ENTROPY PRODUCTION OF QUANTUM MARKOV SEMIGROUPS

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QP 31

Bengaluru, August 13-18, 2010

Outline

1. classical symmetry & detailed balance (reversibility)

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3. symmetry & Markov semigroups (quantum)

4. quantum detailed balance (reversibility)

5. structure of QDB generators

6. entropy production of QMS

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classical symmetry

$\mathcal{A} = L^\infty(E, \mathcal{E}, \mu)$,

$T := (T_t)_{t\geq 0}$ Markov semigroup on $\mathcal{A}$

π invariant density (faithful)

symmetry / reversibility

$$\int_E \mathrm{d}\mu\, \pi g\, T_t f \;=\; \int_E \mathrm{d}\mu\, \pi\, T_t g\, f$$

in an equivalent way

$$\langle g, T_t f\rangle_{L^2(E,\mathcal{E},\mu)} = \langle T_t g, f\rangle_{L^2(E,\mathcal{E},\mu)}$$

Entropy production measures deviation form symmetry

classical entropy production

Forward and backward states on $\mathcal{A} \otimes \mathcal{A}$

$$\overrightarrow{\Pi}_t (g \otimes f) = \int_E \mathrm{d}\mu \, \pi \, g \, T_t f,$$
$$\overleftarrow{\Pi}_t (g \otimes f) = \int_E \mathrm{d}\mu \, \pi \, T_t g \, f.$$

$(X_t)_{t \geq 0}$ Markov process with initial law π and transition semigroup T

$$\overrightarrow{\Pi}_t (g \otimes f) = \mathbb{E}_\pi [g(X_0) f(X_t)]$$
$$\overleftarrow{\Pi}_t (g \otimes f) = \mathbb{E}_\pi [g(X_t) f(X_0)]$$

Relative entropy

$$S\left(\overrightarrow{\Pi}_t \mid \overleftarrow{\Pi}_t\right)$$

Entropy production

$$\lim_{t \to 0^+} \frac{S\left(\overrightarrow{\Pi}_t \mid \overleftarrow{\Pi}_t\right)}{t}$$

densities of $\overrightarrow{\Pi}_t$, $\overleftarrow{\Pi}_t$

$$(T_t f)(x) = \int_E \mu(\mathrm{d}y)\, p_t(x,y) f(y)$$

then

$$\overrightarrow{\Pi}_t\,(g \otimes f)$$
$$= \int_{E\times E} \mu(\mathrm{d}x)\mu(\mathrm{d}y)\, \pi(x) p_t(x,y)\, g(x) f(y)$$

$$\overleftarrow{\Pi}_t\,(g \otimes f)$$
$$= \int_{E\times E} \mu(\mathrm{d}x)\mu(\mathrm{d}y)\, \pi(y) p_t(y,x)\, g(x) f(y)$$

densities w.r.t. $\mu \otimes \mu$

$$\overrightarrow{\Pi}_t \qquad (x,y) \to \pi(x) p_t(x,y)$$
$$\overleftarrow{\Pi}_t \qquad (x,y) \to \pi(y) p_t(y,x)$$

typically *strictly positive* $\mu \otimes \mu$ a.e.

classical explicit formula

Then $S\left(\overrightarrow{\Pi}_t \mid \overleftarrow{\Pi}_t\right)$ is

$$\int \mu(\mathrm{d}x)\mu(\mathrm{d}y)\pi(x)p_t(x,y)\log\left(\frac{\pi(x)p_t(x,y)}{\pi(y)p_t(y,x)}\right)$$

Suppose

$$p_t(x,y) = \delta(x,y) + tq(x,y) + o(t)$$

then $S\left(\overrightarrow{\Pi}_t \mid \overleftarrow{\Pi}_t\right)$, for $t \to 0$ is

$$\approx t\int \mu(\mathrm{d}x)\mu(\mathrm{d}y)\pi(x)q(x,y)\log\left(\frac{\pi(x)q(x,y)}{\pi(y)q(y,x)}\right)$$

The entropy production EP is given by

$$EP = \int \mu(\mathrm{d}x)\mu(\mathrm{d}y)\pi(x)q(x,y)\log\left(\frac{\pi(x)q(x,y)}{\pi(y)q(y,x)}\right)$$

Rem. $EP < \infty \Rightarrow \{\, q(x,y) > 0 \,\text{iff}\, q(y,x) > 0\,\}$

$EP = 0$ iff $\pi(x)q(x,y) = \pi(y)q(y,x)$

Dual semigroup (quantum)

h complex separable Hilbert space

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

ρ faithful normal invariant state

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

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 the commutative 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 $s \neq 1/2$.

