bar\sigma} \hat c^-_{3\bar\sigma} \rangle \langle \hat c^-_{0,3} \hat c^+_{2,\bar\sigma} \rangle$$

$$\langle 2| \hat D^+_{3,\bar\sigma} |\bar\sigma\rangle\langle\bar\sigma| \hat D^-_{2\bar\sigma} |2\rangle\langle 2| \hat D^+_{0\bar\sigma} |\bar\sigma\rangle\langle\bar\sigma| \hat D^-_{1,\bar\sigma} |2\rangle + c.c.$$

$$= \frac{1}{\hbar^4} \lim_{\eta\to 0} \sum_{\alpha\alpha'\bar\sigma} \int_0^\infty d\tau_2' \int_{\tau_2'}^\infty d\tau_1' \int_{\tau_1'}^\infty d\tau' \int d\omega \int d\omega' \, f^+_\alpha(\omega) f^-_{\alpha'}(\omega')$$

$$e^{i/\hbar(-\omega+E_2-E_{\bar\sigma})\tau_1'} e^{i/\hbar(-\omega'+E_2-E_{\bar\sigma})\tau_2'} e^{i/\hbar(\omega'-E_2+E_{\bar\sigma}+i\eta)\tau'}$$

$$T^+_{\alpha\bar\sigma}(2,\bar\sigma)\, T^-_{\alpha'\bar\sigma}(\bar\sigma,2)\, T^+_{\alpha'\bar\sigma}(2,\bar\sigma)\, T^-_{\alpha,\bar\sigma}(\bar\sigma,2) \quad + c.c.$$

$$= -\frac{i}{\hbar} \lim_{\eta\to 0} \sum_{\alpha\alpha'\bar\sigma} \int d\omega \int d\omega' \, f^+_\alpha(\omega) f^-_{\alpha'}(\omega') \, |T^+_{\alpha\bar\sigma}(2,\bar\sigma)|^2 \, |T^+_{\alpha'\bar\sigma}(2,\bar\sigma)|^2$$

$$\frac{1}{-\omega+\omega'+i\eta} \; \frac{1}{-\omega+E_2-E_{\bar\sigma}+i\eta} \; \frac{1}{\omega'-E_2+E_{\bar\sigma}+i\eta} \quad + c.c. \qquad (4.54)$$

where, for the evaluation of the time ordered integration, in the last step, the variable transformation $\tilde\tau_1 = \tau_1'-\tau_2'$, $\tilde\tau = \tau'-\tau_1'$ which decouples the three time integrals, were applied.

The integrals in (4.69) have an analytical solution calculated using the residual integrals. Interestingly, all the 4^{th} order diagrams reduce to expressions involving only 2 types of functions

$$^s X^{pp'}_{dd'}(\mu,\mu',\Delta) \quad \text{and} \quad ^s D^{pp'}_{dd'}(\mu,\mu',\Delta)$$

where $s, p, p', d, d' = \pm$

where

$$ {}^{s}X^{pp'}_{dd'}(\mu,\mu',\Delta) = \frac{\beta}{i\hbar} \lim_{\eta\to 0} \int dx \int dx' \, f^{p}(x)\, f^{p'}(x') \times \tag{4.55} $$

$$ \times \frac{1}{d(x-\mu)+i\eta} \; \frac{1}{dx+d'x'-\Delta+i\eta} \; \frac{1}{d(sx'-\mu')+i\eta} $$

and

$$ {}^{s}D^{pp'}_{dd'}(\mu,\mu',\Delta) = \frac{\beta}{i\hbar} \lim_{\eta\to 0} \int dx \int dx' \, f^{p}(x)\, f^{p'}(x') \times \tag{4.56} $$

$$ \times \frac{1}{d(x-\mu)+i\eta} \; \frac{1}{dx+d'x'-\Delta+i\eta} \; \frac{1}{d(sx-\mu')+i\eta} $$

