Cycle representation and dynamical detailed balance for a class of GKSL generators

Roberto Quezada
(Joint work with L. Accardi and F. Fagnola)

Universidad Autónoma Metropolitana-Iztapalapa
México D. F.

31st Conference on QP and RT,
JNCASR, Bangalore, August 16, 2009

Schedule

1.- Introduction.

2.- Current decomposition for GKSL generators.

3.- A class GKSL generators with a current decomposition.

4.- Cycle decomposition and dynamical detailed balance.

5.- Cycle dynamics and entropy production.

Introduction

Statistical Mechanics (19th century: Maxwell, Boltzmann, Gibbs) separates into two parts: equilibrium and non-equilibrium.

Equilibrium:

Boltzmann: detailed balance.

Kolmogorov: reversibility.

(Kubo-Martin-Schwinger (KMS) condition).

Non-equilibrium: (non-detailed balance, irreversibility)

Dynamical detailed balance.

Entropy production.

Current decomposition for GKSL generators

GKSL have the canonical form

$$\mathcal{L}(x) = \sum_k L_k^* x L_k + G^* x + xG, \quad x \in \mathcal{B}(\mathrm{h}), \tag{1}$$

where $\mathcal{B}(\mathrm{h})$ denotes the von Neumann algebra of all bounded operator on a Hilbert space h, $(L_k)_{k\geq 1}$ is a sequence of possible unbounded operators on h and $-G$ is the generator of a strongly continuous semigroup on h.

The sequence $(L_k)_{k\geq 1}$ and the generator G are related by means of the formula

$$G = \frac{1}{2}\sum_k L_k^* L_k - iH$$

Under suitable conditions one can construct a minimal quantum dynamical semigroup $(\mathcal{T}_t)_{t\geq 0}$ that preserves the identity and hence is a quantum Markov semigroup (QMS).

If we denote by $\mathcal{L}$ the (true) generator of $(\mathcal{T}_t)_{t\geq 0}$, which is an unbounded densely defined operator on $\mathcal{B}(\mathsf{h})$. The domain of this generator is characterized by means of

$$\mathrm{Dom}(\mathcal{L}) = \{x \in \mathcal{B}(\mathsf{h}) : \mathcal{L}(x) \in \mathcal{B}(\mathsf{h})\}, \tag{2}$$

if and only if the corresponding QMS is conservative.

Given a faithful state ρ we consider the Hilbert space $\mathcal{B}(\mathrm{h})$ endowed with the inner product induced by ρ:

$$\langle x, y\rangle_\rho = tr\big(\rho x^* y\big).$$

From now on we will assume that $\mathrm{Dom}(\mathcal{L})$ is dense with the norm-topology induced by the above inner product.

Definition 2.1

Given a faithful state ρ and a $\theta \in [0,1]$, the (ρ,θ)-adjoint $\mathcal{L}^*_{(\rho,\theta)}$ of a GKSL-generator $\mathcal{L}$ is defined for $x \in \mathrm{Dom}(\mathcal{L}^*_{(\rho,\theta)}) := \{x \in \mathcal{B}(\mathrm{h}) : \text{ there exists } z \in \mathcal{B}(\mathrm{h}) \text{ such that } tr\big(\rho^{1-\theta} z^* \rho^\theta y\big) = tr\big(\rho^{1-\theta} x^* \rho^\theta \mathcal{L}(y)\big),\ \forall y \in \mathrm{Dom}(\mathcal{L})\}$ by means of the relation

$$tr\left(\rho^{1-\theta}\left(\mathcal{L}^*_{(\rho,\theta)}(x)\right)^* \rho^\theta y\right) = tr\left(\rho^{1-\theta} x^* \rho^\theta \mathcal{L}(y)\right),\ \ \forall\ \ y \in \mathrm{Dom}(\mathcal{L}) \quad (3)$$

Given a self-adjoint operator H on h such that for some function $\beta : \mathbb{R} \to (0, \infty)$ the operator $e^{-\beta(H)H} \in L_1(\mathrm{h})$, the space of all the operators with finite trace. We denote by $\rho_{\beta,H}$ the state

$$\rho_{\beta,H} = Z_{\beta,H}^{-1} e^{-\beta(H)H}$$

where $Z_{\beta,H} = tr(e^{-\beta(H)H})$.

Definition 2.2

Let H be a self-adjoint operator on h with a discrete spectrum and spectral decomposition

$$H = \sum_m \epsilon_m |\epsilon_m\rangle\langle\epsilon_m|$$

and let $\mathcal{L}$ be a GKSL-generator.

We say that $\mathcal{L}$ have a (H, β)-current decomposition (4), if the state $\rho_{\beta,H}$ is invariant and the $(\rho_{\beta,H}, \theta)$-adjoint $\mathcal{L}^*_{(\rho_{\beta,H},\theta)}$ enjoys the following properties:

(i)

$$\mathcal{L}(x) - \mathcal{L}^*_{(\rho_{H,\beta},\theta)}(x) = 2i[K,x] - \Pi_{\rho_{\beta,H}}(x), \qquad (4)$$

$\forall x \in \mathrm{Dom}(\mathcal{L}) \cap \mathrm{Dom}(\mathcal{L}^*_{(\rho_{\beta,H},\theta)}) \cap \mathrm{Dom}(i[K,\cdot])$. Where K is a self-adjoint operator and $\Pi_{(\rho_{\beta,H},\theta)}(x)$ is CCP map.

$$\Pi_{\rho_{\beta,H}}(x) = \sum_{\{(m,n):\epsilon_m>\epsilon_n\}} (q_{nm}e^{\beta(\epsilon_m)\epsilon_m-\beta(\epsilon_n)\epsilon_n} - q_{mn})E^*_{mn}xE_{mn} + (q_{mn}e^{\beta(\epsilon_n)\epsilon_n-\beta(\epsilon_m)\epsilon_m} - q_{nm})E_{mn}xE^*_{mn}), \qquad (5)$$

with $(E_{mn})_{m,n\geq 0}$ a sequence of rank one operators on h and $(q_{mn})_{m,n\geq 0}$ a sequence of non-negative numbers.

