Currents in some quantum non-equilibrium steady states

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Preliminary definitions and notation

Let $\mathcal{A}$ denote a finite-dimensional C^*-algebra with unit $\mathbb{1}$, regarded as subalgebra of some matrix algebra $\mathcal{M}_n(\mathbb{C})$.
Let τ denote the normalized trace on $\mathcal{A}$ given by $\tau(A) = \mathrm{Tr}[A]/\mathrm{Tr}[\mathbb{1}]$ for all $A \in \mathcal{A}$. Then τ is a faithful state on $\mathcal{A}$. Let $\mathfrak{H}_{\mathcal{A}}$ denote the Hilbert space formed by equipping $\mathcal{A}$ with the normalized Hilbert-Schmidt inner product. That is, for all $A, B \in \mathcal{A}$,

$$\langle A, B\rangle_{\mathfrak{H}_{\mathcal{A}}} = \tau[A^*B] \ .$$

Every linear functional ϕ on $\mathcal{A}$ can be written as

$$\phi(B) = \mathrm{Tr}[AB]$$

for some $A \in \mathcal{A}$ Then $\phi(B) \geq 0$ whenever $B \geq 0$ if and only if $A \geq 0$ in $\mathcal{A}$.

Definition

We define $\mathfrak{S}_+$ to be the set of positive definite elements ρ of $\mathcal{A}$ such that $\mathrm{Tr}[\rho] = 1$, and we refer to $\mathfrak{S}_+$ as the set of faithful states on $\mathcal{A}$ identifying $\rho \in \mathfrak{S}_+$ with the positive linear functional on $\mathcal{A}$ given by

$$\rho(A) = \mathrm{Tr}[\rho A] \ .$$

In other words, $\mathfrak{S}_+$ is the set of of invertible density matrices ρ on $\mathcal{M}_n(\mathbb{C})$ that belong to the subalgebra $\mathcal{A}$. The closure of $\mathfrak{S}_+$ is denoted by $\mathfrak{S}$.

Definition

A *Quantum Markov Semigroup* (QMS) is a continuous one-parameter semigroup of linear transformations $(\mathscr{P}_t)_{t\geq 0}$ on $\mathcal{A}$ such that for each $t \geq 0$, $\mathscr{P}_t$ is completely positive and $\mathscr{P}_t \mathbb{1} = \mathbb{1}$. Associated to any QMS $\mathscr{P}_t = e^{t\mathscr{L}}$, is the dual semigroup $\mathscr{P}_t^\dagger$ acting on $\mathfrak{S}_+$. The QMS $\mathscr{P}_t$ is *ergodic* in case $\mathbb{1}$ spans the eigenspace of $\mathscr{P}_t$ for the eigenvalue 1. In that case, there is a unique invariant state σ.

Characterizations of the generators of quantum Markov semigroups on the C^*-algebra $\mathcal{M}_n(\mathbb{C})$ of all $n \times n$ matrices were given at the same time in 1976 by Gorini, Kossakowski and Sudershan, and by Lindblad in a more general setting (but still assuming norm continuity of the semigroup).

Theorem (GKSL Theorem)

Let $\mathscr{L}$ be a linear map $\mathscr{L}$ on $\mathcal{M}_N(\mathbb{C})$. The $e^{t\mathscr{L}}$ is completely positive if and only if for some completely positive map Φ on $\mathcal{M}_N(\mathbb{C})$ and some $G \in \mathcal{M}_N(\mathbb{C})$

$$\mathscr{L}(A) = (G^*A + AG) + \Phi(A)$$

If further $\mathscr{P}_t\mathbb{1} = \mathbb{1}$, $G^* + G = -\Phi(\mathbb{1})$, and with $K := \frac{1}{2i}(G - G^*)$,

$$\mathscr{L}(A) = \Phi(A) - \frac{1}{2}(\Phi(\mathbb{1})A + A\Phi(\mathbb{1})) - i[K, A] \ .$$

Moreover, it is known that every CP map Φ has a Kraus reprsentation

$$\Phi(A) = \sum_{j=1}^{m} V_j^* A V_j \ .$$

The Kraus representation is *minimal* in case $\{V_1, \ldots, V_m\}$ is linearly independent, and every CP map has a minimal Kraus representation.

Using the Kraus representation, the generator can be written as

$$\mathscr{L}A = \sum_{j=1}^{m} V_j^*[A, V_j] + [V_j^*, A]V_j + i[H, A] \ ,$$

and consequently,

$$\mathscr{L}^\dagger \rho = \sum_{j=1}^{m} [V_j, \rho V_j^*] + [V_j \rho, V_j^*] - i[H, \rho]$$

The terms Φ and G in the decomposition of $\mathscr{L}$ in the Lindblad form are not uniquely determined by $\mathcal{L}$. Indeed, consider any CP map Φ with the Kraus representation as above. Then for any choice of complex numbers $c_1, \dots, c_m$, define $W_j := V_j + c_j\mathbb{1}$, and

$$\Psi(A) := \sum_{j=1}^{m} W_j^* A W_j + \sum_{j=1}^{m} |c_j|^2 A \ .$$

A simple computation shows that

$$\Phi(A) = \Psi(A) - G^* A - AG \qquad \text{where} \qquad G = \sum_{j=1} c_j W_j \ .$$

Consequently, in the Lindblad form, the "Hamiltonian part" $i[H, A]$ is not uniquely determined by $\mathscr{L}$.

