Freudenstadt Lectures on open quantum systems.

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$\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_E \equiv \mathcal{H}_{SE}$ $\mathcal{U}$: unitary on $\mathcal{H}$

Initial state: $\rho \otimes \rho_E$

WaLoG: $\rho_E = |\Omega\rangle\langle\Omega|$ upon possibly changing $\mathcal{H}_E$

(purification; GNS rep.)

$$\Phi(\rho) = \mathrm{Tr}_E\left(\mathcal{U}(\rho \otimes |\Omega\rangle\langle\Omega|)\mathcal{U}^*\right) \quad \text{partial trace.}$$

Let $\{e_j\}$ & $\{f_j\}$ be bases of $\mathcal{H}_S, \mathcal{H}_R$

(both finite-dim.)

For $X \in \mathcal{B}(\mathcal{H}_{SE})$, $\mathrm{Tr}_E X = \sum_j \langle f_j, X f_j \rangle$

where $\langle f_j, X f_j\rangle \in \mathcal{B}(\mathcal{H}_S)$

$$\Rightarrow \quad \Phi(\rho) = \sum_j \langle f_j, \mathcal{U}(\rho \otimes \underbrace{P_\Omega}_{|\Omega\rangle\langle\Omega|})\mathcal{U}^* f_j\rangle$$

$$= \sum_j \langle f_j, \mathcal{U}\Omega\rangle \rho \langle \Omega, \mathcal{U}^* f_j\rangle$$

$$= \sum_j K_j \rho K_j^*$$

where $K_j = \langle f_j, \mathcal{U}\Omega\rangle \in \mathcal{B}(\mathcal{H}_S)$.

$\forall \rho \in \mathcal{B}(\mathcal{H}_S)$,

$$\mathrm{Tr}\, \Phi(\rho) = \mathrm{Tr}_{SE}\, \mathcal{U}(\rho \otimes |\Omega\rangle\langle\Omega|)\mathcal{U}^* = \mathrm{Tr}_S\, \rho$$

so $\mathrm{Tr}\, \Phi(\rho) = \mathrm{Tr} \left(\sum_j K_j^* K_j\right) \rho = \mathrm{Tr}\, \rho$

hence $\mathrm{Tr} \left(\sum_j K_j^* K_j - \mathbb{1}\right) \rho = 0 \quad \forall \rho \in \mathcal{B}(\mathcal{H}_s)$

$$\Rightarrow \quad \sum_j K_j^* K_j = \mathbb{1}.$$

$\Phi(\rho)$ has the following properties:

1. $\mathrm{Tr}\, \Phi(\rho) = 1$ for all density matrices ρ
   [Φ is trace-preserving]

2. $\forall \{p_i\}$, $p_i \geq 0$, $\sum_i p_i = 1$, dmats ρ_i
   $\Phi\left(\sum_i p_i \rho_i\right) = \sum_i p_i\, \Phi(\rho_i)$
   [Φ is convex-linear]

3. Φ is completely positive, meaning that $\forall$ positive operator $A \in \mathcal{B}(\mathcal{H}_s \otimes \mathbb{C}^n)$, $n \geq 0$, $(\Phi \otimes \mathbb{1}_{\mathbb{C}^n})(A)$ is a positive operator on $\mathcal{H}_s \otimes \mathbb{C}^n$.

To see CP: Let $\psi \in \mathcal{H}_s \otimes \mathbb{C}^n$, $A \geq 0$ on $\mathcal{H}_s \otimes \mathbb{C}^n$. Then

$$\langle \psi, (\Phi \otimes \mathbb{1}_{\mathbb{C}^n})(A) \psi \rangle = \sum_j \underbrace{\langle \psi, (K_j \otimes \mathbb{1}_{\mathbb{C}^n}) A (K_j \otimes \mathbb{1}_{\mathbb{C}^n})^* \psi \rangle}_{\geq 0}$$

<u>Theorem</u>. (Kraus representation)

Suppose acts on $\mathcal{H}$ with $\dim \mathcal{H} = d < \infty$. Then there are operators $K_j \in \mathcal{B}(\mathcal{H})$, $j = 1, \dots, d^2$ s.t.

$$\Phi(\rho) = \sum_j K_j \rho K_j^*$$

and $\sum_j K_j^* K_j = \mathbb{1}$.

<u>Proof</u>. Let $\{e_j\}_{j=1}^d$ be an ONB of $\mathcal{H}$ and set

$$\varphi = \sum_j e_j \otimes e_j \qquad \in \mathcal{H} \otimes \mathcal{H}.$$

Define the operator $\sigma = (\Phi \otimes \mathbb{1})\, |\varphi\rangle\langle\varphi|$ on $\mathcal{H} \otimes \mathcal{H}$.
By the CP property of Φ, $\sigma \geq 0$. Thus σ has the decomposition

$$\sigma = \sum_j |s_j\rangle\langle s_j| \qquad (j = 1, \dots, d^2)$$

where $s_j \in \mathcal{H} \otimes \mathcal{H}$ (not necessarily normalized)
Define the map $\mathcal{C} : \mathcal{H} \to \mathcal{H}$ by

$$\mathcal{C}\Big(\sum_j \alpha_j e_j\Big) = \sum_j \bar{\alpha}_j e_j \qquad \text{(complex conj.)}$$

$\forall \psi \in \mathcal{H}$, we have $\mathcal{C}\psi \in \mathcal{H}$ and $\langle \mathcal{C}\psi, s_j \rangle \in \mathcal{H}$
Here, we understand that $\mathcal{C}\psi$ acts on the <u>second</u> factor of $\mathcal{H} \otimes \mathcal{H}$, i.e., $\langle \mathcal{C}\psi, a \otimes b \rangle \equiv a \langle \mathcal{C}\psi, b \rangle$.

$\psi \mapsto \langle \varphi\psi, s_j \rangle$ is linear and so it defines the operator $K_j \in \mathcal{B}(\mathcal{H})$:

$$K_j \psi := \langle \varphi\psi, s_j \rangle = \sum_k \alpha_k \underbrace{\langle e_k, s_j \rangle}$$

$\langle e_k|$ acts on right factor $\mathcal{H}\otimes\mathcal{H}$

Now, $\sum_j K_j |\psi\rangle\langle\psi| K_j^*$

$$= \sum_j |K_j\psi\rangle\langle K_j\psi|$$

check for $s = x\otimes y$:
$K\psi = x \langle \varphi\psi, y\rangle$
$\langle K\psi| = \langle x| \overline{\langle \varphi\psi, y\rangle}$
$= \langle x| \langle y, \varphi\psi\rangle$
$= \langle \underbrace{x\otimes y}_{s}, \varphi\psi\rangle$

$$= \sum_j \langle \varphi\psi, s_j \rangle \langle s_j, \varphi\psi \rangle$$

$$= \langle \varphi\psi, \sigma\, \varphi\psi \rangle$$

$$= \langle \varphi\psi, (\Phi\otimes 1)(|\psi\rangle\langle\psi|)\, \varphi\psi \rangle$$

on second factor

$$= \sum_{k,l} \langle \varphi\psi, \left(\Phi(|e_k\rangle\langle e_l|)\otimes |e_k\rangle\langle e_l|\right) \varphi\psi \rangle$$

$$= \sum_{k,l} \Phi(|e_k\rangle\langle e_l|) \underbrace{\langle \varphi\psi, e_k \rangle}_{\alpha_k} \underbrace{\langle e_l, \varphi\psi \rangle}_{\bar{\alpha}_l}$$

$$= \Phi(|\psi\rangle\langle\psi|).$$

The representation for density matrices $\rho = \sum_k p_k |\psi_k\rangle\langle\psi_k|$ follows from convex linearity

$$\Phi(\rho) = \sum_k p_k\, \Phi(|\psi_k\rangle\langle\psi_k|) = \sum_k p_k \sum_j K_j |\psi_k\rangle\langle\psi_k| K_j^*$$

$$= \sum_j K_j \rho K_j^*. \qquad \square$$

Equivalent representations.

Suppose $\tilde{K}_j := \sum_k U_{jk} K_k$, where U_{jk} is the (j,k)-matrix element of a unitary U.

Then

$$\tilde{\Phi}(\rho) := \sum_j \tilde{K}_j \rho \tilde{K}_j^*$$

$$= \sum_{j,m,n} U_{jm} K_m \rho \left(U_{jn} K_n\right)^*$$

$$= \sum_{m,n} \underbrace{\left(\sum_j U_{jm} \overbrace{\overline{U_{jn}}}^{(U^*)_{nj}}\right)}_{(U^*U)_{nm} = \delta_{nm}} K_m \rho K_n^*$$

$$= \sum_m K_m \rho K_m^*.$$

Hence the $\{\tilde{K}_j\}$ also represent Φ. One can show the converse too:

Suppose $\sum_j K_j \rho K_j^* = \sum_\ell \tilde{K}_\ell \rho \tilde{K}_\ell^*$, $\forall$ states ρ.

Then enlarge the sum with fewer indices by adding zero operators K or $\tilde{K}$, so that both sums have the same number of terms. Then $\tilde{K}_j = \sum_\ell U_{j\ell} K_\ell$, where $U_{j\ell}$ are the matrix elements of a unitary matrix U.

Corollary. Let $\mathcal{H}$ be a finite-dim Hilbert space, and suppose $\Phi : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ is a function. The following are equivalent:

(1) There is a Hilbert space $\mathcal{H}_E$ $(\dim \mathcal{H}_E \le (\dim \mathcal{H})^2)$, and a unitary $\mathcal{U}$ on $\mathcal{H} \otimes \mathcal{H}_E$, s.t.

$$\Phi(\rho) = \mathrm{Tr}_E\, \mathcal{U}\left(\rho \otimes |\Omega\rangle\langle\Omega|\right)\mathcal{U}^*, \ \forall \rho \in \mathcal{B}(\mathcal{H})$$

(2) Φ is linear, CP and trace-preserving.