(ii) $\mathrm{Dom}(\mathcal{L}) \cap \mathrm{Dom}(\mathcal{L}^*_{\rho_{\beta,H}}) \cap \mathrm{Dom}(i[K,\cdot])$ is a core for $\mathcal{L}$, $\mathcal{L}^*_{(\rho_{\beta,H},\theta)}$ and $i[K,\cdot]$ in $\mathcal{B}(\mathsf{h})$, Assume for simplicity that h $= \mathbb{C}^d$. Take $\rho = \rho_{\beta,H} = (\rho_1, \cdots, \rho_n)$, $\rho_n = e^{-\beta(\epsilon_n)\epsilon_n}$. Then, after some computations one can see that (4) reduces to

$$\begin{aligned} &\mathcal{L}(x) - \mathcal{L}^*_{(\rho_{H,\beta},\theta)}(x) \\ =&2i[K,x] - \sum_{\{(m,n):\epsilon_m>\epsilon_n\}} \left(\frac{J_{mn}}{\rho_m} E^*_{mn} x E_{mn} + \frac{J_{nm}}{\rho_n} E_{mn} x E^*_{mn} \right). \end{aligned} \tag{6}$$

Where $J_{mn} = -J_{nm}$ are the currents: $J_{mn} = \rho_m q_{mn} - \rho_n q_{nm}$.

Proposition 1

Assume $\mathsf{h} = \mathbb{C}^n$, *let* $\mathcal{L}$ *be a GKSL generator with a* (H, β)*-current decomposition (4) such that* $E_{nm} = E^*_{mn}$*. Then* $\mathcal{L}$ *is a* $(\rho_{\beta,H}, \theta)$*-detailed balance generator in the sense of Fagnola-Umanità (Alicki, Frigerio) if and only if for all* $x \in \mathcal{B}(\mathsf{h})$,

$$\sum_{\epsilon_m > \epsilon_n} \rho_m \rho_n^{-1} E_{mn} x E^*_{mn} = \sum_{\epsilon_m > \epsilon_n} E^*_{mn} x E_{mn}, \tag{7}$$

where we write simply ρ *instead* $\rho_{\beta,H}$ *and* $\rho_n = e^{-\beta(\epsilon_n)\epsilon_n}$.

Now let us give a necessary and sufficient condition for a GKSL generator to have a current decomposition with the structure (4).

Theorem 2.3

Suppose, that $\mathsf{h} = \mathbb{C}^d$. *Then, the difference* $\mathcal{L} - \mathcal{L}^*_{\rho_{H,\beta}}$ *has the structure (4) if and only if*

(C1) $\rho = \rho_{\beta,H}$ *is a faithful invariant state "generic" i.e.* $\rho_n \rho_m^{-1} = \rho_{n'} \rho_{m'}^{-1}$ *if and only if* $n = n'$ *and* $m = m'$.

(C2) $\mathcal{L}$ *commutes with the modular automorphism* $\sigma_{-i}(x) = \rho x \rho^{-1}$.

Theorems 3.1, 7.1 and Proposition 8.1 in [Fagnola-Umanita]: (ρ, θ)-adjoints coincide, i.e., they are independent of θ. Moreover, under these assumptions, by Prop. 4.4 p. 348, there exists a GKSL representation of $\mathcal{L}$ such that:

- $$\sigma_{-i}(L_k) = \rho L_k \rho^{-1} = \lambda_k L_k, \qquad \text{for all } k. \tag{8}$$

Therefore the L_k are eigenvectors of σ_{-i}.

By (C1), the spectral structure of σ_{-i} is:

- 1 is an eigenvalue with multiplicity d and eigenspace generated by the operators $E_{kk} = |\epsilon_k\rangle\langle\epsilon_k|$ with $k = 1, \ldots, d$,
- each one of the $d^2 - d$ positive values $\rho_n \rho_m^{-1}$, with $n \neq m$, is an eigenvalue with multiplicity 1 and eigenvector $E_{mn} = |\epsilon_n\rangle\langle\epsilon_m|$.

Therefore there exists a GKSL representation of $\mathcal{L}$ with L_k that: either

- Commute with ρ, or
- Are multiples of the E_{mn} with $m \neq n$.

We can then write the generator $\mathcal{L}$ as

$$\mathcal{L}(x) = G^* x + \sum_{m \neq n} q_{mn} E^*_{mn} x E_{mn} + xG, \text{ with } q_{mn} > 0. \qquad (9)$$

The computation of $\mathcal{L}^*_{\rho_{H,\beta}}$ then yields

$$\mathcal{L}^*_{\rho_{H,\beta}}(x) = \mathcal{L}_*(x\rho)\rho^{-1}$$

where $\mathcal{L}_*$ is the pre-dual of $\mathcal{L}$. Hence, using that $E^*_{mn} = E_{nm}$, we can write

$$\begin{aligned}\mathcal{L}(x) - \mathcal{L}^*_{\rho_{H,\beta}}(x) = 2i[K,x] &+ \sum_{\epsilon_m > \epsilon_n} \left(q_{mn} - \rho_n \rho_m^{-1} q_{nm} \right) E^*_{mn} x E_{mn} \\ &+ \sum_{\epsilon_m > \epsilon_n} \left(q_{nm} - \rho_m \rho_n^{-1} q_{mn} \right) E_{mn} x E^*_{mn}.\end{aligned} \tag{10}$$

This is exactly the structure (4).

Conversely, if (4) holds, then the (ρ, θ)-adjoint is a *-map therefore, also the CP maps T_t of the QMS are *-maps and, by a theorem of Majewski and Streater (Theorem 6, p. 7985 in [Majewski-Streater]), T_t as well as its generator commute with the modular automorphism.

The QMS satisfies a $(\rho, 0)$-detailed balance condition in (Fagnola-Umanità) if and only if $\mathcal{L} - \mathcal{L}^*_{(\rho,0)} = 2i[K, \cdot]$. As a consequence of Proposition (1).

