UNIVERSIDADE FEDERAL DO RIO GRANDE DO SUL

Programa de Pós-Graduação em Matemática

Continuous time Thermodynamic Formalism: for the Skorokhod space and for Quantum Markov Semigroups

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Porto Alegre, 2022

Agradecimentos

Gostaria de agradecer ao meu orientador Artur e minha coorientadora Adriana, por diversos cursos que lecionaram, sendo fundamentais na minha formação e agora também colaboradores de pesquisa. Foi uma bela jornada, muito por conta de vocês.

À banca, que contribuiu com valiosas sugestões e observações, incorporadas ao texto.

Aos meus pais, que desde sempre me apoiaram a perseguir o caminho dos estudos, sendo exemplos de perseverança no que fazem. À minha esposa Izabella, minha companheira de vida, que me inspira de diversas formas.

Aos amigos que compartilharam dessa jornada no Campus do Vale. Dividimos inúmeras discussões matemáticas na Sala do café. Obrigado por compartilharem esse entusiasmo com a matemática: Izabella, Marcus, Feltes, Jader, Will, Gleiciano, Pessil e Gustavo Müller. Também aos amigos que celebraram cada pequeno passo, em especial aos que fiz no Grupo Escoteiro Charruas.

À OBMEP e à Leslie Lamport, criador do LaTeX.

I thank Fulbright Commission for the opportunity of an exchange period at the University of Kansas, and Jin Feng for supervising me there. Also Abba, for making our lives so much easier in Lawrence.

“*A Matemática Pura é, à sua maneira,*
a poesia das ideias lógicas.”

Albert Einstein

Tese submetida por Josué Knorst[1], como requisito parcial para a obtenção do grau de Doutor em Ciência Matemática, pelo Programa de Pós-Graduação em Matemática, do Instituto de Matemática e Estatística da Universidade Federal do Rio Grande do Sul.

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Data de Defesa: 1º de Novembro de 2022

[1]Bolsista CAPES - Coordenação de Aperfeiçoamento de Pessoal de Nível Superior

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Chapter 1

Introduction

This thesis consists of two different works with a similar motivation. The common ground for them is the theory of Thermodynamic Formalism, (see, for instance, [LMMS15]). In the classical setting, one seeks the thermodynamical equilibrium states of a system under the action of a potential. This is done by looking for variational principles, where entropy and the Ruelle operator play central roles. An important issue is to introduce an *a priori* probability for defining the Ruelle operator. The two works are extensions of this theory to adjacent subjects.

In Chapter 2, we explore Thermodynamic Formalism on the Skorokhod space $\mathcal{D}$, of right continuous with left limit (càdlàg) trajectories on the circle $\mathbb{S}^1$. The goal, in this case, is to construct the Gibbs states not as probabilities over $\mathbb{S}^1$, but over $\mathcal{D}$.

The Ruelle operator in classical Thermodynamic Formalism seems to be of discrete nature in time, but a natural extension of the concept contemplates the continuous time case (see [BEL08] and [LNT13] for a similar setting). In a formula that resembles the Feynman-Kač formula, we note that the iteration of the Ruelle operator presents an average of the potential A taken over the shift pre-images of a given point.

$$\mathcal{L}_A^n(\varphi)(y) = \int_{\sigma^n(x)=y} e^{A(x)+A(\sigma(x))+\ldots+A(\sigma^{n-1}(x))}\varphi(x)d\mu(x)$$

Notice the similarity between the above and the integral on the right in Figure 1.1 below.

We will take L as a generator of a Markov stationary semigroup which will help us to define an a priori probability on the Skorokhod space. Considering the Time-reversal Markov Process, it gives us a discrete version of Feynman-Kač, a formula that is forward in time. This is the motivation to call this Stochastic Semigroup, $e^{t(L+V)}$, a continuous time Ruelle operator. Recall

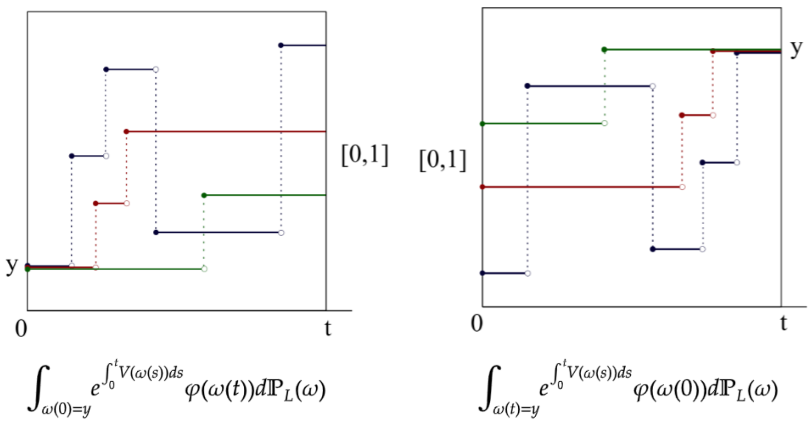


Figure 1.1: Trajectories satisfying $\omega(0) = y$ or $\omega(t) = y$.

that $L : \mathcal{C}(\mathbb{S}^1) \to \mathcal{C}(\mathbb{S}^1)$ acts on continuous functions and $V : \mathbb{S}^1 \to \mathbb{R}$ itself is a Hölder function, that acts by multiplication, $f \in \mathcal{C}(\mathbb{S}^1) \mapsto fV$. Note that the Skorokhod space is a non-compact Polish space.

We then look for a version of the Perron-Ruelle-Frobenius Theorem in this setting, since the introduction of this potential breaks the normalization condition. Restricting to the Hölder potentials and functions, we make use of Krein-Rutman theorem to show the existence of additive eigendata: two positive additive Hölder eigenfunctions, one for $L+V$ and the other for L^*+V, both associated to the same additive positive eigenvalue. With these in hand, we can follow a normalization procedure. More precisely, after finding the eigenprobability, we obtain a normalized Ruelle operator, and then we are able to define a new stationary semigroup (a new time continuous Markov chain taking values in $\mathbb{S}^1$). This stationary continuous Markov chain will be called the Gibbs state (that can be also seen as a probability on the Skohorod space) associated to V (and the a priori infinitesimal generator L).

We also consider a variational principle, where the entropy in the pressure problem is the relative entropy of the probability with respect to the *a priori* probability. Since the relative entropy is related to entropy production, this is also explored and explicitly computed.

In Chapter 3, we study Thermodynamic Formalism in a quantum setting, at continuous time. This means we look at a Quantum Markov Semigroup acting in the space of matrices $M_n(\mathbb{C})$ and its corresponding infinitesimal generator $\mathcal{L} : M_n(\mathbb{C}) \to M_n(\mathbb{C})$. More precisely, we investigate a particular stationary case, the latter meaning the existence of a density ρ such that $\mathcal{L}^*(\rho) = 0$. Following the approach introduced by Schrödinger, this ρ corresponds in the Quantum setting to an invariant (stationary) probability in the classical setting.

In order to analyze a variational principle, it is necessary to define a notion of entropy for density matrices, and also the concept that would correspond to the action of a potential A in this setting. After introducing these concepts we will discuss the existence of an equilibrium state in the set of density matrices. This program ends with the explicit construction of what we called the continuous time equilibrium Quantum Markov Process for the Hamiltonian A. The main idea in this result is to reduce the problem to the "diagonal case", where the computations turned out to be easier.

Regarding the notion of entropy employed in this work, we observe that it is a natural non-commutative extension of the concept of rate function for continuous time Markov chains. In the works of [Kač80] and [Str84], the authors show a simplification of the rate function in case the system is reversible. In the classical case, the terms reversibility and detailed balance are used as synonyms, depending on the approach. In the quantum setting, several analogous notions are studied in the bibliography. The most natural for us, (and most accepted) is what is called σ-Quantum Detailed Balance, which refers to a particular invariant state (stationary density) σ. For a special system with this property, the Heat-semigroup, considered in [CM17], we can show that the same simplification holds, indicating the notion of entropy is consistent. In order to define entropy, a certain kind of a priori probability is necessary, and the choice of σ and $\mathcal{L}$ will help to set this concept. This entropy has no dynamical content. The dynamics is on the continuous time evolution of the semigroup (not at the level of the infinitesimal generator).

To end this introduction, we will now discuss some differences between the two works and future directions. In the second work, the entropy is obtained employing properties of the infinitesimal generator of the system, allowing us to say the generator helps to define the a priori probability, since the entropy can be obtained in a similar way as in Thermodynamic Formalism via the Ruelle operator. Thus, we understand this setting as being in the "log scale". This is in contrast to the second work, where we recognize the Ruelle operator in the semigroup scale, or exponential scale.

A natural question in the quantum setting is to extend the formalism to other Quantum Markov Semigroups with Detailed Balance Condition. The case of Heat-Semigroup was treatable mostly due to the simplicity of the invariant density: the normalized identity. In the trace computations, this was very useful. This topic will be addressed in future work.

For the Skorokhod setting, one can investigate how to extend the presented formalism for potentials V that depend not only on the first coordinate. In classical Thermodynamic Formalism, a potential can depend on all coordinates. It is also of interest to consider an extra parameter β (a constant times the inverse of temperature) in the potential, studying the βV case, and letting β go to infinity, which means sending the temperature to 0. The accumulation points of the sequence of Gibbs states $\mathbb{P}_\beta$ can reveal important thermodynamical information on the system.

⋆⋆⋆

During the Ph.D. degree the following papers were produced: [BKL21b], [BKL21a], [BKL22] and [KLMN22]. The two first are already published at this time, and the last two were submitted to review and are the essence of this thesis. The author thanks Fulbright Commission for the award that let him develop a research project at a university in the U.S.A. During the academic year 2021-2022, the author visited the University of Kansas and develop research in collaboration with Prof. Dr. Jin Feng. This topic will be also addressed in future work.

Chapter 2

Thermodynamic Formalism on the Skorokhod space: the continuous time Ruelle operator, entropy, pressure, entropy production and expansiveness

Abstract

This chapter is part of the work [KLMN22]. Consider the semi-flow given by the continuous time shift $\Theta_t : \mathcal{D} \to \mathcal{D}$, $t \geq 0$, acting on the Skorokhod space $\mathcal{D}$ of *càdlàg* paths (right continuous with left limits) $w : [0, \infty) \to S^1$, where S^1 is the unitary circle (one can also take $[0, 1]$ instead of S^1). We equip the space $\mathcal{D}$ with the Skorokhod metric and we show that the semi-flow is expanding. We also introduce a stochastic semi-group $e^{t\,L}$, $t \geq 0$, where L (the infinitesimal generator) acts linearly on continuous functions $f : S^1 \to \mathbb{R}$. This stochastic semi-group and an initial vector of probability π defines an associated stationary shift-invariant probability $\mathbb{P}$ on the Polish space $\mathcal{D}$. This probability $\mathbb{P}$ will play the role of an *a priori* probability. Given such $\mathbb{P}$ and a Hölder potential $V : S^1 \to \mathbb{R}$, we define a continuous time Ruelle operator, which is described by a family of linear operators $\mathbb{L}^t_V$, $t \geq 0$, acting on continuous functions $\varphi : S^1 \to \mathbb{R}$. More precisely, given any Hölder V and $t \geq 0$, the operator $\mathbb{L}^t_V$, is defined by

$$\varphi \to \psi(y) = \mathbb{L}^t_V(\varphi)(y) = \int_{w(t)=y} e^{\int_0^t V(w(s))\,ds}\, \varphi(w(0))\, d\mathbb{P}(w).$$

We show the existence of an eigenvalue λ_V and an associated Hölder

eigenfunction $\varphi_V > 0$ for the semi-group $\mathbb{L}_V^t$, $t \geq 0$. After a coboundary procedure we obtain another stochastic semi-group, with infinitesimal generator L_V, and this will define a new probability $\mathbb{P}_V$ on $\mathcal{D}$, which we call the Gibbs (or, equilibrium) probability for the potential V. We define entropy, for some shift-invariant probabilities on $\mathcal{D}$, and we consider a variational problem of pressure. Finally, we define entropy production and analyze its relation with time reversal and symmetry of L. We wonder if the point of view described here provides a sketch (as an alternative to the Anosov one) for the chaotic hypothesis for a particle system held in a nonequilibrium stationary state, as delineated by Ruelle, Gallavotti, and Cohen.

