5.5. THE STATIONARY RDM IN FOCK SPACE

We have so far worked in terms of operators only in Liouville space. In particular, we have found the exact equation (5.20) for the stationary RDM

$$\left(\mathcal{L}_S + \tilde{\mathcal{R}}\right) \rho^{\infty} = 0 \qquad (5.20)$$

This equation leads to an (exact) set of coupled equations for the elements $\rho_{aa'}$ of ρ^{∞} in the basis $\{|a\rangle\}$ of the eigenstates of the central system.

As we shall see,

a) conservation of probability

b) symmetries

impose constraints on the elements of the tensor $\tilde{\mathcal{R}}^{\,ba}_{\,b'a'}$ (see (5.27b)) and of $\rho_{aa'}$.

We can express (5.20) in the eigenbasis $\{|a\rangle\}$ of the central system S:

$$\hat{H}_S |a\rangle = E_a |a\rangle$$

where $|a\rangle$ are in general many body states

E.g. SIAM $\{|a\rangle = |0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\}$.

In this basis we have

$$\begin{cases} \rho^{\infty} = \sum_{aa'} \rho_{aa'} |a\rangle\langle a'| & (5.27) \\ \mathcal{K}^{ba}_{b'a'} \equiv \langle b| \left(\tilde{\mathcal{K}}(0)|a\rangle\langle a'|\right) |b'\rangle & (5.27b) \end{cases}$$

Eq. (5.21) thus yields the set of coupled linear eqs for the elements $\rho_{\alpha\beta}$ of the reduced density matrix (RDM)

$$\boxed{0_{bb'} = \langle b|0|b'\rangle = -\frac{i}{\hbar} \sum_{aa'} \delta_{ab}\, \delta_{a'b'} (E_a - E_{a'}) \rho_{aa'} + \sum_{aa'} \mathcal{K}^{ba}_{b'a'} \rho_{aa'}} \quad (5.28)$$

5.5.1 SUM RULE for $\mathcal{K}^{ba}_{ba'}$

Conservation of probability implies $\sum_b \rho_{bb} = 1$. Hence

$$0 = \frac{d}{dt} 1 = \frac{d}{dt} \sum_b \rho_{bb} = \sum_b \dot{\rho}_{bb} = \sum_b \left(\sum_{aa'} \mathcal{K}^{ba}_{ba'} \rho_{aa'} \right) = \sum_{aa'} \left(\sum_b \mathcal{K}^{ba}_{ba'} \right) \rho_{aa'}$$

$\Rightarrow$ since it has to hold true $\forall a, a'$ $\boxed{\sum_b \mathcal{K}^{ba}_{ba'} = 0}$ (5.29)

5.5.2 THE RDM Kernel and its diagrammatic representation

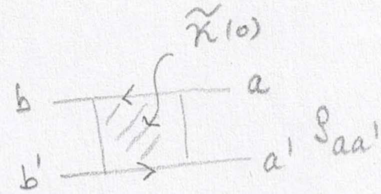
We have defined

$$\left(\tilde{\mathcal{K}}\right)^{ba}_{b'a'} = \langle b| \left(\tilde{\mathcal{K}}(0)\, |a\rangle\langle a'|\right) |b'\rangle$$

Thus, because the kernel $(\mathcal{K})^{ba}_{b'a'}$ governs the stationary dynamics of the RDM it can be viewed as a stationary propagator connecting an initial state $|a\rangle\langle a'|$ of the RDM to a final state $|b\rangle\langle b'|$

Symbolically, the GME (5.26) can be expressed as

$$0_{bb'} = -\frac{i}{\hbar} \sum_{aa'} \delta_{ab}\, \delta_{a'b'}\, (E_a - E_{a'})\, \rho_{aa'} + \sum_{aa'}$$



(5.30)

Here the two arrows indicate propagation according to $\hat{\mathcal{U}}(t)$ from $|a\rangle \to |b\rangle$ (forward propagation) an to $\hat{\mathcal{U}}^{\dagger}(t) = \hat{\mathcal{U}}(-t)$ from $|b'\rangle \to |a'\rangle$ (backward propagation)

since $\hat{\rho}_{tot}(t) = \hat{\mathcal{U}}(t,t_0)\, \hat{\rho}_{tot}(t_0)\, \hat{\mathcal{U}}^{\dagger}(t,t_0)$

The shaded area indicates the action of $\tilde{\mathcal{K}}(0)$. According to the expansion of $\tilde{\mathcal{K}}^{(0)}$ in even powers of d_T, we can see that $\tilde{K}(0)$ includes all possible tunneling events $\begin{cases} a \to b \\ a' \to b' \end{cases}$

In the next sections, a diagrammatic formulation for the elements $(\mathcal{K}^{(2n)})^{ba}_{b'a'}$ of the kernel $\mathcal{K}$ will be provided.