Proof. We've already shown (1) $\Rightarrow$ (2). To show that (2) $\Rightarrow$ (1), use the rep. $\Phi(\rho) = \sum_\alpha K_\alpha \rho K_\alpha^*$. Denote the # of α by N $(\le (\dim \mathcal{H})^2)$. Set $\mathcal{H}_E \cong \mathbb{C}^N$ and let $\{e_\alpha\}$ be an ONB of $\mathcal{H}_E$. Fix any normalized state $\Omega \in \mathcal{H}_E$ and define, $\forall \psi \in \mathcal{H}$:

$$\mathcal{U}\, \psi \otimes \Omega = \sum_\alpha K_\alpha \psi \otimes e_\alpha .$$

Then $\mathrm{Tr}_E\, \mathcal{U}\, |\psi\rangle\langle\psi| \otimes |\Omega\rangle\langle\Omega|\, \mathcal{U}^*$

$$= \mathrm{Tr}_E\, \big|\mathcal{U}\, \psi \otimes \Omega\big\rangle\big\langle \mathcal{U}\, \psi \otimes \Omega\big|$$

$$= \mathrm{Tr}_E \sum_{\alpha,\beta} (K_\alpha \otimes \mathbb{1})\, |\psi \otimes e_\alpha\rangle\langle \psi \otimes e_\beta|\, (K_\beta^* \otimes \mathbb{1}_E)$$

$$= \sum_{\alpha,\beta} K_\alpha |\psi\rangle\langle\psi| K_\beta^* \cdot \underbrace{\mathrm{Tr}_E |e_\alpha\rangle\langle e_\beta|}_{\delta_{\alpha\beta}}$$

It follows that $\forall\ \rho = \sum p_j |\psi_j\rangle\langle\psi_j|$:

$$\Phi(\rho) = \mathrm{Tr}_E\ \mathcal{U}\ \rho \otimes |\Omega\rangle\langle\Omega|\ \mathcal{U}^* .$$

Now $\mathcal{U}$ is defined only on the subspace $\mathcal{H} \otimes |\Omega\rangle\langle\Omega|$.

On this space, $\mathcal{U}$ is unitary:

$$\langle \psi\otimes\Omega,\ \mathcal{U}^*\mathcal{U}\ \psi\otimes\Omega\rangle$$

$$= \sum_{\alpha,\beta} \langle K_\alpha \psi \otimes e_\alpha,\ K_\beta \psi \otimes e_\beta\rangle$$

$$= \sum_\alpha \langle K_\alpha^* K_\alpha \psi, \psi\rangle$$

$$= \langle \psi, \psi\rangle .$$

Then we extend $\mathcal{U}$ to all of

$$\mathcal{H} \otimes \mathcal{H}_E = (\mathcal{H} \otimes \Omega) \oplus \left(\mathcal{H} \otimes (\mathrm{Ran}\, |\Omega\rangle\langle\Omega|)^\perp\right)$$

by setting

$$\left(\begin{array}{c|c} \mathcal{U} & 0 \\ \hline 0 & \mathbb{1} \end{array}\right)$$

(unitary on $\mathcal{H}\otimes\mathcal{H}_E$)

$\square$

A 'generalization' of the Kraus rep. th$^{\underline{m}}$ ($\equiv$ operator sum rep.) is

(1955)

<u>Theorem</u> (Stinespring representation theorem)

Let $\mathcal{A}$ be a C^*-algebra with a unit, let $\mathcal{H}$ be a Hilbert space and let $\Phi : \mathcal{A} \to \mathcal{B}(\mathcal{H})$ be a linear map.
(bdd ops. on $\mathcal{H}$)

Then Φ is completely positive if and only if there is a Hilbert space $\mathcal{K}$, a $*$-representation $\Pi : \mathcal{A} \to \mathcal{B}(\mathcal{K})$ and a bounded linear transformation $V : \mathcal{K} \to \mathcal{H}$ s.t.

$$\Phi(A) = V \, \Pi(A) \, V^* \quad , \quad \forall A \in \mathcal{A}$$

Markovian master equations

Reduced dynamics:

$$\Phi_t(\rho) = \operatorname{Tr}_E\left(e^{-itH}\,\rho\otimes\rho_E\,e^{itH}\right)$$

$\forall t$ fixed, Φ_t is a linear, CP and trace-preserving map on $\mathcal{B}(\mathbb{C}^n) = M_n$ (n×n complex matrices)

Moreover, $\Phi_t\big|_{t=0} = id$.

Any map satisfying these conditions is called a CP dynamical map.

It is not true (generically) that

$$\Phi_{s+t} = \Phi_s \circ \Phi_t$$

because the state at time t, $\Phi_t(\rho)$ depends on the entire history $\{\Phi_r(\rho) : 0 \le r \le t\}$, due to the interaction (and backreaction) with the environment. If the environment correlations decay very fast relative to the change of the system, then one expects that the Markovian property

$\Phi_{s+t} = \Phi_t \circ \Phi_s$ would hold in an approximate sense.

Def. A dynamical map $\{\Phi_t\}_{t\geq 0}$ satisfying the semigroup property $\Phi_{s+t} = \Phi_t \circ \Phi_s$, $s,t \geq 0$, $\Phi_0 = id$, and which is continuous in t, is called a <u>quantum dynamical semigroup</u> (or a <u>markovian semigroup</u>)

The continuity $t \mapsto \Phi_t$ & the fact that $\Phi_0 = id$ implies the existence of a generator L,

$$\Phi_t = e^{tL}, \quad L = \frac{d}{dt}\Big|_0 \Phi_t .$$

Theorem (Gorini-Kossakowski-Sudarshan, 1976)
A linear operator $L: M_N \to M_N$ is the generator of a CP dynamical semigroup of M_N if and only if

$$L\rho = -i[H,\rho] + \sum_{i,j=1}^{N^2-1} c_{ij} \left\{ F_i \rho F_j^* - \frac{1}{2}\left(F_j^* F_i \rho + \rho F_j^* F_i\right)\right\}$$

where (c_{ij}) is a self-adjoint, non-negative matrix.
The H & F_i are arbitrary operators.

One can always choose $H = H^*$, $\operatorname{tr} H = 0$, $\operatorname{tr} F_i = 0$, $\operatorname{Tr}(F_i^* F_j) = \delta_{ij}$.

Derivation of the general form of L

Some linear algebra first.

Let $\{F_\alpha\}_{\alpha=1}^{N^2}$ be an orthonormal basis (ONB) of M_N, i.e., $(F_\alpha, F_\beta) := \operatorname{Tr} F_\alpha^* F_\beta = \delta_{\alpha\beta}$.

Consider the maps

$$\Gamma_{\alpha\beta} : M_N \to M_N, \quad \Gamma_{\alpha\beta} A = F_\alpha A F_\beta^*, \quad \alpha, \beta = 1, \dots, N^2$$

Those are $N^2 \times N^2$ linear maps on the space M_N. We claim that $\{\Gamma_{\alpha\beta}\}_{\alpha,\beta=1}^{N^2}$ is a basis of $\mathcal{B}(M_N)$. To show this, it suffices to prove that the $\Gamma_{\alpha\beta}$ are linearly independent. Let U be the unitary that changes the ONB $\{F_\alpha\}_{\alpha=1}^{N^2}$ of M_N to the ONB $\{E_{ij}\}_{i,j=1}^{N}$ (where E_{ij} is matrix with entry 1 at spot i,j)

Then

$$\sum_{\alpha\beta} c_{\alpha\beta} F_\alpha A F_\beta^* = 0 \iff \sum_{\alpha\beta} c_{\alpha\beta} (UF_\alpha) A (UF_\beta)^* = 0$$

$$\mathcal{U}F_\alpha = \sum_{ij} u_{(ij),\alpha} \; E_{ij} \quad ; \quad \overline{u_{(ij),\alpha}} = (\mathcal{U}^*)_{\alpha,(ij)}$$

And so we want to see that $c_{\alpha\beta} = 0$ whenever, $\forall A$,

$$\sum_{\alpha\beta} \sum_{ij} \sum_{k\ell} c_{\alpha\beta} \; u_{(ij),\alpha} \; E_{ij} A E^*_{k\ell} \; \overline{u_{(k\ell),\beta}}$$

$$\equiv \sum_{ij} \sum_{k\ell} d_{(ij)(k\ell)} \; E_{ij} A \underbrace{E^*_{k\ell}}_{E_{\ell k}} = 0 \qquad (*)$$

here,

$$d_{(ij)(k\ell)} = \sum_{\alpha\beta} (\mathcal{U})_{(ij),\alpha} \; c_{\alpha\beta} \; (\mathcal{U}^*)_{\beta,(k\ell)} = (\mathcal{U}C\mathcal{U}^*)_{(ij),(k\ell)}$$

Clearly $E_{ij} A E_{k\ell} = |e_i\rangle A_{jk} \langle e_\ell|$ and so by choosing suitable $A \in M_N$, we see from $(*)$ that $d_{(ij),(k\ell)} = 0 \;\; \forall (ij), (k,\ell)$. Hence $\mathcal{U}C\mathcal{U}^* = 0$ and so $C = 0$. This shows that $\{\Gamma_{\alpha\beta}\}_{\alpha,\beta=1}^{N^2}$ is a basis of $\mathcal{B}(M_N)$.

Thus, every $\Gamma : M_N \to M_N$ has a unique decomposition

$$\Gamma A = \sum_{\alpha,\beta=1}^{N^2} c_{\alpha\beta} \; F_\alpha A F_\beta^* .$$

If $(\Gamma A)^* = \Gamma A^*$, then C is a self-adjoint matrix.