Quantum detailed balance (QDB)

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

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

Time reversal: antiunitary θ s.t. $\theta^2 = \mathbb{1}$.

$a = a^*$ is *even* (*odd*) if $\theta a \theta^{-1} = a$ ($\theta a \theta^{-1} = -a$)

Ex. Conjugation $\theta u = \bar{u}$.

Def. *Quantum detailed balance condition(s)* with respect to ρ and θ (*QDB-s-*θ), $[\theta, \rho] = 0$,

$$\mathrm{tr}(\rho^s \theta x^* \theta^{-1} \rho^{1-s} \mathcal{T}_t(y)) = \mathrm{tr}(\rho^s \theta\, \mathcal{T}_t(x)^* \theta^{-1} \rho^{1-s}\, y)$$

Ex. Conjugation $\theta u = \bar{u}$, $s = 1/2$

$$\mathrm{tr}(\rho^{1/2} x^{\mathsf{T}} \rho^{1/2} \mathcal{T}_t(y)) = \mathrm{tr}(\rho^{1/2} \mathcal{T}_t(x)^{\mathsf{T}} \rho^{1/2}\, y)$$

x^{T} := transpose

$\overrightarrow{\Omega}_t$ and $\overleftarrow{\Omega}_t$ on $\mathcal{B}(\mathsf{h}) \otimes \mathcal{B}(\mathsf{h})$

$$\begin{aligned} \overrightarrow{\Omega}_t\,(a \otimes b) &= \mathrm{tr}\left(\rho^{1/2} a^{\mathsf{T}} \rho^{1/2} \mathcal{T}_t(b)\right) \\ \overleftarrow{\Omega}_t\,(a \otimes b) &= \mathrm{tr}\left(\rho^{1/2} \mathcal{T}_t(a)^{\mathsf{T}} \rho^{1/2} b\right) \end{aligned}$$

Density of $\overrightarrow{\Omega}_0 = \overleftarrow{\Omega}_0$ w.r.t. Tr on $\mathcal{B}(\mathsf{h}) \otimes \mathcal{B}(\mathsf{h})$

$$\overrightarrow{\Omega}_0\,(a \otimes b) = \langle r, (a \otimes b) r\rangle = \mathrm{Tr}\,(|r\rangle\langle r|(a \otimes b))$$

where

$$r = \sum_k \rho_k^{1/2} e_k \otimes e_k \qquad \rho = \sum_k \rho_k |e_k\rangle\langle e_k|$$

Densities of $\overrightarrow{\Omega}_t$ and $\overleftarrow{\Omega}_t$

$$\begin{aligned} &\overrightarrow{\Omega}_t \qquad && \overrightarrow{D}_t := (I \otimes \mathcal{T}_{*t})\,(|r\rangle\langle r|) \\ &\overleftarrow{\Omega}_t \qquad && \overleftarrow{D}_t := (\mathcal{T}_{*t} \otimes I)\,(|r\rangle\langle r|) \end{aligned}$$

Rem. Other functionals on $\mathcal{B}(\mathsf{h}) \otimes \mathcal{B}(\mathsf{h})$

$a \otimes b \to \mathrm{tr}\,(\rho a b)$ not positive!

$a \otimes b \to \mathrm{tr}\,(\rho a^* b)$ not linear!

entropy production for QMS

$$S\left(\overrightarrow{\Omega}_t | \overleftarrow{\Omega}_t\right) := \mathrm{Tr}\left(\overrightarrow{D}_t\left(\log(\overrightarrow{D}_t) - \log(\overleftarrow{D}_t)\right)\right)$$

$$EP := \lim_{t \to 0^+} \frac{S\left(\overrightarrow{\Omega}_t | \overleftarrow{\Omega}_t\right)}{t}$$

Properties: (1) $EP \geq 0$

(2) $EP = 0$ if and only if $\overrightarrow{\Omega}_t = \overleftarrow{\Omega}_t \ \forall t$