5.5.3 SUPER SELECTION RULE for $\rho_{aa'}$

Eq. (5.26) involves both diagonal elements of ρ (populations) as well as off-diagonal elements (coherences).

Even if in the transient evolution all elements $\rho_{aa'}(t)$ are involved, in the stationary limit $t \to \infty$ the RDM has a block diagonal structure, whereby the blocks are determined by the quantum numbers conserved by $\hat{H}_{TOT}$ and $\hat{H}_S$.

Example: $\hat{H}_{TOT}$ conserves the particle nr. $\hat{N}_{TOT}$ and $[\hat{H}_S, \hat{N}_S]=0$

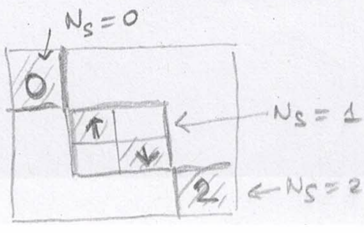
$$\Rightarrow \quad \langle a' | \rho^{\infty} | a \rangle \propto \delta_{N_a, N_{a'}}$$

Example: $\hat{H}_{TOT}$ conserves spin along z, $\hat{S}^z_{TOT}$ and $[\hat{H}_S, \hat{S}^z_S]=0$

$$\Rightarrow \quad \langle a' | \rho^{\infty} | a \rangle \propto \delta_{S_a, S_{a'}}$$

This is because one obtains a decoupled set of eqs. for populations and coherences, whereby the coherences decay exponentially to 0 when $t \to \infty$ (cf. spin-boson model) (cf. next page)

Example: SIAM

$\rho_{aa'} =$ 

$$\rho^{\infty} = \sum_a \rho_{aa} |a\rangle\langle a|$$

<u>Proof.</u>

Consider e.g. the 2nd order GME in interaction picture

$$\dot{\hat{\rho}}_I(t) = -\frac{1}{\hbar^2}\int_0^t dt'\, \mathrm{Tr}_B\left\{\left[\hat{H}_{T,I}(t), \left[\hat{H}_{T,I}(t'), \hat{\rho}_I(t')\otimes\hat{\rho}_B\right]\right]\right\}$$

Because of particles and spin conservation in the reservoirs,

- $$\mathrm{Tr}_B\left\{\hat{C}^{p}_{\vec{k}\sigma}(t)\,\hat{C}^{p'}_{\vec{k}'\sigma'}(t')\right\} = \mathrm{Tr}_B\left\{\hat{C}^{p}_{\vec{k}\sigma}(t)\,\hat{C}^{\bar{p}}_{\vec{k}\sigma}(t')\right\}\delta_{\vec{k}\vec{k}'}\,\delta_{\sigma\sigma'}\,\delta_{\bar{p}p'}$$

- Because of spin and particles conservation by $\hat{H}_T$, this also implies a corresponding arrangement of dot operators <u>which conserves spin and particles</u>

  $\Rightarrow$ block structure

Let us check (cf. sheet 13) on the example of the SIAM

$$\dot{\hat{\rho}}_I(t) = -\frac{1}{\hbar^2}\sum_{\sigma}\sum_{e}|T_e|^2\int_0^t dt'\Big[\underbrace{F^+_e(t-t')\,\hat{d}_\sigma(t)\,\hat{d}^+_\sigma(t')\,\hat{\rho}_I(t')}_{(I)}$$

$$+\underbrace{F^-_e(t-t')\,\hat{d}_\sigma(t)\,\hat{d}^+_\sigma(t')\,\hat{\rho}_I(t')}_{II} - \underbrace{(F^+_e(t-t'))^*\,d_\sigma(t)\,\hat{\rho}_I(t')\,d^+_\sigma(t')}_{III}$$

