Open Quantum Systems: Linblad Master Equation and Vectorisation

Linblad Master Equation

- Markovian – the environment has no memory, so the system evo. is not dependent on history, but current state alone.

- Recall that the total system's Hilbert space is $\mathcal{H}_{sys} \otimes \mathcal{H}_{env}$, and for Linblad, we want to trace out the env. from the sys total, such that:

$$\rho_{sys} = Tr_{env}(\rho_{total})$$

- In this way, Linblad eqn governs the reduced dynamics of ρ_{sys}.

Fock-Liouville Hilbert Space: Liouville Operator

- Recall: $\rho^\dagger = \rho$
  $\langle\psi|\rho|\psi\rangle \geq 0$ for all $|\psi\rangle$ positive semi-definiteness
  $Tr(\rho) = 1$.

- Using these properties, linear combinations of ρ_i are proven to be valid density matrices.

- This allows us to define a linear (Hilbert) space of matrices, converting ρs to vectors.

$$\rho \rightarrow |\rho\rangle\rangle$$

- This space is the Fock-Liouville Space (FLS), where the scalar prod. of matrices is defined as:

$$\langle\langle\phi|\rho\rangle\rangle = Tr[\phi^\dagger\rho]$$

- Using the Von Neumann Equation, we can express time evolution in terms of Liouvillian Operator:

$$\frac{d|\rho\rangle\rangle}{dt} = -i[H,\rho] \equiv \mathcal{L}\rho$$

$\begin{pmatrix}\rho_{00} \\ \rho_{01} \\ \vdots\end{pmatrix}$ where e.g. $\mathcal{L} = \begin{bmatrix} 0 & i\Omega & -i\Omega & 0 \\ i\Omega & iE & 0 & -i\Omega \\ -i\Omega & 0 & -iE & i\Omega \\ 0 & -i\Omega & i\Omega & 0 \end{bmatrix}$ → One form of $\hat{\mathcal{L}}$

space

map is a synonym for func, maps input to output space.

CPT Maps

- ~~One way of deriving~~ We want to find the most general Markovian transformation set between density matrices, and what is the corresponding dynamical equation.
- Recall: Q sys evolves either by coherent evo, or measurement collapse.

- Thus, we're looking for a map that transforms ρs to ρs. i.e. $\mathcal{V} : \rho(\mathcal{H}) \longrightarrow \rho(\mathcal{H})$.

- The map must fulfill: Trace preservation $Tr[\mathcal{V}A] = Tr[A]$
  Completely +ve.

- Hence, we're looking for Completely Positive Trace-preserving Maps.

- There are two main properties of CPT maps:

$\boxed{1.}$ map is positive if $\forall A \in \underbrace{B(\mathcal{H})}_{\text{set of bounded lin. operators}}$ s.t. $A \geqslant 0 \rightarrow \mathcal{V}A \geqslant 0$.

for all operators A in

$\forall A \in$ For all operators in $B(\mathcal{H})$
$B(\mathcal{H})$ (the set of bounded linear operators on a Hilbert space $\mathcal{H}$)
s.t. such that
$A \geqslant 0$ A is positive semi-definite,
$\mathcal{V}A \geqslant 0$ the map $\mathcal{V}$ takes A and returns $\mathcal{V}A$ which is also positive semi-definite.

more rigorous

⇒ i.e. map is positive if positive op ⟶ positive op.

$\boxed{2.}$ A map is completely positive if $\forall A \in \mathbb{N}$, $\mathcal{V} \otimes \mathbb{1}_n$ is positive.

$\forall A \in \mathbb{N}$ For all operators in natural number set (i.e for all nat nos.)
$\mathcal{V} \otimes \mathbb{1}_n$ The map acts only on the system and not on env.

⇒ i.e. A map is CP if it stays +ve even when the sys is entangled with smth else.

e.g. matrix transpose is not a CP map.

positive refers to eigenvals. being -ve.

- Imposing these two conditions, we can derive a master equation as a generator of a CPT Markovian map.

<u>Linblad Derivation from Open Quantum Theory</u>

- The most common derivation is based on OQT, such that the Linblad is an effective EoM.

- We start by noting $\mathcal{H}_T = \mathcal{H} \otimes \mathcal{H}_E$, and that the evolution of the total system is given by VN Equation:

$$\dot{\rho}_T(t) = -i\,[H_T, \rho_T(t)]$$

- Since we're interested in the system without env, <u>we trace out</u>* ~~total~~ env, $\rho(t) = Tr_E(\rho_T)$.

