CYCLE DECOMPOSITION OF

QUANTUM MARKOV SEMIGROUPS

AND

NON-EQUILIBRIUM PHENOMENA

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Free Probabilities, Operator Spaces and von Neumann Algebras

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Outline

- irreversible evolution (Markov)

  $\searrow$ semigroup of (completely) positive maps

- stationary regime

  $\searrow$ invariant state ρ for c.p. maps $\mathcal{T}_t$

- equilibrium regime

  $\searrow$ $\mathcal{T}_t$ symmetric ($\mathcal{T}_t = \widetilde{\mathcal{T}}_t$ ρ-dual)

- non-equilibrium regime

  ... lack of good characterisations

Outline - 2

Proposal: find good representations of

$$\mathcal{L} - \widetilde{\mathcal{L}}$$

generators of $(\mathcal{T}_t)$ and $(\widetilde{\mathcal{T}}_t)$

Models:

- Spohn - Lebowitz, **CMP 54** (1977)
- Gallavotti - Cohen, **JSP 80** (1995)
- Rey-Bellet - Thomas, **CMP 215** (2000), **CMP 225** (2002)
- Accardi - Imafuku, `quant-ph/0209088` (2002)

Common feature:

$\mathcal{L} - \widetilde{\mathcal{L}}$ must show *micro-currents*.

Reversible Markov Chains

$T = (T_{ij})_{i,j\in E}$ stochastic matrix

$$T_{ij} > 0, \qquad \sum_{j\in E} T_{ij} = 1,$$

E countable.

$\pi = (\pi_j)_{j\in E}$ faithful invariant distribution

$$\pi_i > 0, \ \sum_{j\in E} \pi_j = 1, \quad \pi_j = \sum_{k\in E} \pi_k T_{kj}$$

Def. (T, π) is *reversible* (or π is an equilibrium distribution for T) if

$$\pi_i T_{ij} = \pi_j T_{ji}, \quad \forall i, j \quad (\textit{detailed balance})$$

Rem. Scalar product on $L^2(E; \pi)$

$$\langle g, f\rangle = \sum_{j\in E} \pi_j \bar{g}_j f_j$$

(T, π) is *reversible* if and only if

$$\langle g, Tf\rangle = \langle Tg, f\rangle$$

Reversible MC - time continuous case

$T(t) := (T_{ij}(t))_{i,j\in E}$ transition op. at time t

$$T_{ij}(t) \geq 0, \quad \sum_{j\in E} T_{ij}(t) = 1,$$

semigroup prop. $T(t+s) = T(t)T(s)$, $t, s \geq 0$

Generator $Q = (q_{ij})_{i,j\in E}$

$$q_{ij} = \lim_{t\to 0^+} \frac{T_{ij}(t) - \delta_{ij}}{t}$$

$$\pi_i T_{ij}(t) = \pi_j T_{ji}(t) \ \forall t \quad \Leftrightarrow \quad \pi_i q_{ij} = \pi_j q_{ji}$$

π-**dual** $\widetilde{T}$

$$\langle g, T(t)f\rangle = \sum_{j\in E} \pi_i \bar{g}_i T_{ij}(t) f_j = \langle \widetilde{T}(t)g, f\rangle$$

$$\boxed{\widetilde{T}(t)g = \pi^{-1} T^*(t)(\pi g)}$$

Deviation from equilibrium

"distance" between T and $\widetilde{T}$

"distance" between Q and $\widetilde{Q}$

$$M_\pi Q \qquad M_\pi \widetilde{Q} = Q^* M_\pi$$

$$(i,j) \to \pi_i q_{ij} \qquad (i,j) \to \pi_j q_{ji}$$

$$\uparrow \qquad\qquad \uparrow$$

forward backward

probability densities on $E \times E$

Equilibrium-deviation can be "measured" by

1) numerical index: *relative entropy*,

2) currents $\pi_i q_{ij} - \pi_j q_{ji} = (M_\pi Q - Q^* M_\pi)_{ij}$,

3) structure of $M_\pi Q - Q^* M_\pi$.

Cycle decomp. of classical Markov chains

Finite Markov Chain, transition matrix (q_{ij})

Defn. A n-cycle is n-tuple of transitions

$$i_1 \to i_2 \to \cdots \to i_n \to i_{n+1} = i_1$$

$i_1, \ldots, i_n$ distinct.