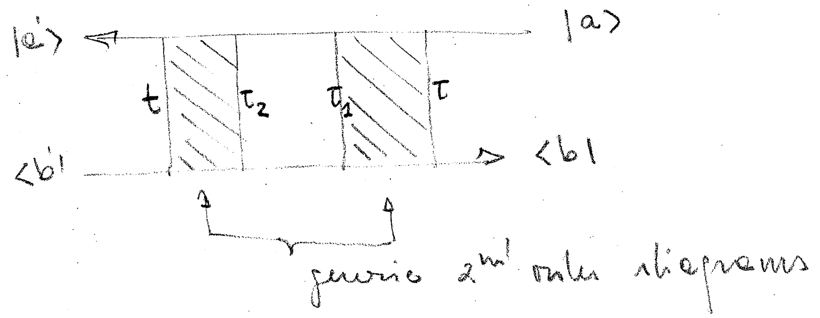
Interestingly, the Liouville space approach will reveal that there are formally only 2 classes of diagrams associated to the 2 functions above.

4.2.4 Diagrammatic representation of K_c

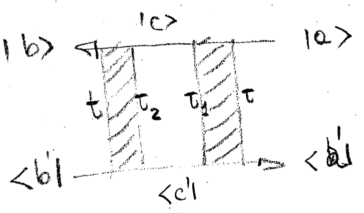
The correction kernel due to non-secular terms reads

$$ \tilde{K}_c = - \tilde{K}^{(2)}_{sn} \left(\tilde{K}_0\right)^{-1}_{nn} \tilde{K}^{(2)}_{ns} $$

This kernel can be seen as a sum of REDUCIBLE fourth order diagrams. Specifically, let's consider the most generic reducible 4^{th} order graph



The diagram above can be translated into the analytic expression



$$= \sum_{cc'} \langle b| U_0(t,0) \int_0^t d\tau_2\, K_I^{(2)}(t,\tau_2) \Big[U_0^+(\tau_2,0) \int_0^{\tau_2} d\tau_1\, U_0(\tau_2,\tau_1) |c\rangle$$

$$\langle c| U_0(\tau_1,0) \int_0^{\tau_1} d\tau\, K_I^{(2)}(\tau_1,\tau) \left[U_0^+(\tau,0) |a\rangle\langle a'| U_0(\tau,0) \right] U_0^+(\tau_1,0) |c'\rangle$$

$$\langle c'| U_0^+(\tau_2,\tau_1)\, U_0(\tau_2,0) \Big] U_0^+(t,0) |b'\rangle \tag{4.57}$$

where one recognizes a sequence of nested operations:

i) $|a\rangle\langle a'| \longrightarrow U_0^+(\tau,0)|a\rangle\langle a'| U_0(\tau,0)$ Schr. to interaction picture

ii) $\int_0^{\tau_1} d\tau\, K_I^{(2)}(\tau_1,\tau)[\quad]$ application of 2^{nd} order Kernel in interaction picture.

iii) $U_0(\tau_1,0)[\quad] U^+(\tau_1,0)$ Interaction to Schr. picture at time τ_1

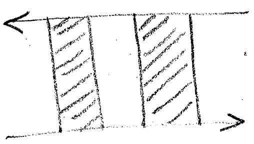
iv) $\int_0^{\tau_2} d\tau_1\, U_0(\tau_2,\tau_1)[\quad] U_0^+(\tau_2,\tau_1)$ Evolution in the Schr. picture from τ_1 to τ_2
The integral simply ensures that one integrates over all possible cases.

v) $U_0^+(\tau_2,0)[\quad] U_0(\tau_2,0)$ Schr. $\rightarrow$ interaction picture at time τ_2

vi) $\int_0^t d\tau_2\, K_I^{(2)}(t,\tau_2)[\quad]$ application of the 2^{nd} order Kernel in I picture

vii) $U_0(t,0)[\quad] U_0^+(t,0)$ Back to Schr. picture at time t.