2.1 Introduction

We consider the semi-flow given by the continuous time shift $\Theta_t : \mathcal{D} \to \mathcal{D}$, $t \geq 0$, acting on the Skorokhod space $\mathcal{D}$ of *càdlàg* paths (right continuous with left limits) $w : [0, \infty) \to S^1$, where S^1 is the unitary circle (one can take $[0, 1]$ instead of S^1). We will prefer to state the results in $[0, 1]$. The set $\mathcal{D}$ is equipped with the Skorokhod metric. The Skorokhod space $\mathcal{D}$ is a noncompact Polish space. We will show that continuous time shift Θ_t, $t \geq 0$, is expanding (see Proposition 2.6.1).

Continuous time Stochastic Processes X_t, $t \geq 0$, taking values on $[0, 1]$ are described by probabilities $\mathbb{P}$ on $\mathcal{D}$. To say that the process is stationary is equivalent to saying that the associated probability $\mathbb{P}$ is invariant for the action of the shift Θ_t, $t \geq 0$.

The results presented in the initial part of our work are in some way related to [BEL08], [LNT13], [LMN22] and [LN15]. Our main purpose here is to describe a version of Thermodynamic Formalism for semi-flows specified by infinitesimal generators. More precisely, in section 2.3 we follow the program of introducing a Ruelle operator from a potential and an *a priori* probability (in a similar fashion as in [BCL+11], [LMMS15], [BEL08] and [LNT13]).

We introduce a stochastic semi-group $e^{t\,L}$, $t \geq 0$, where L (the infinitesimal generator) acts on continuous functions $f : [0, 1] \to \mathbb{R}$. This stochastic semi-group and an initial vector of probability π defines an associated stationary shift-invariant probability $\mathbb{P}$ on the $\mathcal{D}$ (see [Lid19]). This probability $\mathbb{P}$ will play the role of an *a priori* probability (a continuous time version of the point of view of [LMMS15] and [BCL+11]).

Given the *a prori* probability $\mathbb{P}$ on $\mathcal{D}$ and a Hölder continuous potential $V : [0, 1] \to \mathbb{R}$, we define the Ruelle operator $\mathbb{L}_V^t$, $t \geq 0$, in such way that for

$\varphi : [0,1] \to \mathbb{R}$, we get $\mathbb{L}_V^t(\varphi) = \psi$, $t \geq 0$, when

$$\varphi \to \psi(y) = \mathbb{L}_V^t(\varphi)(y) = \int_{w(t)=y} e^{\int_0^t V(w(s))\,ds}\, \varphi(w(0))\, d\mathbb{P}(w). \tag{2.1}$$

The above expression can be recognized as in Feynman-Kac form if the infinitesimal generator is symmetric according to Lemma 1 in Section 2.3 and figure 2.1 (see also [LMN22]).

The Feynmann-Kac formula is the partial differential equation

$$\frac{\partial u}{\partial t} + Lu + V\,u = 0.$$

General results for continuous-time Markov chains that were specially designed to be applicable to our setting appear on [MN22].

Note that expression (2.1) depends also on L (because $\mathbb{P}$ depends on L).

From the *a priori* probability $\mathbb{P}$ on $\mathcal{D}$, in section 2.4 we are able to introduce the concepts of entropy, for a certain class of shift-invariant probabilities on $\mathcal{D}$, and pressure for a potential $V : [0,1] \to \mathbb{R}$ (see Definition 2.4.1 and expression (2.40)). For the existence of an eigenvalue and a positive eigenfunction for the Ruelle operator (see Theorem 1), an assumption on the regularity of the potential V will be required (Hölder or Lipschitz continuous will be enough) as discussed in Proposition 2.3.4 in section 2.3. Example 3 presents explicit expressions for the eigenvalue and the eigenfunction $f : [0,1] \to \mathbb{R}$ solutions for a certain class of infinitesimal generators L and quadratic potentials V. In the Appendix Section 2.7 we show that this regularity assumption is necessary. From L and V, after a kind of coboundary procedure, we obtain another stochastic semi-group, with infinitesimal generator L_V, and this will define a new probability $\mathbb{P}_V$ on $\mathcal{D}$, which we call the equilibrium probability for the potential V (see Definitions 2.3.5, 2.3.9, 2.3.8, Lemma 2 and expressions (2.26) and (2.25)). The initial stationary vector of probability for such a process is given by Proposition 2.3.6. A nice formula related to the main eigenvalue is given by (2.41). Note that V is completely independent of the dynamics of the shift Θ_t, $t \geq 0$, and the *a priory* probability defined by L.

We define entropy production in section 2.5 and we discuss some properties related to time-reversal and the symmetry of the infinitesimal generator L (see Propositions 2.5.2 e 2.5.4). Related results for continuous time quantum channels (where the infinitesimal generator is a Lindbladian) appear in [BKL22].

In [Coh97], [Gal99], [Rue96], [ABR14] and [Rue15], the authors use an idea of Ruelle's as a guiding principle to describe nonequilibrium stationary states in general. The purpose is a better understanding of a model for the chaotic hypothesis for a single (moving) particle system held in a nonequilibrium stationary state. This model is described by properties of SBR probabilities for Axiom A (or Anosov) systems and entropy production rate (see also [JQQ00], [MNS09],[MN02] and [Pol14]). In this case, the potential is fixed as the Lyapunov exponent. The reason for such interest is that the real physical problem behaves, in many respects, as if they were Anosov systems as far as their properties of physical interest are concerned. We wonder if our setting, where V is general, also provides a sketch (as an alternative for the Anosov one) for the chaotic hypothesis.

The original article has two extra Appendix sections of technical nature and they have the purpose of analyzing some integral kernels which naturally appear in our reasoning. The interested reader can find them [KLMN22].

In Appendix 2.8 we present the details of the claims mentioned in Example 1 which describes in explicit form an interesting working case.

Some of our results are related to the ones in [DV75], [Kif90a], [Kif90b], [MNS09], [MN02], [LMN22], [JQQ00], [Gom01], [LT18] and [LM22a].

2.2 Motivation and Preliminaries

To motivate our reasoning, we will begin with a review of some basic and simple properties of Markov chains taking values on $[0,1]$ (in a similar fashion one considers the case where the process is taking values in S^1.

Consider $P(x,y)>0$, $P:[0,1]\times[0,1]\to\mathbb{R}$ continuous such that for all $y\in[0,1]$

$$\int P(x,y)\ dx = 1. \tag{2.2}$$

Note that is not true that the supremum of P is smaller than 1.

Let $\theta:[0,1]\to\mathbb{R}$ be a strictly positive function such that

$$\iint P(x,y)\theta(y)\ dx\ dy = 1,$$

and also that for any x

$$\int P(x,y)\theta(y)dy = \theta(x). \tag{2.3}$$

The function θ is the initial invariant vector of probability for a stationary discrete-time Markov chain with values on $[0,1]$.

The above reasoning was just to explain what is a line sum 1 stochastic matrix with values on $[0,1]$. In analogy with Markov chains with finite state space, $P(x,y)$ should be seen as a matrix with entries in $[0,1]\times[0,1]$ where x is in the vertical axis and y is in the horizontal axis (see [LMST09] for related results).

We define the infinitesimal generator L acting on the left in **periodic** functions $f:[0,1]\to\mathbb{R}$, by

$$L(f)(y)=\int f(x)P(x,y)d\,x-f(y),$$

which by (2.2) means

$$L(f)(y)=\int\big[f(x)-f(y)\big]P(x,y)d\,x \tag{2.4}$$

Note that $L(1)=0$.

We call L the *a priori* infinitesimal generator.

Later we consider (see the expression (2.25)) the action of infinitesimal generators of the form

$$f\to\gamma(y)\int\big[f(x)-f(y)\big]\,P(x,y)dx, \tag{2.5}$$

where γ is positive, as in [LNT13].

We will consider $L:\mathcal{L}^2(dx)\to\mathcal{L}^2(dx)$ and the dual $L^*:\mathcal{L}^2(dx)\to\mathcal{L}^2(dx)$, which acts on probability densities $g:[0,1]\to\mathbb{R}$ by

$$L^*(g)(x)=\int P(x,y)g(y)d\,y-\ g(x). \tag{2.6}$$

Now setting $\mu(dx)=\theta(x)dx$, the probability measure with density θ, we get $L^*(\theta)=0$, by (2.3). In this context, this means that μ is invariant for the action of L^*.

L and L^* are bounded operators.

Note that for any f,g we have for $\mathcal{L}^2$ inner product

$$<g,L(f)>=<L^*(g),f>.$$

L acts on (the left) functions $f:[0,1]\to\mathbb{R}$ (on the variable y) and L^* acts on (the right) densities $g(x)dx$ (or on probabilities).

A nice reference for continuous time processes with infinitesimal generator L is [DV75], where it is considered a strongly continuous semigroup mapping T^t, $t\geq 0$, acting on the set of continuous functions f on compact manifold, satisfying for all $t \geq 0$: $T^t(f)$ is a positive function, if f is positive and $T^t 1 = 1$.

The operator e^{tL}, for fixed $t \geq 0$, is an integral operator, that is, there exists a function $K_t : [0,1] \times [0,1] \to \mathbb{R}^+$ such that

$$e^{t\,L}(f)(y) = \int f(x) K_t(x,y) dx + e^{-t} f(y).$$

The function $K_t : [0,1] \times [0,1] \to \mathbb{R}^+$ satisfies the following equations (see appendix 1):

$$\frac{d}{dt} K_t(x,y) = \int K_t(x,z) P(z,y) dz - K_t(x,y) + e^{-t} P(x,y), \qquad (2.7)$$

$$\begin{aligned} \frac{d}{dt} K_t(x,y) &= L(K_t(x,\cdot))(y) + e^{-t} P(x,y) \\ &= L^*(K_t(\cdot,y))(x) + e^{-t} P(x,y), \end{aligned}$$

and

$$\frac{d}{dt} K_t(x,y) = \int K_t(z,y) P(x,z) dz - K_t(x,y) + e^{-t} P(x,y).$$

Example 1. *Take $P(x,y) = \cos[(x-y)2\pi]/2 + 1$. This P is symmetric and continuous on $[0,1]$. Since $\int \cos[(x-y)2\pi] dx = 0$, for any $y \in [0,1]$ we get that $\int P(x,y) dx = 1$.*

$K_t(x,y), t \geq 0$ can be explicitly expressed by

$$K_t(x,y) = 2\cos(2\pi(x-y))(e^{-3t/4} - e^{-t}) + (1 - e^{-t}).$$

The Lebesgue probability dx is the unique invariant probability. The proofs of these claims are presented in Appendix section 2.8.

$\diamondsuit$

For each t fixed, $K_t(x,y)$ can be seen as a matrix with entries in $[0,1] \times [0,1]$, where x is in the vertical axis and y in the horizontal axis.

We denote by $\mathcal{D}$ the Skorokhod space of *càdlàg* paths (right continuous with left limits) $w : (0,\infty) \to [0,1]$ (see [EK86] for general properties)

The continuous time shift $\Theta_t : \mathcal{D} \to \mathcal{D}$, $t \geq 0$, is defined in such way that, $\Theta_t(w_a) = w_b$, if for all $s \geq 0$, we have $w_b(s) = w_a(s+t)$.

We say that a probability P on $\mathcal{D}$ is invariant for the semi-flow $\Theta_t : \mathcal{D} \to \mathcal{D}$, $t \geq 0$, if for all measurable set $C \subset \mathcal{D}$, and any $t \geq 0$, we have that $P(C) = P(\,(\Theta_t)^{-1}(C)\,)$.

The kernel K_t , $t \geq 0$, defines a Markov Process X_t, $t \geq 0$, with values on $[0,1]$. Given an initial density function φ_0 on $[0,1]$, this Markov Process determines a probability $\mathbb{P}$ on $\mathcal{D}$. For example, for the cylinder set $C = \{X_0 \in (a_0, b_0), X_{t_1} \in (a_1, b_1), X_{t_2} \in (a_2, b_2), X_{t_3} \in (a_3, b_3)\}$ we get that

$$\mathbb{P}(C) = \int_{a_0}^{b_0} \int_{a_1}^{b_1} \int_{a_2}^{b_2} \int_{a_3}^{b_3} K_{t_1}(x_0, x_1)\, K_{t_2-t_1}(x_1, x_2)\, K_{t_3-t_2}(x_2, x_3)$$

$$\times\, \varphi_0(x_0)\, dx_3\, dx_2\, dx_1\, dx_0.$$

Given L (as in (2.4)) assume that there exists a positive continuous density function $\theta : [0,1] \to \mathbb{R}$, such that, for any continuous function $f : [0,1] \to \mathbb{R}$ we get

$$\int L(f)(x)\theta(x)dx = 0. \tag{2.8}$$

Moreover, we assume that L is such that the above-defined θ is unique.