Corollary 2.4

(Fagnola-Umanità) Under the assumptions of Theorem 2.3, the GKSL generator $\mathcal{L}$ satisfies a $(\rho, 0)$-detailed balance condition if and only if Fagnola-Umanità's condition for existence of a privileged representation holds, i.e., there exists a unitary operator $(u_{kj})_{1\leq k,j\leq d}$ such that with $\lambda_k = \rho_m \rho_n^{-1}$ and $L_k = E_{mn}$

$$\lambda_k^{\frac{1}{2}} L_k^* = \sum_j u_{kj} L_j, \quad \forall\, k. \tag{11}$$

A class of GKSL generators with a current decomposition

The stochastic limit shows:

- If a quantum system with discrete spectrum Hamiltonian H, interacts with a reservoir (field) in an equilibrium state of inverse temperature β, then (under general conditions) the GKSL generator of the system has an equilibrium state $\rho_{H,\beta}$.

Idea:

- Replace the equilibrium state of the reservoir by a non-equilibrium state, then one should obtain a non-equilibrium invariant state $\rho_{H,\beta}$ of the GKSL generator.

This idea was realized by Accardi and Imafuku and yield to a class of generators that have a GKSL representation of the form

$$\mathcal{L}(x) = i[\Delta, x] - \sum_{\omega \in F} \Big(\Gamma_{-,\omega} \big(\frac{1}{2}\{E_\omega^* E_\omega, x\} - E_\omega^* x E_\omega \big) + \Gamma_{+,\omega} \big(\frac{1}{2}\{E_\omega E_\omega^*, x\} - E_\omega x E_\omega^* \big) \Big), \tag{12}$$

which are canonically associated with Hamiltonian

$$H_S = \sum_m \epsilon_m |\epsilon_m\rangle\langle\epsilon_m|, \tag{13}$$

because $E_\omega = |\epsilon_l\rangle\langle\epsilon_m|$, for $\epsilon_l, \epsilon_m \in \mathrm{Spec}(H_S)$ such that $\epsilon_m - \epsilon_l = \omega > 0$.

It is assumed that the Hamiltonian is generic, i.e., with the notations

$$F = \{\omega = \epsilon_r - \epsilon_{r'} : \epsilon_r, \epsilon_{r'} \in \mathrm{Spec}(H_S)\},$$
$$F_\omega = \{\epsilon_{r'} \in \mathrm{Spec}(H_S) : \epsilon_{r'} - \omega \in \mathrm{Spec}(H_S)\}. \qquad (14)$$

(1) The spectrum $\mathrm{Spec}(H_S)$ is not degenerate.

(2) For any ω, $|F_\omega| = 1$, i.e., there exists a unique pair of energy levels(1
$\epsilon_l, \epsilon_m \in \mathrm{Spec}(H_S)$ such that $\omega = \epsilon_m - \epsilon_l$.

$$\Delta = i \sum_{\omega \in F} \sum_{j=1,2} \Big(\mathrm{Im}(\gamma_{-j,\omega}) E_\omega^* E_\omega - \mathrm{Im}(\gamma_{+j,\omega}) E_\omega E_\omega^* \Big), \tag{16}$$

$$\Gamma_{\pm,\omega} = 2\mathrm{Re}\big(\sum_{j=1,2} \gamma_{\pm j,\omega} \big) \geq 0, \ \ \text{for} \ \ \omega > 0, \ \ \Gamma_{\pm,\omega} = 0, \ \ \text{for} \ \ \omega \leq 0. \tag{17}$$

The physical information is contained in the generalized susceptivities (or transport coefficients):

$$\begin{aligned}\gamma_{-,j,\omega} =&\pi \int dk|g_{j,\omega}(k)|^2 \frac{e^{\beta_j(\omega_j(k)-\mu_j)}}{e^{\beta_j(\omega_j(k)-\mu_j)}-1}\delta(\omega_j(k)-\omega)- \\ & iP.P. \int dk \frac{|g_{j,\omega}(k)|^2}{\omega_j(k)-\omega} \frac{e^{\beta_j(\omega_j(k)-\mu_j)}}{e^{\beta_j(\omega_j(k)-\mu_j)}-1},\end{aligned} \tag{18}$$

$$\begin{aligned}\gamma_{+,j,\omega} =&\pi \int dk|g_{j,\omega}(k)|^2 \frac{1}{e^{\beta_j(\omega_j(k)-\mu_j)}-1}\delta(\omega_j(k)-\omega)- \\ & iP.P. \int dk \frac{|g_{j,\omega}(k)|^2}{\omega_j(k)-\omega} \frac{1}{e^{\beta_j(\omega_j(k)-\mu_j)}-1}, \quad j=1,2.\end{aligned} \tag{19}$$

The minimal QMS

One can construct the minimal semigroup associated with this class of generators, observe that the completely positive part is

$$\Phi(x) = \sum_{\omega \in F} \left(\Gamma_{-,\omega} E_\omega^* x E_\omega + \Gamma_{+,\omega} E_\omega x E_\omega^* \right),$$

and $G = -\frac{1}{2}\Phi(I) + i\Delta$.

The minimal semigroup is conservative, hence it is a QMS.

Proposition 2

Any GKSL generator of the form (12) commutes with the modular automorphism $\sigma_{-i}(x) = \rho_{\beta,H} x \rho_{\beta,H}^{-1}$, *i.e.,* $\mathcal{L} \circ \sigma_{-i} = \sigma_{-i} \circ \mathcal{L}$.

Proof: Define $q_{nl} = \Gamma_{-,\epsilon_n - \epsilon_l}$ and $q_{ln} = \Gamma_{+,\epsilon_n - \epsilon_l}$. Hence we can write

$$\mathcal{L}(x) = \Phi(x) + G^* x + xG,$$

where

$$\Phi(x) = \sum_{\{(n,l):\epsilon_n > \epsilon_l\}} \left(L_{nl}^* x L_{nl} + L_{ln}^* x L_{ln} \right), \quad L_{nl} = q_{nl}^{\frac{1}{2}} E_{nl}, \; L_{ln} = q_{ln}^{\frac{1}{2}} E_{nl}^*;$$

$$G = -\frac{1}{2}\Phi(I) - i\Delta,$$

and the sum is finite.