- We further <u>separate</u> the total Hamiltonian into system and environment parts:

measure of sys-env int. strength

$$H_T = \underbrace{H_S \otimes \mathbb{1}_E}_{\text{affects only system}} + \underbrace{\mathbb{1}_S \otimes H_E}_{\text{affects only env.}} + \alpha \underbrace{H_I}_{\text{interaction part}}$$

- We can <u>decompose</u> H_I: $\quad H_I = \sum_i S_i \otimes E_i \quad$ where $S_i \in B(\mathcal{H})$, $E_i \in B(\mathcal{H}_E)$ (1)

- We now <u>switch</u> into the interaction picture, where ρs evolve w/ time, i.e. H_I while operators evolve with sys and env H:

$$\hat{O}(t) = e^{i(H+H_E)t}\, O\, e^{-i(H+H_E)t}$$

and
$$\dot{\rho}_T(t) = -i\alpha\,[\hat{H}_I(t), \rho_T(t)] \tag{2}$$

- <u>Integrate</u> above to get:

$$\rho_T(t) = \rho_T(0) - i\alpha \int_0^t ds\,[\hat{H}_I(s), \hat{\rho}_T(s)] \tag{3}$$

$\boxed{\text{ASSUMPTION 1}}$: Env and sys are uncorrelated at $t=0$. Weak Coupling Regime.
$$\rho_T(0) = \rho(0) \otimes \rho_E(0)$$

* Underlined double means key step in derivation

- Since the integration is currently non-Markovian (integration between 0 and t), we can avoid this history dependence by <u>subbing</u> (3) → (2):

$$\frac{d\tilde{\rho}(t)}{dt} = -i\alpha\,[H_I(t), \rho_T(0)] - \alpha^2 \int_0^t ds\,[H_I(t)[H_I(s), \rho_T(s)]] \quad (4)$$

- We <u>apply substitution a second time</u> to get an $\mathcal{O}(\alpha^3)$ term:

$$\frac{d\hat{\rho}(t)}{dt} = \text{''} - \alpha^2 \text{''} \int_0^t ds\,[\hat{H}_I(t), [H_I(s), \rho_T(t)]] + \mathcal{O}(\alpha^3) \quad (5)$$

$\mathcal{O}(\alpha^3) \to 0$

ASSUMPTION 2: α, interaction strength sys-env, is small

- Thus, ignore $\mathcal{O}(\alpha^3)$.

- Since we want EoM for ρ, <u>trace out</u> environment:

$$\frac{d\rho(t)}{dt} = Tr_E\left[\frac{d\rho_T(t)}{dt}\right] = -i\alpha\,Tr_E\,[H_I(t), \rho_T(0)] - \alpha^2\int_0^t ds\,Tr_E\,[H_I(t),[H_I(s), \rho_T(t)]] \quad (6)$$

- We still haven't got an effectively closed t-evo for $\rho(t)$ since we have $\rho_T(t)$ dependence. We <u>use</u> assumption 1 again and apply assumption 3:

ASSUMPTION 3: Initial state of env. is thermal, can be described by $\rho_E(0)$ of a particular form.

- Now, we can calc. 1st element rhs of (6) using (1):

$$Tr_E\,[H_I(t), \rho_T(0)] = \sum_i \Big(S_i(t)\rho(0)\,Tr_E\,[E_i(t)\,\rho_E(0)] - \rho(0)S_i(t)\,Tr_E\,[\rho_E(0)E_i(t)]\Big) \quad (7)$$

ASSUMPTION 4: $\langle E_i\rangle = Tr\,[E_i\rho_E(0)] = 0$ for all i.

- Not a strong assumption. If H doesn't fulfill A4 then <u>rewrite</u>:

$$H_T = \Big(H + \alpha\sum_i\langle E_i\rangle S_i\Big) + H_E + \alpha\sum S_i \otimes (E_i - \langle E_i\rangle) \quad (8)$$

· From (8), we see that it is still equal to original H_T, as $\langle E_i \rangle S_i$'s cancel. System dynamics don't change, so assume $\langle E_i \rangle = 0$.

· Using cyclic property of Trace, (8) = 0, so (6) is:

$$\dot{\rho}(t) = -\alpha \int_0^t ds \, Tr_E \left([H_I(t), [H_I(s), \rho_T(t)]] \right) \quad (9)$$

ASSUMPTION 5: Correlation time scales and env. relaxation t-scales are much less than system time-scale. Env. is thermal, always decoupled from state:

$$\rho_T(t) = \rho(t) \otimes \rho_E(0)$$

⇒ The correlation timescale refers to the amount of time sys and env are entangled. Since weak coupling regime (α small), only sometimes entangled during evolution ($\tau_{corr}, \tau_{rel} \ll \tau_{sys}$).