$$-\underbrace{(F^-_e(t-t'))^*\,d^+_\sigma(t)\,\hat{\rho}_I(t')\,d_\sigma(t')}_{IV} + h.c.\Big] \qquad (*)$$

where
$$\begin{cases} F^+_e(t-t') = \sum_{\vec{k}}\mathrm{Tr}_B\left\{\hat{C}^+_{e\vec{k}\sigma}(t)\,\hat{C}_{e\vec{k}\sigma}(t')\,\hat{\rho}_B\right\} \\ F^-_e(t-t') = \sum_{\vec{k}}\mathrm{Tr}_B\left\{\hat{C}_{e\vec{k}\sigma}(t)\,\hat{C}^+_{e\vec{k}\sigma}(t')\,\hat{\rho}_B\right\} \end{cases}$$ ← check

Project (*) in the eigenbasis of the central system

$$\langle a|\dot{\hat{\rho}}_I(t)|a'\rangle = \int dt' \underbrace{\langle a|\hat{d}_\sigma(t)\,\hat{d}^+_\sigma(t')\,\hat{\rho}_I(t')|a'\rangle}_{(I)} F^+_{\cdot\cdot}$$

(II), (III), (IV)

- Consider contribution (I)

$$\sum_b \underbrace{\langle a|\hat{d}_\sigma(t)\,d^+_\sigma(t')|b\rangle}\langle b|\hat{\rho}_I(t')|a'\rangle$$

↳ since $d_\sigma d^+_\sigma$ conserves particles and the S_z component of the spin, $|a\rangle$ and $|b\rangle$ belong to the subspace with equal N_S, S^z_S

Similar holds for (II).

- Consider contribution (III). Also here the combination d, d^+ conserves particle

$$\langle a|\hat{d}_\sigma(t)\,\rho_I(t')\,\hat{d}^+_\sigma(t')|a'\rangle$$

$$= \sum_{bb'} \langle a|d_\sigma(t)|b\rangle\langle b|\rho_I(t')|b'\rangle\langle b'|d^+_\sigma(t')|a'\rangle$$

In this case $\begin{cases} |b'\rangle \text{ has one particle more than } |a'\rangle \\ |b\rangle \text{ " " " " } |a\rangle \end{cases}$

2) E.g. diagonal elements in $\{|N, S^z\rangle\}$ representation coupled among themselves as well the off-diagonal.
similarly for IV.

- Finally, one should show that given initial off-diagonal elements in particle number

$|a\rangle = |N, i\rangle, \quad |a'\rangle = |N', j\rangle \qquad N \neq N'$

one should show that $\quad \rho^{\infty}_{aa'} = 0 \quad (**)$

This happens e.g. if

$$\dot{\rho}_{aa'}(t) = -C\, \rho_{aa'}(t) \Rightarrow \rho_{aa}(t) = e^{-ct}$$

This latter fact $(**)$ is more complicated to show. See e.g. the spin-boson problem,

5.6 CURRENT FORMULA

The current formula is straightforward from the definition

$$I(t) = I_L(t) = \langle \hat{I}_L(t) \rangle = \mathrm{Tr}\{\hat{\rho}_{tot}(t)\, \hat{I}_L\}$$

where the current operator at the left lead is $\hat{I}_L(t) = e\dot{\hat{N}}_L(t)$, i.e.

$$\hat{I}_L = +\frac{ie}{\hbar}[\hat{H}_{TL}, \hat{N}_L]$$

since $\hat{I}_L$ is linear in $\hat{H}_{TL}$ and thus does not conserve particles in lead L

$$I(t) = \mathrm{Tr}\{\hat{\rho}_{tot}(t)\,\hat{I}_L\} \underset{\uparrow \atop 1=P+Q}{=} \mathrm{Tr}\{Q\hat{\rho}_{tot}(t)\,\hat{I}_L\} \quad (5.31)$$

i.e., only the entangled part $Q\hat{\rho}_{tot}(t)$ contributes.