Let L be the generator of the CP dynamical semigroup Φ_t. Note that then

(1) $\mathrm{Tr}(LA) = 0 \quad \forall A \in M_N$ (Φ_t trace preserving)

(2) $(LA)^* = LA^*$

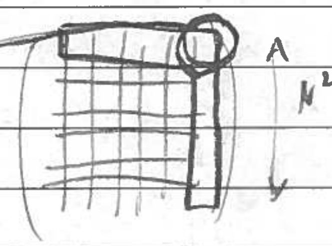
($A = P_1 - P_2 + i(P_3 - P_4)$, $P_j \geq 0$

$\Rightarrow \Phi_t(A) = \Phi_t(P_1) - \Phi_t(P_2) + i\left(\Phi_t(P_3) - \Phi_t(P_4)\right)$

and all $\Phi_t(P_j) \geq 0$. This gives $\Phi_t(A)^* = \Phi_t(A^*)$

and (2) follows by differentiation)

Choose an ONB $\{F_\alpha\}_{\alpha=1}^{N^2}$ of M_N with $F_{N^2} = \frac{1}{\sqrt{N}}$. Then we have



$$LA = \sum_{\alpha,\beta=1}^{N^2} c_{\alpha\beta} F_\alpha A F_\beta^*$$

$$= \frac{1}{N} c_{N^2N^2} A + \frac{1}{\sqrt{N}} \sum_{\alpha=1}^{N^2-1} \left\{ c_{\alpha N^2} F_\alpha A + c_{N^2\alpha} A F_\alpha^* \right\} \tag{5.1}$$

$$+ \sum_{\alpha,\beta=1}^{N^2-1} c_{\alpha\beta} F_\alpha A F_\beta^*.$$

Set
$$F = \frac{1}{\sqrt{N}} \sum_{\alpha=1}^{N^2-1} c_{\alpha N^2} F_\alpha = X + iY, \quad X = X^*, \; Y = Y^*$$

The r.h.s. of (5.1) is

$$\frac{c_{N^2N^2}}{N} A + (X+iY)A + A(X-iY)$$

$$= -i[H, A] + \{G, A\}, \quad \text{where}$$

$$H = -Y = -\mathrm{Im}\, F = \frac{-1}{2i}(F - F^*), \quad G = \frac{1}{2N} c_{N^2N^2} \mathbb{1} + \underbrace{\tfrac{1}{2}(F + F^*)}_{X}$$

Since $\mathrm{Tr}(LA)=0$ we get

$$0 = \mathrm{Tr}\left(2GA + \sum_{\alpha,\beta=1}^{N^2-1} c_{\alpha\beta} F_\beta^* F_\alpha A\right) \quad \forall A \in M_N$$

$$\Rightarrow \quad G = -\frac{1}{2} \sum_{\alpha,\beta=1}^{N^2-1} c_{\alpha\beta} F_\beta^* F_\alpha$$

So finally

$$LA = -i[H,A] + \frac{1}{2} \sum_{\alpha,\beta=1}^{N^2-1} c_{\alpha\beta}\left(-F_\beta^* F_\alpha A - A F_\beta^* F_\alpha + 2F_\alpha A F_\beta^*\right)$$

Note that $\mathrm{Tr}\, H = 0$ since $\mathrm{Tr}\, F_\alpha = 0$, $\alpha = 1, \dots, N^2-1$
(as $F_\alpha \perp F_{N^2} = \frac{1}{\sqrt{N}}$.)

One can also show that $C = (c_{\alpha\beta})$ is a positive definite matrix (all eigenvalues are ≥ 0).

As C is self-adjoint, it can be diagonalized unitarily:

$$C = UDU^*, \quad D = \mathrm{diag}(d_1, \dots, d_{N^2-1})$$

$$c_{\alpha\beta} = (UDU^*)_{\alpha\beta} = \sum_{i=1}^{N^2-1} u_{\alpha i}\, d_i\, (U^*)_{i\beta}$$

$$= \sum_{i=1}^{N^2-1} d_i\, u_{\alpha i}\, \overline{u_{\beta i}}$$

Then

$$\sum_{\alpha,\beta} c_{\alpha\beta} \left\{ F_\alpha \rho F_\beta^* - \frac{1}{2}\left(F_\beta^* F_\alpha \rho + \rho F_\beta^* F_\alpha \right) \right\}$$

$$= \sum_{i=1}^{N^2-1} \left\{ V_i \rho V_i^* - \frac{1}{2}\left(V_i^* V_i \rho + \rho V_i^* V_i \right) \right\}$$

where $V_i = \sqrt{d_i} \sum_\alpha u_{\alpha i} F_\alpha$. Thus we arrive at the "diagonal" form of L:

$$L\rho = -i[H,\rho] + \sum_{i=1}^{N^2-1} V_i \rho V_i^* - \frac{1}{2}\left(V_i^* V_i \rho + \rho V_i^* V_i \right)$$

The <u>adjoint L^*</u> is defined by

$$\mathrm{Tr}\, A^* L B = \mathrm{Tr}\, (L^* A) B \qquad \forall A, B \in M_N$$

One readily finds

$$L^* A = i[H,A] + \sum_{i,j=1}^{N^2-1} c_{ij} \left\{ F_j^* \rho F_i - \frac{1}{2}\left(F_j^* F_i A + A F_j^* F_i \right) \right\}$$

or in diagonal form

$$L^* A = i[H,A] + \sum_{i=1}^{N^2-1} V_i^* A V_i - \frac{1}{2}\left(V_i^* V_i A + A V_i^* V_i \right)$$

<u>Note that $L^* \mathbb{1} = 0$</u> (so Φ_t has at least one invariant state)

Approach to equilibrium

Consider the generator L of a CP dyn. semigroup in diagonal form,

$$L\rho = -i[H,\rho] + \sum_{j\in J}\left\{ V_j \rho V_j^* - \frac{1}{2}\left(V_j^* V_j \rho + \rho V_j^* V_j\right)\right\}$$

We call the dynamical semigroup $\Phi_t = e^{tL}$ <u>relaxing</u> if there is a density matrix ρ_0 s.t.

$$\lim_{t\to\infty} \Phi_t(\rho) = \rho_0 \qquad \forall \text{ state } \rho.$$

How can we detect from the diagonal form of L if Φ_t is relaxing?

<u>Theorem</u> (Spohn 1977)

If the vector space $\mathcal{K} = \operatorname{span}\{V_j\}_{j\in J}$ has a basis of self-adjoint operators (inner product: $\langle A,B\rangle = \operatorname{Tr} A^* B$) and if $(\{V_j\}_{j\in J})'' = \mathcal{B}(\mathcal{H})$ (double commutant), then Φ_t is relaxing.

Proof. Let $\{F_1, \dots, F_p\}$ be a self-adjoint basis of $\mathcal{K}$.
Expand V_j in this basis:

$$V_j = \sum_{m=1}^{p} v_{jm} F_m \qquad \left(v_{jm} = \langle F_m, V_j \rangle \right)$$

Then we have

$$L\rho = -i[H, \rho] + \sum_{m,n=1}^{p} b_{mn} \left\{ F_m \rho F_n^* - \frac{1}{2}\left(F_n^* F_m \rho + \rho F_n^* F_m \right) \right\}$$

where

$$b_{mn} = \sum_j \langle F_m, V_j \rangle \overline{\langle F_n, V_j \rangle}$$

$$= \langle F_m, \left(\sum_j V_j V_j^* \right) F_n \rangle$$

Now the matrix $B \equiv (b_{mn})$ is strictly positive: $\forall \vec{x} = (x_1, \dots, x_p) \in \mathbb{C}^p$

$$\langle \vec{x}, B\vec{x} \rangle = \sum_{m,n} \overline{x_m} b_{mn} x_n$$

$$= \sum_j \langle G, V_j V_j^* G \rangle \qquad \left(G = \sum_{m=1}^{p} x_m F_m \right)$$

$$= \sum_j \| V_j^* G \|^2 \geq 0$$

And if $\vec{x} \in \operatorname{Ker} B$, then $V_j^* G = 0$ $\forall j$, so $\operatorname{Tr} V_j^* G = 0$ $\forall j$, hence $\langle K, G \rangle = 0$ $\forall K \in \mathcal{K}$. Since $G \in \mathcal{K}$, we have $G = 0$, so $x_m = 0$ $\forall m$. Thus B is strictly positive.

Let $\alpha > 0$ be smaller than the smallest eigenvalue of B and define L_2 by

$$L_2 \rho = \frac{\alpha}{2} \sum_{m=1}^{p} F_m \rho F_m - \frac{1}{2}\left(F_m F_m \rho + \rho F_m F_m \right)$$

Then $L_1 := L - L_2$ is given by

$$L_1 \rho = -i[H, \rho] + \sum_{m,n=1}^{p} c_{mn} \left\{ F_m \rho F_m - \frac{1}{2}\left(F_m F_m \rho + \rho F_m F_m \right) \right\}$$

where $\quad c_{mn} = b_{mn} - \frac{\alpha}{2} \delta_{mn} \quad$ (Kronecker)

Then $(c_{mn}) \geq 0$ and hence L_1 is the generator of a CP dynamical semigroup (by Gorini-Kossakowski-Sudarshan)

Note that

$$\mathrm{Tr}(A^* L_2 A) = \frac{\alpha}{2} \sum_{m=1}^{p} \mathrm{Tr}\Big(A^* F_m A F_m - \frac{1}{2}\left\{ A^* F_m F_m A + A^* A F_m F_m \right\} \Big)$$

$$= \frac{\alpha}{4} \sum_{m=1}^{p} [A^*, F_m][A, F_m]$$

$$= -\frac{\alpha}{4} \sum_{m=1}^{p} ([A, F_m])^* [A, F_m] \leq 0$$

Hence $L_2 \rho = 0 \Leftrightarrow [F_m, \rho] = 0 \ \forall m \Rightarrow [V_j, \rho] = 0 \ \forall j$

and so $\rho \propto \mathbb{1}$ (since $(\mathrm{span}\, V_j)' = \mathbb{C}\mathbb{1}$)

Consider the decomposition $\mathcal{B}(\mathcal{H}) = \mathcal{A} \oplus \{\mathbb{C}\mathbb{1}\}$

$\left(\mathcal{A} = (\mathbb{C}\mathbb{1})^{\perp}\right)$. Then operators $\mathcal{L}$ on $\mathcal{B}(\mathcal{H})$ have

decompositions

$$\mathcal{L} = \left(\begin{array}{c|c} \tilde{\mathcal{L}} & * \\ \hline * & * \end{array}\right) \begin{array}{l} \updownarrow \mathcal{A} \\ \updownarrow \mathbb{C}\mathbb{1} \end{array}$$

1×1 block

(i.e. $\tilde{\mathcal{L}}$ is the projection of $\mathcal{L}$ to $\mathcal{A}$).

The operator L_2 is self-adjoint and $L_2 \mathbb{1} = 0$.

From the above we have $\operatorname{spec}(\tilde{L}_2) \subset (-\infty, -\lambda]$, some $\lambda > 0$.

Also, since $L_1^* \mathbb{1} = 0$, we have

$$L_1^* = \left(\begin{array}{c|c} \tilde{L}_1^* & \begin{matrix} 0 \\ \vdots \\ 0 \end{matrix} \\ \hline * & 0 \end{array}\right), \text{ so } \quad L_1 = \left(\begin{array}{c|c} \tilde{L}_1 & * \\ \hline 0 \cdots 0 & 0 \end{array}\right)$$

This shows that L_1 leaves $\mathcal{A}$ invariant and $L_1|_{\mathcal{A}} = \tilde{L}_1$.