· Under assumption 5 A5, $\rho_T(t) \to \rho(t) \otimes \rho_E(0)$. Still non markovian, however. To circumvent, realize kernel in integration decays fast and we can extend lim → ∞. Change variables $s \to t - s$:

Redfield Equation
$$\dot{\rho}(t) = -\alpha^2 \int_0^\infty ds \, Tr_E \left([H_I(t), [H_I(s-t), \rho(t) \otimes \rho_E(0)]] \right) \quad (10)$$

· This however doesn't fulfill complete positivity! We need to apply RWA:

ASSUMPTION 6: Rotating Wave Approximation using spectrum of the superoperator:

$$\mathcal{H} A \equiv [H, A]$$

· Eigenvec of superop. forms complete basis of $\mathcal{B}(\mathcal{H})$, so:

$$S_i = \sum_\omega S_i(\omega), \text{ where } [H, S_i(\omega)] = -\omega S_i(\omega) \text{ and } [H, S_i^\dagger(\omega)] = \omega S_i^\dagger(\omega) \quad (11)$$

· To apply, we want to <u>change back to Schrö picture</u>, done by $\hat{S}_k = e^{iHt} S_k e^{-iHt}$, for H_I:

$$\Rightarrow \quad H_I(t) = \sum_{k,\omega} e^{-i\omega t} S_k(\omega) \otimes E_k(t) = \sum_{k,\omega} e^{i\omega t} S_k^\dagger(\omega) \otimes E_k^\dagger(t).$$

⇒ Combine with (10) by first <u>expanding commutators</u>
⇒ Use $S_k(\omega)$ for $H_I(t-s)$, $S_k^\dagger(\omega')$ for $H_I(t)$, trace permutation and $[H_E, \rho_E^{(0)}] = 0$.

$$\dot{\rho}(t) = \sum_{\substack{\omega,\omega' \\ k,l}} \Big(e^{i(\omega'-\omega)t} \Gamma_{kl}(\omega) \left[S_l(\omega)\hat{\rho}(t), S_k^\dagger(\omega') \right] + e^{i(\omega-\omega')t} \Gamma_{lk}^*(\omega') \left[S_l(\omega), \hat{\rho}(t) S_k^\dagger(\omega') \right] \Big) \quad (12)$$

where $\underbrace{\Gamma_{kl}(\omega)}_{\text{contains environment effect}} = \int_0^\infty ds\, e^{i\omega s} \mathrm{Tr}_E \left(E_k^\dagger(t) E_I(t-s) \rho_E(0) \right)$

⇒ <u>Apply A6.</u>, $|\omega - \omega'| \gg \alpha^2$, so don't contribute, but only $\omega = \omega'$ contribute, to get simpler $\dot{\rho}(t)$.

⇒ Divide dynamics to Hamiltonian and non-Hamiltonian by splitting $\Gamma_{kl}(\omega)$ into Hermitian, non-Hermitian using:

$$\Gamma_{kl}(\omega) = \frac{1}{2}\gamma_{kl}(\omega) + i\pi_{kl} \quad (13)$$

where $\pi_{kl}(\omega) \equiv -\frac{i}{2}\left(\Gamma_{kl}(\omega) - \Gamma_{kl}^*(\omega) \right)$,

$$\gamma_{kl}(\omega) \equiv \Gamma_{kl}(\omega) + \Gamma_{kl}^*(\omega) = \int_{-\infty}^{\infty} ds\, e^{i\omega s} \mathrm{Tr} \left(E_k^\dagger(s) E_l \hat{\rho}_E(0) \right)$$

⇒ Using these definitions, transform back to SE pic.

$$\dot{\rho}(t) = -i\left[H + H_{LS}, \rho(t) \right] + \sum_{\omega,k,l} \gamma_{kl}(\omega) \times \left(S_l(\omega)\rho(t) S_k^\dagger(\omega) - \frac{1}{2}\left\{ S_k^\dagger S_l(\omega), \rho(t) \right\} \right) \quad (14)$$

· In (14), Ham. dynamics influenced by $\underbrace{H_{LS} = \sum_{\omega,k,l} \pi_{kl}(\omega) S_k^\dagger(\omega) S_l(\omega)}_{\text{Lamb-Shift Hamiltonian}}$

- Lamb-Shift H_{LS} renormalises energy levels. $\dot{\rho}(t)$ is now Markovian, but not in Linblad form.