The weak coupling limit

One way in which QMS arise in the description of physical systems if through the *weak coupling limit*. Let $\mathcal{H}$ be a finite dimension Hilbert space and H a self adjoint operator on $\mathcal{H}$, which is the Hamiltonian of a quantum system on $\mathcal{H}$. Let $\mathcal{K}$ be the Fock space for one Boson degree of freedom in $L^2(\mathbb{R}^3)$. Let K be the Hamiltonian for this system which may be the second quantization of the free Hamiltonian $-\Delta$ on $L^2(\mathbb{R}^3)$.

One way to couple the system and the bath is by defining an interaction Hamiltonan using the anhilation and creation operators for the bath and an arbitrary operator B on $\mathcal{H}$:

$$H_I = B \otimes a^\dagger(\phi) + B^* \otimes a(\phi)$$

where ϕ is a test function.

For each $\lambda > 0$, define the Hamiltonian

$$H_\lambda = H \otimes \mathbb{1} + \mathbb{1} \otimes K + \lambda H_I \ .$$

Also, let ω_β be the equilibrium state of the reservoir at inverse temperature β.

Define the map $U_t^{(\lambda)}$ on $\mathscr{B}(\mathcal{H} \otimes \mathcal{K})$ by

$$U_t^{(\lambda)} X = e^{-itH_\lambda} X e^{itH_\lambda}$$

for all $X \in \mathscr{B}(\mathcal{H} \otimes \mathcal{K})$. Then under certain regularity conditions, Davies proved that for each fixed $\tau > 0$, and all $\rho \in \mathfrak{S}_+$

$$\lim_{\lambda \to 0} \mathrm{Tr}_{\mathcal{K}} \left[U^{(0)}_{-\lambda^{-2}\tau} \left(\mathrm{Tr}_{\mathcal{K}} [U^{(\lambda)}_{-\lambda^{-2}\tau}(\rho \otimes \omega_\beta)] \right) \otimes \omega_\beta \right] = e^{\tau \mathscr{L}^\dagger}$$

where $\mathscr{L}^\dagger$ is the generator of a quantum dynamical semigroup. The quantum dynamical semigroups that arise in this way have a very special structure. Of course, $\mathscr{L}^\dagger$ is determined by H, K, β, B and ϕ. There is an explicit formula for $\mathscr{L}^\dagger$, but it is complicated. Here are the key facts.

Let $\{e_1, \ldots, e_n\}$ be the distinct eigenvalues of H. Let P_j be the projector onto the eigenspace corresponding to the eigenvalue e_j. Then

$$H = \sum_{j=1}^{n} e_j P_j$$

is the canonical decomposition of H. Define the derivation on $\mathscr{B}(\mathcal{H})$ by

$$D_H(X) = [H, X] = HX - XH \ .$$

Let $\{u_1, \ldots, u_N\}$ be an orthonormal basis of H consisting of eigenvectors of H; that is $Hu_j = e_j u_j$ where each $\lambda_j \in \{e_1, \ldots, e_n\} = \mathrm{Spec}(H)$. Then

$$\{|u_i\rangle\langle u_j| \ : \ 1 \leq i, j \leq N\}$$

is an orthonormal basis for $\mathscr{B}(\mathcal{H})$ equipped with the Hilbert-Schmidt inner product, and

$$D_H(|u_i\rangle\langle u_j|) = (\lambda_i - \lambda_j)|u_i\rangle\langle u_j| \ .$$

It follows that

$$\mathrm{Spec}(D_H) = \{\ \omega \ : \ \omega = e_j - e_k \ , \ e_j, e_k \in \mathrm{Spec}(H)\}$$

which is known as the set of *Bohr frequencies* of H.

Then for each $\omega \in \mathrm{Spec}(D_H)$, define

$$V_\omega := \sum_{j,k\ :\ e_k - e_j = \omega} P_{e_j} B P_{e_k} = V^*_{-\omega} \ .$$

Also define for real some constants $a(\beta, \omega)$

$$\begin{aligned} \mathscr{L}_\omega(A) &:= e^{-\beta\omega/2}\Big(V^*_\omega [A, V_\omega] + [V^*_\omega, A] V_\omega \Big) \\ &+ e^{\beta\omega/2}\Big(V_\omega [A, V^*_\omega] + [V_\omega, A] V^*_\omega \Big) \\ &+ ia(\beta,\omega)[(V^*_\omega V_\omega + V_\omega V^*_\omega), A] \ . \end{aligned}$$

Then for non-negative constants $c(\beta, \omega)$,

$$\mathscr{L} = \sum_{\omega \in \mathrm{Spec}(D_H)\ ,\ \omega \geq 0} c(\beta,\omega) \mathscr{L}_\omega \ .$$

The corresponding formulas for the dynamical semigroup generators then are

$$\begin{aligned}\mathscr{L}_\omega^\dagger(\rho) &:= e^{-\beta\omega/2}\Big([V_\omega\rho, V_\omega^*] \\ &+ [V_\omega, \rho V_\omega^*]\Big) + e^{\beta\omega/2}\Big([V_\omega^*\rho, V_\omega] + [V_\omega^*, \rho V_\omega]\Big) \\ &- ia(\beta,\omega)[(V_\omega^* V_\omega + V_\omega V_\omega^*), A]\ .\end{aligned}$$

As Davies showed, one has $\mathscr{L}^\dagger\sigma_\beta = 0$ where β is the inverse temperature of the bath and

$$\sigma_\beta = \frac{1}{Z_\beta} e^{-\beta H}\ .$$

Moreover, this special class of QMS belongs to a larger class satisfying certain conditions that are quantum analogs of the classical *detailed balance condition.*

Before going into the specific structure of this class of QMS, we discuss the questions we would like to treat.