Thm. (*Cycle decomposition*)

$$\boxed{\pi_i q_{ij} = \sum_{c \in \mathcal{C}} w_c J_c(i,j)}$$

- $\mathcal{C}$ family of cycles,
- J_c (shift $i_1 \to i_2 \to \cdots \to i_n$) passage matrix

  $J_c(h,k) = 1$ if $h = i_\ell, k = i_{\ell+1}$ for some ℓ
  $J_c(h,k) = 0$ otherwise

- $w_c > 0$ constants

Corollary

$$\boxed{\pi_i q_{ij} - \pi_j q_{ji} = \textstyle\sum_{c\in\mathcal{C}} w_c \left(J_c(i,j) - J_{c^-}(i,j)\right)}$$

where c^- is the reverse of the cycle c.

Rem. Defining

$$\begin{aligned} \bar{J}_c(h,k) = J_c(h,k) = 1 \quad &\text{if} \quad h = i_\ell, k = i_{\ell+1} \\ \bar{J}_c(h,k) = \delta_{hk} \qquad &\text{otherwise} \end{aligned}$$

(completion of J_c to a full permutation matrix) $\bar{J}_{c^-} = \bar{J}_c^{-1}$ and the unitary matrices $\bar{J}_c$ define automorphisms of $\ell^\infty(E)$.

$$M_\pi Q - Q^* M_\pi = \sum_{c\in\mathcal{C}} w_c \left(\bar{J}_c - \bar{J}_{c^-}\right)$$

Non-equilibrium

<u>*Simplest model:*</u> $E = \{1, 2, 3\}$

$$Q = \begin{pmatrix} -1 & 1 & 0 \\ 0 & -1 & 1 \\ 1 & 0 & -1 \end{pmatrix}, \quad \tilde{Q} = \begin{pmatrix} -1 & 0 & 1 \\ 1 & -1 & 0 \\ 0 & 1 & -1 \end{pmatrix}$$

$$Q - \tilde{Q} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

1 cycle, $Q - \tilde{Q} =$right shift - left shift, $w_c = 1$

<u>*Further models:*</u>

"distance" from equilibrium related to: minimal number of cycles, values w_c, ...

noncommutative versions ...

Quantum Markov Semigroups

h complex separable Hilbert space

$\mathcal{T} = (\mathcal{T}_t)_{t\geq 0}$ semigroup of completely positive, identity preserving maps on $\mathcal{B}(\mathsf{h})$.

ρ faithful normal invariant state

$$\mathrm{tr}(\rho\mathcal{T}_t(x)) = \mathrm{tr}(\rho x) \quad \forall t \quad \text{i.e.} \quad \mathcal{T}_{*t}(\rho) = 0$$

$\mathcal{T}_* = (\mathcal{T}_{*t})_{t\geq 0}$ predual semigroup.

Dual semigroup(s) $\widetilde{\mathcal{T}}$ with respect to ρ

$$\begin{aligned} \mathrm{tr}(\rho\widetilde{\mathcal{T}}_t(x)y) &= \mathrm{tr}(\rho x\mathcal{T}_t(y)) \qquad \text{or} \\ \mathrm{tr}(\rho^s\widetilde{\mathcal{T}}_t(x)\rho^{1-s}y) &= \mathrm{tr}(\rho^s x\rho^{1-s}\mathcal{T}_t(y)) \quad s\in[0,1] \end{aligned}$$

$$\boxed{\widetilde{\mathcal{T}}_t(x) = \rho^{-(1-s)}\mathcal{T}_{*t}(\rho^{1-s}x\rho^s)\rho^{-s}}$$

Contrary to comm. case $\widetilde{\mathcal{T}}$ may not be $*$-map, i.e. $\widetilde{\mathcal{T}}_t(a)^* \neq \widetilde{\mathcal{T}}_t(a^*)$ for some a if $s \neq 1/2$.

When is $\widetilde{\mathcal{T}}$ a QMS for $s = 0$?

$$\widetilde{\mathcal{T}}_t(x) = \rho^{-1}\mathcal{T}_{*t}(\rho x)$$

$$\begin{aligned}(\widetilde{\mathcal{T}}_t(x))^* = \widetilde{\mathcal{T}}_t(x^*) \ &\Rightarrow \ \widetilde{\mathcal{T}}_t(x) = \mathcal{T}_{*t}(x\rho)\rho^{-1} \\ &\Rightarrow \ \rho^{-1}\mathcal{T}_{*t}(\rho x) = \mathcal{T}_{*t}(x\rho)\rho^{-1} \\ &\Rightarrow \ \rho^{-1}\mathcal{T}_{*t}(\rho x\rho^{-1})\rho = \mathcal{T}_{*t}(x)\end{aligned}$$

If $\quad \sigma_t(a) := \rho^{it}a\rho^{-it} \qquad$ then

$\mathcal{T}_{*t} \circ \sigma_{-i} = \sigma_{-i} \circ \mathcal{T}_{*t}$ and $\mathcal{T}_t \circ \sigma_{-i} = \sigma_{-i} \circ \mathcal{T}_t$

Thm. (F-G-K-V) (under some assumptions) $\widetilde{\mathcal{T}}$ is a QMS if and only if $\mathcal{T}_t \circ \sigma_{-i} = \sigma_{-i} \circ \mathcal{T}_t$.