Definition 2.2.1. *Given L (as in (2.4)) and an initial density $\varphi_0 = \theta$ satisfying (2.8), we get a continuous time stationary Markov process X_t, $t \geq 0$, with values on $[0,1]$ (see [BGL13],[Bob05] or [Lid19]). This process defines a probability $\mathbb{P} = \mathbb{P}_{L,\theta}$ on the Skorokhod space $\mathcal{D}$. This probability $\mathbb{P}$ is invariant for the shift Θ_t, $t \geq 0$.*

Consider an infinitesimal generator L (where L is given by (2.4)) for the semigroup $e^{t\,L}$, $t \geq 0$. This semigroup satisfies $e^{t\,L}(1) = 1$. Moreover, $e^{t\,L^*}(\theta) = \theta$, where L^* was given by (2.6) and θ satisfies (2.8).

Now we take a continuous function $V : [0,1] \to \mathbb{R}$, which will be called a potential. In Statistical Mechanics $H = -e^V$ should correspond in some sense to the Hamiltonian. For some results, we will assume that V is of Hölder class.

By definition, the operator $L + V : \mathcal{L}^2(dx) \to \mathcal{L}^2(dx)$ (acting on the left on functions on the variable y) is such that

$$(L+V)(f)(y) = g(y) = \int \big[f(x) - f(y)\big] P(x,y)\; d\,x + V(y)f(y).$$

The dual operator acts (on the right) on density functions g on the variable x

$$(L^* + V)(g)(x) = f(x) = \int P(x,y)g(y)d\,y - \; g(x) + V(x)\, g(x).$$

If $P(x,y)$ is symmetric the spectral properties of L and L^* is the same.

Example 2. $P(x,y) = \cos[(x-y)2\pi]/2+1$ *and* $V(y) = (y-1/2)^2$.
Then,

$$(L+V)(f)(y) = \int f(x)[\,\cos[(x-y)2\pi]/2+1\,]\,d\,x - f(y) + (y-1/2)^2\, f(y).$$

$\diamondsuit$

Now consider the semigroup $e^{t\,(L+V)}$. By Feynman-Kac (see [Str84] or [BGL13]), we can write

$$e^{t\,(L+V)} f(x) = \mathbb{E}_x\Big[e^{\int_0^t V(X_r)dr} f(X_t)\Big],$$

where X_t, $t \geq 0$, is the Markov process with infinitesimal generator L. This semigroup is not a stochastic semigroup.

This operator is an integral operator, that is, there exist $K_t^V : [0,1] \times [0,1] \to \mathbb{R}^+$, such that,

$$e^{t\,(L+V)}(f)(y) = \int f(x) K_t^V(x,y) dx + e^{-t} e^{tV(y)} f(y).$$

The function $K_t^V : [0,1]\times[0,1] \to \mathbb{R}^+$ satisfies the following equation (see Appendix 1 and 2 in [KLMN22])

$$\begin{aligned}\frac{d}{dt} K_t^V(x,y) &= (L+V)(K_t^V(x,\cdot))(y) + e^{t(V(x)-1)} P(x,y)\\ &= (L+V)^*(K_t^V(\cdot,y))(x) + e^{t(V(y)-1)} P(x,y).\end{aligned}$$

2.3 Ruelle Operator

We denoted by $\mathcal{D} := \mathcal{D}\big([0,+\infty),[0,1]\big)$ the path space of *càdlàg* trajectories taking values in $[0,1]$ (see [Lid19]). This space is endowed with the Skorokhod metric.

Remember that the flow $\Theta_t : \mathcal{D} \to \mathcal{D}$, $t \geq 0$, satisfies: given t we have that $\Theta_t(w_1) = w_2$, if for all $s \geq 0$, $w_2(s) = w_1(s+t)$.

We assume in this section that L is of the form (2.4).

Lemma 1. *If L is symmetric, then*

$$\int_{w(0)=y} e^{\int_0^t V(w(s))\,ds}\, \varphi(w(t))\, d\mathbb{P}_L(w) = \int_{w(t)=y} e^{\int_0^t V(w(s))\,ds}\, \varphi(w(0))\, d\mathbb{P}_L(w). \tag{2.9}$$

A more general version of the above result appears in the Appendix. This Lemma, in particular, is an immediate consequence of (2.52) for $T = t$.

Definition 2.3.1. *Given L and V, consider, for each fixed t, the continuous time Ruelle operator $\mathbb{L}_V^t$, $t \geq 0$, where $\mathbb{L}_V^t : C^0[0,1] \to C^0[0,1]$, associated to V (in a similar way to [BEL08]): in this case for $t \geq 0$ we denote $\mathbb{L}_V^t(\varphi) = \psi$, when*

$$\varphi \to \psi(y) = \int_{w(0)=y} e^{\int_0^t V(w(s))\,ds}\, \varphi(w(t))\, d\mathbb{P}_L(w),$$

that is,

$$\varphi \to \psi(y) = \mathbb{L}_V^t(\varphi)(y) = e^{t(L+V)}(\varphi)(y), \tag{2.10}$$

where $\varphi, \psi : [0,1] \to \mathbb{R}$.

This operator (which was considered in similar cases in [BEL08] and [LNT13]) is the continuous time version of the classical Ruelle operator (discrete time case). Indeed, Lemma 1 confirms the claim and figure 2.1 schematically support this statement.

The left-hand side of expression (2.9) is more suitable for the Feynman-Kac formula.

According to our notation the continuous time Ruelle operator $\mathbb{L}_V^t$, $t \geq 0$, is a family of linear operators indexed by t.

Definition 2.3.2. *Given L and $V : [0,1] \to \mathbb{R}$ we say that the familiy of Ruelle operators $\mathbb{L}_V^t$, $t \geq 0$, is normalized if $\mathbb{L}_V^t(1) = 1$, for all $t \geq 0$.*

Given L, in case V is constantly equal to zero, the family of Ruelle operators $\mathbb{L}_0^t, t \geq 0$, is normalized.

In this case $\mathbb{L}_0^t(f) = g$, when

$$f \to g(y) = \int_{w(0)=y} f(w(t))\, d\mathbb{P}_L(w) = e^{tL}(f)(y) = \mathbb{L}_0^t(f)(y),$$

where $f, g : [0,1] \to \mathbb{R}$ are periodic.

Definition 2.3.3. *Given L and V we say that $f : [0,1] \to \mathbb{R}$ is an eigenfunction of the continuous time Ruelle operator $\mathbb{L}_V^t$, $t \geq 0$, associated to the eigenvalue $\lambda \in \mathbb{R}$, if for all $t \geq 0$,*

$$\mathbb{L}_V^t(f) = e^{\lambda t} f. \tag{2.11}$$

In order to find eigenfunctions, we have to analyze the properties of the operator $L + V$ and $L^* + V$.

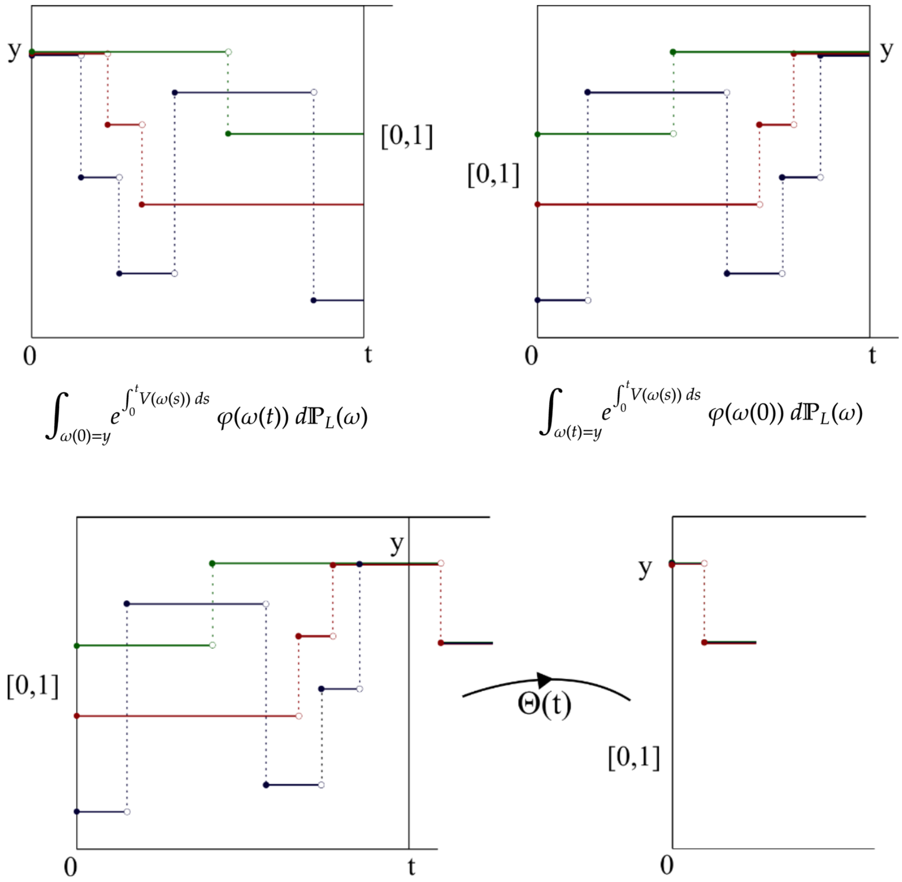


Figure 2.1: The point $y \in [0, 1]$ is the value at time $t = 0$ of the path obtained as the image - by the continuous time shift Θ_t - of the set of paths described above.

Assume that the positive function $f : [0, 1] \to \mathbb{R}$ is such that

$$(L + V)(f) = \lambda f, \tag{2.12}$$

then, for all $t \geq 0$,

$$e^{t\,(L+V)}(f) = e^{t\,\lambda} f, \tag{2.13}$$

that is, $f : [0, 1] \to \mathbb{R}^+$ is an eigenfunction (for the semigroup generated by the infinitesimal generator $L + V$) associated with the eigenvalue $\lambda \in \mathbb{R}$.

We say that such λ (which can be positive or negative) is the main eigenvalue for $L + V$.

Example 3. *Consider the periodic function* $g(x) = \frac{6}{7}(1 + x\,(1-x))$ *and* $P(x,y)$ *defined for* $x, y \in [0,1]$ *(or, in* $S^1 \times S^1$*), by*

$$P(x,y) = g(x+y), \text{ if } (x+y) < 1, \text{ and } P(x,y) = g(x+y-1), \text{ if} (x+y) \geq 1. \tag{2.14}$$

One can show that the kernel P *is symmetric and therefore the corresponding density* θ *satisfying* (2.3) *is equal to* 1*. Consider now the function* $V : S^1 = [0,1) \to \mathbb{R}$*, given by* $V(y) = 1 + \frac{1}{7}y\,(1-y)$*. Taking*

$$\lambda = \frac{1}{70}(35 + \sqrt{1345}) \text{ and } y \to f(y) = \frac{1}{10}(35 + \sqrt{1345}) + (1-y)y > 0,$$

we get for all $y \in S^1$

$$(L+V)(f)(y) \;=\; \int_0^1 P(x,y) f(x)dx - f(y) + V(y)\,f(y) = \lambda\, f(y), \tag{2.15}$$

and therefore, f *and* λ *solve* (2.12) *for such* P *and* V*.*

As P *is symmetric the function* $f : S^1 \to \mathbb{R}$ *also solves*

$$(L^* + V)(f) = \lambda f.$$

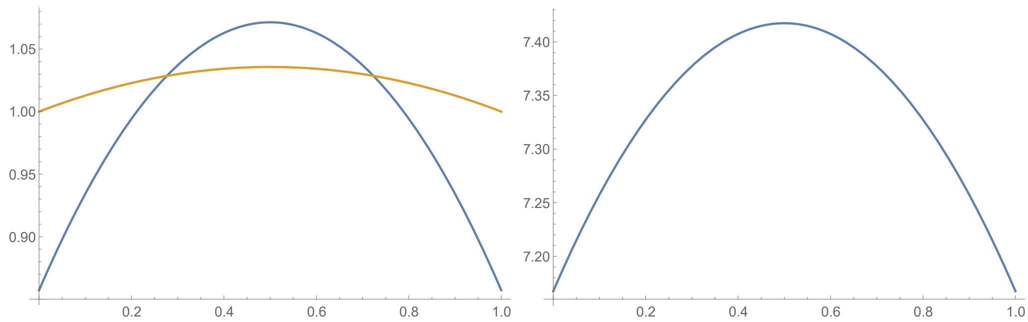


Figure 2.2: On the left, functions g (blue) and V (orange); On the right, eigenfunction f.