Currents and heat flow

We would like to investigate systems that are coupled to two or more thermal reservoirs at different temperatures. Let us focus on two reservoirs with two (inverse) temperatures $\beta_1 > \beta_2$. Then in equilibrium, one might expect that heat would flow through the system from the hot reservoir to the cold reservoir.

$j = 1, 2$, let $\mathscr{L}_{(j)}$ denote an ergodic QMS generator satisfying detailed balance for the Gibbs state

$$\sigma_{\beta_j} = \frac{1}{Z_{\beta_j}} e^{-\beta_j H} \ .$$

Define

$$\mathscr{L}_{1,2} := \mathscr{L}_{(1)} + \mathscr{L}_{(2)} \ .$$

Assume that $\mathscr{L}_{1,2}$ is ergodic. Define $\sigma_{1,2}$ to be the unique steady state; i.e., the unique solution in $\mathfrak{S}_+$ of $\mathscr{L}_{1,2}^\dagger \rho = 0$.

Then (Lebowitz and Spohn 1978) the amount of heat flowing into the system from the hot reservoir is

$$\langle J \rangle = \mathrm{Tr}[\sigma_{1,2}\mathscr{L}_{(1)}H] \ .$$

Unfortunately, much is known about $\sigma_{1,2}$ in general. When H has non-degenerate spectrum, then it turns out that $\sigma_{1,2}$ is a function of H. However, in the models of interest, the spectrum of H is far from degenerate.

We next discuss one model treated recently by Fagnola, Poletti and Sasso (2021). The system is a spin chain in which $\mathcal{H}$ is the n-fold tensor product of $\mathbb{C}^2$ with itself, and the Hamiltonian H is given by

$$H = \sum_{j=1}^{n-1} \sigma_j^z \sigma_{j+1}^z \ .$$

Let $|1\rangle =: \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and let $|-1\rangle =: \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. An orthonormal basis of eigenvectors of H is given by

$$\psi_\alpha = \otimes_{j=1}^n |\alpha(j)\rangle$$

where $\alpha \in \{-1, 1\}^n$.
Define k_α to be the cardinality of the set

$$\{\ 1 \leq j \leq n-1\ :\ \alpha(j+1) \neq \alpha(j)\}\ .$$

Then

$$H\psi_\alpha = e_\alpha \psi_\alpha$$

where $e_\alpha = n - 1 - 2k_\alpha$.
Notice that all of the eigenfunctions are simple tensor products; there is no entanglement.

It would be more interesting to consider a Hamiltonian of the form

$$H = \sum_{j=1}^{n-1} (\sigma_j^z \sigma_{j+1}^z + a\sigma_j^x \sigma_{j+1}^x) \ .$$

for non-zero a. But then we lack an explicit diagonalization, and it is difficult to write down the QMS generators arising through weak coupling limits and hence to evaluate the current.

For $a = 0$, Fagnola, Poletti and Sasso show that when the two ends of the chain are connected to heat baths at two different temperatures, and $n > 2$, there is no heat flow. This is not surprising. Their process is far from ergodic and the two ends of the chain are unaware of each other.

Our goal here is to introduce a model in which we can prove that heat does flow from the hot bath to the cold. We will use a quantum analog of a thermostated kinetic model studied by Carlen, Esposito, Lebowitz, Marra and Mouhot (2019).

But before coming to this, we study the structure of the rather small class of QMS arising through weak coupling limits. We are particularly interested in when the the stationary states resulting from coupling a system to two (or more) baths at different temperatures will be a function of the Hamiltonian.

A key property of the class of QMS arising as weak coupling limits is that they satisfy the *detailed balance condition*.

Detailed balance

We begin by recalling the notion of detailed balance in a classical setting. Let $P_{i,j}$ be the Markov transition matrix for a Markov chain on a finite state space S with elements $\{x_1, \ldots, x_n\}$. Suppose that σ is a probability density on S that is invariant under this transition function: $\sigma_j = \sum_{i=1}^n \sigma_i P_{i,j}$ for all i. The transition matrix satisfies the *detailed balance condition with respect to* σ in case

$$\sigma_i P_{i,j} = \sigma_j P_{j,i} \qquad \text{for all } i, j \ . \tag{$*$}$$

Let X_n be the Markov process started from the initial distribution σ, so that the process is stationary. Let Pr be measure on the path space of the process. Then $(*)$ is equivalent to

$$\mathrm{Pr}\{X_n = i, X_{n+1} = j\} = \mathrm{Pr}\{X_n = j, X_{n+1} = i\} \qquad \text{for all } i, j \text{ and all } n \ .$$

In other words, (X_n, X_{n+1}) has the same joint distribution as (X_{n+1}, X_n), so that $(*)$ characterizes *time reversal invariance*.