Let $\Phi_{nl}(x) = L_{nl}^* x L_{nl} + L_{ln}^* x L_{ln}$.
Since $E_{nl}^* E_{nl} = |\epsilon_n\rangle\langle\epsilon_n|$ and $E_{nl} E_{nl}^* = |\epsilon_l\rangle\langle\epsilon_l|$, then $\Phi(I)$ and Δ are diagonal operators. Hence G and G^* commute with ρ.
Hence it suffices to prove that Φ commutes with σ_{-i}.

$$\text{For all,} \quad \theta \in [0,1]: \quad \begin{aligned} [E_{nl}, \rho^\theta] &= (\rho_n^\theta - \rho_l^\theta) E_{nl}, \\ [E_{nl}^*, \rho^\theta] &= (\rho_l^\theta - \rho_n^\theta) E_{nl}^*. \end{aligned} \tag{20}$$

Using these relations, simple computations show that for all (n, l) such that $\epsilon_n > \epsilon_l$ we get

$$
\begin{aligned}
\Phi_{nl}(\rho x \rho^{-1}) =& L_{nl}^* \rho x \rho^{-1} L_{nl} + L_{ln}^* \rho x \rho^{-1} L_{ln} \\
=& q_{nl} \rho_n (\rho_l^{-1} - \rho_n) E_{nl}^* x E_{nl} + q_{nl} (\rho_l - \rho_n) \rho_l^{-1} E_{nl}^* x E_{nl} \\
&+ q_{ln} \rho_l (\rho_n^{-1} - \rho_l^{-1}) E_{nl} x E_{nl}^* + q_{ln} (\rho_n - \rho_l) \rho_n^{-1} E_{nl} x E_{nl}^* \\
=& \rho \Phi_{nl}(x) \rho^{-1}.
\end{aligned}
\tag{21}
$$

The commutativity of Φ with the modular automorphism follows from the above relations.
Therefore all GKSL generators of this class have a current decomposition.

Cycle decomposition and dynamical detailed balance

Assume the (ρ, θ)-adjoint does not depend on θ. Therefore it suffices to consider the case $\theta = 0$ and talk about ρ-dynamical detailed balance. To avoid technical difficulties, we take $\mathsf{h} = \mathbb{C}^d$, (or equivalently, for the class (12), $S = \mathrm{Spect}(H_S)$ is not degenerate and finite).

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$$
\begin{aligned}
&\mathcal{L}(x) - \mathcal{L}^*_{(\rho_{H,\beta},\theta)}(x) \\
=&2i[K, x] - \sum_{\{(m,n):\epsilon_m > \epsilon_n\}} \left(\frac{J_{mn}}{\rho_m} E^*_{mn} x E_{mn} + \frac{J_{nm}}{\rho_n} E_{mn} x E^*_{mn} \right).
\end{aligned} \tag{22}
$$

Cycle: any finite collection $c = \{\epsilon_0, \ldots, \epsilon_s\}$ of different elements of S, $s \geq 2$ and $\epsilon_0 = \epsilon_s$.

Proposition 3

(Kalpazidou) If ξ is an irreducible, stationary Markov chain with finite state space S, Q-matriz $Q = (q_{i,j})_{i,j \in S}$ stationary distribution $\Pi = (\pi_i)_{i \in S}$. Then for every cycle $c = (\epsilon_0, \ldots, \epsilon_s)$ there exists $\lim_{t\to\infty} \frac{w_{c,t}(\omega)}{t} = w_c$ a.s., where $w_{c,t}(\omega)$ denotes the times that the cycle c appears in the trajectory ω up to time t and

$$w_c = (-1)^{s-1} q_{\epsilon_0,\epsilon_2} q_{\epsilon_2,\epsilon_3} \cdots q_{\epsilon_{s-1},\epsilon_s} q_{\epsilon_s,\epsilon_0} \frac{\tilde{D}(\{i_0, \ldots, i_s\}^c)}{\sum_{j \in S} \tilde{D}(\{j\}^c)}. \qquad (23)$$

Theorem 4.1

*(Kalpazidou)***(Cycle deomposition)** *If ξ is as in previous Propostion, then for every $\epsilon_i, \epsilon_j \in S$*

$$J_{ij} = \pi_i q_{i,j} - \pi_j q_{j,i} = \sum_{c \in \mathcal{C}_\infty} (w_c - w_{c_-}) J_c(i,j). \quad (24)$$

In Kalpazidou-Qians notations: w_c are the cycle “skipping rates", $\mathcal{C}_\infty$ is the set of cycles and $J_c(m,n)$ is the passage function for the cycle c, i.e., $J_c(m,n) = 1$ if the edge $(\epsilon_m, \epsilon_n) \in c$ and zero otherwise.

An immediate consequence of Kalpazidou's cyclic decomposition for the currents J_{nm} is:

Proposition 4

Let $S = \mathcal{S}pect(H_S)$ be not degenerate and finite. Let the diagonal restriction of the QMS, with generator of the form (12), be a finite Markov chain irreducible, recurrent and stationary with faithful invariant state (measure) $\rho_{H,\beta}$. Then

$$\mathcal{L}(x) - \mathcal{L}^*_{(\rho_{H,\beta},\theta)}(x) = 2i[K, x]$$

$$- \sum_{c \in \mathcal{C}_\infty} (w_c - w_{c_-}) \sum_{\{(m,n):\epsilon_m > \epsilon_n\}} J_c(m,n)\left(\rho_m^{-1} E^*_{mn} x E_{mn} - \rho_n^{-1} E_{mn} x E^*_{mn}\right).$$

Moreover one can prove.

Theorem 4.2

The following are equivalent:

(i) *The generator* $\mathcal{L}$ *is* 0*-detailed balance,*

(ii) *The classical Markov chain is reversible,*

(iii) *The classical Markov chain is in detailed balance,*

(iv) *The classical generator* $Q = (q_{i,j})_{i,j\in S}$ *satisfies Kolmogorov's reversibility condition:*

$$q_{\epsilon_0,\epsilon_1} q_{\epsilon_1,\epsilon_2} \cdots q_{\epsilon_{s-1},\epsilon_s} = q_{\epsilon_s,\epsilon_{s-1}} \cdots q_{\epsilon_2,\epsilon_1} q_{\epsilon_1,\epsilon_0}$$

for any cycle $\{\epsilon_0, \ldots, \epsilon_s\}$.

(v) $w_c = w_{c_-}, \ \forall c \in \mathcal{C}_\infty$,

(vi) *The classical entropy production rate* $e_p = 0$.