Replacing the expression for the entangled part,

$$Q\hat{\rho}_{tot}(t) = G_Q(t)\,Q\hat{\rho}_{tot}(0) + G_Q(t)\int_0^t ds\, G_Q(-s)\, Q\mathcal{L}_{tot}\, P\hat{\rho}_{tot}(s),$$

yields

$$I(t) = \underbrace{\mathrm{Tr}\{\hat{I}_L G_Q(t)\, Q\hat{\rho}_{tot}(0)\}}_{=0}$$

$$+ \mathrm{Tr}\{\hat{I}_L G_Q(t)\int_0^t ds\, G_Q(-s)\, Q\mathcal{L}_{tot}\, P\hat{\rho}_{tot}(s)\}$$

$$= \mathrm{Tr}\{P\hat{I}_L \int_0^t ds\, \bar{G}_Q(t-s)\, Q\mathcal{L}_{tot}\, P\hat{\rho}_{tot}(s)\}$$

↑ same as for Eq. (5.9)

with $\bar{G}_Q(t) = e^{(\mathcal{L}_0 + Q\mathcal{L}_T Q)t}$

$$= \mathrm{Tr}\{P\hat{I}_L \int_0^t ds\, \bar{G}_Q(t-s)\, Q\mathcal{L}_T P\, \hat{\rho}_{tot}(s)\}$$

$$\equiv \mathrm{Tr}\{\int_0^t ds\, \mathcal{K}^+_{PL}(t-s)\, P\hat{\rho}_{tot}(s)\}$$

← the meaning of "+" will become clear later

finally

$$\boxed{I_L(t) = \mathrm{Tr}_S\{\int_0^t ds\, \mathcal{K}^+_{I_L}(t-s)\, \hat{\rho}(s)\}} \quad (5.32)$$

where we introduced the current kernel for the left lead

$$\boxed{\mathcal{K}^+_{I_L}(t-s)\,\hat{\rho}(s) = \mathrm{Tr}_B\{\hat{I}_L\, \bar{G}_Q(t-s)\, \mathcal{L}_T\, \hat{\rho}_S(s) \times \hat{\rho}_B\}} \quad (5.33)$$

Note the similarity with the kernel $\mathcal{K}(t-s)\hat{\rho}(s)$ in (5.13):

$\mathcal{K} \to \mathcal{K}^+_{I_L}$ upon replacing the leftmost $\mathcal{L}_T \to \hat{I}_L$!

5.6.2 STATIONARY CURRENT

From the Dyson series for $\bar{G}_Q(t)$ it immediately follows the series expression for $\mathcal{K}_L(t)$. Further, since we are interested in the stationary current we find

$$\boxed{I^\infty = \mathrm{Tr}_S\{\tilde{K}^+_{I_L}\,\rho^\infty\} = \sum_b \Big(\sum_{aa'} (\tilde{\mathcal{K}}^+_{I_L})^{ba}_{ba'}\,\rho_{aa'}\Big)} \qquad (5.34)$$

eigenbasis $\{|a\rangle\}$ of S , $\rho^\infty = \sum_{aa'} \rho_{aa'} |a\rangle\langle a'|$

and also

$$\boxed{I^\infty = \mathrm{Tr}_S\,\mathrm{Tr}_B\,\Big\{\hat{I}_L \sum_{m=0}^{\infty} (\tilde{G}_0\Sigma_Q)^{2m}\,\tilde{G}_0\,\mathcal{L}_T\,\rho^\infty \otimes \rho_B\Big\}} \qquad (5.35)$$

Again (5.31) allows a systematic perturbation theory.

<u>Second order current</u>

$$\boxed{I^{(2)} = \mathrm{Tr}_S\,\mathrm{Tr}_B\,\{\hat{I}_L\,\tilde{G}_0\,\mathcal{L}_T\,\hat{\rho}^\infty \otimes \hat{\rho}_B\}} \qquad (5.36)$$

<u>4th order contribution to the current</u>

$$\boxed{I^{(4)} = \mathrm{Tr}_S\,\mathrm{Tr}_B\,\{\hat{I}_L\,\tilde{G}_0\,\Sigma_Q\,\tilde{G}_0\,\Sigma_Q\,\tilde{G}_0\,\mathcal{L}_T\,\rho^\infty \otimes \hat{\rho}_B\}} \qquad (5.37)$$

etc.