There is another characterization of detailed in terms of self-adjointness: The matrix P is self-adjoint on $\mathbb{C}^n$ equipped with the inner product

$$\langle f, g\rangle_\sigma = \sum_{k=1}^{n} \sigma_k \overline{f_k} g_k \ ,$$

if and only if $(*)$ is satisfied.

There are a number of different ways one might generalize this inner product to the quantum setting:

Definition

Let $\sigma \in \mathfrak{S}_+$ be a non-degenerate density matrix. For each $s \in \mathbb{R}$, and each $A, B \in \mathcal{A}$, define

$$\langle A, B\rangle_s = \mathrm{Tr}[(\sigma^{(1-s)/2} A \sigma^{s/2})^* (\sigma^{(1-s)/2} B \sigma^{s/2})] = \mathrm{Tr}[\sigma^s A^* \sigma^{1-s} B] \ .$$

The *Gelfand-Naimark-Segal* (GNS) inner product is the the $\langle \cdot, \cdot \rangle_1$ inner product, while the *Kubo-Martin-Schwinger* (KMS) inner product is the the $\langle \cdot, \cdot \rangle_1$ inner product.

Another inner product that arises in physics is the *Bogoliubov-Kubo-Mori* (BKM) inner product,

$$\int_0^1 \mathrm{Tr}[B^*\sigma^s A\sigma^{1-s}]\mathrm{d}s \ .$$

Let $\mathcal{L}(\mathcal{M}_N(\mathbb{C}))$ denote the linear operators on $\mathcal{M}_N(\mathbb{C})$, or, what is the same thing in this finite dimensional setting, on $\mathfrak{H}$. Throughout this paper, a dagger is always used to denote the adjoint with respect to the inner product on $\mathfrak{H}$. That is, for $\Phi \in \mathcal{L}(\mathcal{M}_N(\mathbb{C}))$, $\Phi^\dagger$ is defined by

$$\langle \Phi^\dagger(B), A\rangle_{\mathfrak{H}} = \langle B, \Phi(A)\rangle_{\mathfrak{H}}$$

for all A, B.

Definition (Modular operator and modular group)

Let $\sigma \in \mathfrak{S}_+$. Define a linear operator Δ_σ on $\mathfrak{H}$ by

$$\Delta_\sigma(A) = \sigma A \sigma^{-1}$$

for all $A \in \mathcal{A}$. Δ_σ is called the *modular operator*. The *modular generator* is the self-adjoint element $h \in \mathcal{A}$ given by

$$h = -\log \sigma \ .$$

The *modular automorphism group* α_t on $\mathcal{A}$ is the group defined by

$$\alpha_t(A) = e^{ith} A e^{-ith} \ .$$

A linear operator $\mathscr{K}$ on $\mathcal{A}$ is *positivity preserving* in case $\mathscr{K} A \geq 0$ whenever $A \geq 0$. A linear operator $\mathscr{K}$ on $\mathcal{A}$ is *Hermitian* in case $(\mathscr{K} A)^* = \mathscr{K} A^*$, or, equivalently, in case $\mathscr{K} A$ is self-adjoint whenever A is self-adjoint. Any positivity preserving operator is Hermitian.

When $\mathscr{P}_t = e^{t\mathscr{L}}$ is a Hermitian semigroup, then its generator

$$\mathscr{L} = \lim_{t\to 0} t^{-1}(\mathscr{P}_t - I)$$

is Hermitian as well.

Let $\sigma \in \mathfrak{S}_+$ and note that $(\Delta_\sigma A)^* = \Delta_\sigma^{-1}(A^*)$ for all $A \in \mathcal{A}$. Moreover, for all $A, B \in \mathcal{A}$,

$$\mathrm{Tr}[A^*\Delta_\sigma B] = \mathrm{Tr}[(\Delta_\sigma A)^* B] \quad \text{and} \quad \mathrm{Tr}[A^*\Delta_\sigma A] = \mathrm{Tr}[|\sigma^{1/2}A\sigma^{-1/2}|^2] \ ,$$

so that Δ_σ is a positive operator on $\mathfrak{H}_\mathcal{A}$.

It turns out that self-adjointness with respect to the GNS inner product, or indeed with respect to $\langle \cdot, \cdot \rangle_s$ for any $s \neq 1/2$ implies self-adjointness with respect to $\langle \cdot, \cdot \rangle_s$ for all s, and hence other inner products such as the BKM inner product. The first part of the following theorem is due to Alicki with further contributions by Fagnola and Umanita.

Theorem

Let $\sigma \in \mathfrak{S}_+$ be a non-degenerate density matrix, and let $\mathscr{K}$ be any operator on $\mathcal{A}$. Then:

(1) If $\mathscr{K}$ is self-adjoint with respect to the GNS inner product $\langle \cdot, \cdot \rangle_1$, and $\mathscr{K} A^* = (\mathscr{K} A)^*$ for all $A \in \mathcal{A}$, then $\mathscr{K}$ commutes with the modular operator Δ_σ and moreover, $\mathscr{K}$ is self-adjoint with respect to $\langle \cdot, \cdot \rangle_s$ for all $s \in [0, 1]$.