Thus $\tilde{L} = \tilde{L}_1 + \tilde{L}_2$ leaves $\mathcal{A}$ invariant. Let $\| \, \|_{\mathcal{A}}$ be the norm restricted to $\mathcal{A}$. Then

$$\| e^{t\tilde{L}_1} \|_{\mathcal{A}} \le 1$$ (since e^{tL_1} is a CP semigroup and hence contracting, and leaves $\mathcal{A}$ invariant)

$$\| e^{t\tilde{L}_2} \|_{\mathcal{A}} \le e^{-\lambda t}$$ (by the above: $\tilde{L}_2 = \tilde{L}_2^*$, spec $\le -\lambda$)

Therefore, by Trotter's formula,

$$e^{t\tilde{L}} = \lim_{n\to\infty} \left(e^{\frac{t}{n}\tilde{L}_1}\right)^n \left(e^{\frac{t}{n}\tilde{L}_2}\right)^n,$$

we get $\|e^{t\tilde{\mathcal{L}}}\|_* \leq e^{-\lambda t}$, some $\lambda > 0$.

Hence $\operatorname{spec}(\tilde{\mathcal{L}}) \subset \{x+iy : x \leq -\lambda\}$. Again,

since

$$L = \left(\begin{array}{c|c} \tilde{L} & \\ \hline 0 \text{ --- } 0 & 0 \end{array}\right) \qquad (L^* \mathbb{1} = 0)$$

the characteristic equation shows that the spect of L is that of $\tilde{L}$ with exactly one simple eigenvalue zero added. This shows the theorem. $\square$

<u>Note</u>: To conclude the relaxing property from the knowledge that $\operatorname{spec}(L) = \underbrace{\{0\}}_{\text{simple}} \cup \{z_1, \dots, z_q\}$, $\operatorname{Im} z_q < 0$, one expands L into its Jordan block form

$L = \sum_k z_k P_k + N_k$. The usual thing.

A more general result (with a seemingly more difficult proof) is given by Frigerio (1977)

Consider the generator in the form

$$L\rho = \sum_{j>0} V_j^* A V_j + K^* A + KA$$

(see the construction of L, p.5), acting on a finite-dim. Hilbert space.

<u>Theorem</u> (Frigerio 1977)

If $\{V_j\}' = \mathbb{C}\mathbb{1}$, then e^{tL} is relaxing.

<u>Rem.</u> The difference w/ Spohn's result: the V_j are different. Spohn uses that span$\{V_j\}$ has self-adjoint basis.

Microscopic derivation of the markovian master equation

Weak coupling limit

$$\underbrace{H = H_S + H_R}_{H_0} + V \quad , \qquad V = A \otimes B$$

(could take $\sum_\alpha A_\alpha \otimes B_\alpha$)

Interaction picture $\rho_I(t) = e^{itH_0} \rho(t) e^{-itH_0}$

$$\Rightarrow \quad \partial_t \rho_I(t) = i\left[H_0, \rho_I(t)\right] - i e^{-itH_0}\left[H, \rho(t)\right] e^{itH_0}$$

$$= -i\left[V_I(t), \rho_I(t)\right]$$

So $$\rho_I(t) = \underbrace{\rho_I(0)}_{=\rho(0)} - i\int_0^t \left[V_I(s), \rho_I(s)\right] ds$$

$$\Rightarrow \quad \partial_t \rho_I(t) = -i\left[V_I(t), \rho(0)\right] - \int_0^t \left[V_I(t), \left[V_I(s), \rho_I(s)\right]\right] ds.$$

We assume that $\rho(0) = \hat{\rho}(0) \otimes \rho_B$

↑ system initial state.

Then
$$\mathrm{Tr}_B \, -i\,[V_I(t), \overset{\overset{\hat{\rho}(0)\otimes\rho_B}{\downarrow}}{\rho(0)}]$$

$A_I(t)\otimes B_I(t)$

$$= -i\,[A_I(t), \hat{\rho}(0)]\, \mathrm{Tr}_B(\rho_B B_I(t))$$

$$-i\, A_I(t)\,\hat{\rho}(0)\, \underbrace{\mathrm{Tr}_B[B_I(t), \rho_B]}_{=0}$$

$$= 0$$

provided
$$\mathrm{Tr}_B(\rho_B \, B_I(t)) = 0,$$

which is what we assume. By taking the partial trace over the bath we obtain ($\hat{\rho}_I$: red. syst. dmat in int. picture)

$$\partial_t \hat{\rho}_I(t) = -\int_0^t \mathrm{Tr}_B\,[V_I(t), [V_I(s), \rho_I(s)]]\, ds.$$

Born approximation: the statistical properties of the (huge) bath are unaffected by the (weak) interaction with the (small) system: $\rho_I(s) \approx \hat{\rho}_I(s)\otimes\rho_B$

Then
$$\partial_t \hat{\rho}_I(t) = -\int_0^t \mathrm{Tr}_B\,[V_I(t), [V_I(s), \hat{\rho}_I(s)\otimes\rho_B]]\, ds$$

One can calculate (expand) the integrand.

$$\mathrm{Tr}_B \left[V_I(t), \left[V_I(s), \hat{\rho}_I(t-s) \otimes \rho_B \right] \right]$$

$$= \mathcal{O}_1(s,t) \; \mathrm{Tr}_B \left(\rho_B \, B_I(t) \, B_I(s) \right)$$
$$+ \mathcal{O}_2(s,t) \; \mathrm{Tr}_B \left(\rho_B \, B_I(s) \, B_I(t) \right)$$

where $\mathcal{O}_1$, $\mathcal{O}_2$ are ops. acting on the system. Suppose that ρ_B is stationary w.r.t. its free dynamics. Then the correlation functions

$$C_B(t-s) = \mathrm{Tr}_B \left(\rho_B \, B_I(t) \, B_I(s) \right)$$

depend only on the difference $t-s$. One expects (assumes) that C_B decay quickly relative to the change of $\hat{\rho}_I(s)$.

For thermal reservoirs, the correlation function C_B decays exponentially $\propto e^{-t/\tau_{th}}$, with thermal correlation time $\tau_{th} = \frac{\hbar}{2\pi k T}$.

Let τ_{OSR} (open syst. relax.) be the characteristic time-scale over which the open system, i.e., $\hat{\rho}_I(t)$ varies appreciably.

In the regime $\tau_{OSR} \gg \tau_{th}$ (system is slow relative to reservoir evol.) one may thus approximate $\hat{\rho}_I(s)$ by $\hat{\rho}_I(t)$ in the above integral, i.e., {the Markov approximation

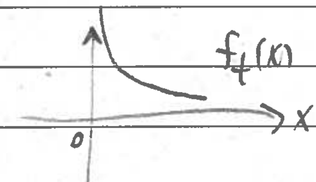
$$\partial_t \hat{\rho}_I(t) = -\int_0^t \mathrm{Tr}_B \left[V_I(t), \left[V_I(s), \hat{\rho}_I(t) \otimes \rho_B \right] \right] ds$$

$$\overset{\text{change of var.}}{=} -\int_0^t \mathrm{Tr}_B \left[V_I(t), \left[V_I(t-s), \hat{\rho}_I(t) \otimes \rho_B \right] \right] ds$$

This is called the Redfield equation.

Calling the last integrand $f_t(t-s)$ we must consider $\int_0^t f_t(t-s) ds = \int_0^t f_t(x) dx$.

Then, since $f_t(x) \sim e^{-x/\tau_{th}}$



if we consider $t \gg \tau_{th}$, we do not make an appreciable mistake if we extend the integral to $\int_0^\infty f_t(x) dx$

(However, for $t \ll \tau_{th}$ this approx. is not valid — one says that times of the order of the correlation time of the bath (or shorter) are not resolved in this approximation). We obtain the Markovian quantum master equation

$$\partial_t \hat{\rho}_I(t) = -\int_0^\infty \mathrm{Tr}_B \left[V_I(t), \left[V_I(t-s), \hat{\rho}_I(t) \otimes \rho_B \right] \right] ds.$$

We have

$$\partial_t \hat{\rho}_I(t) = \int_0^\infty \mathrm{Tr}_B \Big\{ V_I(t-s) \left(\hat{\rho}_I(t) \otimes \rho_\beta\right) V_I(t)$$
$$- V_I(t) V_I(t-s) \hat{\rho}_I(t) \otimes \rho_\beta \Big\} + h.c.$$

Next, let P_E be the projection onto the eigenspace of H_S associated to the eigenvalue E. We have

$$\mathbb{1} = \sum_E P_E$$

and so

$$A_I(t) = \sum_{E,E'} P_E A_I(t) P_{E'}$$
$$= \sum_{E,E'} e^{it(E-E')} P_E A P_{E'}$$
$$= \sum_{\omega \in \Omega} e^{-i\omega t} \sum_{\{E,E' : E'-E=\omega\}} P_E A P_{E'}$$

where the sum over the ω is over all Bohr energies

$$\omega \in \Omega := \{ E - F : E, F \in \mathrm{spec}(H_S) \}.$$

$$\Rightarrow \quad A_I(t) = \sum_\omega e^{-i\omega t} A(\omega) \quad , \text{ where}$$

$$A(\omega) := \sum_{\{E,E' : E'-E=\omega\}} P_E A P_{E'} .$$

Note that $A(\omega)^* = \sum_{\{E,E' : E'-E=\omega\}} P_{E'} A P_E = A(-\omega)$.