Definition 4.3

The entropy production rate for a stationary classical Markov chain:

$$e_p = \lim_{t\to\infty} \frac{1}{t} H(\mathbb{P}_{[0,t]}, \mathbb{P}^{-}_{[0,t]}),$$

where $H(\mathbb{P}_{[0,t]}, \mathbb{P}^{-}_{[0,t]})$ is the relative entropy of $\mathbb{P}$ with respect to $\mathbb{P}^{-}$ restricted to the σ-algebra $\mathcal{F}_0^t$.

$$H(\mu, \lambda) = \begin{cases} \int_M \log \frac{d\mu}{d\lambda}(x)\mu(dx) & \text{if } \mu \ll \lambda \text{ and } \log \frac{d\mu}{d\lambda} \in L_1(\mu) \\ +\infty & \text{otherwise} \end{cases}$$

Proposition 5

Assume $S = Spect(H_S)$ is not degenerate and finite, the diagonal restriction of a GKSL generator $\mathcal{L}$ of the form (12) is the generator of a irreducible, recurrent and stationary classical Markov chain with a faithful invariant state (measure) ρ. If $\mathcal{L}$ has a current decomposition (6) with currents J_{nm} satisfying Ohm's law:

$$\sum_n J_{nm} = \sum_n J_{mn},$$

for every m, then all currents are integral multiples of certain real constants.

An idea of the proof:
Under the above assumptions, in predual representation equation (6) takes the form

$$\sum_{\{(m,n):\epsilon_m>\epsilon_n\}} \left(\frac{J_{mn}}{\rho_m} E_{mn}\rho E^*_{mn} + \frac{J_{nm}}{\rho_n} E^*_{mn}\rho E_{mn}\right) = 0. \tag{26}$$

Equivalently,

$$\sum_{\{(m,n):\epsilon_m>\epsilon_n\}} J_{nm}\Big(|\epsilon_m\rangle\langle\epsilon_m| - |\epsilon_n\rangle\langle\epsilon_n|\Big) = 0. \tag{27}$$

The above equation (27) yields to a system of homogeneous d linear equations for the currents J_{mn}. Indeed, (27) together with the relations $J_{mn} = -J_{nm}$ yields the system of d equations in $\frac{d^2-d}{2}$ indeterminates (currents):

$$\begin{aligned} J_{01} + J_{02} + J_{03} + \cdots + J_{0d} &= 0 \\ -J_{01} + J_{12} + J_{13} + \cdots + J_{1d} &= 0 \\ -J_{02} - J_{12} + J_{23} + \cdots + J_{2d} &= 0 \\ &\vdots \\ -J_{0d} - J_{1d} - J_{2d} + \cdots - J_{(d-1)d} &= 0. \end{aligned} \quad (28)$$

Consider the oriented graph with set of vertices S and oriented edges

$$E = \{(\epsilon_i, \epsilon_j) : \epsilon_i < \epsilon_j, \epsilon_i, \epsilon_j \in S\}.$$

The incidence matrix of this oriented graph coincides with the matrix M of system (28). A function $Z : E \to \mathbb{Z}$ is called an integral cycle if it satisfies Ohm's law. Moreover it is well known that the set of cycles (cycle space) coincides with the null space of the incidence matrix. Therefore any solution $J = (J_{01}, \cdots, J_{0d}, J_{12}, \cdots, J_{1d}, \cdots, J_{(d-1)d})$ of (28) can be written in the form $J = aZ$ where Z is an integral cycle and a is a real constant.

- detailed balance condition holds if and only if $J_{mn} = 0$ for all m, n.

If $J_{nm} \neq 0$ for some edge (ϵ_n, ϵ_m), then there is a integral cycle Z on the graph for which $J_{nm} = aZ(\epsilon_n, \epsilon_m)$ and the corresponding vector of currents $J = aZ$, $a \neq 0$. Collecting all of these non-trivial cycles we obtain a sub-graph $\mathcal{C}$ whose complexity measures the deviation from detailed balance.

- For instance, if these sub-graph is connected, there is only one non-zero constant a.
- Otherwise there may be two or more different constants.

The sub-graph $\mathcal{C}$ consist of the set of cycles that does not satisfies Kolmogorov's reversibility condition.

Definition 4.4

Assume $h = \mathbb{C}^d$. A QMS $\mathcal{T}$ with an invariant state ρ and a KGSL generator $\mathcal{L}$ that commutes with the modular automorphism, satisfies a ρ-dynamical detailed balance condition with “complexity" n if and only if $\mathcal{L}$ has a ρ-current decomposition (6) with a subgraph $\mathcal{C}$ of non-trivial cycles with n connected components.

Example: non-equilibrium stationary state for a quantum spin chain

We apply this approach to a quantum spin chain interacting with two non-equilibrium boson fields at different temperatures. The Hamiltonian of the spin chain is defined by means of

$$H_S = \lambda_1 \sigma_1^z + \lambda_2 \sigma_2^z + (1+\gamma)\sigma_1^x \sigma_2^x + (1-\gamma)\sigma_1^y \sigma_2^y, \qquad (29)$$

where λ_1, λ_2 and γ are real numbers,

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

And we set σ_1^z for $\sigma^z \otimes I$.