(2) If $\mathscr{K}$ commutes with the Δ_σ, and if $\mathscr{K}$ is self-adjoint with respect to $\langle \cdot, \cdot \rangle_s$ for some $s \in [0, 1]$, then $\mathscr{K}$ is self-adjoint with respect to $\langle \cdot, \cdot \rangle_s$ for all $s \in [0, 1]$.

Every QMS $\mathscr{P}_t = e^{t\mathscr{L}}$ is self-adjointness preserving: $\mathscr{P}_t A^* = (\mathscr{P}_t A)^*$. Thus, when $\mathscr{P}_t$ satisfies the σ detialed balalnce condition, it follows that

$$e^{it'h}(\mathscr{P}_t(A))e^{-it'h} = \mathscr{P}_t(e^{it'h}Ae^{-it'h})$$

for all t, t' and all $A \in \mathcal{A}$. In this generality, this is due to Alicki, and it means that $\mathscr{P}_t$ commutes with the time-translation governed by the Hamiltonian h corresponding to the state σ. Furthermore, when $\mathscr{P}_t$ is self adjoint with respect to $\langle \cdot, \cdot \rangle_s$, then for all $A \in \mathcal{A}$,

$$0 = \langle \mathscr{L}(1)A \rangle_s = \langle \mathbb{1}, \mathscr{L}(A) \rangle_s = \mathrm{Tr}[\sigma \mathscr{L}(A)] = \mathrm{Tr}[\mathscr{L}^\dagger(\sigma)A] \ .$$

Since this is true for all A, $\mathscr{L}^\dagger \sigma = 0$. Hence either condition for detailed balance implies that σ is stationary for $\mathscr{P}_t$.

Since a QMS $\mathscr{P}_t = e^{t\mathscr{L}}$ on $\mathcal{A}$ that satisfies the σ-DBC for some $\sigma \in \mathfrak{S}_+(\mathcal{A})$ has a generator $\mathscr{L}$ that commutes with the modular operator Δ_σ, and since Δ_σ is positive with respect to the GNS inner product, Δ_σ and $\mathscr{L}$ can be simultaneously diagonalized. The diagonalization of Δ_σ reduces immediately to the diagonalization of σ: Let $\sigma = e^{-h}$ be a density matrix on $\mathbb{C}^n$. Let $\{\phi_1, \dots, \phi_n\}$ be an orthonormal basis of $\mathbb{C}^n$ consisting of eigenvectors of $h = -\log \sigma$: $h\eta_j = \lambda_j \eta_j$. For $\alpha = (\alpha_1, \alpha_2) \in \{(i,j) \ : 1 \le i,j \le n\}$, define numbers

$$\omega_\alpha = \lambda_{\alpha_1} - \lambda_{\alpha_2} \ ,$$

and rank-one operators F_α given by $F_\alpha = |\phi_{\alpha_1}\rangle\langle\phi_{\alpha_2}|$. Evidently

$$\Delta_\sigma F_\alpha = e^{-\omega_\alpha} F_\alpha \qquad \text{and} \qquad F_\alpha^* = F_{\alpha'} \quad \text{where} \quad \alpha' = (\alpha_2, \alpha_1) \ .$$

QMS generators satisfying detailed balance

We make $\mathcal{L}(\mathcal{M}_N(\mathbb{C}))$ into a Hilbert space by equipping it with the normalized Hilbert-Schmidt inner product. Throughout this paper, this Hilbert space is denoted by $\widehat{\mathfrak{H}}$. The following formula for the inner product in $\widehat{\mathfrak{H}}$ is often useful. Let $\{F_{i,j}\}_{1\leq i,j\leq N}$ be any orthonormal basis for $\mathfrak{H}$. Then for Φ and $\Psi \in \widehat{\mathfrak{H}}$,

$$\langle \Psi, \Phi \rangle_{\widehat{\mathfrak{H}}} = \frac{1}{N^2} \sum_{i,j=1}^{N} \langle \Psi(F_{i,j}), \Phi(F_{i,j}) \rangle_{\mathfrak{H}} \ .$$

Definition

Define $\widehat{\mathfrak{H}}_{\mathcal{S}}$ to be the subspace of $\widehat{\mathfrak{H}}$ consisting of all operators Φ of the form

$$\Phi(A) = XA + AY$$

for some $X, Y \in \mathcal{M}_N(\mathbb{C})$.

Lemma (Amorim Carlen 2021)

For each $s \in [0,1]$, both $\widehat{\mathfrak{H}}_{\mathcal{S}}$ and $\widehat{\mathfrak{H}}_{\mathcal{S}}^{\perp}$ are invariant under the operation of taking the adjoint with respect to the inner product $\langle \cdot, \cdot \rangle_s$. Moreover, if $\{V_1, \dots, V_M\}$ is linearly independent in $\mathcal{M}_N(\mathbb{C})$, the map $A \mapsto \sum_{j=1}^{M} V_j^* A V_j$ belongs to $\widehat{\mathfrak{H}}_{\mathcal{S}}^{\perp}$ if and only if $\mathrm{Tr}[V_j] = 0$ for each j.