Then we get

$$\partial_t \hat{\rho}_I(t) = \int_0^\infty \Big\{ \sum_{\omega,\omega'} e^{-i\omega(t-s)} A(\omega) \hat{\rho}_I(t) e^{-i\omega' t} A(\omega') \times \mathrm{Tr}_B\big(B_I(t-s) \rho_B B_I(t) \big)$$

$$- \sum_{\omega,\omega'} e^{-i\omega t} e^{-i\omega'(t-s)} A(\omega) A(\omega') \hat{\rho}_I(t) \times \mathrm{Tr}_B\big(B_I(t) B_I(t-s) \rho_B \big) \Big\}$$

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

Now with $A(\omega') = A(-\omega')^*$ and a change of variable $\omega' \to -\omega'$ in the sum:

$$\partial_t \hat{\rho}_I(t) = \sum_{\omega,\omega'} e^{-i(\omega-\omega')t} A(\omega) \hat{\rho}_I(t) A(\omega')^* \times \int_0^\infty e^{i\omega s} \mathrm{Tr}_B\big(B_I(t-s) \rho_B B_I(t) \big) ds$$

$$- \sum_{\omega,\omega'} e^{-i(\omega'-\omega)t} A(\omega)^* A(\omega') \hat{\rho}_I(t) \times \int_0^\infty e^{i\omega' s} \mathrm{Tr}_B\big(B_I(t) B_I(t-s) \rho_B \big) ds$$

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

$$\Rightarrow \quad \partial_t \hat{\rho}_I(t) = \sum_{\omega,\omega'} e^{-i(\omega-\omega')t} \, \Gamma(\omega)$$

$$\times \left\{ A(\omega) \hat{\rho}_I(t) A(\omega')^* - A(\omega')^* A(\omega) \hat{\rho}_I(t) \right\}$$

$$+ h.c. \qquad (7.1)$$

where
$$\Gamma(\omega) := \int_0^\infty e^{i\omega s} \langle B_I(t) \, B_I(t-s) \rangle \, ds$$

bath average w.r.t. ρ_B

Assuming that ρ_B is stationary w.r.t. the dynamics generated by H_B, the reservoir correlation function is

$$\langle B_I(t) \, B_I(t-s) \rangle = \langle B(s) \, B \rangle, \quad B(s) = e^{isH_B} B e^{-isH_B}$$

is independent of t.

Note: (7.1) is not of Lindblad form yet (Dümcke & Spohn 1979, see Breuer & Petruccione p.132)

Rotating wave approximation

Call τ_S, the "system time scale", (defined as) the typical value of $\frac{1}{\omega-\omega'}$, where $\omega \neq \omega'$ are Bohr frequencies of the system. Under the condition

$$\tau_S \ll \tau_{OSR}$$

the oscillation in $e^{-i(\omega-\omega')t}$ is very rapid relative to the change of $\hat{\rho}_I(t)$ and we can neglect the terms where $\omega \neq \omega'$. Then

$$\partial_t \hat{\rho}_I(t) = \sum_\omega \Gamma(\omega) \left\{ A(\omega)\hat{\rho}_I(t) A(\omega)^* - A(\omega)^* A(\omega) \hat{\rho}_I(t) \right\} + h.c.$$

This is the RWA.

$\langle B(-s) B \rangle$ by stationarity

$$\mathrm{Re}\,\Gamma(\omega) = \frac{1}{2} \int_0^\infty \left\{ e^{i\omega s} \langle B(s) B \rangle + e^{-i\omega s} \langle B\, B(s) \rangle \right\} ds$$

$$= \frac{1}{2} \int_{\mathbb{R}} e^{i\omega s} \langle B(s) B \rangle \, ds$$

$$\equiv \frac{1}{2} \gamma(\omega)$$

$$\mathrm{Im}\,\Gamma(\omega) = \frac{1}{2i} \int_0^\infty \left\{ e^{i\omega s} \langle B(s) B \rangle - e^{-i\omega s} \langle B(-s) B \rangle \right\}$$

$$= \frac{1}{2i} \int_{\mathbb{R}} e^{i\omega s} \,\mathrm{sgn}(s) \langle B(|s|) B \rangle \, ds \equiv S(\omega)$$

So $\Gamma(\omega) = \frac{1}{2} \gamma(\omega) + i S(\omega)$

F.T. of bath correlation function

Thus

$$\partial_t \hat{\rho}_I(t) = \sum_\omega \frac{1}{2}\gamma(\omega)\Big\{ 2A(\omega)\hat{\rho}_I(t)A(\omega)^* - A(\omega)^*A(\omega)\hat{\rho}_I(t) - \hat{\rho}_I(t)A(\omega)^*A(\omega)\Big\}$$

$$+ \sum_\omega i S(\omega)\Big\{ -A(\omega)^*A(\omega)\hat{\rho}_I(t) + \hat{\rho}_I(t)A(\omega)^*A(\omega)\Big\}$$

Set $$H_{LS} = \sum_\omega S(\omega)\, A(\omega)^*A(\omega)$$

(Lamb shift Hamiltonian) and

$$\mathcal{D}(\rho) = \sum_\omega \gamma(\omega)\Big\{ A(\omega)\rho A(\omega)^* - \frac{1}{2}\big(A(\omega)^*A(\omega)\rho + \rho A(\omega)^*A(\omega)\big)\Big\}$$

(dissipator). We have arrived at the Lindblad form of the Markovian master equation:

$$\partial_t \hat{\rho}_I(t) = -i\,[H_{LS}, \hat{\rho}_I(t)] + \mathcal{D}(\hat{\rho}_I(t))$$

Undo the interaction picture:

$$\hat{\rho}(t) = e^{-itH_S}\hat{\rho}_I(t)\,e^{itH_S}, \text{ so}$$

$$\partial_t \hat{\rho}(t) = -i[H_S, \hat{\rho}(t)] + e^{-itH_S}\underbrace{\big(\partial_t \hat{\rho}_I(t)\big)}_{-i[H_{LS},\hat{\rho}_I(t)] + \mathcal{D}(\hat{\rho}_I(t))} e^{itH_S}$$

Note that $[H_S, H_{LS}] = 0$ as

$$H_S A(\omega) = \sum_{\{E,E' : E'-E=\omega\}} E \, P_E A P_{E'}$$

$$A(\omega) H_S = \sum_{\{E,E' ; E'-E=\omega\}} P_E A P_{E'} E'$$

$$\Rightarrow \quad [H_S, A(\omega)] = -\omega A(\omega).$$

Then $[H_S, H_{LS}] = 0$ follows.

Next,

$$\mathcal{D}(\hat{\rho}_I(t)) = \sum_\omega \gamma(\omega) \Big\{ A(\omega) e^{itH_S} \hat{\rho}(t) e^{-itH_S} A(\omega)^* - \frac{1}{2}\Big(A(\omega)^* A(\omega) e^{itH_S} \hat{\rho}(t) e^{-itH_S} + e^{itH_S} \hat{\rho}(t) e^{-itH_S} A(\omega)^* A(\omega)\Big)\Big\}$$

We have $e^{-itH_S} A(\omega) e^{itH_S} = e^{-i\omega t} A(\omega)$ and so

$$e^{-itH_S} \mathcal{D}(\rho) e^{itH_S} = \mathcal{D}(e^{-itH_S} \rho e^{itH_S}).$$

Thus

$$e^{-itH_S} \mathcal{D}(\hat{\rho}_I(t)) e^{itH_S} = \mathcal{D}(\hat{\rho}(t)).$$

(Rem: the above means $\alpha^t_{syst} \circ \mathcal{D} = \mathcal{D} \circ \alpha^t_{syst}$)

We get the markovian master equation in Lindblad form (in "original", not "interaction" picture)

$$\partial_t \hat{\rho}(t) = -i\left[H_S + H_{LS}, \hat{\rho}(t)\right] + \mathcal{D}(\hat{\rho}(t)).$$

Note: $\gamma(\omega) \geq 0$. To see this we use Bochner's theorem saying that the F.T. of a function f is positive if we have: $\forall n$, $\forall t_1, \dots, t_n$, the $n \times n$ matrix $a_{k\ell} = f(t_k - t_\ell)$ is a positive matrix.

Here, $\forall n$, $\vec{x} = (x_1, \dots, x_n) \in \mathbb{C}^n$:

$$\langle \vec{x}, (a)\vec{x} \rangle = \sum_{k,\ell} \bar{x}_k \underbrace{\langle B(t_k - t_\ell) B \rangle}_{= \langle B(t_k) B(t_\ell) \rangle \text{ (stat.!)}} x_\ell$$

$$= \left\langle \left(\sum_k x_k B(t_k) \right)^* \left(\sum_k x_k B(t_k) \right) \right\rangle \geq 0$$

Résumé

- Born approximation ("weak coupling") $\rho(t) \approx \hat{\rho}(t) \otimes \rho_B$
- Markov approx: locality in time imposed and "integration limit pushed to ∞".

  validity: if $\tau_{th} \ll \tau_{OSR}$ (bath modes are fast)

- RWA: suppress rapid osc.

  valid: if $\tau_S \ll \tau_{OSR}$ (system time scale fast) def = p.7

Pauli master equation for populations

Let P_E be the spectral proj. assoc. to eval E of H_S.

Note that

$$P_E A(\omega) P_{E'} = \begin{cases} 0 & \text{if } E'-E \neq \omega \\ P_E A(\omega) P_{E+\omega} & \text{if } E'-E=\omega \end{cases}$$

Thus

$$P_E A(\omega) \rho \overbrace{A(-\omega)}^{A(\omega)^*} P_E$$

$$= P_E A(\omega) P_{E+\omega} \rho P_{E+\omega} A(-\omega) P_E$$

and

$$P_E \overbrace{A(-\omega)}^{A(\omega)^*} A(\omega) \rho P_E = P_E A(-\omega) P_{E-\omega} A(\omega) \rho P_E$$

$$= P_E A(-\omega) P_{E-\omega} A(\omega) P_E \rho P_E$$

It follows that the equations of motion of $\{P_E \rho(t) P_E\}_{E \in \mathrm{spec}(H)}$ are closed. If all E are simple, then the values of the diagonal of $\rho(t)$ depend only on the initial values of the diagonal.

In other words, the populations evolve as a group.

Assume all eigenvalues of H_S are simple and list them: $\operatorname{spec} H_S = \{E_1, \dots, E_N\}$, $H_S \varphi_{E_n} = E_n \varphi_{E_n}$, $\{\varphi_n\}$ an ONB.