- We can prove matrix formed by $\gamma_{kl}(\omega)$ is positive, so can be diagonalised, and we can find a unitary operator $O\gamma_{kl}(\omega)O^{+} = \mathrm{diag}\{d_1(\omega), \ldots\}$.

- Finally, we reach the general Linblad master equation:

$$\dot{\rho}(t) = -i\left[H + H_{LS}, \rho(t)\right] + \sum_{i,\omega}\left(L_i(\omega)\rho(t)L_i^{+}(\omega) - \frac{1}{2}\left\{L_i^{+}L_i(\omega), \rho(t)\right\}\right)$$
$$\equiv \mathcal{L}\rho(t).$$

- Assuming only 1 ω (simplification), we get:

$$\boxed{\dot{\rho}(t) = -i\left[H + H_{LS}, \rho(t)\right] + \sum_i\left(L_i\rho(t)L_i^{+} - \frac{1}{2}\left\{L_i^{+}L_i, \rho(t)\right\}\right) \equiv \mathcal{L}\rho(t)}$$

L_i are jump operators, governing the dissipative processes such as decay.

<u>Summary of Derivation</u>

1. VN Eqn: $\dot{\rho}_T(t) = -i\left[H_T, \rho_T(t)\right] \equiv \mathcal{L}\rho(t)$

2. Trace out environment definition is $\rho(t) = Tr_E(\rho_T(t))$

3. Separate H_T into H_{sys}, H_{env}, H_I.

4. Decompose H_I

5. Swith $\dot{\rho}_T(t)$ into interaction picture and integrate for $\rho_T(t)$.

6. Sub $\rho_T(t) \to \dot{\rho}_T(t)$ twice and ignore $\mathcal{O}(\alpha^3)$ terms by applying A2

7. Trace out ρ_{Env} from $\dot{\rho}_T(t)$

8. Use A1, A3, calc. 1st element of step 7 rhs

9. Use A4 to simplify $\dot{\rho}(t) = Tr_E\left(\frac{d\rho_T(t)}{dt}\right)$

10. Use A5 to say $\rho_T(t) \rightarrow \rho(t) \otimes \rho_E(0)$.

11. Realise integration kernel decays fast enough, extend limits of integration to infinity, $s \rightarrow t-s$ to get Redfield Equation.

12. We want to apply RWA (A6) for complete positivity, and to do so, change back to Schrödinger picture ~~form~~:

a. $\hat{S}_K = e^{iHt} S_K e^{-iHt}$ for H_I.

b. Expand Redfield eqn in terms of commutators using:

i. $S_K(\omega)$ for $H_I(t-s)$
ii. $S_K^\dagger(\omega')$ for $H_I(t)$
iii. Trace permutativity
iv. $[H_E, \rho_E] = 0$.

c. Apply A6, $|\omega - \omega'| \gg \alpha^2$

d. Divide dynamics into Hamiltonian/non-Hamiltonian by splitting $\Gamma_{KL}(\omega)$ into Hermitian / non-Hermitian

e. Using $\Gamma_{KL}(\omega)$, $\Pi_{KL}(\omega)$, $\gamma_{KL}(\omega)$ to transform back into S picture.

13. Prove $\gamma_{KL}(\omega)$ is positive, and $O\gamma_{KL}(\omega)O^\dagger = \text{diag}\{d_1(\omega), d_2(\omega)\ldots\}$.

14. Assume only one regular frequency to remove ω out of sum.

$$\dot{\rho}(t) = -i[H + H_{LS}, \rho(t)] + \sum_{i,(\omega)} L_i(\omega)\rho(t)L_i^\dagger(\omega) - \frac{1}{2}\{L_i^\dagger L_i(\omega), \rho(t)\}$$

$$\equiv \mathcal{L}\rho(t) \quad //.$$

Properties of Linblad Equation

Property 1: Under Linblad dynamics, if L_i are Hermitian,

$$P = \frac{d}{dt}\left(\mathrm{Tr}(\rho^2)\right) \leq 0.$$

Property 2: Linblad master eqn invariant under unitary transforms of L_i :

unitary matrix.

$$\sqrt{\Gamma_i}\, L_i \rightarrow \sqrt{\Gamma_i'}\, L_i' = \sum_j v_{ij} \sqrt{\Gamma_j}\, L_j$$

Vectorisation

- Using the idea that matrices form themselves a vector space, we may define a Hilbert space of matrices which convert density matrices to vectors.
- This space is the Fock-Liouville Space (FLS).

$$|i\rangle\langle j| \longrightarrow |j\rangle \otimes |i\rangle \quad \text{Vectorisation}$$

- So then : $\quad \rho = \sum_{ij} \rho_{i,j} |i\rangle\langle j|$

$$\mathrm{vec}(\rho) = \sum_{i,j} \rho_{ij} \, |j\rangle \otimes |i\rangle$$

$$\mathrm{vec}\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix}$$

$$\rho \rightarrow |\rho\rangle\rangle$$

- This essentially maps/flattens an operator, i.e. reduces rank by 1.
- Before looking at what it does to super-operators, let's look at 2 key properties of vectorisation.