Now consider any QMS generator $\mathscr{L}$. By the *LGKS* Theorem, $\mathscr{L}$ has the form

$$\mathscr{L}(A) = (G^* A + AG) + \Psi(A)$$

where Ψ is CP. Let $\Psi(A) = \sum_{j=1}^{M} V_j^* A V_j$ be a minimal Kraus representation of Ψ. Replacing each V_j by $V_j - \mathrm{Tr}[V_j]\mathbb{1}$, and absorbing the difference into G, we may assume that $\mathrm{Tr}[V_j] = 0$ for each j. By the lemma, $\Psi \in \widehat{\mathfrak{H}}_{\mathcal{S}}^{\perp}$. Making this choice for Ψ gives a *canonical decomposition* of $\mathscr{L}$ into its components in $\widehat{\mathfrak{H}}_{\mathcal{S}}$ and $\widehat{\mathfrak{H}}_{\mathcal{S}}^{\perp}$, and if $\mathscr{L}$ is self-adjoint on $\mathcal{H}_s$, each of these pieces must be *individually* self-adjoint on $\mathcal{H}_s$.

Theorem (Amorim Carlen 2021)

The extremal rays in the cone of CP maps that are self-adjoint on $\mathcal{H}_s$, $s \neq \frac{1}{2}$, are precisely the maps of the form

$$\Phi(A) = e^{\omega/2} V^* A V + e^{-\omega/2} V A V^*$$

where $\Delta V = e^{\omega} V$, $\omega > 0$, or of the form

$$\Phi(A) = VAV \ ,$$

$\Delta V = V = V^*$ In particular, every CP map that is self-adjoint on $\mathcal{H}_s$ is a positive linear combination of such operators.

Theorem (Amorim Carlen 2021)

There is a one-to-one correspondence between QMS generators $\mathscr{L}$ that are GNS self adjoint and CP maps Φ that are GNS self adjoint. The corresondence identifies Φ with the generator $\mathscr{L}_\Phi$ where

$$\mathscr{L}_\Phi(A) = G^*A + AG + \Phi(A)$$

where $G = H + iK$ with $H = -\frac{1}{2}\Phi(\mathbb{1})$.
The dual semigroup generator is given by

$$\mathscr{L}^\dagger_{\Phi,H}(\rho) = G\rho + \rho G^* + \Phi^\dagger(\rho)$$

Theorem (Amorim Carlen 2021)

Let $\mathfrak{K}$ be the real vector space consisting of all $V \in \mathcal{M}_N(\mathbb{C})$ such that $\Delta^{-1/2} V = V^*$. The extremal elements Φ of cone of QMS generators that are self adjoint for the KMS inner product are precisely the elements of the form

$$\Phi(A) = V^* A V \ , \qquad V \in \mathfrak{K} \ .$$

Every map in CP that is self adjoint for the KMS inner product is a positive linear combination of at most N^2 such maps.

Form here we deduce a result that complements an earlier theorem of Fagnola and Umanita giving necessary and sufficient conditions for a QMS generator $\mathscr{L}$ to be KMS self adjoint:

Theorem (Amorim Carlen 2021)

There is a one-to-one correspondence between the cone of CP maps Ψ *that are KMS self adjoint and the cone of QMS generators* $\mathscr{L}$ *that are KMS self adjoint. The correspondence identifies* Ψ *with* $\mathscr{L}_\Psi$ *where*

$$\mathscr{L}_\Psi(A) = G^* A + AG + \Psi(A)$$

where $G = H + iK$, H *and* K *self-adjoint and given by* $H := \frac{1}{2}\Psi(\mathbb{1})$ *and*

$$K := \frac{1}{i}\int_0^\infty e^{-t\sigma^{1/2}}(\sigma^{1/2}H - H\sigma^{1/2})e^{-t\sigma^{1/2}}\mathrm{d}t\ .$$

The extreme points of the cone of QMS generators that are KMS self adjoint are precisely the generators of the form

$$\mathscr{L}(A) := G^* A + AG + V^* AV$$

where $\Delta^{-1/2}V = V^*$ *and where* $G = H + iK$.

Restriction to invariant subalgebras

Let $\mathcal{A}$ be a unital C^*-algebra, and let $\sigma \in \mathfrak{S}_+(\mathcal{A})$. Let A_1, A_2 be eigenvectors of Δ_σ: $\Delta_\sigma(A_j) = \lambda_j A_j$, $j = 1, 2$. Then $\lambda_1, \lambda_2 > 0$, and since the modular operator is an automorphism,

$$\Delta_\sigma(A_1 A_2) = \Delta_\sigma(A_1)\Delta_\sigma(A_2) = \lambda_1 \lambda_2 A_1 A_2 \ .$$

That is, the product of eigenvectors of Δ_σ is again an eigenvector of Δ_σ, and moreover, the eigenspace of Δ_σ for the eigenvalue 1 is an algebra.