Call $$p_n(t) = \langle \varphi_{E_n}, \hat{\rho}(t) \varphi_{E_n} \rangle. \qquad \text{(population)}$$

$$\partial_t p_n(t) = -i \underbrace{\langle \varphi_{E_n}, [H_S + H_{LS}, \hat{\rho}(t)] \varphi_{E_n} \rangle}_{=0} + \langle \varphi_{E_n}, \mathcal{D}(\hat{\rho}(t)) \varphi_{E_n} \rangle$$

$$= \sum_\omega \gamma(\omega) \Big\{ \langle \varphi_{E_n}, A(\omega) \rho A(\omega)^* \varphi_{E_n} \rangle - \frac{1}{2}\Big(\langle \varphi_{E_n}, A(\omega)^* A(\omega) \rho \varphi_{E_n} \rangle + \langle \varphi_{E_n}, \rho A(\omega)^* A(\omega) \varphi_{E_n} \rangle \Big) \Big\}$$

In $$\langle \varphi_{E_n}, A(\omega) \rho A(\omega)^* \varphi_{E_n} \rangle = \sum_k \underbrace{\langle \varphi_{E_n}, A(\omega) \varphi_{E_k} \rangle}_{E_k - E_n = \omega} \underbrace{\langle \varphi_{E_k}, \rho A^*(\omega) \varphi_{E_n} \rangle}$$

selects a single k: for if

$E_k - E_n = E_{k'} - E_n \Rightarrow E_k = E_{k'}$
$\Rightarrow k = k'$

Hence $\sum_\omega$ can be replaced by

$\sum_k$ and $\omega = E_{kn}$

We get

$$\partial_t p_n(t) = \sum_k \gamma(E_{kn}) \, [A]_{nk} \, \overbrace{\rho_{kk}}^{p_k(t)} \, [A]_{kn}$$

$$\underbrace{\quad}_{E_k - E_n = -\omega}$$

$$-\frac{1}{2} \sum_k \gamma(E_{nk}) \quad [A]_{nk} [A]_{kn} \; p_n(t)$$

$$-\frac{1}{2} \sum_k \gamma(E_{nk}) \quad p_n(t) \; [A]_{n,k} [A]_{kn}$$

$E_n - E_k = \omega$

$$\partial_t p_n(t) = \sum_k \Big\{ \gamma(E_{kn}) \; |\langle \varphi_{E_k}, A \varphi_{E_n} \rangle|^2 \; p_k(t)$$

$$- \gamma(E_{nk}) \; |\langle \varphi_{E_k}, A \varphi_{E_n} \rangle|^2 \; p_n(t) \Big\}$$

Define $\quad \Pi_{k \to n} := \gamma(E_k - E_n) \; |\langle \varphi_{E_k}, A \varphi_{E_n} \rangle|^2$, so

$$\partial_t p_n(t) = \sum_k \left(p_k(t) \, \Pi_{k \to n} - p_n(t) \, \Pi_{n \to k} \right)$$

This is called the <u>Pauli master equation</u>. It describes a classical markov process with time-independent <u>transition rates</u> $\Pi_{k \to n}$.

(Note transition <u>probability</u> is defined by:

$$P(k \to \ell) = \Pi_{k \to \ell} \quad \text{if } k \neq \ell$$

$$P(k \to k) = 1 - \sum_{\ell \neq k} \Pi_{k \to \ell}$$

and satisfies $\quad \sum_\ell P(k \to \ell) = 1, \quad \forall k$)

Therefore, the proba $\mathbb{P}(k \to \ell)$ $(k \neq \ell)$

is just $\underbrace{\gamma(E_k - E_\ell)}_{\text{bath contrib.}} \underbrace{|\langle \varphi_{E_k}, A \varphi_{E_\ell} \rangle|^2}_{\text{system contrib.}} \geq 0$

$\updownarrow$

Real part of F.T. of bath correl. function.

For a thermal bath, we have

$$\gamma(-\omega) = \frac{1}{2} \int_{\mathbb{R}} e^{-i\omega s} \langle B(s) B \rangle ds$$

$$= \frac{1}{2} \int_{\mathbb{R}} e^{i\omega s} \langle B B(s) \rangle ds$$

$$\overset{(\text{KMS})}{=} \frac{1}{2} \int_{\mathbb{R}} e^{i\omega s} \langle B(s - i\beta) B \rangle ds$$

$$= \frac{1}{2} \int_{\mathbb{R}} e^{i\omega(s-i\beta)} e^{i\omega i\beta} \langle B(s-i\beta) B \rangle ds$$

$$= e^{-\beta\omega} \gamma(\omega)$$

So $\gamma(-\omega) = e^{-\beta\omega} \gamma(\omega)$. It follows that

$$\Pi_{n \to k} = \gamma(E_{nk}) \, |[A]_{nk}|^2 = e^{\beta E_{nk}} \gamma(E_{kn}) \, |[A_{kn}]|^2$$
$$= e^{\beta E_{nk}} \, \Pi_{k \to n}, \text{ or,}$$

$$\Pi_{k \to n} \, e^{-\beta E_k} = \Pi_{n \to k} \, e^{-\beta E_n}. \quad \text{(Detailed balance condition)}$$

Using the detailed balance condition, we find a stationary solution for the populations:

$$\partial_t p_n(t) = 0 \quad \forall n \quad \Leftrightarrow$$

$$\sum_k \left\{ \Pi_{k\to n}\, e^{-\beta E_k}\, e^{\beta E_k} p_k - \Pi_{n\to k}\, e^{-\beta E_n}\, e^{\beta E_n} p_n \right\} = 0 \quad \forall n$$

$$\Leftrightarrow \quad \sum_k a_{kn} \left(e^{\beta E_k} p_k - e^{\beta E_n} p_n \right) = 0 \qquad \forall n,$$

where $a_{kn} = \Pi_{k\to n}\, e^{-\beta E_k} = \Pi_{n\to k}\, e^{-\beta E_n}$.

A solution is $\qquad e^{\beta E_k} p_k - e^{\beta E_n} p_n = 0 \qquad \forall k, \forall n,$

or,

$$p_k = c \cdot e^{-\beta E_k}, \quad \forall k$$

which is the Gibbs distribution.

Construction of a spatially infinitely extended reservoir.

First consider a finite box $\Lambda \subset \mathbb{R}^3$, $|\Lambda| = L^3$.

Put non-interacting particles in the box.

$$\mathcal{H}_\Lambda = \mathcal{F}\left(L^2(\Lambda, d^3x) \right) \qquad \text{Fock space}$$

$$H = d\Gamma\left(-\Delta\restriction_\Lambda \right) \qquad -\Delta\restriction_\Lambda \text{ with periodic BC.}$$

(or $\sqrt{|\Delta|}$, or $f(\Delta)$...)

Pick momenta $k_1, \dots, k_p$

(Each $k_j = (k_j^x, k_j^y, k_j^z)$; $k_j^\# \in \frac{\mathbb{Z}}{\pi L}$)

numbers $n_1, \dots, n_p$. The state having n_j particles in Λ with momenta k_j is

$$\Psi_\Lambda = \frac{1}{\sqrt{n_1! \cdots n_p!}} \; a^*(f_V^1)^{n_1} \cdots a^*(f_V^p)^{n_p} \Omega,$$

where Ω is the vacuum of $\mathcal{F}$ and

$$f_V^j(x) = \frac{1}{\sqrt{|V|}} e^{i k_j x}.$$

Let $\rho_j = n_j / |V|$ be the density of states in Λ having momentum k_j.

The expectation functional is given by

$$f \mapsto E_V(f) = \langle \Psi_V, W(f)\Psi_V \rangle \qquad (f \text{ cpct support})$$

where $\qquad W(f) = e^{i\varphi(f)} = e^{\frac{i}{\sqrt{2}}(a^*(f)+a(f))}$

is the Weyl operator.

The infinite volume limit: $|V| \to \infty$ and

$\rho_j \to \rho(k)$ momentum density distribution, namely, $\rho(k)\,d^3k$ is the number of particles per unit volume in direct space, having momentum in d^3k.

Araki-Woods (JMP 1963):

$$\lim_{|V|\to\infty} E_V(f) = E_\rho(f) = e^{-\frac{1}{4}\langle \hat{f}, (1+\rho)\hat{f}\rangle}$$

Given a mom. density distr. ρ, let

$$CCR_\rho = \{ C^* \text{ algebra generated by } W(f),\ f \text{ s.t. } \langle \hat{f}, (1+\rho)\hat{f}\rangle < \infty \}.$$

Then

$$E_\rho(f) = \omega_\rho(W(f))$$

defines a state on CCR_ρ, namely, the spatially infinitely extended reservoir state with mom. density distribution $\rho(k)$.

One verifies that the GNS rep. of the state is given by

$$\mathcal{H}_R = \mathcal{F}(L^2(\mathbb{R}^3, d^3k)) \otimes \mathcal{F}(L^2(\mathbb{R}^3, d^3k))$$

$$\Omega = \Omega_F \otimes \Omega_F \qquad (\Omega_F \text{ the "Fock" vacuum in } \mathcal{F})$$

$$\pi_\rho : CCR_\rho \to \mathcal{B}(\mathcal{H}) \quad \text{rep. map}$$

$$\pi_\rho(W(f)) = W_F(\sqrt{1+\rho}\, f) \otimes W(\sqrt{\rho}\, \bar{f})$$

One has $\omega_\rho(W(f)) = \langle \Omega, \pi_\rho(W(f))\Omega\rangle_{\mathcal{H}_R}$

This rep. is regular, meaning that $t \mapsto \pi_\rho(W(tf))$ is differentiable on a dense set and so we obtain the represented field operator

$$\Phi_\rho(f) := -i\partial_t|_0 \, \pi_\rho(W(f))$$

$$= \Phi_F(\sqrt{1+\rho}\, f) \otimes \mathbb{1} + \mathbb{1} \otimes \Phi_F(\sqrt{\rho}\, \bar{f})$$

and the represented creation & annihilation ops

$$a^*_\rho(f) = \frac{1}{\sqrt{2}}\left(\Phi_\rho(f) - i\, \Phi_\rho(if)\right)$$

$$= a^*_F(\sqrt{1+\rho}\, f) \otimes \mathbb{1} + \mathbb{1} \otimes a_F(\sqrt{\rho}\, \bar{f})$$

Equilibrium state: $\rho(k) = \dfrac{1}{e^{\beta\omega(k)} - 1}$

Planck's black body radiation. Photon: $\omega(k) = |k|$

Free reservoir dynamics: Bogoliubov transfo $f \to e^{i\omega t} f$

$$\pi_\rho\left(W(e^{i\omega t} f)\right) = W_F\left(e^{i\omega t}\sqrt{1+\rho}\, f\right) \otimes W_F\left(e^{-i\omega t}\sqrt{\rho}\, \bar{f}\right)$$

$$= e^{itH_R} W_F\left(\sqrt{1+\rho}\, f\right) e^{-itH_R}$$

$$\otimes\, e^{-itH_R} W_F\left(\sqrt{\rho}\, \bar{f}\right) e^{itH_R}$$

$$= e^{itL_R}\, \pi_\rho\left(W(f)\right) e^{-itL_R}$$

where $L_R = H_R \otimes \mathbb{1} - \mathbb{1} \otimes H_R$, $\quad H_R = d\Gamma(\omega)$