$\boxed{\text{Property 1:}}$ Inner product to define the vector space.

$$\langle\langle \sigma | \rho \rangle\rangle = Tr(\sigma^\dagger \rho) = vec(\sigma)^\dagger vec(\rho)$$

⇒ identity operator is interesting :

$$vec(I) = \sum_i |i\rangle \otimes |i\rangle = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}_{etc}$$ so it is maximally entangled Bell state that is unnormalised

⇒ But, $Tr(\rho) = vec(I)^\dagger vec(\rho) = 1$.

$\boxed{\text{Property 2:}}$ $vec(ABC) = (C^T \otimes A)vec(B)$

Let's use P2 to look at superoperator products:

⇒ a superoperator product looks like ~~this~~:

$$S[\rho] = \sum_k K_k \rho K_k^\dagger$$ → kraus decomp.

⇒ So : $$vec(S[\rho]) = \sum_k (K_k^* \otimes K_k) vec(\rho)$$
$$= \sum_k (K_k^* \otimes K_k) |\rho\rangle\rangle$$

⇒ I.e. the superoperator becomes a matrix in FLS !

Applying this to our Linblad Master Equation (Markovian) :

$$\boxed{\frac{d}{dt}|\rho\rangle\rangle = \hat{\mathcal{L}}|\rho\rangle\rangle}$$ Vectorisation form of Linblad Master Equation.

$$\frac{d}{dt}\begin{bmatrix} \dot{a} \\ \dot{b} \\ \dot{c} \\ \dot{d} \end{bmatrix} = \begin{bmatrix} & \mathcal{L} & \end{bmatrix}\begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix}$$

where $$\boxed{\hat{\mathcal{L}} = -i(I \otimes H - H^T \otimes I) + \sum_k \gamma_k \left(L_k^* \otimes L_k - \frac{1}{2} I \otimes L_k^\dagger L_k - \frac{1}{2}(L_k^\dagger L_k)^T \otimes I\right)}$$

Special Properties of $\hat{\mathcal{L}}$

- Recall, for vectorised Linblad master equation, solutions take the form of ordinary differential equations' solutions.

$$|\rho(t)\rangle\rangle = e^{\hat{\mathcal{L}}t}|\rho(0)\rangle\rangle$$

- ~~Generally~~ $\hat{\mathcal{L}}$ may <u>not</u> be diagonalisable, but assume it <u>is</u>. Since it's not Hermitian, different lhs, rhs eigenvectors:

$$\hat{\mathcal{L}}x_\alpha = \lambda_\alpha x_\alpha$$
$$y_\alpha^\dagger \hat{\mathcal{L}} = \lambda_\alpha y_\alpha^\dagger$$
$$\hat{\mathcal{L}} = S\overbrace{\Lambda}^{\text{diagonal matrix}}\underbrace{S^{-1}}_{\text{rows are } y_\alpha^\dagger} = \sum_\alpha \lambda_\alpha x_\alpha y_\alpha^\dagger$$

$\underbrace{S}_{\text{rows are } x_\alpha}$

- This is useful when we want to write the matrix exp, as:

$$e^{\hat{\mathcal{L}}t} = Se^{\Lambda t}S^{-1} = \sum_\alpha e^{\lambda_\alpha t}x_\alpha y_\alpha^\dagger$$

- Let's look at trace preservation of vectorisation.

$$0 = \frac{d}{dt}\left(\mathrm{vec}(I)^\dagger \mathrm{vec}(\rho)\right) = \mathrm{vec}(I)^\dagger \hat{\mathcal{L}}\,\mathrm{vec}(\rho)$$

- Must be true for all density matrices so $\mathrm{vec}(I)^\dagger \mathcal{L} = 0$.

- This eventually leads to the result:

"Any trace-preserving Liouvillian <u>must</u> have a zero eigenvalue. rhs eigenvector is the steady-state, lhs eigenvector is the identity."