Definition (Modular subalgebra)

Let $\mathcal{A}$ be a unital C^*-algebra, and let $\sigma \in \mathfrak{S}_+(\mathcal{A})$. The *$\sigma$-modular subalgebra of $\mathcal{A}$*, denoted $\mathcal{A}_\sigma$, is the C^*-subalgebra of $\mathcal{A}$ consisting of the eigenspace of Δ_σ with eigenvalue 1, which is the same thing as the commutant of $\{\sigma\}$. Let $\mathcal{C}_\sigma$ denote the commutative subalgebra of $\mathcal{A}_\sigma$ consisting of complex functions of σ. That is, $\mathcal{C}_\sigma$ is the smallest C^* subalgebra of $\mathcal{A}$ containing σ and $\mathbb{1}$.

If $\mathscr{P}_t$ satisfies detailed balance with respect to σ, then $\mathcal{A}_\sigma$ is invariant under $\mathscr{P}_t$, but it need not be commutative. On the other hand $\mathcal{C}_\sigma$ is always commutative, but need not be invariant under $\mathscr{P}_t$.

If the spectrum of H is non-degenerate, then $\mathcal{C}_\sigma = \mathcal{A}_\sigma$ is generated by $\{ \ |u_j\rangle\langle u_j| \ : \ 1 \le j \le n \ \}$ where $\{u_1, \dots, u_n\}$ is an orthonormal basis consisting of eigenvectors of σ.

Unfortunately, the Hamiltonians, and hence the Gibbs states that are of interest to us very rarely have non-degenrate spectrum. Pursuing the rare case where H does have non-degenerate spectrum, consider two inverse temperatures $\beta_1 > \beta_2$. For $j = 1, 2$, let $\mathscr{L}_{(j)}$ denote an ergodic QMS generator satisfying detailed balance for the Gibbs state

$$\sigma_{\beta_j} = \frac{1}{Z_{\beta_j}} e^{-\beta_j H} \ .$$

Since the algebra $\mathcal{A}_\sigma$ is generated by $\{\ |u_j\rangle\langle u_j|\ :\ 1 \le j \le n\ \}$ where $\{u_1, \dots, u_n\}$ is an orthonormal basis consisting of eigenvectors of H, it is independent of the inverse temperature β. Call this commutative algebra $\mathcal{C}$.

Then since $\mathcal{C}$ is invariant under both $\mathscr{L}_{(1)}$ and $\mathscr{L}_{(2)}$, it is invariant under

$$\mathscr{L}_{1,2} := \mathscr{L}_{(1)} + \mathscr{L}_{(2)}\ .$$

Hence the unique invariant state $\sigma_{1,2}$ for the QMS generated by $\mathscr{L}_{1,2}$ lies in $\mathcal{C}$, and therefore it is a function of H.

Theorem

For a Hamiltonian H and two inverse temperatures $\beta_1 > \beta_2$, and for or $j = 1, 2$, let $\mathscr{L}_{(j)}$ denote an ergodic QMS generator satisfying detailed balance for the Gibbs state

$$\sigma_{\beta_j} = \frac{1}{Z_{\beta_j}} e^{-\beta_j H} \ .$$

Define $\mathscr{L}_{1,2} := \mathscr{L}_{(1)} + \mathscr{L}_{(2)}$. Then $\mathcal{A}_{\sigma_{\beta_1}} = \mathcal{A}_{\sigma_{\beta_2}} = \mathcal{B}$
If H has disjoint spectrum, then the unique invariant state $\sigma_{1,2}$ of the QMS generated by $\mathscr{L}_{1,2}$ has the form $\sigma_{1,2} = f(H)$ for some function f.
Without any restriction on H, $\sigma_{1,2}$ lies in the algebra $\mathcal{B}$.

The N-particle binary collision model

Consider a d-dimensional Hilbert space $\mathcal{H}$ and a single particle Hamiltonian h with d distinct eigenvalues $e_0, \dots, e_{d-1}$. Let $\{\psi_0, \dots, \psi_{d-1}\}$ be an orthonormal basis for $\mathcal{H}$ with $h\psi_j = e_j\psi_j$ for all $0 \leq j \leq d-1$. The corresponding N-particle Hamiltonian on $\mathcal{H}_N = \otimes^N \mathcal{H}$ is given by

$$H_N = \sum_{j=1}^{N} I \otimes \cdots \otimes h \otimes \cdots \otimes I$$

where h is in the jth position. The eigenvalues of H_N are indexed by the multindices $\alpha \in \{0, \dots, d-1\}^N$, and are given by

$$e(\alpha) = e_{\alpha_1} + \cdots e_{\alpha_N} \quad \text{where} \quad \alpha_j \in \{0, \dots, d-1\} \ , \ j = 1, \dots, N \ .$$

Defining

$$\Psi_\alpha := \psi_{\alpha_1} \otimes \cdots \otimes \psi_{\alpha_N} \ ,$$

$\{\Psi_\alpha \ : \ \alpha \in \{0, \dots d-1\}^N\}$ is an orthonormal basis of $\mathcal{H}_N$ consisting of eigenvectors of H_N. For a multiindex α, and $k \in \{0, \dots, d-1\}$ define

$$k_m(\alpha) = \#\{1 \le j \le N \ \ \alpha_j = m \ \}$$

where for a set A, $\#A$ denotes the cardinality of A. Thus, a second expression for $e(\alpha)$ is