Reservoir correlation function

$$\langle \Phi_\rho(e^{i\omega s} f)\, \Phi_\rho(f) \rangle = \frac{1}{2} \Big\langle \left[a^*_\rho(e^{i\omega s} f) + a_\rho(e^{i\omega s} f)\right]$$

$$\times \left[a^*_\rho(f) + a_\rho(f) \right] \Big\rangle$$

$$= \frac{1}{2} \Big\langle \Omega_F \otimes \Omega_F, \left[\mathbb{1} \otimes a_F\left(\sqrt{\rho}\, e^{-i\omega s} \bar{f}\right) + a_F\left(\sqrt{1+\rho}\, e^{i\omega s} f\right) \right]$$

$$\times \left[a^*_F\left(\sqrt{1+\rho}\, f\right) \otimes \mathbb{1} + \mathbb{1} \otimes a^*_F\left(\sqrt{\rho}\, \bar{f}\right) \right] \Omega_F \otimes \Omega_F \Big\rangle$$

$$= \frac{1}{2} \left\langle \sqrt{\rho}\, e^{-i\omega s} \bar{f}, \sqrt{\rho}\, \bar{f} \right\rangle + \frac{1}{2} \left\langle \sqrt{1+\rho}\, e^{i\omega s} f, \sqrt{1+\rho}\, f \right\rangle$$

$$= \frac{1}{2} \langle f, \left(e^{i\omega s} \rho + e^{-i\omega s} (1+\rho) \right) f \rangle$$

Fourier transfo: $\delta(x) = \frac{1}{2\pi} \int_{\mathbb{R}} e^{ix\xi} d\xi$, so

$$\Gamma(\mu) = \int_0^\infty e^{i\mu s} \langle \Phi_\rho(e^{i\omega s} f) \Phi_\rho(f) \rangle ds$$

$$\gamma(\mu) = 2 \operatorname{Re} \Gamma(\mu) = \int_{\mathbb{R}} e^{i\mu s} \langle \Phi_\rho(e^{i\omega s} f) \Phi_\rho(f) \rangle$$

$$= \pi \langle f, \left(\delta(\mu + \omega(k)) \rho(k) + \delta(\mu - \omega(k)) (1 + \rho(k)) \right) f \rangle$$

For $\omega(k) = |k|$ & $\rho(k) = \rho(|k|)$:

$$\gamma(\mu) = \begin{cases} \pi \mu^2 (1 + \rho(\mu)) \int_{S^2} |f(\mu, \Sigma)|^2 d\Sigma, & \mu > 0 \\ \pi \mu^2 \rho(|\mu|) \int_{S^2} |f(|\mu|, \Sigma)|^2 d\Sigma, & \mu < 0 \\ \pi \mu^2 (1 + 2\rho(\mu)) \int_{S^2} |f(\mu, \Sigma)|^2 d\Sigma \Big|_{\mu = 0}, & \mu = 0 \end{cases}$$

In equilibrium: $\rho(\mu) = \frac{1}{e^{\beta\mu} - 1}$ we get

$$\gamma(\mu) = \frac{\pi \mu^2}{|1 - e^{-\beta\mu}|} \int_{S^2} |f(|\mu|, \Sigma)|^2 d\Sigma \quad \text{for } \mu \neq 0$$

and

$$\gamma(0) = \pi \lim_{\mu \to 0} \mu^2 \coth\left(\frac{\beta\mu}{2}\right) \int_{S^2} |f(|\mu|, \Sigma)|^2 d\Sigma$$

For $|f(|\mu|,\Sigma)| \sim \frac{1}{\sqrt{|\mu|}}$ as $\mu \sim 0$ we get

$$\gamma(0) \propto \frac{\pi}{\beta}$$

<u>Coupling of a spin to the ∞ extended heat bath</u>

Condensate

The markovian master equation, with $\rho_B = |\Omega\rangle\langle\Omega|$ a valid density matrix acting on $\mathcal{F}\otimes\mathcal{F}$. This is precisely what we did before. The derivation has a chance of being correct, since indeed the correlation function of the bath do decay (∞ volume!)

$$H = \frac{a}{2}\overset{\begin{pmatrix}1&0\\0&-1\end{pmatrix}}{\sigma_z} + L_R + \lambda \underbrace{\overset{\begin{pmatrix}0&1\\1&0\end{pmatrix}}{\sigma_x}}_{A} \otimes \underbrace{\Phi_\rho(f)}_{B} \quad \text{on} \quad \mathbb{C}^d \otimes \underbrace{\mathcal{F}\otimes\mathcal{F}}_{\infty \text{ res.}}$$

$\Omega = \{-a, 0, a\}$ system Bohr frequencies

"$A(\omega)$":

$$\sigma_x(a) = P_\downarrow \sigma_x P_\uparrow = |\downarrow\rangle\langle\uparrow| \quad (\sigma_z|\uparrow\rangle = |\uparrow\rangle)$$

$$\sigma_x(-a) = P_\uparrow \sigma_x P_\downarrow = |\uparrow\rangle\langle\downarrow|$$

$$\sigma_x(0) = P_\uparrow \sigma_x P_\uparrow + P_\downarrow \sigma_x P_\downarrow = 0.$$

$$\Rightarrow \mathcal{D}(\rho) = \gamma(a)\left(|\downarrow\rangle\langle\uparrow|\rho|\uparrow\rangle\langle\downarrow| - \tfrac{1}{2}|\uparrow\rangle\langle\uparrow|\rho - \tfrac{1}{2}\rho|\uparrow\rangle\langle\uparrow|\right)$$
$$+ \gamma(-a)\left(|\uparrow\rangle\langle\downarrow|\rho|\downarrow\rangle\langle\uparrow| - \tfrac{1}{2}|\downarrow\rangle\langle\downarrow|\rho - \tfrac{1}{2}\rho|\downarrow\rangle\langle\downarrow|\right)$$

$$\partial_t \, \rho_{\uparrow\downarrow}(t) = -i \, \langle \uparrow | \, [H_S + H_{LS}, \rho(t)] \, | \downarrow \rangle$$

$$-\frac{1}{2}\gamma(a)\, \rho_{\uparrow\downarrow}(t) - \frac{1}{2}\gamma(-a)\, \rho_{\uparrow\downarrow}(t)$$

$$= -i\,(a + \lambda^2 e)\, \rho_{\uparrow\downarrow} - \frac{1}{2}\big(\gamma(a) + \gamma(-a)\big)\, \rho_{\uparrow\downarrow}$$

(Lamb shift)

$$\delta := \gamma(a) + \gamma(-a) = \coth\left(\frac{\beta a}{2}\right) \cdot \pi a^2 \int_{S^2} |f(a, z)|^2 \, dz > 0$$

$$\Rightarrow \quad \underline{\rho_{\uparrow\downarrow}(t) = e^{-it(a + \lambda^2 e)} \, e^{-\frac{\lambda^2}{2}\delta t} \, \rho_{\uparrow\downarrow}(0)}$$

__Decoherence:__ $\rho_{\uparrow\downarrow}(t) \to 0$ as $t \to \infty$ at rate $\tau_{deco} \propto \frac{1}{\lambda^2 \delta}$.

Dynamics of diagonal:

$$\partial_t \, \rho_{\uparrow\uparrow} = -\gamma(a)\, \rho_{\uparrow\uparrow} + \gamma(-a)\, \rho_{\downarrow\downarrow} \qquad \rho_{\uparrow\uparrow} + \rho_{\downarrow\downarrow} = 1$$

$$= \gamma(-a) - \big(\gamma(a) + \gamma(-a)\big)\, \rho_{\uparrow\uparrow}$$

stat. soln:

$$\rho_{\uparrow\uparrow} = \frac{\gamma(-a)}{\gamma(a) + \gamma(-a)} = \frac{1}{\frac{\gamma(a)}{\gamma(-a)} + 1}$$

$$= \frac{1}{\frac{e^{\beta a} - 1}{1 - e^{-\beta a}} + 1} = \frac{e^{-\beta a/2}}{e^{-\beta a/2} + e^{\beta a/2}}$$

<u>Thermalization</u> Gibbs ✓

The Gibbs state is reached exp. quickly with decay rate $\gamma(a)+\gamma(-a) = \lambda^2 \delta$ (twice as fast as decoherence rate)

Rigorous analysis of the dynamics of open quantum systems: spectral approach.

System: N-dimensional pure state space $\mathbb{C}^N$

reservoir: ∞ extended free Bose gas in thermal equilibrium.

Hamiltonian:

represented field op.

$$H = H_S + L_R + \lambda\, G \otimes \Phi_\beta(g)$$

acting on $\mathbb{C}^N \otimes \mathcal{F} \otimes \mathcal{F}$ ∞ volume reservoir state space.

Physical observables: $\mathfrak{A} = \mathcal{B}(\mathcal{H}_S) \otimes \mathcal{W}$

where $\mathcal{W} = \Pi_\rho(CCR)$ is the represented Weyl algebra.

Evolution of $A \in \mathfrak{A}$:

$$\langle A \rangle_t = \mathrm{Tr}_{S+R}\left(\rho \otimes |\Omega\rangle\langle\Omega|\; e^{itL} A e^{-itL}\right)$$

$$= \sum_{k,l} \langle \varphi_k, \rho\, \varphi_l \rangle \langle \varphi_l \otimes \Omega,\; e^{itH} A e^{-itH} \varphi_k \otimes \Omega \rangle$$

where $\{\varphi_k\}$ is an ONB of $\mathbb{C}^N$, typically the eigenfans of H_S. The general idea is to link the behaviour in t to the spectrum of H.