<u>FAZIT</u>

$\Rightarrow$ According to (5.31) the elements $\rho_{aa'}$ of the stationary RDM as well as the current kernel elements $\tilde{\mathcal{K}}^{+\,ba}_{L\,ba'}$ are needed

5.6.3 Relation between current and density matrix kernels $\tilde{\mathcal{K}}^{+}_{I_L}$, $\tilde{\mathcal{K}}$

From Eqs. (5.25) and (5.30) we find for the two kernels the exact expressions

$$\begin{cases} \tilde{K}(0)\rho^{\infty} = \mathrm{Tr}_B\{\mathcal{L}_T \tilde{G}_Q(0)\mathcal{L}_T\, \rho^{\infty}\otimes\rho_B\} \\ \\ \tilde{K}^{+}_{I_L}(0)\rho^{\infty} = \mathrm{Tr}_B\{\hat{I}_L\, \tilde{G}_Q(0)\mathcal{L}_T\, \rho^{\infty}\otimes\rho_B\} \end{cases}$$

where
$$\begin{cases} \mathcal{L}_T\{\cdot\} = -\frac{i}{\hbar}[\hat{H}_T,\cdot] = \sum_{\alpha=L,R} -\frac{i}{\hbar}[\hat{H}_{T\alpha},\cdot] \\ \hat{I}_L = +\frac{ie}{\hbar}[\hat{H}_{TL},\hat{N}_L] \end{cases}$$

Thus both $\mathcal{L}_T$ and $\hat{I}_L$ involve the tunneling Hamiltonian.

Further, for noninteracting leads and tunneling Hamiltonians of the generic form

$$\hat{H}_{T\alpha} = \sum_{\vec{k}\sigma i}\left(t_{\alpha\vec{k}\sigma i}\, c^{\dagger}_{\alpha\vec{k}\sigma}\, d_{i\sigma} + t^{*}_{\alpha\vec{k}\sigma i}\, d^{\dagger}_{i\sigma}\, c_{\alpha\vec{k}\sigma}\right)$$

$$\Rightarrow \boxed{\hat{H}_{T\alpha} \equiv \hat{h}^{out}_{T\alpha} + \hat{h}^{in}_{T\alpha} = \sum_{p=in,out}\hat{h}^{p}_{T\alpha}}\,,\quad \left(\hat{h}^{in}_{T\alpha}\right)^{*} = \hat{h}^{out}_{T\alpha}$$

we have seen that (cf. $\hat{h}^{out}_{TL} = \hat{L}$, $\hat{h}^{in}_{TL} = \hat{L}^{+}$ in (4.116)

$$\boxed{\hat{I}_L = -\frac{ie}{\hbar}\left(\hat{h}^{out}_{TL} - \hat{h}^{in}_{TL}\right) = -\frac{ie}{\hbar}\sum_{p=in,out}(-p)\,\hat{h}^{p}_{TL}}$$

in = +
out = −

To account for the differences between the actions of the Liouvillian superoperator $\mathcal{L}_T$ and an operator like $\hat{I}_L$ we introduce the notation

$$\mathcal{L}_T \hat{X} = -\frac{i}{\hbar}[\hat{H}_T, \hat{X}] = -\frac{i}{\hbar}(\hat{H}_T\hat{X} - \hat{X}\hat{H}_T)$$

Thus we define

$$\mathcal{L}_T \hat{X} := \hat{H}_T^+ X - \hat{H}_T^- X = \sum_\nu \nu \hat{H}_T^\nu \hat{X} \qquad (5,38)$$

That it is, in general

$$\begin{cases} \hat{A}^+ \hat{X} \equiv \hat{A}\hat{X} \\ \hat{A}^- \hat{X} \equiv \hat{X}\hat{A} \end{cases} \qquad (5.39)$$