More generally, given V *of the form* $V(y) = r + s\,y(1-y)$*, and the quadratic density* $g(x) = \frac{d + c\,x(1-x)}{d + c/6}$ *(defining* P *as in* (2.14)*), one can find a density* f *of the form* $f(y) = a + b\,y(1-y)$*, such that, for some* λ *we get* (2.15)*.*

$\diamondsuit$

Given λ as in (2.12), if $g(y) > 0$ is such that

$$(L^* + V)(g) = \lambda g, \tag{2.16}$$

then, for all $t \geq 0$,

$$e^{t\,(L^*+V)}(g) = e^{t\,\lambda} g,$$

that is $g : [0,1] \to \mathbb{R}^+$ is an eigenfunction (for the semigroup generated by the infinitesimal generator $L^* + V$) associated to the eigenvalue $\lambda \in \mathbb{R}$. It is natural to assume the normalization condition $\int g(y)dy = 1$ so we can see g as a density.

Note that we ask for f and g to have the same eigenvalue λ.

A natural normalization assumption for f is to assume that

$$\int f(x)g(x)dx = 1. \tag{2.17}$$

In this case $\pi(x) = f(x)g(x)$ is a density on $[0,1]$, and this will be important later (see proposition 2.3.6).

Compare all this with pages 52-54 in [Kač80] and around page 113 in [Str84].

We want to show that given L and V one can find a solution for (2.12). This will follow from Krein-Rutman Theorem (see [Dei85] and [LMST09]).

Theorem 1. *Assume that $V : [0,1] \to \mathbb{R}$ is Hölder , then, there exist $\lambda \in \mathbb{R}$, $\ell : [0,1] \to \mathbb{R}^+$ and $r : [0,1] \to \mathbb{R}^+$, where ℓ, r are also Hölder (in particular $\ell, r \in \mathcal{L}^2(dx)$), such that,*

$$\ell\,(L+V) = \lambda \ell$$

and

$$(L+V)r = \lambda r.$$

Proof. The action of $\ell \to \ell\,(L+V)$ (acting on the left side) can be seen as the action on the dual, i.e., $\ell \to (L^* + V)\,\ell$ (acting on the right side). Consider $\mathcal{H}_\alpha$ the Banach space of Hölder continuous real functions on $[0,1]$ with constant α and the norm

$$\|h\|_\alpha = \|h\| + \sup_{x \neq y} \frac{|h(y) - h(x)|}{|y-x|^\alpha}.$$

The above supremum is denoted as $Höl_h$. Let $K \subset \mathcal{H}_\alpha$ be the cone of positive α-Hölder functions in $[0,1]$. The interior of K, denoted K^o, is the set of strictly positive α-Hölder functions. We will use item (a) in Theorem 19.3 in [Dei85].

Indeed, consider $z = \|V\| + 1$. We claim that $(L + V + zI)$ is a strongly positive operator (take non-null positive functions to strictly positive functions). Then, from Krein-Rutman Theorem (see Theorem 19.3 page 228 in

[Dei85]) there exists a unique eigenfunction r for $(L+V+zI)$ in the set K^o. The same is true for the left eigenfunction ℓ.

We now check the assumptions of Krein-Rutman theorem. Notice that $-\|V\| \leq V(x)$ and therefore $V(x)+z-1 \geq 0$ for all $x \in [0,1]$. It follows that

$$(L+V+zI)f(x) = \int f(y)P(y,x)dy + (V(x)+z-1)f(x) \geq \int f(y)P(y,x)dy.$$

We started with $f(y) \geq 0$ and $P(y,x) > 0$, for every $x, y \in [0,1]$. For $f \neq 0$, by continuity there exists an open set in which f is strictly positive and then $(L+V+zI)f(x) > 0$. This means $(L+V+zI)(K\backslash\{0\}) \subset K^o$.

Now to see that the operator is compact, consider $f \in B_\alpha(1)$, the unitary ball of $\mathcal{H}_\alpha$. Then $\|f\| \leq 1$, $H\ddot{o}l_f \leq 1$ and

$$|(L+V+zI)f(y) - (L+V+zI)f(x)| \leq |Lf(y) - Lf(x)|$$
$$+|V(y)f(y) - V(x)f(x)| + z|f(y) - f(x)|$$
$$\leq \int |f(w)||P(w,y) - P(w,x)|\, dw + (z+1)|f(y) - f(x)| +$$
$$|V(y)||f(y) - f(x)| + |f(x)||V(y) - V(x)|.$$

Since $P : [0,1]^2 \to \mathbb{R},\ V : [0,1] \to \mathbb{R}$ are continuous and therefore uniformly continuous, given $\varepsilon > 0$, there exists $\delta > 0$ such that $|x-y| < \delta \Rightarrow |P(w,y) - P(w,x)| < \frac{\varepsilon}{3}$ for every $w \in [0,1]$ and $|V(y) - V(x)| < \frac{\varepsilon}{3}$. If we take δ small enough to have $\delta^\alpha < \frac{\varepsilon}{3(z+1+\|V\|)}$ also, we get

$$|(L+V+zI)f(y) - (L+V+zI)f(x)| \leq \frac{2\varepsilon}{3} + (z+1+\|V\|)|f(y) - f(x)|$$
$$\leq \frac{2\varepsilon}{3} + (z+1+\|V\|)|y-x|^\alpha < \varepsilon.$$

This means that $(L+V+zI)(B_\alpha(1))$ is equicontinuous. It is bounded also, since $L+V+zI$ is bounded by $1+2\|V\|$, and finally the operator is compact. The same analysis can be done for $L+V+zI$ acting on the right, which is equivalent to the action of L^*+V+zI.

From the above we get the existence of $\ell, r : [0,1] \to (0,\infty)$ and a λ which satisfy

$$(L+V-\lambda I)\, r = 0, \tag{2.18}$$

and

$$\ell(L+V-\lambda I) = 0, \tag{2.19}$$

by Krein-Rutman (as in [1]).

□

We denote by ℓ_V, r_V and $\lambda(V)$ the solutions of the above equations.

We consider normalization conditions: $\int r_V(y)dy = 1$ and (see (2.17))

$$\int r_V(x)\ell_V(x)dx = 1. \tag{2.20}$$

The equation for the above right eigenfunction $r = r_V$ is

$$\int r(x)P(x,y)\,dx - (\,1 + \lambda(V)\; - \;V(y))\,r(y) = 0. \tag{2.21}$$

for any y.

The equation for the above left eigenfunction $\ell = \ell_V$ is

$$\int P(x,y)\ell(y)\,dy - (\,1 + \lambda(V)\; - V(x))\,\ell(x) = 0, \tag{2.22}$$

for any x.

It follows from the existence of ℓ satisfying (2.19) and the above that:

Proposition 2.3.4. *Given L and the Hölder continuous function $V : [0,1] \to \mathbb{R}$ there exists f and λ, such that,*

$$\mathbb{L}_V^t(f) = e^{\lambda t} f. \tag{2.23}$$

For all $y, z \in [0,1]$, $t \geq 0$ and $f \in C_b([0,1])$, define

$$\gamma_V(y) = 1 + \lambda(V) - V(y), \qquad Q_V(z,y) = \frac{r(z)P(z,y)}{r(y)\gamma_V(y)}, \tag{2.24}$$

$$\mathcal{L}_V(f)(y) = \gamma_V(y)\int [f(z) - f(y)]Q_V(z,y)\,dz \tag{2.25}$$

and

$$\mathcal{P}_t^V(f)(y) = \frac{e^{t(L+V)}(rf)(y)}{e^{\lambda(V)\,t}\,r(y)}. \tag{2.26}$$

Lemma 2. *The operator $\mathcal{P}_t^V$, defined in (2.26), is the semi-group associated to the infinitesimal generator $\mathcal{L}_V$, defined in (2.25), that is,*

$$\lim_{t\to 0} \frac{\mathcal{P}_t^V(f)(y) - f(y)}{t} = \mathcal{L}_V(f)(y).$$

Proof. Since

$$\gamma_V(y) = \int r(z) \tfrac{P(z,y)}{r(y)} \, dz,$$

we have

$$\int Q_V(z,y) \, dz = \int \frac{r(z)P(z,y)}{r(y)\gamma_V(y)} \, dz = 1. \tag{2.27}$$

We can rewrite $\frac{\mathcal{P}_t^V(f)(y)-f(y)}{t}$ as

$$\frac{1}{e^{\lambda_V t} r(y)} \Big(\frac{e^{t(L+V)}(rf)(y) - r(y)f(y)}{t} \Big) + f(y) \Big(\frac{e^{-\lambda(V)\, t} - 1}{t} \Big).$$

Taking limit as $t \to 0$, we get $\frac{1}{r(y)}(L+V)(rf)(y) - \lambda(V)f(y)$. Using (2.24), the last expression becomes

$$\int [f(z) - f(y)] \, \frac{r(z)}{r(y)} \, P(z,y) \, dz = \mathcal{L}^V f(y).$$

$\square$

The semigroup $e^{t\,\mathcal{L}_V}, t \geq 0$, is normalized.

Definition 2.3.5. *The continuous Markov chain process with values on* $[0,1]$ *and infinitesimal generator* $\mathcal{L}_V$ *has an initial stationary positive density* $\pi_V : [0,1] \to \mathbb{R}$. *We denote the associated stationary continuous time Markov chain by* X_t^V, $t \geq 0$. *We call such Process the* **Gibbs Markov Process for the potential** V *(see section in 3 in [LNT13]).*

In Proposition 2.3.6 we show that $\pi_V = \ell_V \, r_V$, where the normalization conditions (2.20) are assumed to be satisfied.

Note that from (2.27) we get that $Q_V(x,y)$, $x, y \in [0,1]$, defines a continuos time Markov chain with a generator L of the form (2.4) where we replace P by Q_V.

Then, multiplying (2.22) by $\ell(y)$ and integrating over y we get

$$\iint r(x)P(x,y)\ell(y) \, dy \, dx + \int V(x)r(x)\ell(x) \, dx = \lambda + 1. \tag{2.28}$$

Note that when P is symmetric we have from (2.28) that $\ell = r$ and

$$\iint r(x)P(x,y)r(y) \, dy \, dx + \int V(x)r^2(x) \, dx = \lambda + 1. \tag{2.29}$$

The above reasoning is similar to section 5 in [LNT13].

Lemma 3. *The dual of the operator* $\mathcal{L}_V$*, defined in* (2.25) *is the operator*

$$g \to \mathcal{L}_V^*(g)(z) = \int \gamma_V(y) g(y) Q_V(z,y) dy - \gamma_V(z)\, g(z). \tag{2.30}$$

Proof. Given the functions f, g we get

$$\int \mathcal{L}_V(f)(y)\, g(y)\, dy = \int [\gamma_V(y) \int [f(z) - f(y)] Q_V(z,y)\, dz\,]\, g(y) dy =$$

$$\iint \gamma_V(y) f(z) g(y)\, Q_V(z,y)\, dz\, dy - \int \gamma_V(y) f(y) g(y)\, [\int Q_V(z,y)\, dz]\, dy =$$

$$\int f(z)\, [\int \gamma_V(y)\, g(y)\, Q_V(z,y)\, dy\,]\, dz - \int f(z)\ \gamma_V(z)\, g(z)\, dz =$$

$$\int f(z)\, [\int \gamma_V(y)\, g(y)\, Q_V(z,y)\, dy\ -\ \gamma_V(z)\, g(z)\,] dz = \int f(z)\, \mathcal{L}_V^*(g)(z)\, dz.$$

□

Given the the Markov Process X_t^V, $t \geq 0$, with infinitesimal generator $\mathcal{L}_V$, we ask: how to get the stationary initial probability $\pi_V = \pi : [0,1] \to \mathbb{R}$.

We assume that $\int r_V(z) dz = 1$ and, moreover, that $\int \ell_V(z) r_V(z) dz = 1$.

Proposition 2.3.6. *The density* $\pi_V(z) = \ell_V(z)\, r_V(z)$ *satisfies* $\mathcal{L}_V^*(\pi_V) = 0$.