Considering only the Schr. picture



$$= \langle b| \int_0^t d\tau_2\, K^{(2)}(t-\tau_2) \Big[\int_0^{\tau_2} d\tau_1\, U_0(\tau_2-\tau_1) \int_0^{\tau_1} d\tau\, K^{(2)}(\tau_1-\tau) \big[|a\rangle\langle a'|\big] U_0^+(\tau_2-\tau_1) \Big] \tag{4.58}$$

that is, 3 convoluted operations on the operator $|a\rangle\langle a'|$. In Laplace space they will then result into the product of operations

$$\tilde{K}^{aa'}_{bb'} = \sum_{\substack{cc'\\dd'}} \tilde{K}^{(2)\,cc'}_{bb'}\, \tilde{K}_0^{hl\,dd'}{}_{cc'}\, \tilde{K}^{(2)\,aa'}_{dd'}$$

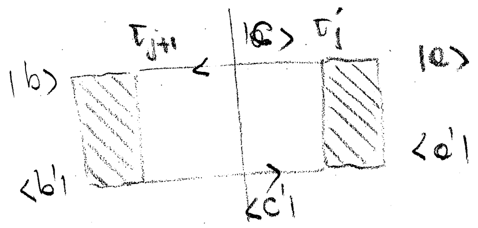
where, in order to obtain the identification of K_0^{nl}

$$\tilde{K}_0^{nl}{}^{dd'}_{cc'} = \lim_{\lambda\to 0}\int_0^\infty d\tau\; e^{-\lambda\tau}\,\langle c|\,U_0(\tau,0)\,|d\rangle\langle d'|\,U_0^+(\tau,0)\,|c'\rangle$$

$$= \lim_{\lambda\to 0}\int_0^\infty d\tau\;\delta_{cd}\,\delta_{d'c'}\;e^{-\frac{i}{\hbar}(E_d-E_{d'})\tau-\lambda\tau} = -\frac{\hbar}{i}\,\frac{1}{E_{d'}-E_d}\,\delta_{cd}\,\delta_{c'd'} \qquad (4.59)$$

in other terms $\left(\tilde{K}_0^{nl}\right)^{dd'}_{cc'} = -\left[\left(K_0\right)^{dd'}_{cc'}\right]^{-1}$.

Notice that the calculated non-local Kernel also follows from the diagrammatic rules in energy space



has an extra contribution $-\frac{i}{\hbar}\frac{1}{E_c-E_{c'}}$

The prefactor $-\frac{\hbar}{i}$ of the analytical calculation is needed to compensate the excess of $-\frac{i}{\hbar}$ factors from the 2 2^{nd} order Kernels.

Notice: the nl diagram does not diverge since it is only considered for states with different energies

4.3 Fourth order GME: physical interpretation

The first physical property which can be extracted from the diagrammatic analysis is the probability conservation. $\sum_a \rho_{red,aa}(t) = 1$ $\forall t$ which ensures that the physical system is in a certain state at every moment. A direct consequence $\sum_b \dot{\rho}_{red,bb} = 0$. The stationary limit of the GME reads:

$$0 = -\frac{i}{\hbar}\sum_{aa'} \delta_{ab}\delta_{a'b'}(E_a - E_{a'})\rho^{stat}_{aa'} + \sum_{aa'} \tilde{K}^{aa'}_{bb'}\rho^{stat}_{aa'}$$

If we take $b'=b$ we obtain thus the sum rule for the Kernel:

$$\left(\sum_b \tilde{K}^{aa'}_{bb}\right) = 0 \qquad \forall\, aa' \qquad (4.60)$$

Notice that (4.60) ensures that a non-trivial solution $\rho^{stat}_{aa'}$ exists but the trace condition makes it unique. Eq. (4.60), with $a=a'$ suggest the existence of gain-loss pairs which balance each other.