Thm. (Majewski-Streater, J Phys A **31** '88) $\widetilde{\mathcal{T}}$ is a QMS if and only if $\widetilde{\mathcal{T}}$ is a $*$-map. In this case $\mathcal{T}_t \circ \sigma_z = \sigma_z \circ \mathcal{T}_t$ ($|z| \leq 1/2$) and duals of $\mathcal{T}$ for $s \in [0, 1]$ coincide.

Quantum detailed balance (QDB)

QMS $\mathcal{T}$ with dual $\widetilde{\mathcal{T}}$ which is still a QMS and

$$\mathcal{L}(a) - \widetilde{\mathcal{L}}(a) = 2i\,[K, a]\,, \qquad K = K^*.$$

Remark 1. ρ is invariant state for $\mathcal{T}$ and $\widetilde{\mathcal{T}}$. Consequence $[K, \rho] = 0$.

Remark 2. In the commutative case there is no derivation $a \to i\,[K, a]$ because derivations $\delta : \ell^\infty(E) \to \ell^\infty(E)$ (E discrete!) are trivial.

$$\begin{aligned} &\delta(1_{\{j\}}) = \delta(1_{\{j\}}^2) = 2\delta(1_{\{j\}})1_{\{j\}} \\ \Rightarrow\ &\delta(1_{\{j\}}) = \varphi_j 1_{\{j\}}, \quad 0 = \delta(1) = \sum_j \varphi_j 1_{\{j\}} \end{aligned}$$

Remark 3. $\widetilde{\mathcal{L}} = \mathcal{L} - 2i[K, \cdot]$ is conditionally completely positive $\Rightarrow \widetilde{\mathcal{T}}$ is a QMS and both $\widetilde{\mathcal{T}}_t$, $\widetilde{\mathcal{L}}$ commute with σ_{-i}

Generators commuting with σ_{-i}

Theorem (FF-VU, **IDAQP** '07) A generator $\mathcal{L}$ commutes with σ_{-i} if and only if

$$\mathcal{L}(a) = G^* a + \Phi(a) + aG$$

1) $[G, \rho] = 0$,
2) Φ completely positive commuting with σ_{-i},
3) structure $\Phi(a) = \sum_\ell L_\ell^* a L_\ell$ where

$$\sigma_{-i}(L_\ell) = \lambda_\ell L_\ell,\ \lambda_\ell > 0,$$

4) G and Φ with the above properties are unique.

Indeed, G is unique up to irI with $r \in \mathbb{R}$.

Corollary. If $\mathcal{L}$ commutes with σ_{-i} then

$$\widetilde{\mathcal{L}}(a) = Ga + \widetilde{\Phi}(a) + aG^*$$

where

$$\widetilde{\Phi}(a) = \sum_\ell \lambda_\ell^{-1} L_\ell a L_\ell^*$$

Deviation from q-detailed balance

$$\begin{aligned}\mathcal{L}(a) &= G^*a + \Phi(a) + aG \\ \widetilde{\mathcal{L}}(a) &= Ga + \widetilde{\Phi}(a) + aG^*\end{aligned}$$

$$\Phi(a) = \sum_\ell L_\ell^* a L_\ell \qquad \widetilde{\Phi}(a) = \sum_\ell \lambda_\ell^{-1} L_\ell a L_\ell^*$$

Putting $G - G^* = 2iK$, (K self-adjoint)

$$\mathcal{L}(a) - \widetilde{\mathcal{L}}(a) - 2i[K,a] = \Phi(a) - \widetilde{\Phi}(a)$$

Deviation from QDB: $\Phi - \widetilde{\Phi}$

Commutative inspiration:

write it as difference of automorphisms ...