Proof. From (2.24) and (2.21) we get for any point z

$$\begin{aligned}
\mathcal{L}_V^*(\pi_V)(z) &= \int \gamma_V(y) \ell_V(y) r_V(y) Q_V(z,y) dy - \gamma_V(z)\, \ell_V(z) r_V(z) \\
&= \int \gamma_V(y) \ell_V(y) r_V(y) \frac{r_V(z)\, P(z,y)}{r_V(y) \gamma_V(y)} dy - \gamma_V(z)\, \ell_V(z) r_V(z) \\
&= \int r_V(z)\, P(z,y)\, \ell_V(y) dy - \gamma_V(z)\, \ell_V(z) r_V(z) \\
&= r_V(z) [\int P(z,y)\, \ell_V(y) dy - \gamma_V(z)\, \ell_V(z)\,] \\
&= r_V(z)\, 0 \\
&=\ 0.
\end{aligned}$$

□

From the above we get for any z

$$\int \frac{\gamma_V(y)}{\gamma_V(z)} \ell_V(y) r_V(y) Q(z,y) dy =\ \ell_V(z) r_V(z) \tag{2.31}$$

Corollary 2.3.7. *Given V we get for any $t \geq 0$ and continuous function $\varphi : [0,1] \to \mathbb{R}$:*

$$\mathcal{P}_t^V(\varphi)(x) = \mathbb{E}_x \left[e^{\int_0^t V(X_s)\, ds} \; \frac{r_V(X_t)}{e^{t\,\lambda(V)}\, r_V(x)}\, \varphi(X_t)\right] \tag{2.32}$$

Moreover,

$$\mathcal{P}_t^V(1) = e^{t\,\mathcal{L}_V}(1) = 1 \tag{2.33}$$

and

$$(\mathcal{P}_t^V)^*(\pi_V) = e^{t\,\mathcal{L}_V^*}(\pi_V) = \pi_V. \tag{2.34}$$

The expected value calculated above is relative to the *a priori* probability P on the Skorokhod space.

Definition 2.3.8. *The Markov Process X_t^V, $t \geq 0$ will be called the* **Gibbs stochastic process** *associated with $V : [0,1] \to \mathbb{R}$ (where the a priori P on $\mathcal{S}$ was given via the infinitesimal generator L which was fixed).*

Definition 2.3.9. *Given L and $V : [0,1] \to \mathbb{R}$, the associated probability $\mathbb{P}_V$ on the space $\mathcal{D}$ obtained from the* **Gibbs Markov Process** *X_t^V, $t \geq 0$ (with infinitesimal generator $\mathcal{L}_V$ and the stationary probability π_V) will be called the* **Gibbs probability for the interaction** *V (and the a priori infinitesimal generator L). $\mathbb{P}_V$ is invariant for the shift $\Theta_s, s \geq 0$.*

In the case $V = 0$ (and the Ruelle operator is normalized) $\mathbb{P}_0$ is the probability $\mathbb{P} = \mathbb{P}_L$ of Definition 2.2.1.

From [DV75],

$$\lim_{t\to\infty} \frac{1}{t} \log \sup_x \mathbb{E}_x \left[e^{\int_0^t V(w(s))\, ds}\right] = \lambda_V.$$

2.4 Relative Entropy, Pressure and the equilibrium state for V

The results of this section in some sense are similar to the ones in [LNT13].

Given the inifinitesimal generators L_1 and L_2 (of the form (2.4)) consider the corresponding stationary probabilities μ_1 and μ_2 on $[0,1]$.

We denote by $\mathbb{P}_{L_1}$ and $\mathbb{P}_{L_2}$ the corresponding associated Θ_t-invariant probabilities on the Skorokhod space, $t \geq 0$.

Definition 2.4.1. *The relative entropy (or Kullback-Leibler divergence) of* $\mathbb{P}_{L_1}$ *and* $\mathbb{P}_{L_2}$ *is the value*

$$\frac{1}{T}H_T(\mathbb{P}_{L_2}|\mathbb{P}_{L_1}) \;=-\,\frac{1}{T}\int_{\mathcal{D}}\log\left(\frac{d\mathbb{P}_{L_2}}{d\mathbb{P}_{L_1}}\Big|_{\mathcal{F}_T}\right)(\omega)\, d\mathbb{P}_{L_1}(\omega) \tag{2.35}$$

Consider the infinitesimal generator $\tilde{\mathcal{L}}$, which acts on bounded mensurable functions $f:[0,1]\to\mathbb{R}$ as

$$\tilde{\mathcal{L}}(f)(x) = \int \big[f(y)-f(x)\big]\tfrac{\phi(y)}{\phi(x)}P(y,x)\,dy\,.$$

To rewrite the operator above we consider

$$\tilde{\gamma}(x) := \frac{1}{\phi(x)}\int \phi(y)P(y,x)dy \tag{2.36}$$

and $\tilde{Q}(y,x) := \frac{\phi(y)}{\phi(x)\tilde{\gamma}(x)}P(y,x)$. Then

$$\tilde{\mathcal{L}}(f)(x) = \tilde{\gamma}(x)\int \big[f(y)-f(x)\big]\tilde{Q}(y,x)\,dy\,.$$

The invariant probability for $\tilde{\mathcal{L}}$ is

$$\tilde{\mu}(dy) = \frac{\phi(y)\tilde{r}_\phi(y)}{\|\phi\|_2\|r_\phi\|_2}dy \tag{2.37}$$

where $\tilde{r}_\phi$ satisfies

$$\frac{1}{\tilde{r}_\phi(x)}\int P(x,z)\tilde{r}_\phi(z)dz = \tilde{\gamma}(x) = \frac{1}{\phi(x)}\int \phi(y)P(y,x)dy.$$

The probability $\tilde{\mathbb{P}}_{\tilde{\mu}}$ on $\mathcal{D}$ is called admissible, if it is induced by the continuous time Markov chain with infinitesimal generator $\tilde{\mathcal{L}}$ and the initial measure $\tilde{\mu}$. We point out that $\tilde{\mu}$ is invariant for this chain.

Given a Lipschitz function $V:[0,1]\to\mathbb{R}$, note that $\mathbb{P}^V_{\mu_V}$ is induced by the continuous time Markov chain with infinitesimal generator $\mathcal{L}^V$ and invariant probability μ_V is admissible.

Define

$$\frac{1}{T}H_T(\tilde{\mathbb{P}}_{\tilde{\mu}}|\mathbb{P}_{\tilde{\mu}}) \;=-\,\frac{1}{T}\int_{\mathcal{D}}\log\left(\frac{\mathrm{d}\tilde{\mathbb{P}}_{\tilde{\mu}}}{\mathrm{d}\mathbb{P}_{\tilde{\mu}}}\Big|_{\mathcal{F}_T}\right)(\omega)\,\mathrm{d}\tilde{\mathbb{P}}_{\tilde{\mu}}(\omega)\,, \tag{2.38}$$

for $\tilde{\mathbb{P}}_{\tilde{\mu}}$ admissible and $\mathbb{P}_{\tilde{\mu}}$ the probability on $\mathcal{D}$ induced by the continuous time Markov chain with infinitesimal generator L, defined in (2.4), and initial probability $\tilde{\mu}$.

It is possible to compute

$$\log\left(\frac{\mathrm{d}\tilde{\mathbb{P}}_{\tilde{\mu}}}{\mathrm{d}\mathbb{P}_{\tilde{\mu}}}\Big|_{\mathcal{F}_T}\right)(\omega) \;=\; \int_0^T [1-\tilde{\gamma}(\omega_s)]\,\mathrm{d}s + \big[\log\big(\phi(\omega_T)\big) - \log\big(\phi(\omega_0)\big)\big]\,.$$

Then

$$H(\tilde{\mathbb{P}}_{\tilde{\mu}}|\mathbb{P}_{\tilde{\mu}}) \;=\; \int [\tilde{\gamma}(x)-1]\,\mathrm{d}\tilde{\mu}(x). \tag{2.39}$$

Note that

$$H(\mathbb{P}^V_{\mu_V}|\mathbb{P}_{\mu_V}) = \lambda_V - \int V(x)\,\mathrm{d}\mu_V(x)\,.$$

We denote the Pressure (or, Free Energy) of V as the value

$$\mathbf{P}(V) := \sup_{\substack{\tilde{\mathbb{P}}_{\tilde{\mu}}\\ \text{admissible}}} \left\{ H(\tilde{\mathbb{P}}_{\tilde{\mu}}|\mathbb{P}_{\tilde{\mu}}) \;+\; \int V(x)\,\mathrm{d}\tilde{\mu}(x)\right\}. \tag{2.40}$$

Using (2.39), the pressure of V, $\mathbf{P}(V)$, is equal to

$$\sup_{\substack{\tilde{\mathbb{P}}_{\tilde{\mu}}\\ \text{admissible}}} \int [\tilde{\gamma}(x) - 1 + V(x)]\,\mathrm{d}\tilde{\mu}(x).$$

Recalling the definition of $\tilde{\gamma}$, in (2.36), and $\tilde{\mu}$, in (2.37), we have

$$\sup_{\phi>0} \int (L+V)(\tfrac{\phi}{\|\phi\|_2})(x)\tfrac{\tilde{r}_\phi}{\|\tilde{r}_\phi\|_2}(x)dx \;=\lambda. \tag{2.41}$$

Indeed, first we can assume $\|\tilde{r}_\phi\|_2 = 1$.

We can also assume ϕ is such that $\int \frac{\phi(x)}{|\phi|^2}\tilde{r}_\phi(x)dx = 1$.

2.5 Time-Reversal Process and entropy production

Related results can be find in [WQ18], [JQQ00], [JQQ06], [LM22b], [MN02] and [MNS09].

Before we begin the study of duality on the Skorokhod space we will state the results for the detailed balance condition when the continuous time Markov Chain takes values on $\{1,2..,k\}$. Denote by $\sigma = (\sigma_1, ..., \sigma_k)$ the initial invariant probability for the line sum zero matrix $W = (W_{i,j})_{i,j=1,..,k}$.

The detailed balance condition for W is: for all $i, j = 1, ..., k$

$$\sigma_i W_{i,j} = \sigma_j W_{j,i}.$$

Consider the inner product

$$\langle x, y \rangle_\sigma = \sum_{j=1}^{k} \sigma_j x_j y_j.$$

It is easy to see that W satisfies the detailed balance condition, if and only if, W is self-adjoint for the inner product $\langle ., . \rangle_\sigma$.

We assume in this section that L is of the form (2.4).

In this section, we consider that the time parameter is bounded, $t \in [0, T]$ for a fixed $T > 0$, in order to explore the time-reversal process. As mentioned before, we have that μ is somehow invariant with respect to L^*:

$$\int Lf(x)\mu(dx) = \iint [f(y) - f(x)]\, P(y, x)dy\ \theta(x)dx$$
$$= \int f(y) \int P(y, x)\theta(x)dx\ dy - \int f(x) \int P(y, x)dy\ \theta(x)dx$$
$$= \int f(y)\theta(y)dy - \int f(x)\theta(x)dx = 0.$$

More precisely, $L^*(\theta) = 0$, where L^* acts on $\mathcal{L}^2(dx)$. We will consider the dual process associated with μ in what follows. The substantial change is that our reference measure which was simply Lebesgue measure dx becomes now $\theta(x)dx$. Taking that into account, the inner product in this new space is given by

$$\langle f, g \rangle_\mu = \int f(x)g(x)\mu(dx) = \int f(x)g(x)\theta(x)dx.$$

The dual operator for L (using $\langle f, g \rangle_\mu$), will be denoted by $\mathfrak{L}^* : \mathcal{L}^2(\mu) \to \mathcal{L}^2(\mu)$. One can show that

$$(\mathfrak{L}^* g)(x) = \int [g(y) - g(x)]\ \frac{\theta(y)}{\theta(x)}\ P(x, y)dy.$$

To verify this, notice that

$$\langle Lf, g \rangle_\mu = \int Lf(x)g(x)\theta(x)dx$$

$$= \iint f(y)P(y,x)g(x)dy\ \theta(x)dx - \int f(x)g(x)\ \theta(x)dx$$

$$= \iint g(x)P(y,x)\theta(x)dx\ f(y)dy - \int f(x)g(x)\ \theta(x)dx$$

$$= \iint g(y)P(x,y)\theta(y)dy\ f(x)dx - \int f(x)g(x)\ \theta(x)dx$$

$$= \iint g(y)P(x,y)\frac{\theta(y)}{\theta(x)}dy\ f(x)\theta(x)dx - \int g(x)\ f(x)\theta(x)dx.$$

$$= \int \left[\int g(y)P(x,y)\frac{\theta(y)}{\theta(x)}dy - g(x)\right]\ f(x)\theta(x)dx$$

From (2.3) we have $\int P(x,y)\theta(y)dy = \theta(x)$. Thus, $\int P(x,y)\frac{\theta(y)}{\theta(x)}dy = 1$ and

$$\begin{aligned}\langle Lf, g\rangle_\mu &= \iint [g(y)-g(x)]P(x,y)\frac{\theta(y)}{\theta(x)}dy\ f(x)\theta(x)dx \\ &= \iint [g(y)-g(x)]P^*(y,x)dy\ f(x)\theta(x)dx,\end{aligned}$$

where $P^*(y,x) = P(x,y)\frac{\theta(y)}{\theta(x)}$. To fix ideas, we write again the expression for $\mathfrak{L}^*$:

$$(\mathfrak{L}^* g)(x) = \int (g(y)-g(x))P^*(y,x)dy = \int (g(y)-g(x))P(x,y)\frac{\theta(y)}{\theta(x)}dy$$

Notice that we write L^* for the dual over $\mathcal{L}^2(dx)$ and $\mathfrak{L}^*$ for the one over $\mathcal{L}^2(\mu)$.