Example

For $\lambda_1\lambda_2 < 1 - \gamma^2$ the spectral representation of the above Hamiltonian is given by

$$H_S = \sum_{l=0}^{3} \epsilon_l |\epsilon_l\rangle\langle\epsilon_l|, \tag{30}$$

where $\epsilon_0 = -\sqrt{(\lambda_1 - \lambda_2)^2 + 4}$, $\epsilon_1 = -\sqrt{(\lambda_1 + \lambda_2)^2 + 4\gamma^2}$, $\epsilon_2 = -\epsilon_1$, $\epsilon_3 = -\epsilon_0$ and with respect to the basis $e_- \otimes e_+$, $e_- \otimes e_-$, $e_+ \otimes e_+$, $e_+ \otimes e_-$, where $e_\pm$ are unit vectors in $\mathbb{C}^2$ such that $\sigma^x e_\pm = e_\mp$ and $\sigma^y e_\pm = \pm i e_\mp$, the coordinates of $(|\epsilon_j\rangle)_{0\leq j\leq 3}$ are

Example

$$
\begin{aligned}
|\epsilon_0\rangle &= c_0^{-\frac{1}{2}}\left(0, 2, (\lambda_1 - \lambda_2) - \sqrt{(\lambda_1 - \lambda_2)^2 + 4}, 0\right), \\
|\epsilon_1\rangle &= c_1^{-\frac{1}{2}}\left(2\gamma, 0, 0, (\lambda_1 + \lambda_2) - \sqrt{(\lambda_1 + \lambda_2)^2 + 4\gamma^2}\right), \\
|\epsilon_2\rangle &= c_2^{-\frac{1}{2}}\left(2\gamma, 0, 0, (\lambda_1 + \lambda_2) + \sqrt{(\lambda_1 + \lambda_2)^2 + 4\gamma^2}\right), \\
|\epsilon_3\rangle &= c_3^{-\frac{1}{2}}\left(0, 2, (\lambda_1 - \lambda_2) + \sqrt{(\lambda_1 - \lambda_2)^2 + 4}, 0\right),
\end{aligned}
\tag{31}
$$

Example

$$
\begin{aligned}
c_0 &= c_0(\lambda_1, \lambda_2) = 4 + \left((\lambda_1 - \lambda_2) - \sqrt{(\lambda_1 - \lambda_2)^2 + 4}\,\right)^2, \\
c_1 &= c_1(\lambda_1, \lambda_2) = 4\gamma^2 + \left((\lambda_1 + \lambda_2) - \sqrt{(\lambda_1 + \lambda_2)^2 + 4\gamma^2}\,\right)^2, \\
c_2 &= c_2(\lambda_1, \lambda_2) = 4\gamma^2 + \left((\lambda_1 + \lambda_2) + \sqrt{(\lambda_1 + \lambda_2)^2 + 4\gamma^2}\,\right)^2, \\
c_3 &= c_3(\lambda_1, \lambda_2) = 4 + \left((\lambda_1 - \lambda_2) + \sqrt{(\lambda_1 - \lambda_2)^2 + 4}\,\right)^2.
\end{aligned}
\tag{32}
$$

Notice that $\epsilon_0 < \epsilon_1 < \epsilon_2 < \epsilon_3$ and the set of Bohr frequencies is given explicitly by

$$F = \{\omega = \epsilon_r - \epsilon_{r'} : \epsilon_r, \epsilon_{r'} \in \mathrm{Spec}(H_S)\} = \{\omega_{10}, \omega_{20}, \omega_{30}, \omega_{21}\}, \quad (33)$$

with $\omega_{10} = \epsilon_1 - \epsilon_0, \omega_{20} = \epsilon_2 - \epsilon_0, \omega_{30} = \epsilon_3 - \epsilon_0, \omega_{21} = \epsilon_2 - \epsilon_1$; $\omega_{31} = \epsilon_3 - \epsilon_1 = \omega_{20}$, and $\omega_{32} = \epsilon_3 - \epsilon_2 = \omega_{10}$. Hence we are in the case of a non-generic Hamiltonian. For simplicity we will write simply $\omega_1 = \omega_{10}, \ \omega_2 = \omega_{20}, \ \omega_3 = \omega_{30}, \ \omega_4 = \omega_{21}, \ \omega_5 = \omega_{31}$ and $\omega_6 = \omega_{32}$.

The interaction of the spin chain with the two non-equilibrium boson fields is described by the Hamiltonian

$$\begin{aligned} H =& H_0 + \lambda \sum_{j=1,2} H_{I_j}, \quad (\lambda \text{ is a coupling constant}), \\ H_0 =& H_S + H_B, \\ H_B =& \sum_j \int \omega_j(k) a^\dagger_{j,k} a_{j,k}, \quad [a_{j,k}, a^\dagger_{j',k'}] = \delta_{jj'}\delta(k-k'), \\ H_{I_j} =& \int dk \left(g_j(k) D_j a^\dagger_{j,k} + g^*_j(k) D^\dagger_j a_{j,k} \right), \end{aligned} \quad (34)$$

where $D_j = \sigma_j^-$, $\sigma^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$, $a_{j,k}$ and $a^\dagger_{j,k}$ are the annihilation and creation operators of the j-th field ($j = 1, 2$) and $g_j(k)$ is a form factor.

The initial state of each field is a Gibbs state at constant temperature β_j^{-1} and chemical potential μ_j with respect to the free Hamiltonian (in this example we assume $\mu_j = 0, \ \ j = 1, 2$), i.e., the mean zero gauge invariant Gaussian state with correlations

$$\begin{aligned} \langle a^{\dagger}_{j,k} a_{j',k'} \rangle =& \delta_{jj'} N(k; \beta_j) \delta(k - k'), \\ N(k; \beta_j) =& \frac{1}{e^{\beta_j \omega_j(k)} - 1}. \end{aligned} \tag{35}$$

Example

The Schrödinger equation in the interaction picture is

$$\frac{d}{dt}U_t^{(\lambda)} = -i\lambda H_I(t)U_t^{(\lambda)}, \quad U_t^{(\lambda)} = e^{itH_0}e^{-itH_0}, \tag{36}$$

$$H_I(t) = \sum_{j=1,2} e^{itH_0}H_{I_j}e^{-itH_0} =$$

$$\sum_{j=1,2}\sum_{\omega\in F}\sum_{l,m}\int dk\Big(g_{j;l,m}(k)E_\omega(l,m)a_{j,k}^\dagger e^{i(\omega_j(k)-\omega)t} + g_{j;l,m}^*(k)E_\omega^\dagger(l,m)a$$

$$g_{j;l,m}(k) = g_j(k)\langle\epsilon_l, D_j\epsilon_m\rangle,$$

$$E_\omega(l,m) = \sum_{\epsilon_r\in F_\omega}\langle\epsilon_r-\omega|\epsilon_l\rangle\langle\epsilon_m|\epsilon_r\rangle|\epsilon_r-\omega\rangle\langle\epsilon_r|,$$

$$\omega = \epsilon_m-\epsilon_l, \quad \epsilon_m > \epsilon_l; \; F_\omega = \{\epsilon_{r'}\in \mathrm{Spec}(H_S) : \epsilon_{r'}-\omega \in \mathrm{Spec}(H_S)$$