(3) $EP = 0$ if and only if

$$(I \otimes \mathcal{L}_*)(D) = (\mathcal{L}_* \otimes I)(D)$$

Example: 3-cycle

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

$Se_j = e_{j+1}$ (mod 3) shift

example: (quantum) 3-cycle

$$\mathcal{L}(a) = \alpha\, S^* a S + (1-\alpha)\, S a S^* - a, \qquad \alpha \in]0,1[$$

invariant state: $\rho = \frac{\mathbb{1}}{3}$ (normalized trace)
adjoint w.r.t. any s ($[\rho, a] = 0\ \forall a \in \mathcal{B}(\mathsf{h})$)

$$\widetilde{\mathcal{L}}(a) = \alpha\, S a S^* + (1-\alpha)\, S^* a S - a$$

$\mathcal{T}$, $\widetilde{\mathcal{T}}$ are QMSs, QDB does not hold if $\alpha \neq 1/2$

$$\mathcal{L}(a) - \widetilde{\mathcal{L}}(a) = (2\alpha - 1)\,(S^* a S - S a S^*)$$

Explicit computation of $\overrightarrow{D}_t$ and $\overleftarrow{D}_t$ yields

$$EP = (2\alpha - 1) \log\left(\frac{\alpha}{1-\alpha}\right)$$

Coincides with the classical EP of the Markov semigroup acting on diagonal matrices.

Generic QMSs

$\mathsf{h} = \ell^2(\mathbb{N};\mathbb{C})$, $(e_j)_{j\geq 1}$ o.n. basis,

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

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

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

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

$$\mu_j = \sum_k \varphi_{jk} \quad \Rightarrow \quad \mathcal{L}(\mathbb{1}) = 0$$

Invariant state

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

Properties. (1) Restriction to diagonal matrices defines a classical Markov semigroup.

(2) EP of the QMS and its classical restriction coincide.

GKSL form

h complex separable Hilbert,

$\mathcal{T} = (\mathcal{T}_t)_{t\geq 0}$ CP-semigroup on $\mathcal{B}(\mathsf{h})$,

norm continuous, unital ($\mathcal{T}_t(\mathbb{1}) = \mathbb{1}\ \forall t \geq 0$),

$\mathcal{T}_t$ normal.

Thm (GKSL)

$$\begin{aligned} \mathcal{L}(a) &= G^*a + \Phi(a) + aG, \\ \Phi(a) &:= \sum_j L_j^* a L_j \end{aligned}$$

where

1. $G, L_j \in \mathcal{B}(\mathsf{h})$, $\quad G^* + \sum_j L_j^* a L_j + G = 0$,

2. $\sum_j L_j^* L_j$ strongly convergent.

GKSL form & fixed normal state

We can write

$$G = -\frac{1}{2}\sum_j L_j^* L_j - iH, \qquad H = H^*$$

We can choose L_j with $\mathrm{tr}(\rho L_j) = 0$ and

$\mathbb{1}, L_1, L_2, \ldots$ linearly independent (min)

If L'_j also satisfy $\mathrm{tr}(\rho L'_j) = 0$, (min) and

$$\begin{aligned}\mathcal{L}(a) &= G^* a + \textstyle\sum_j L_j^* a L_j + aG \\ \mathcal{L}(a) &= G'^* a + \textstyle\sum_j L'^*_j a L'_j + aG'\end{aligned}$$

then $\exists$ a unitary (u_{jk}) s.t.

$$L'_j = \sum_k u_{jk} L_k, \qquad H' = H + c\mathbb{1},$$

(special GKSL).

Decomposition

$$\mathcal{L}(a) = \mathcal{L}_0(a) + i[H, a].$$

EP explicit formula

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

$\rho = \sum_k \rho^{1/2} |e_k\rangle\langle e_k|$ invariant state

$r = \sum_k \rho_k^{1/2} |e_k \otimes e_k\rangle\langle e_k \otimes e_k|, \qquad D = |r\rangle\langle r|$

$$\overrightarrow{D}_t = (I \otimes \mathcal{T}_{*t})(D) \qquad \overleftarrow{D}_t = (\mathcal{T}_{*t} \otimes I)(D),$$
$$\overrightarrow{D}'_t = \frac{d}{dt}(I \otimes \mathcal{T}_{*t})(D) \qquad \overleftarrow{D}'_t = \frac{d}{dt}(\mathcal{T}_{*t} \otimes I)(D)$$