Having discussed that, we turn now into defining the Time-Reversal process, associated with the stationary Markov Process (X_t,μ) and an interval of time $[0,T]$. The new process is then denoted by $(\hat{X}_t)$ and satisfies

$$\mathbb{E}_\mu[\,g(\hat{X}_0)f(\hat{X}_t)] := \mathbb{E}_\mu[\,g(X_T)f(X_{T-t})].$$

It has transition family $\hat{P}_t$ satisfying

$$\int g(x)(\hat{P}_t f(x))\ d\mu(x) := \mathbb{E}_\mu[\,g(X_T)f(X_{T-t})],\ \forall f,g \in \mathcal{L}^2(\mu).$$

This object is not at all new. In fact, notice that

$$\mathbb{E}_\mu[\,g(X_T)f(X_{T-t})] = \mathbb{E}_\mu[\,f(X_{T-t})\,\mathbb{E}_\mu[g(X_T)|\mathcal{F}_{T-t}]\,]$$

$$= \mathbb{E}_\mu[f(X_{T-t})\,\mathbb{E}_{X_{T-t}}[\,g(X_t)]\,] = \mathbb{E}_\mu[f(X_0)\,\mathbb{E}_{X_0}[\,g(X_t)]\,]$$
$$= \int f(x)\,\mathbb{E}_x[\,g(X_t)]\,d\mu(x)$$
$$= \int f(x)\,P_t(g(x))\,d\mu(x).$$

Since the last is true for all $f, g \in \mathcal{L}^2(\mu)$, we already get that $\hat{P}_t = P_t^*$, the transition family of $\mathfrak{L}^* : \mathcal{L}^2(\mu) \to \mathcal{L}^2(\mu)$. This also means that $\hat{L}f(x) = \mathfrak{L}^* f(x)$, $dx - a.s.$, where $\hat{L}$ is the infinitesimal generator of the semigroup $\hat{P}_t$.

For a fixed $T > 0$, we are interested in the quantity $\frac{1}{T} H_T(\mathbb{P}_\mu|\hat{\mathbb{P}}_\mu)$ where $H_T(.|.)$ is the relative entropy between two probability measures over the space of trajectories $\mathcal{D}(S, [0,T])$. Recall the definition

$$H_T(\mathbb{P}_\mu|\hat{\mathbb{P}}_\mu) := \int_{\mathcal{D}} \log \left.\frac{d\mathbb{P}_\mu}{d\hat{\mathbb{P}}_\mu}\right|_{\mathcal{F}_T} d\mathbb{P}_\mu.$$

The general formula of the above Radon-Nykodin derivative for a càdlàg process with general state space S is given by

$$\left.\frac{d\mathbb{P}_\mu}{d\hat{\mathbb{P}}_\mu}\right|_{\mathcal{F}_T} = \exp\left\{\int_0^T [\hat{\lambda}(X_s) - \lambda(X_s)]ds + \sum_{s\leq T} \log\left(\frac{\lambda(X_{s^-})}{\hat{\lambda}(X_{s^-})}\,\frac{dP}{d\hat{P}}(X_{s^-}, X_s)\right)\right\} \tag{2.42}$$

Above, for each fixed $x \in S$, $\frac{dP}{d\hat{P}}(x, y)$ is the Radon-Nykodin derivative of $P(x, dy)$ with respect to $\hat{P}(x, dy)$. The summation over $s \leq T$ stands for all jumps until time T. Here we are omitting technicalities that guarantee the existence of this derivative

For the processes we are considering, we have $\lambda(x) = \hat{\lambda}(x) = 1$ and

$$\hat{P}(x, dy) = P^*(x, dy) = P^*(y, x)dy = P(x, y)\frac{\theta(y)}{\theta(x)}dy$$

$$\Rightarrow \frac{dP}{d\hat{P}}(X_{s^-}, X_s) = \frac{P(X_s, X_{s^-})\theta(X_{s^-})}{P(X_{s^-}, X_s)\theta(X_s)}.$$

After these simplifications, we get

$$H_T(\mathbb{P}_\mu|\hat{\mathbb{P}}_\mu) = \mathbb{E}_\mu\left[\sum_{s\leq T} \log\left(\frac{P(X_s, X_{s^-})\theta(X_{s^-})}{P(X_{s^-}, X_s)\theta(X_s)}\right)\right]$$
$$= \mathbb{E}_\mu\left[\sum_{s\leq T} \log\left(\frac{P(X_s, X_{s^-})}{P(X_{s^-}, X_s)}\right) + \log(\theta(X_{s^-})) - \log(\theta(X_s))\right].$$

Notice the telescopic summation

$$\sum_{s\leq T}\mathbb{E}_\mu[\,\log\theta(X_{s^-})-\log\theta(X_s)]=\mathbb{E}_\mu[\,\log\theta(X_0)-\log\theta(X_T)]=0,$$

since μ is invariant. Therefore, it is natural to consider the expression

$$\mathbb{E}_\mu\left[\sum_{s\leq T}\log\left(\frac{P(X_s,X_{s^-})}{P(X_{s^-},X_s)}\right)\right].$$

For this one, we use the underlying structure of the Markov chain given by P. Invoking the jump times T_n and the skeleton ξ_n of the discrete time Markov chain, we write

$$\sum_{n=0}^{\infty}\mathbb{E}_\mu\left[\sum_{s\leq T}\log\left(\frac{P(X_s,X_{s^-})}{P(X_{s^-},X_s)}\right)\mathbf{1}_{[T_n\leq T\leq T_{n+1}]}\right]$$

If until T there are no jumps, then we will simply get 0 from the expression above. This means that the summation could start at the first jump, $n=1$.

$$=\sum_{n=1}^{\infty}\mathbb{E}_\mu\left[\sum_{k=0}^{n-1}\log\left(\frac{P(\xi_{k+1},\xi_k)}{P(\xi_k,\xi_{k+1})}\right)\mathbf{1}_{[T_n\leq T\leq T_{n+1}]}\right]$$

To simplify the calculations below, we denote for every $n\geq 1$, $\varphi(x_0,...,x_n):=\sum_{k=0}^{n-1}\log\frac{P(x_{k+1},x_k)}{P(x_k,x_{k+1})}$. Then

$$H_T(\mathbb{P}_\mu|\hat{\mathbb{P}}_\mu)=\sum_{n=1}^{\infty}\int d\mu(x_0)\int P(x_1,x_0)dx_1\int...\int P(x_n,x_{n-1})\,dx_n\,\varphi(x_0,...,x_n)$$

$$\times\int_0^\infty ds_0\;e^{-s_0}...\int_0^\infty ds_n\;e^{-s_n}\;\mathbf{1}_{[0\leq T-\sum_{i=0}^{n-1}s_i\leq s_n]}. \tag{2.43}$$

Above, the first line covers spatial integrals that involve P. The second line integrals are independent of P and are easier to compute now. Notice that

$$\int_0^\infty ds_n e^{-s_n}\;\mathbf{1}_{[0\;\leq T-\sum_{i=0}^{n-1}s_i\;\leq\;s_n]}\;=\;\int_{T-\sum_{i=0}^{n-1}s_i}^\infty ds_n e^{-s_n}\;\mathbf{1}_{[0\;\leq T-\sum_{i=0}^{n-1}s_i]}$$

$$=e^{-(T-\sum_{i=0}^{n-1}s_i)}\,\mathbf{1}_{[0\leq T-\sum_{i=0}^{n-1}s_i]}\;=\;e^{-T}\;e^{\sum_{i=0}^{n-1}s_i}\,\mathbf{1}_{[0\leq T-\sum_{i=0}^{n-1}s_i]}.$$

The second line in (2.43) becomes

$$e^{-T}\int_0^{\infty}...\int_0^{\infty} ds_0...ds_{n-1}\ \mathbf{1}_{[\sum_{i=0}^{n-1} s_i\leq T]},$$

where the integrals can be recognized as a fraction (exactly $\frac{1}{2^n}$) of the volume of the ball in the $\mathbb{R}^n$ with 1-norm and radius T. This means those integrals sum up to $\frac{1}{2^n}\frac{2^n}{n!}T^n$. Thus, the entire second line of (2.43) is equal to $e^{-T}\ \frac{T^n}{n!}$.

The first line in (2.43) is

$$\sum_{n=1}^{\infty}\sum_{k=0}^{n-1}\int d\mu(x_0)\int P(x_1,x_0)dx_1\int...\int P(x_n,x_{n-1})\,dx_n\ \log\frac{P(x_{k+1},x_k)}{P(x_k,x_{k+1})}. \tag{2.44}$$

To illustrate what happens in general, we will analyze the term of $k=0$ of the above sum, for general n:

$$\int d\mu(x_0)\int P(x_1,x_0)\ \log\frac{P(x_1,x_0)}{P(x_0,x_1)}dx_1\left[\int P(x_2,x_1)\,dx_2\,...\int P(x_n,x_{n-1})\,dx_n\right]$$

The integrals inside [ ] are all equal to 1. This happens in general for the integrals where the variable of integration is x_i for $k+1<i\leq n$. We can rewrite the general term of (2.44) as

$$\int d\mu(x_0)\int P(x_1,x_0)dx_1\int...\int P(x_k,x_{k-1})\,dx_k\int\log\frac{P(x_{k+1},x_k)}{P(x_k,x_{k+1})}P(x_{k+1},x_k)\,dx_{k+1}.$$

Now we will handle those integrals of variables x_i with $i<k$. This is allowed since there are no functions that depend on $x_0,...,x_{k-1}$ on the right. Notice that

$$\begin{aligned}&\int d\mu(x_0)\int P(x_1,x_0)dx_1\int P(x_2,x_1)dx_2\int...\int P(x_k,x_{k-1})\,dx_k\\ &=\iint\theta(x_0)P(x_1,x_0)dx_0\ dx_1\int P(x_2,x_1)dx_2\int...\int P(x_k,x_{k-1})\,dx_k\\ &=\int\theta(x_1)dx_1\int P(x_2,x_1)dx_2\,...\int P(x_k,x_{k-1})\,dx_k\\ &=\int d\mu(x_1)\int P(x_2,x_1)dx_2\int...\int P(x_k,x_{k-1})\,dx_k\end{aligned}$$

$$\cdots$$

$$= \int d\mu(x_{k-1}) \int P(x_k, x_{k-1})\, dx_k$$

$$= \iint \theta(x_{k-1}) P(x_k, x_{k-1})\, dx_{k-1}\, dx_k$$

$$= \int \theta(x_k)\, dx_k.$$

After all of this, (2.44) becomes

$$\int \theta(x_k) dx_k \int \log \frac{P(x_{k+1}, x_k)}{P(x_k, x_{k+1})} P(x_{k+1}, x_k)\, dx_{k+1}$$

$$= \int \theta(x) dx \int \log \frac{P(y,x)}{P(x,y)} P(y,x)\, dy$$

$$= \iint \log \frac{P(y,x)}{P(x,y)}\ P(y,x)\ dy\ d\mu(x).$$

Therefore,

$$H_T(\mathbb{P}_\mu | \hat{\mathbb{P}}_\mu) = \sum_{n=1}^{\infty} e^{-T}\ \frac{T^n}{n!}\ \sum_{k=0}^{n-1} \iint \log \frac{P(y,x)}{P(x,y)}\ P(y,x)\ dy\ d\mu(x)$$

$$= \sum_{n=1}^{\infty} e^{-T}\ \frac{T^n}{(n-1)!} \iint \log \frac{P(y,x)}{P(x,y)}\ P(y,x)\ dy\ d\mu(x)$$

$$= T \iint \log \frac{P(y,x)}{P(x,y)}\ P(y,x)\ dy\ d\mu(x)$$

and finally, the entropy production rate is

$$ep = \lim_{T\to\infty} \frac{1}{T}\ H_T(\mathbb{P}_\mu | \hat{\mathbb{P}}_\mu) = \iint \log \frac{P(y,x)}{P(x,y)}\ P(y,x)\ dy\ d\mu(x). \tag{2.45}$$

Notice that $P(x,y) = P(y,x) \Rightarrow ep = 0$.