Hence

$$\boxed{\mathcal{L}_T \hat{X} = \sum_{\alpha=L,R} \sum_{p=in,out} -\frac{i}{\hbar}[\hat{h}^p_{T\alpha}, \hat{X}] = -\frac{i}{\hbar}\sum_{\alpha,p,\nu} \nu \hat{h}^{p\nu}_{T\alpha}\hat{X}} \qquad (5.40)$$

and

$$\boxed{\hat{I}_L \hat{X} = \hat{I}_L^+ \hat{X} = \frac{ie}{\hbar}\sum_p (-p)\,\hat{h}^{p+}_{TL}\hat{X}} \qquad (5.41)$$

here is the meaning of "+" in the current kernel $\tilde{\mathcal{K}}_L^+$

2> We need the building blocks $Tr_B\{\hat{h}^{p\nu}_{T\alpha}\hat{X}\}$!!!

with $\hat{X} = \tilde{G}_Q(0)\mathcal{L}_T\hat{\rho}^\infty \otimes \hat{\rho}_B$

We shall use the Dyson eq. for $\tilde{G}_Q(0)$ to get a diagrammatic expansion of such building blocks.

To proceed use also the additional properties

$$X^{\nu} Y^{\nu} = \nu (XY)^{\nu} \quad (a) \qquad \text{and} \qquad X^{\nu} Y^{\nu'} = -\nu\nu' Y^{\nu'} X^{\nu} \quad (b)$$

which are useful when working with objects like $\hat{h}^{\,in/out}_{T\alpha}$

which is composed of $c^{p} d^{\bar{p}}$ operators.

Explicitly,

$$\hat{h}^{in}_{T\alpha} = \hat{h}^{+}_{T\alpha} = \sum_{\vec{k}\sigma i} t^{*}_{\alpha\vec{k}\sigma i} d^{+}_{i\sigma} c_{\alpha\vec{k}\sigma} \equiv \sum_{\vec{k}\sigma} D^{+}_{\alpha\vec{k}\sigma} C^{-}_{\alpha\vec{k}\sigma} = -\sum_{\vec{k}\sigma} C^{-}_{\alpha\vec{k}\sigma} D^{+}_{\alpha\vec{k}\sigma}$$

$$D^{+}_{\alpha\vec{k}\sigma} = \sum_{i} t^{*}_{\alpha\vec{k}\sigma i} d^{+}_{i\sigma} = \left(D^{-}_{\alpha\vec{k}\sigma}\right)^{*}$$

$$\hat{h}^{out}_{T\alpha} = \hat{h}^{-}_{T\alpha} = \sum_{\vec{k}\sigma i} t_{\alpha\vec{k}\sigma i} c^{+}_{\alpha\vec{k}\sigma} d_{i\sigma} \equiv \sum_{\vec{k}\sigma} C^{+}_{\alpha\vec{k}\sigma} D^{-}_{\alpha\vec{k}\sigma}$$

Thus

$$\boxed{\hat{h}^{p}_{T\alpha} = -\sum_{\vec{k}\sigma} p\, C^{\bar{p}}_{\alpha\vec{k}\sigma} D^{p}_{\alpha\vec{k}\sigma}} \quad (5.42)$$

and

property (a)

$$\boxed{\hat{h}^{p\nu}_{T\alpha} = -\sum_{\vec{k}\sigma} (-p)\nu\, C^{\bar{p}\nu}_{\alpha\vec{k}\sigma} D^{p\nu}_{\alpha\vec{k}\sigma}} \quad (5.43)$$

from (5.34)

$$\Rightarrow \boxed{d_T \hat{X} = -\frac{i}{\hbar} \sum_{\nu\alpha p} \sum_{\vec{k}\sigma} p\, C^{p\nu}_{\alpha\vec{k}\sigma} D^{\bar{p}\nu}_{\alpha\vec{k}\sigma} \hat{X}} \quad (5.44)$$

Similarly,

$$\boxed{\hat{I}_L \hat{X}} = -\frac{ie}{\hbar} \sum_p (-p)\, \hat{h}^{p+}_{TL} \hat{X} \underset{(5.43)}{=} \boxed{-\frac{ie}{\hbar} \sum_p \sum_{\vec{k}\sigma} C^{p+}_{L\vec{k}\sigma} D^{\bar{p}+}_{L\vec{k}\sigma} \hat{X}}$$

(5.45)

↳ Comparing (5.38) and (5.39) we see that in the expression for $\hat{I}_L \hat{X}$

i) $\nu = +$

ii) $\alpha = L$

iii) outgoing $\bar{p} = -$ and ingoing $\bar{p} = -$ processes carry the same overall sign