4.3.1 Gain-loss pairs

Let us consider once again the AIM and restrict ourselves to the case of non-polarized or parallel polarized leads, such that spin coherences can be excluded and we can restrict to populations only.

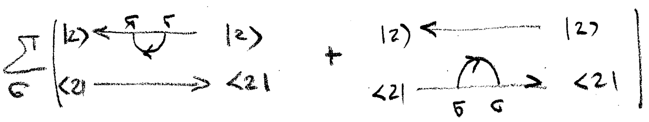
The GME assumes the form:

$$\begin{cases} \dot P_0 = \underbrace{-\left(\sum_\sigma \Gamma^{0\to\sigma} + \Gamma^{0\to 2}\right)}_{\tilde K^{00}_{00}} P_0 + \sum_\sigma \underbrace{\Gamma^{\sigma\to 0}}_{\tilde K^{\sigma\sigma}_{00}} P_\sigma + \underbrace{\Gamma^{2\to 0}}_{\tilde K^{22}_{00}} P_2 \\ \dot P_\sigma = \underbrace{-\left(\Gamma^{\sigma\to 0} + \Gamma^{\sigma\to\bar\sigma} + \Gamma^{\sigma\to 2}\right)}_{\tilde K^{\sigma\sigma}_{\sigma\sigma}} P_\sigma + \underbrace{\Gamma^{0\to\sigma}}_{\tilde K^{00}_{\sigma\sigma}} P_0 + \underbrace{\Gamma^{\bar\sigma\to\sigma}}_{\tilde K^{\bar\sigma\bar\sigma}_{\sigma\sigma}} P_{\bar\sigma} + \underbrace{\Gamma^{2\to\sigma}}_{\tilde K^{22}_{\sigma\sigma}} P_2 \\ \dot P_2 = \underbrace{-\left(\sum_\sigma \Gamma^{2\to\sigma} + \Gamma^{2\to 0}\right)}_{\tilde K^{22}_{22}} P_2 + \sum_\sigma \underbrace{\Gamma^{\sigma\to 2}}_{\tilde K^{\sigma\sigma}_{22}} P_\sigma + \underbrace{\Gamma^{0\to 2}}_{\tilde K^{00}_{22}} P_0 \end{cases} \qquad (4.61)$$

Where $P_{0/\sigma/2}$ is the probability of occupation of the corresponding AIM eigenstate $|0\rangle$, $|\sigma\rangle$, $|2\rangle$. $\Gamma^{\alpha\to\beta}$ is the rate of transfer of the probability from state $|\alpha\rangle$ to $|\beta\rangle$. Below we identify the different components of the Kernel. Notice (4.76) can be interpreted in Markov approx, or alternatively simply the GME up to a given perturbative order for the stationary p stat, if LHS = 0. If we write (4.75) for $\alpha\alpha$'s 22

$$\underbrace{\tilde K^{22}_{22}}_{\text{loss for } |2\rangle} = -\underbrace{\left(\tilde K^{22}_{00} + \sum_\sigma \tilde K^{22}_{\sigma\sigma}\right)}_{\text{gain (for } |0\rangle \text{ and for } |\sigma\rangle) \text{ from } |2\rangle} \qquad (4.62)$$

The Kernel element $\tilde K^{22}_{22}$ enters in (4.76) as a depopulating rate for state $|2\rangle$. $\tilde K^{22}_{00}$ populates $|0\rangle$ from $|2\rangle$ and $\tilde K^{22}_{\sigma\sigma}$ populates $|\sigma\rangle$ from $|2\rangle$. This relation is valid at each order. In particular, to 2nd order $\left(\Gamma^{(2)}\right)^{2\to 0} = \left(\tilde K^{(2)}\right)^{22}_{00} = 0$

$\left(K^{(2)}\right)^{22}_{22} = \sum_\sigma$  (4.63)

$\left(K^{(2)}\right)^{22}_{\sigma\sigma} =$