Proposition 2.5.1. *In the above conditions, $ep \geq 0$, for all transition functions $P(x,y) > 0$.*

Proof. Since $\mathfrak{L}^*(\mu) = 0$, we have that $\int L(f)\, d\mu = 0$, for every continuous function f. For $f = -\log \circ \theta$, we have that

$$\iint [\log(\theta(x)) - \log(\theta(y))]\, P(y,x)\, dy\ d\mu(x) = 0. \tag{2.46}$$

Therefore, we can include this term into the entropy production rate of (2.45) as

$$ep = \iint \log\left[\frac{P(y,x)\theta(x)}{P(x,y)\theta(y)}\right]\ P(y,x)\ dy\ d\mu(x)$$

$$= \iint \left[\frac{P(y,x)\theta(x)}{P(x,y)\theta(y)}\right] \log\left[\frac{P(y,x)\theta(x)}{P(x,y)\theta(y)}\right]\ P(x,y)\frac{\theta(y)}{\theta(x)}\ dy\ d\mu(x)$$

Since $\iint P(x,y)\frac{\theta(y)}{\theta(x)}\ dy\ d\mu(x) = \int 1\, d\mu(x) = 1$, we can use this as a probability measure (in fact it is $P^*(y,x)\ dy\ d\mu(x)$) in order to apply the Jensen inequality for the convex function $\psi(x) = x \log x$ on $\mathbb{R}_+$. In this way,

$$\psi\left(\int \left[\frac{P(y,x)\theta(x)}{P(x,y)\theta(y)}\right] P(x,y)\frac{\theta(y)}{\theta(x)}\ dy\ d\mu(x)\right)$$

$$\leq \int \psi\left[\frac{P(y,x)\theta(x)}{P(x,y)\theta(y)}\right] P(x,y)\frac{\theta(y)}{\theta(x)}\ dy\ d\mu(x) = ep.$$

Finally,

$$ep \geq \psi\left(\int P(y,x)\ dy\ d\mu(x)\right) = \psi(1) = 0.$$

The idea here was similar to the one in Lemma 3.3 in [PP90]. □

Proposition 2.5.2. $ep^* = \lim_{T\to\infty} \frac{1}{T} H_T(\hat{\mathbb{P}}_\mu | \mathbb{P}_\mu) = ep.$

Proof. Recall that $P^*(y,x) = P(x,y)\theta(y)/\theta(x)$. The calculation in (2.46) allows us to add a term into ep:

$$ep = \iint \log\frac{P(y,x)}{P(x,y)}\ P(y,x)\, dy\ d\mu(x) + \iint [\log(\theta(x) - \log(\theta(y))]\, P(y,x)\, dy\ d\mu(x)$$

$$= \iint \log\frac{P(y,x)\theta(x)}{P(x,y)\theta(y)}\ P(y,x)\, dy\ d\mu(x)$$

$$= \iint \log\frac{P(y,x)}{P^*(y,x)}\ P(y,x)\, dy\ d\mu(x).$$

In the formula above, we can recognize the transition functions, $P(y,x)$ and $P^*(y,x)$, associated to the processes $\mathbb{P}_\mu$ and $\hat{\mathbb{P}}_\mu$, respectively. Now, to proceed the change to $H_T(\hat{\mathbb{P}}_\mu, \mathbb{P}_\mu)$, we change the role of them:

$$ep^* = \iint \log \frac{P^*(y,x)}{P(y,x)} \, P^*(y,x) \, dy \, d\mu(x) = \iint \log \frac{P(x,y)\theta(y)}{P(y,x)\theta(x)} \, P^*(y,x) \, dy \, d\mu(x)$$

$$= \iint \log \frac{P(x,y)}{P(y,x)} \, P^*(y,x) \, dy \, d\mu(x) + \iint [\log\theta(y) - \log\theta(x)] \, P^*(y,x) \, dy \, d\mu(x)$$

$$= \iint \log \frac{P(x,y)}{P(y,x)} \, P(x,y) \frac{\theta(y)}{\theta(x)} \, dy \, d\mu(x)$$

$$= \iint \log \frac{P(x,y)}{P(y,x)} \, P(x,y) \; dx \; d\mu(y) = ep.$$

$\square$

Remmark 2.5.3. *In case one wants to symmetrize the process generated by L by taking the average $\frac{L+\mathfrak{L}^*}{2}$, the following would apply. Consider the transition function for this operator*

$$Q(y,x) = \frac{P(y,x)}{2} + \frac{P(x,y)\theta(y)}{2\theta(x)} = \frac{P(y,x)\theta(x) + P(x,y)\theta(y)}{2\theta(x)}.$$

Notice that

$$\int Q(y,x)dy = \frac{1}{2}\int P(y,x)dy + \frac{1}{2\theta(x)}\int P(x,y)\theta(y)dy = 1$$

and

$$Q(x,y) = Q(y,x)\frac{\theta(x)}{\theta(y)}.$$

We arrive at an equation that can be understood as a balance condition:

$$Q(x,y)\theta(y) = Q(y,x)\theta(x) \tag{2.47}$$

We already knew that $\frac{L+\mathfrak{L}^*}{2}$ is symmetric by construction, but the above is sufficient to conclude the symmetry for any operator.

Proposition 2.5.4. *Every operator $\mathcal{A}$ which has a transition function Q that satisfies the balance condition (2.47) is symmetric in $\mathcal{L}^2(\mu)$.*

Proof. Indeed,

$$\int (\mathcal{A}f)(x)\, g(x)\, d\mu(x)$$

$$= \iint [f(y) - f(x)] Q(y,x)\, dy\ g(x)\theta(x) dx$$

$$= \iint [f(y) - f(x)]\, g(x)\, Q(y,x)\theta(x) dy\, dx$$

$$= \iint [f(y) - f(x)]\, g(x)\, Q(x,y)\theta(y) dy\, dx$$

$$= \iint f(y)g(x)\ Q(x,y)\theta(y)\, dy\, dx - \int f(x)g(x)\theta(x) \int Q(y,x)\, dy\, dx$$

$$= \iint f(y)g(x)\ Q(x,y)\theta(y)\, dy\, dx - \int f(x)g(x)\theta(x)\, dx$$

$$= \iint f(y)g(x)\ Q(x,y)\theta(y)\, dy\, dx - \int f(y)g(y)\theta(y)\, dy$$

$$= \iint f(y)[g(x) - g(y)]\ Q(x,y)\theta(y)\, dy\, dx$$

$$= \int f(y) \int [g(x) - g(y)]\ Q(x,y) dx\ \theta(y)\, dy$$

$$\int f(y)\, (\mathcal{A}g)(y)\, d\mu(y).$$

□

2.6 Expansiveness of the semi-flow Θ_t, $t \geq 0$, on $\mathcal{D}$

From now on we assume in this section that L is of the form (2.4).

In this section, we consider the Skorokhod space $\hat{\mathcal{D}}$ of paths $w : (-\infty, \infty) \to \mathbb{R}$ continuous at right and with limit at left (also called *càdlàg*).

$\hat{\Theta}_t$, $t \in \mathbb{R}$, denotes the bidirectional flow on $\hat{\mathcal{D}}$, acting on w by translation to the left on time t. That is, for fixed t, then $\tilde{w} = \hat{\Theta}_t(w)$ is such that $\tilde{w}(s) = w(s+t)$.

Let $\mathcal{D}$, the set of path $w_2 : [0, \infty) \to \mathbb{R}$ continuous at right and with limit at left.

Θ_t, $t \geq 0$, denotes the shift on $\mathcal{D}$, acting on w_2 by translation to the left on time t. That is, for fixed t, then $\tilde{w}_2 = \Theta_t(w_2)$ is such that $\tilde{w}_2(s) = w_2(s+t)$.

Let $\mathcal{D}^*$, the set of path $w_1 : (0, \infty) \to \mathbb{R}$ continuous at left and with limit at right.

It is necessary to make our notation clearer: by $w =< w_1|w_2 >= (w_1, w_2)$ we mean a path $w : \mathbb{R} \to \mathcal{D}$ such that $w(t) = w_2(t)$ for $t \geq 0$ and $w(t) = w_1(-t)$ for $t < 0$. In our notation $w_1 : [0, \infty) \to \mathbb{R}$ is continuous at left and with limit at right, and $w_2 : (0, \infty) \to \mathbb{R}$ is continuous at right and with limit at left.

Using the above notation we can write $\hat{\mathcal{D}}$, the Skorokhod space of *càdlàg* paths $w : (-\infty, \infty) \to \mathbb{R}$, as $\hat{\mathcal{D}} = \mathcal{D}^* \times \mathcal{D}$. A typical path in $\hat{\mathcal{D}}$ will be written in the form $w =< w_1|w_2 >= (w_1, w_2) \in \mathcal{D}^* \times \mathcal{D}$. By convention, w_1 will be at left of $t = 0$ and w_2 at right of $t = 0$.

Denote, for $s \geq 0$,

$$(w_1|_t w_2)(s) = \begin{cases} w_1(t-s), & s < t \\ w_2(s-t), & s \geq t \end{cases}.$$

We denote by $\Pi_1 : \mathcal{D}^* \times \mathcal{D} \to \mathcal{D}^*$ the projection $\Pi_1(w) = \Pi_1(< w_1|w_2 >) = w_1$. If we denote by $\Pi_2 : \mathcal{D}^* \times \mathcal{D} \to \mathcal{D}$ the projection $\Pi_2(w) = \Pi_2(< w_1|w_2 >) = w_2$, then $(w_1|_t w_2) = \Pi_2(\hat{\Theta}_{-t}(w_1, w_2))$.

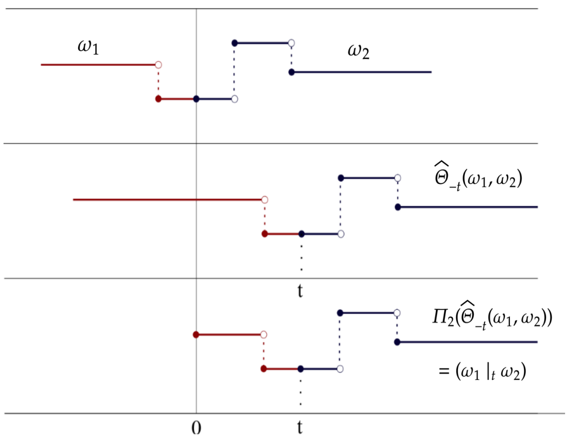


Figure 2.3: The bilateral shift and the projection Π_2

We will show that the semi-flow Θ_t, $t \geq 0$, is *expanding* (see (2.49)).

Proposition 2.6.1. *The continuous time shift Θ_t, $t \geq 0$, acting on the Skorokhod space $\mathcal{D}$ equipped with the Skorokhod metric is expanding: given paths w_1, w_2 and t*

$$d\left((w_1|_t w_2), (w_1|_t w_2')\right) \leq \int_t^\infty e^{-u} du = e^{-t}. \tag{2.48}$$

Proof. Notice that $|A(w_1|_t w_2) - A(w_1|_t w_2')| \le C_A d\left((w_1|_t w_2), (w_1|_t w_2')\right)$, where $d(x, y)$ denotes the Skorokhod distance on $\mathcal{D}$. This is the distance between two paths that coincides until time t. Recall the definition of the Skorokhod distance

$$d(x, y) = \inf_{\lambda \in \Lambda} \left[\gamma(\lambda) \wedge \int_0^\infty e^{-u} d(x, y, \lambda, u) du\right].$$

Above, the Λ set is for the continuous functions such that the below function γ is finite.