The presence of two terms $e^{\pm itH}$ in $\langle A \rangle_t$ is a problem. For instance, think of $H = -\Delta$ on $\mathbb{R}^3$, then $e^{\pm itH} f$ converges to zero locally only ($\| \chi_\Omega e^{\pm itH} f \| \to 0$, $\chi_\Omega = \chi_\Omega(x)$ indicator of a cpct $\Omega \subset \mathbb{R}^3$). This is due to dispersiveness and hence "motion to infinity". But clearly $e^{\pm itH} f$ does not converge to zero strongly, as $\| e^{\pm itH} f \| = \| f \|$. Similarly, we cannot expect to obtain good convergence properties in $\langle A \rangle_t$ unless A is somehow localized in a compact region. However, typically we want $A = A_S \otimes \mathbb{1}_R$ which is not localized at all in the reservoir part. To overcome this problem, we modify the generator of dynamics (H) into a "full" Liouville operator in such a way that one of the propagators ($e^{\pm itL}$) disappears.

Let ρ be a density matrix on $\mathbb{C}^N$ and $A \in \mathcal{B}(\mathbb{C}^N)$ an observable. Then

$$\operatorname{Tr} \rho A = \operatorname{Tr} \sqrt{\rho} A \sqrt{\rho} =: \langle \sqrt{\rho}, A \sqrt{\rho} \rangle_2 ,$$

where $\langle A, B\rangle_2 = \mathrm{Tr}\, A^* B$ makes $\mathbb{C}^N$ into a Hilbert space.

We define the map $T : \mathcal{B}(\mathbb{C}^N) \to \mathbb{C}^N \otimes \mathbb{C}^N$ by

$$T\, |\varphi\rangle\langle\psi| = \varphi \otimes \mathcal{C}\psi$$

and linear extension, where $\mathcal{C}$ is an anti-linear involution ($\mathcal{C}^2 = \mathbb{1}$). Then T is an isometric isomorphism.

One usually chooses $\mathcal{C}$ to be the operation of complex conjugation of coordinates in the eigenbasis $\{\varphi_n\}$ of H_S. The Gibbs state $\rho_\beta = \frac{1}{Z_\beta} e^{-\beta H_S}$ is then represented by

$$T\rho_\beta = \sum_{n=1}^{N} \frac{e^{-\beta E_n/2}}{\sqrt{Z_\beta}}\, \varphi_n \otimes \varphi_n = \Omega_{S,\beta}.$$

One easily verifies that $\forall A_S \in \mathcal{B}(\mathbb{C}^N)$:

$$\mathrm{Tr}\, \rho_S A_S = \langle \Omega_{S,\beta}, (A_S \otimes \mathbb{1})\, \Omega_{S,\beta}\rangle_{\mathbb{C}^N \otimes \mathbb{C}^N}$$

Set $\quad \Pi_S(A) = A \otimes \mathbb{1} \quad$ (Π_S is rep. of $\mathcal{B}(\mathbb{C}^N)$)

Note that $\quad \Pi_S(e^{itH_S} A e^{-itH_S}) = e^{itL_S}\, \Pi_S(A)\, e^{-itL_S}$,

where

$$L_S = H_S \otimes \mathbb{1} - \mathbb{1} \otimes H_S$$

The additional term $-\mathbb{1}\otimes H_S$ that L has relative to $H_S\otimes\mathbb{1}$ is chosen so that $L_S\,\Omega_{S,\beta}=0$. (One could implement the system dynamics with $H_S\otimes\mathbb{1}-\mathbb{1}\otimes X$, for a general s.t. X)

The uncoupled system-reservoir dynamics is given by the propagator e^{-itL_0},

$$L_0 = L_S + L_R,$$

having the property that $L_0\,\Omega_{S,\beta}\otimes\Omega_R = 0$.

The coupled dynamics is then generated by

$$\widetilde{L} = L_0 + \lambda\, G\otimes\mathbb{1}_{\mathbb{C}^N}\otimes\Phi_\beta(g).$$

In other words, $\forall A\in\mathcal{A}$,

$$\langle A\rangle_t = \langle \Psi_0,\ e^{it\widetilde{L}} A\, e^{-it\widetilde{L}}\,\Psi_0\rangle_{\mathbb{C}^N\otimes\mathbb{C}^N\otimes\mathcal{F}\otimes\mathcal{F}},$$

where Ψ_0 is the vector representing the initial system-reservoir state.

Let $\mathfrak{M}$ be the weak closure of $\mathcal{A} = \mathcal{B}(\mathbb{C}^N) \otimes 1\!\!1 \otimes \mathcal{W}$ in $\mathcal{B}(\mathbb{C}^N \otimes \mathcal{F} \otimes \mathcal{F})$, or, $\mathfrak{M} = \mathcal{A}''$ (double commutant).
One verifies that $\alpha_0^t(\cdot) = e^{itL_0} \cdot e^{-itL_0}$ and $\alpha_\lambda^t(\cdot) = e^{it\tilde{L}} \cdot e^{-it\tilde{L}}$ are both σ-weakly continuous groups of $*$-automorphisms of $\mathfrak{M}$. Moreover,

$$\Omega_{SR,0} = \Omega_{S,\beta} \otimes \Omega_R$$

is a (β, α_0^t)-KMS state. By Araki's perturbation theory of KMS states, the vector

$$\Omega_{SR,\lambda} = \frac{e^{-\beta \tilde{L}/2}\, \Omega_{SR,0}}{\| e^{-\beta\tilde{L}/2}\, \Omega_{SR,0} \|}$$

defines a $(\beta, \alpha_\lambda^t)$-KMS state. (The equilibrium state of the interacting system.) Associated to $\Omega_{SR,\lambda}$ is a modular conjugation $J = J_S \otimes J_R$, given by

$$J_S\, \varphi \otimes \chi = \mathcal{C}\chi \otimes \mathcal{C}\varphi \quad , \quad \forall \varphi, \psi \in \mathbb{C}^N$$

and where $\mathcal{C}$ is the cplx conjugation in the eigenbasis of H_S
and

$$J_R \quad \psi_n(k_1, \dots, k_n) \otimes \varphi_m(k_1, \dots, k_m)$$

$$= \overline{\varphi_m}(k_1, \dots, k_m) \otimes \overline{\psi_n}(k_1, \dots, k_n)$$

The Tomita-Takesaki theorem asserts that

$$J \mathcal{M} J = \mathcal{M}' \quad \text{(commutant algebra)}$$

Next, by using the Trotter product formula, one sees that

$$\forall A \in \mathcal{M}: \quad e^{it\tilde{L}} A e^{-it\tilde{L}} = e^{it(\tilde{L} - JVJ)} A e^{-it(L - JVJ)}$$

Namely, adding an element of the commutant to the generator of dynamics does <u>not</u> change the dynamics.

The standard Liouvillean is denoted by

$$L = \tilde{L} - \lambda JVJ = L_0 + \lambda V - \lambda JVJ,$$

where $\quad V = G \otimes 1\!\!1 \otimes \Phi_\beta(g)$.

The advantage of adding $-\lambda JVJ$ is that

$$L \, \Omega_{SR,\lambda} = 0$$

(To see this: $\quad L \, \Omega_{SR,\lambda} \propto (\overbrace{L_0 + \lambda V}^{\tilde{L}} - \lambda JVJ) \, e^{-\beta \tilde{L}/2} \, \Omega_{SR,0}$

$$= \underbrace{e^{-\beta\tilde{L}/2} \tilde{L} \, \Omega_{SR,0}}_{\lambda e^{-\beta\tilde{L}/2} V \Omega_{SR,0}} - \lambda e^{-\beta\tilde{L}/2} \underbrace{e^{\beta(L_0+V)/2} JVJ \, e^{-\beta(L_0+V)/2}}_{e^{\beta L_0/2} JVJ \, e^{-\beta L_0/2}} \Omega_{SR,0}$$

$$= \lambda e^{-\beta\tilde{L}/2} V \Omega_{SR,0} - \lambda e^{-\beta\tilde{L}/2} \underbrace{J e^{-\beta L_0/2} V \Omega_{SR,0}}_{= V^* \Omega_{SR,0} = V \Omega_{SR,0}}$$

$\Delta^{1/2}_{R,0}$

$= 0 \quad)$

Since $\Omega_{SR,\lambda}$ is a KMS state of $\mathfrak{M}$, the set

$$\mathcal{D} := \mathfrak{M}' \Omega_{SR,\lambda} \text{ is dense in } \mathbb{C}^N \otimes \mathbb{C}^N \otimes \mathcal{F} \otimes \mathcal{F}.$$

Let $\Psi_0 = B' \Omega_{SR,\lambda} \in \mathcal{D}$ be an initial state. Observables $A \in \mathfrak{M}$ then evolve as

$$\langle A \rangle_t = \langle \Psi_0, e^{itL} A e^{-itL} \Psi_0 \rangle$$

$$= \langle \Psi_0, B' e^{itL} A \Omega_{SR,\lambda} \rangle$$

as $e^{itL} A e^{-itL} B' = B' e^{itL} A e^{-itL}$ & $L \Omega_{SR,\lambda} = 0$.

This formula is suitable for spectral analysis since a single propagator e^{itL} appears.

<u>Spectral analysis of Liouville operators</u>

$$L = L_0 + \lambda V - \lambda J V J, \quad V = G \otimes 1\!\!1_{\mathbb{C}^N} \otimes \Phi_\beta(g)$$

$$L_0 = L_S + L_R, \qquad L_S = H_S \otimes 1\!\!1 - 1\!\!1 \otimes H_S \quad \text{on } \mathbb{C}^N \otimes \mathbb{C}^N$$

$$L_R = H_R \otimes 1\!\!1 - 1\!\!1 \otimes H_R \quad \text{on } \mathcal{F} \otimes \mathcal{F}$$

Resolvent representation:

$$\langle A \rangle_t = \langle \Psi_0, B' e^{itL} A \Omega_{SR,\lambda} \rangle$$

$$= \frac{-1}{2\pi i} \int_{\mathbb{R}-i\eta} e^{itz} \langle \Psi_0, B'(L-z)^{-1} A \Omega_{SR,\lambda} \rangle \, dz.$$

$(\eta > 0)$

Spectral deformation: convenient unitary transformation

$$\mathcal{F}(L^2(\mathbb{R}^3, d^3k)) \otimes \mathcal{F}(L^2(\mathbb{R}^3, d^3k))$$

$$\cong \mathcal{F}(L^2(\mathbb{R}^3, d^3k) \oplus L^2(\mathbb{R}^3, d^3k))$$

$$\cong \mathcal{F}(L^2(\mathbb{R} \times S^2, du \times d\Sigma))$$