Non commutative examples

Two-level systems

$\mathsf{h} = \mathbb{C}^2$. $\mathcal{T}$, $\widetilde{\mathcal{T}}$ are QMS iff

$$\begin{aligned}\mathcal{L}(a) &= i[H,a] - \frac{\eta^2}{2}\left(L^2 a - 2LaL + aL^2\right) \\ &\quad -\frac{\lambda^2}{2}\left(\sigma^-\sigma^+ a - 2\sigma^- a\sigma^+ + a\sigma^-\sigma^+\right) \\ &\quad -\frac{\mu^2}{2}\left(\sigma^+\sigma^- a - 2\sigma^+ a\sigma^- + a\sigma^+\sigma^-\right),\end{aligned}$$

with $[L,\rho] = 0 = [H,\rho]$, $\eta, \lambda, \mu \geq 0$ and

$$\sigma^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad \sigma^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix},$$

Consequence: QDB holds.

As in the commuative case!

Three-level system

$\widetilde{\mathcal{T}}$ QMS; no q-detailed balance

$\mathsf{h} = \mathbb{C}^3 \qquad (e_1, e_2, e_3)$ basis,

$$Se_j = e_{j+1} \qquad \text{(mod 3)}$$

$$\mathcal{L}(a) = S^* a S - a$$

$\rho = \frac{\mathrm{I}}{3}$ (normalized trace)

$$\widetilde{\mathcal{L}}(a) \;=\; SaS^* \,-\, a$$

$\mathcal{T}$, $\widetilde{\mathcal{T}}$ are QMSs, QDB does not hold

$$\mathcal{L}(a) - \widetilde{\mathcal{L}}(a) = S^* a S - S a S^*$$

Non-equilibrium $(\mathcal{T}, \rho)$: classification

Natural generalisation: for $x \in \mathcal{B}(\mathsf{h})$ write

$$\rho^{\frac{1}{2}} \left(\mathcal{L}(x) - \widetilde{\mathcal{L}}(x) - 2i[H, x]\right) \rho^{\frac{1}{2}}$$

equal to

$$\rho^{\frac{1}{2}} \left(\Phi(x) - \widetilde{\Phi}(x)\right) \rho^{\frac{1}{2}}$$

in the form

$$\sum_{c \in \mathcal{C}} w_c \left(U_c^* x U_c - U_c x U_c^*\right)$$

with

- U_c unitary
- $w_c > 0$

Generic QMSs - d levels

$\mathsf{h} = \mathbb{C}^d$, $\quad (e_j)_{1\leq j\leq d}$ o.n. basis, $\quad E_k^j = |e_k\rangle\langle e_j|$

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

$$Ge_j = -\left(\frac{\mu_j}{2} + i\kappa_j\right) e_j, \qquad He_j = i\kappa_j\, e_j$$

$$\Phi(x) = \sum_{j,k} \varphi_{jk} |e_j\rangle\langle e_k|x|e_k\rangle\langle e_j|$$

where $\mu_j, \varphi_{jk} > 0$, $\kappa_j \in \mathbb{R}$

$$\mu_j = \sum_k \varphi_{jk} \quad \Rightarrow \quad \mathcal{L}(I) = 0$$

Invariant state

$$\rho = \sum_j \rho_j |e_j\rangle\langle e_j|$$

Rem. Generic QMSs form an open dense set in the class of QMSs obtained from the stochastic (weak-coupling) limit.

Generic QMSs - d levels (cont.)

Putting

$$w_{jk} := \rho_j \varphi_{jk} - \rho_k \varphi_{kj}$$

we can write $\rho^{\frac{1}{2}} \left(\Phi(x) - \widetilde{\Phi}(x) \right) \rho^{\frac{1}{2}}$ as

$$\sum_{j<k<d} w_{jk} \left(\frac{1}{d} \sum_{m=1}^{d} \left(U_m^{(jk)*} x U_m^{(jk)} - U_m^{(jk)} x U_m^{(jk)*} \right) \right)$$

where

$$\begin{aligned} U_m^{(jk)} &= \mathrm{e}^{\frac{2\pi i}{d} mj} |e_k\rangle\langle e_j| + \mathrm{e}^{\frac{2\pi i}{d} mk} |e_d\rangle\langle e_k| \\ &+ \mathrm{e}^{\frac{2\pi i}{d} md} |e_k\rangle\langle e_d| + \sum_{h \neq j,k,d} \mathrm{e}^{\frac{2\pi i}{d} mh} |e_h\rangle\langle e_h| \end{aligned}$$

Impossible to write $\rho^{\frac{1}{2}} \left(\Phi(x) - \widetilde{\Phi}(x) \right) \rho^{\frac{1}{2}}$ as

$$\sum_{j<k<d} w_{jk} \left(V^{(jk)*} x V^{(jk)} - V^{(jk)} x V^{(jk)*} \right)$$

for unitaries $V^{(jk)}$.