Example

With Δ, $\gamma_{\pm,j,\omega}$ given by (16), (18) and (19), respectively. Taking $g_j(k) = e^{-\frac{1}{2}|k|^2}$, $j = 1, 2$ using (19), (18) and (38), after some computation we get for $\lambda_1\lambda_2 < 1 - \gamma^2$ and $d = 3$

Example

The restriction of the predual GKSL generator to the diagonal sub-algebra, coincides with the generator of a classical Markov chain (or Q-matrix) given by

$$Q = \begin{pmatrix} -(q_{01}+q_{03}) & q_{01} & 0 & q_{03} \\ q_{10} & -(q_{10}+q_{12}) & q_{12} & 0 \\ 0 & q_{21} & -(q_{21}+q_{23}) & q_{2} \\ q_{30} & 0 & q_{32} & -(q_{30}+q_{32}) \end{pmatrix}.$$

Example

$$q_{10} = \Gamma_{-,\epsilon_1-\epsilon_0} = 4\pi^2 \frac{(c_1 - 4\gamma^2)}{c_0 c_1} \omega_1 e^{-\omega_1} \Big(4 \frac{e^{\beta_1\omega_1}}{e^{\beta_1\omega_1} - 1} + (c_0 - 4)^2 \frac{e^{\beta_2\omega_1}}{e^{\beta_2\omega_1} - 1}\Big),$$

$$q_{01} = 4\pi^2 \frac{(c_1 - 4\gamma^2)}{c_0 c_1} \omega_1 e^{-\omega_1} \Big(\frac{4}{e^{\beta_1\omega_1} - 1} + \frac{(c_0 - 4)^2}{e^{\beta_2\omega_1} - 1}\Big), \quad (39)$$

$$q_{20} = 8\pi^2 \frac{(c_2 - 4\gamma^2)^2}{c_0 c_2} \omega_2 e^{-\omega_2} \Big(4 \frac{e^{\beta_1\omega_2}}{e^{\beta_1\omega_2} - 1} + (c_0 - 4)^2 \frac{e^{\beta_2\omega_2}}{e^{\beta_2\omega_2} - 1}\Big),$$

$$q_{02} = 8\pi^2 \frac{(c_2 - 4\gamma^2)^2}{c_0 c_2} \omega_2 e^{-\omega_2} \Big(\frac{4}{e^{\beta_1\omega_2} - 1} + \frac{(c_0 - 4)^2}{e^{\beta_2\omega_2} - 1}\Big),$$

Example

$$q_{31} = 8\pi^2 \frac{4\gamma^2}{c_1 c_3}\omega_2 e^{-\omega_2}\left((c_3-4)^2\frac{e^{\beta_1\omega_2}}{e^{\beta_1\omega_2}-1} + 4\frac{e^{\beta_2\omega_2}}{e^{\beta_2\omega_2}-1}\right),$$

$$q_{13} = 8\pi^2 \frac{4\gamma^2}{c_1 c_3}\omega_2 e^{-\omega_2}\left(\frac{(c_3-4)^2}{e^{\beta_1\omega_2-1}} + \frac{4}{e^{\beta_2\omega_2}-1}\right),$$

$$q_{32} = 8\pi^2 \frac{1}{c_2 c_3}\omega_1 e^{-\omega_1}\left((c_3-4)^2\frac{e^{\beta_1\omega_1}}{e^{\beta_1\omega_1}-1} + 16\gamma^2\frac{e^{\beta_2\omega_1}}{e^{\beta_2\omega_1}-1}\right),$$

$$q_{23} = 8\pi^2 \frac{1}{c_2 c_3}\omega_1 e^{-\omega_1}\left(\frac{(c_3-4)^2}{e^{\beta_1\omega_1}-1} + \frac{16\gamma^2}{e^{\beta_2\omega_1}-1}\right).$$

And all remaining $q_{ij}'s$ equal zero.

Example

The classical Markov chain with the above Q-matrix is irreducible, i.e., starting from any ϵ_j it is possible to reach any ϵ_k with positive probability. Moreover it has an invariant measure, that we identify with the generalized Gibbs state ρ.

Example

To identify the cycles that does not satisfy Kolmogorov's reversibility condition, one can use formula 23 in, to evaluate the cycle skipping rates in terms of the matrix elements of Q. It follows that for all cycles we have $w_c = w_{c_-}$ with the exception of the cycle $c = (0, 2, 3, 1)$. Therefore Kolmogorov's reversibility condition does not hold for this cycle. Moreover we can prove the following.

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Proposition 6

Kolmogorov's reversibility condition holds for the cycle $(0, 2, 3, 1)$, *i.e.,*

$$q_{02}q_{23}q_{31}q_{10} = q_{01}q_{13}q_{32}q_{20},$$

for all values of ω_1, ω_2*; if and only if the boson fields are at the same temperature,* $\beta_1^{-1} = \beta_2^{-1}$.

Corollary 4.5

If $\beta_1^{-1} \neq \beta_2^{-1}$ then the GKSL generator of the QMS associated with the above spin chain, satisfies a ρ-dynamical detailed balance with constant non-zero currents $J_{ij} = \pm J_{01}$.

Proof.