$$e(\alpha) = \sum_{m=0}^{d-1} k_m(\alpha) e_k \ .$$

We consider energy conserving binary collisions: If before a collision the state of the system is $|\Psi_\gamma\rangle\langle\Psi_\gamma|$, then after the collision it is given by a density matrix ρ all of whose eigenstates are are linear combinations of vectors the form Ψ_δ where for some $i < j$, $\delta_\ell = \gamma_\ell$ for $\ell \notin \{i, j\}$, and

$$e_{\gamma_i} + e_{\gamma_j} = e_{\delta_i} + e_{\delta_j}$$

Suppose that the spectrum of h is such that the spectrum of H_2 on $\mathcal{H} \otimes_{\rm sym} \mathcal{H}$ is non-degenerate. Then for any $0 \le m_1, m_2, m_3, m_4 \le d-1$,

$$e_{m_1} + e_{m_2} = e_{m_3} + e_{m_4} \iff \{m_1, m_2\} = \{m_3, m_4\} \ .$$

Suppose further that the pair of equations

$$\sum_{m=1}^{d-1} k_m e_n = E \quad \text{and} \quad \sum_{m=1}^{d-1} k_m \ = \ N$$

has exactly one solution for each E in the spectrum of $\mathcal{H}_N$. Then γ and δ can only differ differ by a pair transposition. (This is generic.)

The collision rules induce a graph structure on $\mathcal{V}_N := \{0, \dots d-1\}^N$: We say that $\gamma, \delta \in \mathcal{V}_N$ are **adjacent** if they differ by a pair transposition $\pi_{i,j}$ for some $i < j$. If γ is adjacent δ, we write $[\gamma, \delta]$ to denote the corresponding edge in $\mathcal{E}_N$. Note that $[\gamma, \delta] = [\delta, \gamma]$. **We denote this graph by $\mathcal{G}_N$.**

The connected components of $\mathcal{G}_N$ are indexed by the $\mathbf{k} = (k_0, \dots, k_{d-1})$ such that $\sum_{m=1}^{d-1} k_m = N$, and the corresponding vertex set, $\mathcal{V}_{N,\mathbf{k}}$ consists of all α such that $k_j(\alpha) = k_j$ for each $j = 0, \dots, d-1$.

A Quantum Kac model

Let $(\mathcal{C}, \mathrm{d}\nu)$ be some probability space, and let $c \mapsto U_{(i,j),\mathbf{k}}(c)$ be a measurable map from $\mathcal{C}$ into unitaries on $\mathcal{H}_{N,\mathbf{k}}$ such that $U_{(i,j),\mathbf{k}}(c)$ commutes with H_N and acts as the identity on all factors except for i, j. Define

$$\Phi(X) := \binom{N}{2}^{-1} \sum_{i<j} \int_{\mathcal{C}} U^*_{(i,j),\mathbf{k}}(c) X U_{(i,j),\mathbf{k}}(c) \mathrm{d}\nu \ .$$

Define

$$\mathcal{K} := N(\Phi(X) - X) \ .$$

Then

$$e^{t\mathcal{K}}(X) = e^{-tN} \sum_{j=0}^{\infty} \frac{(tN)^j}{j!} \Phi^j(X) \ .$$

For simplicity, consider the uniform quantum Kac model, averaging uniformly over all kinematically possible collisions just as in the original Kac model.

That is, for each $i < j$, let $\mathcal{U}_{i,j}$ be the group of unitaries U acting trivially on all factors except the i and j factors, and further such that U commutes with H_N. Let $\mu_{i,j}$ be the uniform Haar measure on this group. We then set

$$\Phi_{i,j}(X) := \int_{\mathcal{C}} U^*_{(i,j),\mathbf{k}}(c) X U_{(i,j),\mathbf{k}}(c) \mathrm{d}\nu = \int_{\mathcal{U}_{i,j}} U^* X U \mathrm{d}\mu_{i,j}(U) \ .$$

Then $\Phi_{i,j}$ is a "pinching operation" and so $\Phi_{i,j}(X)$ is a positive linear combination of operators of the form PXP where P is a spectral projection of the partial Hamiltonian for particles i and j. From here it is easy to write down a Kraus representation for Φ, and hence a Lindblad representation for $\mathcal{K}$.

The Kac generator $\mathcal{K}$ is not ergodic: Define $\mathcal{H}_{N,\mathbf{k}}$ is the eigenspace of H_N corresponding to the level populations specified by $\mathbf{k}$. Then the algebra $\mathscr{B}(\mathcal{H}_{N,\mathbf{k}})$ is invariant, and Restricted to each $\mathscr{B}(\mathcal{H}_{N,\mathbf{k}})$, $e^{t\mathcal{K}}$ is ergodic, and there is a spectral gap independent of N, and more surprisingly, $\mathbf{k}$, except in the trivial cases when $\mathbf{k}$ has only one non-zero entry, and shown by Carlen and Loss, who in fact prove a logarithmic Sobolev inequality.

One obtains an interesting model by adding to this one an interaction with two heat baths exactly as in the model considered by Fagnola, Poletti and Sasso. As opposed to their model, there are two "Lindbladian" dynamics involved. However, the one involved in the Kac model come from something other than the weak coupling limit: It arises in a kinetic model in which most of the time particles are not interacting, but occasionally, a pair come close to one another and interact. In an appropriate scaling limit, the interaction is instantaneous.

Thank you for your Interest!