By conditional complete positivity

$$D^\perp \overrightarrow{D}'_0 D^\perp \geq 0, \qquad D^\perp \overleftarrow{D}'_0 D^\perp \geq 0$$

Prop. If both are > 0 and

$$D^\perp \overrightarrow{D}'_0 D = D^\perp \overleftarrow{D}'_0 D, \quad D \overrightarrow{D}'_0 D^\perp = D \overleftarrow{D}'_0 D^\perp$$

then $EP =$

$$\boxed{\mathrm{Tr}\left(D^\perp \overrightarrow{D}'_0 D^\perp \left(\log(D^\perp \overrightarrow{D}'_0 D^\perp) - \log(D^\perp \overleftarrow{D}'_0 D^\perp)\right)\right)}$$

EP formula - 2

$$\langle r, (I \otimes \Phi_*)(D) r \rangle = \sum_\ell |\mathrm{tr}(\rho L_\ell)|^2$$

shifting L_ℓ to $L_\ell - \mathrm{tr}(\rho L_\ell)\mathbb{1}$ we find

$$D(I \otimes \Phi_*)(D) D = 0.$$

Then, with the new L_ℓ's,

$$\begin{aligned} \overrightarrow{D}'_0 - \overleftarrow{D}'_0 &= D^\perp(\mathbb{1} \otimes G)D - D^\perp(G \otimes \mathbb{1})D \\ &+ D(\mathbb{1} \otimes G^*)D^\perp - D(G^* \otimes \mathbb{1})D^\perp \\ &+ D^\perp \left((I \otimes \Phi_*)(D) - (\Phi_* \otimes I))(D)\right) D^\perp \end{aligned}$$

and the following are equivalent

(1) $D^\perp(\mathbb{1} \otimes G)D = D^\perp(G \otimes \mathbb{1})D$

(2) $\rho^{1/2} G^\mathsf{T} = G \rho^{1/2}$

$$\mathrm{Tr}\left(D^\perp \overrightarrow{D}'_0 D^\perp \left(\log(D^\perp \overrightarrow{D}'_0 D^\perp) - \log(D^\perp \overleftarrow{D}'_0 D^\perp)\right)\right)$$

SQDB generators, $s = 1/2$, θ conjugation

$$\mathrm{tr}\left(\rho^{1/2} a^{\mathsf{T}} \rho^{1/2} \mathcal{L}(b)\right) = \mathrm{tr}\left(\rho^{1/2} \mathcal{L}(a)^{\mathsf{T}} \rho^{1/2} b\right)$$

represent $\mathcal{L}$ is GKSL form with $\mathrm{tr}(\rho L_\ell) = 0$

Thm (FF-VU) This SQDB condition holds if and only if

(1) $\rho^{1/2} G^{\mathsf{T}} = G \rho^{1/2}$,

(2) $\mathrm{Lin}\{L_\ell \rho^{1/2} \mid \ell \geq 1\} = \mathrm{Lin}\{\rho^{1/2} L_\ell^{\mathsf{T}} \mid \ell \geq 1\}$
(in Hilbert-Schmidt ops on h)

(3) (trace class) operators

$$C_{jk} := \mathrm{tr}(\rho L_k^* L_j), \quad R_{jk} := \mathrm{tr}(\rho^{1/2} L_j^* \rho^{1/2} L_k^{\mathsf{T}})$$

commute and $C^{-1} R$ is unitary self-adjoint.

SQDB $s = 1/2$, θ & $EP = 0$

(1) $\Leftrightarrow D^{\perp}(\mathbb{1} \otimes G)D = D^{\perp}(G \otimes \mathbb{1})D$,

(2) $\Leftrightarrow D^{\perp}(I \otimes \Phi_*(D))D^{\perp}$ and $D^{\perp}(\Phi_*(D) \otimes I)D^{\perp}$ have the same support

(3) $\Leftrightarrow \exists$ a unitary self-adjoint $(u_{\ell j})$ s.t.

$$\rho^{1/2} L_{\ell}^{\top} = \sum_{j} u_{\ell j} L_j \rho^{1/2}$$

Open problem: EP formula when

$$D^{\perp}(\mathbb{1} \otimes G)D \neq D^{\perp}(G \otimes \mathbb{1})D$$

Thank you