If $\beta_1^{-1} \neq \beta_2^{-1}$, then Kolmogorov's reversibility condition is violated for the cycle $(0, 2, 3, 1)$ i.e.,

$$q_{02}q_{23}q_{31}q_{10} \neq q_{01}q_{13}q_{32}q_{20}. \tag{40}$$

Then, associated with this cycle is the solution of system (28): $J_{20} = -J_{01}, \;\; J_{13} = J_{01}, \;\; J_{32} = -J_{01}$ and all remaining J_{mn}'s equal zero. This proves the corollary. □

The invariant state ρ is a solution of the linear system,

$$\mathcal{M}\rho = \mathrm{j}, \tag{41}$$

with $\mathrm{j} = J_{01}(1, -1, 1, -1)$ and

$$\mathcal{M} = \begin{pmatrix} -q_{01} & q_{10} & 0 & 0 \\ -q_{02} & 0 & q_{20} & 0 \\ 0 & -q_{13} & 0 & q_{31} \\ 0 & 0 & -q_{23} & q_{32} \end{pmatrix}.$$

Example

Direct computations show that the unique solution of (41) has the explicit form $\tilde{\rho} = (\rho_0, \rho_1, \rho_2, \rho_3)$, with

$$
\begin{aligned}
\rho_0 &= \frac{(q_{13}q_{20}q_{32} + q_{10}(q_{23}q_{31} + q_{20}(q_{31} + q_{32})))J_{01}}{\mathrm{Det}(\mathcal{C})},\\
\rho_1 &= \frac{(q_{02}q_{23}q_{31} + q_{01}(q_{23}q_{31} + q_{20}(q_{31} + q_{32})))J_{01}}{\mathrm{Det}(\mathcal{C})},\\
\rho_2 &= \frac{(q_{01}q_{13}q_{32} + q_{02}(q_{13}q_{32} + q_{10}(q_{31} + q_{32})))J_{01}}{\mathrm{Det}(\mathcal{C})},\\
\rho_3 &= \frac{(q_{02}(q_{10} + q_{13})q_{23} + q_{01}q_{13}(q_{20} + q_{23}))J_{01}}{\mathrm{Det}(\mathcal{C})}.
\end{aligned}
\tag{42}
$$

Where

$$\mathrm{Det}(\mathcal{C}) = q_{02}q_{23}q_{31}q_{10} - q_{01}q_{13}q_{32}q_{20}.$$

The value of the current J_{01} is obtained in terms of the $q'_{ij}s$ from the normalization condition $\mathrm{tr}(\tilde{\rho}) = 1$.

If a generic QMS $(\mathcal{T}_t)_{t\geq 0}$ is irreducible and has an invariant measure ρ, then this state is the unique $\mathcal{T}_t$-invariant state and

$$\lim_{t\to\infty} \mathcal{T}_{*t}(\sigma) = \rho, \tag{43}$$

for every initial normal state. σ.

Hence, as a consequence of the above result, the QMS associated with our quantum spin chain is ergodic, in the sense that any initial normal state is driven by the QMS towards the dynamical equilibrium steady state ρ.

Cycle dynamics and entropy production

Our analysis of the cycle decomposition of a GKSL generator satisfying a ρ-dynamical detailed balance reveals that, in a non-equilibrium stationary state of the small system coupled to the environment, there exists a dynamics associated with the set $\mathcal{C}$ of cycles violating Kolmogorov's reversibility condition. This section is devoted to an initial study of this cycle dynamics.

The first important question is give a physical meaning to the map $\Pi_{\rho_{H,\beta}}$ in current decomposition (4). First of all notice that this is a CCP map, i.e., a quantum object. One can compute explicitly $\Pi_{\rho_{H,\beta}}$ in the case of the spin chain of Example 1 above. In this case $\Pi_{\rho_{H,\beta}}$ is not identically zero, it has a non-trivial contribution coming from the cycle $(0, 2, 3, 1)$. Moreover, denoting by $\Pi_{\rho_{H,\beta},*}$ its predual, one can show that $\Pi_{\rho_{H,\beta},*}(\rho_{H,\beta})$ is the diagonal matrix

$$\begin{pmatrix} w_{(0231)} - w_{(1320)} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -w_{(0231)} + w_{(1320)} \end{pmatrix}.$$

A naive interpretation of this quantity is the following: $\Pi_{\rho_{H,\beta}}(\rho_{H,\beta})$ represents the net current (or flow of energy) between the fields through the small system, i.e., the spin chain. Indeed, at level ϵ_0, the spin chain is taken a quantity $w_{(0231)} - w_{(1320)}$ of energy from environment at temperature $\beta_1^{-1} > \beta_2^{-1}$, the same quantity is transfer to environment at temperature β_2^{-1} at level ϵ_3. The quantity $w_{(0231)} - w_{(1320)}$ can be computed explicitly in terms of the matrix elements q_{mn} of the classical generator Q, i.e., in terms of the temperatures β_1^{-1}, β_2^{-1}.

For an irreducible and stationary continuous time Markov chain, the notion of entropy production was defined by the Qian's and collaborators, see Chapter 2 in [Qian's et al], in terms of the relative entropy of the probabilities of the Markov chain and its time reversed. This entropy production rate has a simple expression in terms of the cycle skipping rates w_c of cycles in $\mathcal{C}$, indeed,

$$e_p = \frac{1}{2} \sum_{c \in \mathcal{C}_\infty} (w_c - w_{c_-}) \log(\frac{w_c}{w_{c_-}}). \tag{44}$$

One can evaluate the entropy production for the spin chain. Indeed, a direct computation show that

$$\begin{aligned} e_p =& (w_{(0231)} - w_{(0132)}) \log \frac{w_{(0231)}}{w_{(0132)}} \\ =& -\frac{q_{02}q_{23}q_{31}q_{10} - q_{01}q_{13}q_{32}q_{20}}{\sum_{j=0}^{3} \tilde{D}(\{j\}^c)} \log \frac{q_{02}q_{23}q_{31}q_{10}}{q_{01}q_{13}q_{32}q_{20}}; \end{aligned} \tag{45}$$

where

$$\begin{aligned} \tilde{D}(\{0\}^c) &= q_{13}q_{20}q_{32} + q_{10}q_{23}q_{31} + q_{10}q_{20}q_{31} + q_{10}q_{20}q_{32} \\ \tilde{D}(\{1\}^c) &= q_{02}q_{23}q_{31} + q_{01}q_{23}q_{31} + q_{01}q_{20}q_{31} + q_{01}q_{20}q_{32} \\ \tilde{D}(\{2\}^c) &= q_{01}q_{13}q_{32} + q_{02}q_{13}q_{32} + q_{02}q_{10}q_{31} + q_{02}q_{10}q_{32} \\ \tilde{D}(\{3\}^c) &= q_{02}q_{10}q_{23} + q_{02}q_{13}q_{23} + q_{01}q_{12}q_{20} + q_{01}q_{13}q_{23}. \end{aligned} \tag{46}$$

Therefore, entropy production is non-zero since Kolmogorov's

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