So, if we choose λ as the identity function, we get

$$\gamma(\lambda) := \sup_{t \ge 0} \text{ ess } |\log \lambda'(t)| = 0.$$

Then

$$d((w_1|_t w_2), (w_1|_t w_2')) \le \int_0^\infty e^{-u} d((w_1|_t w_2), (w_1|_t w_2'), \lambda, u)\, du$$

$$= \int_0^\infty e^{-u} \sup_{s \ge 0} q\left((w_1|_t w_2)(s \wedge u), (w_1|_t w_2')(\lambda(s) \wedge u)\right) du$$

$$= \int_0^\infty e^{-u} \sup_{s \ge 0} q\left((w_1|_t w_2)(s \wedge u), (w_1|_t w_2')(s \wedge u)\right) du,$$

where $q = r \wedge 1$ with r denoting the metric on the state space, i.e., Lebesgue in $[0, 1]$. For $u < t$, the distance q above is $q(w_1(s \wedge u), w_1(s \wedge u)) = 0$. Furthermore, the distance q is upper bounded by 1. Then,

$$d\left((w_1|_t w_2), (w_1|_t w_2')\right) \le \int_t^\infty e^{-u} du = e^{-t}. \tag{2.49}$$

□

Proposition 2.6.2. *For a fix Lipschitz function $A : \mathcal{D} \to \mathbb{R}$ and a path $w_2' \in \mathcal{D}$ denote $W_{t_1}^0 = W_{A,t_1,w_2'}^0 : \mathcal{D}^* \times \mathcal{D} \to \mathbb{R}$ the function given by*

$$W^0(w_1, w_2)_{A,t_1,w_2'} = W_{t_1}^0(w_1, w_2) := \sum_{n=1}^\infty A(w_1|_{nt_1} w_2) - A(w_1|_{nt_1} w_2'). \tag{2.50}$$

Then, W^0 is well defined.

Proof. As consequence of (2.49), we have

$$|W_{t_1}^0(w_1, w_2)| \le \sum_{n=1}^\infty |A(w_1|_{nt_1} w_2) - A(w_1|_{nt_1} w_2')| \le C_A \sum_{n=1}^\infty e^{-nt_1} < \infty,$$

for $t_1 > 0$. We conclude that $W^0_{t_1}$ given by the expression (2.50) is well defined.

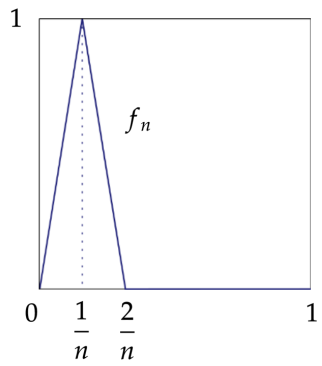
□

2.7 Appendix - The need for Lipschitz or Hölder class on Theorem 1

We present an example of the operator $L+V+zI$ with domain the whole space of continuous functions. Without the restriction on the variation of the functions, we cannot assure that the operator is compact and therefore, we cannot use Krein-Rutman theorem.

Let $f_n : [0,1] \to \mathbb{R}$ be defined as

$$f_n(x) = \begin{cases} nx & 0 \leq x < \frac{1}{n} \\ 2 - nx & \frac{1}{n} \leq x < \frac{2}{n} \\ 0 & \frac{2}{n} \leq x \leq 1 \end{cases}$$



The key idea here is that the set $\{f_n\}$ is contained in the unitary ball of $C_0([0,1])$, but it does not admit a uniform bound M on the variation, i.e., $|f_n(y) - f_n(x)| \leq M|y-x|$, for all n, x, y.

Take $P(x,y) \equiv 1$. Then

$$Lf_n(y) = \int f_n(x)dx - f_n(y) = \frac{1}{n} - f_n(y).$$

For $V(x) = (x - 1/2)^2$ and $z = 1 + \|V\|_\infty$, we get

$$g_n(y) := (L + V + zI)f_n(y) = \frac{1}{n} + f_n(y)[V(y) + z - 1]$$

$$= \frac{1}{n} + f_n(y)(V(y) + \|V\|_\infty) = \frac{1}{n} + f_n(y)(y^2 - y + 1/2).$$

If $L + V + zI$ is compact, $\{g_n\}$ must admit a convergent subsequence, since $\{f_n\}$ is a bounded sequence. Without loss of generality, we assume that such subsequence g_{n_k} is rewritten as g_n.

It is a Cauchy sequence: take $\epsilon = \frac{1}{4}$. There must be a N s.t. $m, n \geq N \Rightarrow \|g_n - g_m\|_\infty < \frac{1}{4}$. Notice that $f_n(\frac{1}{n}) = 1$ and $f_n(x) = 0$, for $x \geq \frac{2}{n}$. For $m \geq 2n$, we have $f_m(\frac{1}{n}) = 0$, since $\frac{1}{n} = \frac{2}{2n} \geq \frac{2}{m}$. So,

$$\left| g_n\left(\frac{1}{n}\right) - g_m\left(\frac{1}{n}\right)\right| = \left|1\left(\frac{1}{n^2} - \frac{1}{n} + \frac{1}{2}\right) + \frac{1}{n} - 0 - \frac{1}{m}\right|$$

$$= \left|\frac{1}{2} + \frac{1}{n^2} - \frac{1}{m}\right| > \frac{1}{2} - \frac{1}{m}.$$

The latter contradicts $\|g_n - g_m\|_\infty < \frac{1}{4}$ for $n \geq 2$.

2.8 Appendix - Proofs of claims of Example 1

In this appendix we will show the proofs of the claims mentioned in Example 1.

First, we will show that

$$K_t(x, y) = 2\cos(2\pi(x - y))(e^{-3t/4} - e^{-t}) + (1 - e^{-t}).$$

Note that $P(x, y) = \cos[(x - y)2\pi]/2 + 1$ is symmetric and continuous on $[0, 1]$. Also, note that

$$\int \cos(2\pi(x - z)) \cdot \cos(2\pi(z - y))\, dz = \frac{1}{2}\cos(2\pi(x - y))$$

$$\Rightarrow P^2(x, y) := \int P(x, z)P(z, y)\, dz = \frac{\cos(2\pi(x - y))}{8} + 1$$

We state: $P^n(x, y) = \frac{\cos(2\pi(x-y))}{2^{2n-1}} + 1$. We proceed by induction.

$$P^n(x, y) = \int P^{n-1}(x, z)P(z, y)dz$$

$$= \int \left(\frac{\cos(2\pi(x-z))}{2^{2n-3}} + 1 \right) \left(\frac{\cos(2\pi(z-y))}{2} + 1 \right) dz$$
$$= \frac{1}{2^{2n-2}} \int \cos(2\pi(x-z)) \cdot \cos(2\pi(z-y))\, dz + 1$$
$$= \frac{\cos(2\pi(x-y))}{2^{2n-1}} + 1.$$

We continue to find $K_t(x, y)$. We refer to the appendix 1 for the general case.

$$Q_k(x,y) := \sum_{j=1}^{k} (-1)^{k-j} \binom{k}{j} P^j(x,y)$$

$$= \sum_{j=1}^{k} (-1)^{k-j} \binom{k}{j} \left(\frac{\cos(2\pi(x-y))}{2^{2j-1}} + 1 \right)$$

$$= 2\cos(2\pi(x-y)) \sum_{j=1}^{k} (-1)^{k-j} \binom{k}{j} \frac{1}{2^{2j}} + \sum_{j=1}^{k} (-1)^{k-j} \binom{k}{j}$$

$$= 2\cos(2\pi(x-y)) \left[(-1)^{k+1} + \left(-\frac{3}{4} \right)^k \right] + (-1)^{k+1}$$

$$= (2\cos(2\pi(x-y)) + 1)(-1)^{k+1} + 2\cos(2\pi(x-y)) \left(-\frac{3}{4} \right)^k$$

Finally,

$$K_t(x,y) = \sum_{k=1}^{\infty} \frac{t^k}{k!} Q_k(x,y)$$

$$= (2\cos(2\pi(x-y)) + 1) \sum_{k=1}^{\infty} \frac{t^k}{k!} (-1)^{k+1} + 2\cos(2\pi(x-y)) \sum_{k=1}^{\infty} \frac{t^k}{k!} \left(-\frac{3}{4} \right)^k$$
$$= (2\cos(2\pi(x-y)) + 1)(1 - e^{-t}) + 2\cos(2\pi(x-y))(e^{-3t/4} - 1)$$
$$= 2\cos(2\pi(x-y))(e^{-3t/4} - e^{-t}) + (1 - e^{-t}).$$

This way,

$$e^{tL} f(y) = e^{-t} f(y) + \int f(x) K_t(x,y) dx$$

$$= e^{-t} f(y) + (1 - e^{-t}) \int f(x) dx + 2(e^{-3t/4} - e^{-t}) \int f(x) \cos(2\pi(x-y)) dx.$$

Since $P(x,y) = P(y,x)$, we have $L = L^*$ and the normalized eigenfunctions are precisely the eigendensities. By construction, $L^*(1) = L(1) = 0$, so 1 is an eigenfunction, for which we get dx, the Lebesgue probability is invariant. Given the simplicity of P we can go further and find that they are unique.

Continuous functions $f : \mathbb{S}^1 \to \mathbb{R}$ can be seen as periodic functions $f : \mathbb{R} \to \mathbb{R}$ with period 1, so that we can employ Fourier Series. Write

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos(2\pi n x) + \sum_{n=1}^{\infty} b_n \sin(2\pi n x),$$

where $a_0 = 2\int f(x)dx$, $a_n = 2\int f(x)\cos(2\pi n x)dx$ and $b_n = 2\int f(x)\sin(2\pi n x)dx$. Notice $\cos(2\pi(x-y)) = \cos(2\pi x)\cos(2\pi y) + \sin(2\pi x)\sin(2\pi y)$. Then

$$Lf(y) = \int f(x)dx + \frac{1}{2}\int f(x)\cos(2\pi(x-y))dx - f(y)$$

$$= \frac{a_0}{2} + \frac{1}{2}\cos(2\pi y)\frac{a_1}{2} + \frac{1}{2}\sin(2\pi y)\frac{b_1}{2} - f(y).$$

Therefore, $Lf = 0$ if and only if

$$f(y) = \frac{a_0}{2} + \cos(2\pi y)\frac{a_1}{4} + \sin(2\pi y)\frac{b_1}{4}. \tag{2.51}$$

and from this follows $a_1 = a_1/4$, $b_1 = b_1/4$ and $a_n = b_n = 0$, $\forall n \geq 2$. Conclusion: $Lf = 0 \Rightarrow f \equiv \frac{a_0}{2}$, constant. This means that the only eigendensity of the operator e^{tL} is that of Lebesgue measure dx.

2.9 Appendix 5 - Another look of Feynman-Kac formula for symmetrical L

Consider X_t a continuous time process with state space S and infinitesimal generator L. Let f and V be two functions on S taking values on $\mathbb{R}$. For any fixed $T > 0$, we denote by $\hat{X}_s = X_{T-s}$ the time-reversal process and by $\hat{L}$ it's generator. For this process $\hat{X}$, we have that, by Feynman-Kac, the function

$$u_t(x) = \hat{\mathbb{E}}_x\left[e^{\int_0^t V(\hat{X}_s)ds} f(\hat{X}_t)\right]$$

is the solution of the partial differential equation

$$\begin{cases} \partial_t u_t(x) = \hat{L}u_t(x) + V(x)u_t(x)\,, & t \in (0,T] \\ u_0(x) = f(x) \end{cases}.$$

If L is symmetric, i.e., $\hat{L} = L$, this partial differential equation is the same for the original process X, whose known solution, by Feynman-Kac, is

$$v_t(x) = \mathbb{E}_x \left[e^{\int_0^t V(X_s) ds} f(X_t) \right].$$

Then, for any $t \in (0, T]$, we have that $v_t = u_t$. Looking to the paths, we get

$$\int_{w(0)=x} e^{\int_0^t V(w(s)) ds} f(w(t)) d\mathbb{P}(w) = \int_{w(T)=x} e^{\int_0^t V(w(T-s)) ds} f(w(T-t)) d\mathbb{P}(w).$$

Making a change of variables, we can rewrite this expression as

$$\int_{w(0)=x} e^{\int_0^t V(w(s)) ds} f(w(t)) d\mathbb{P}(w) = \int_{w(T)=x} e^{\int_{T-t}^T V(w(s)) ds} f(w(T-t)) d\mathbb{P}(w). \tag{2.52}$$

Data sharing not applicable to this article as no datasets were generated or analysed during the current study.

On behalf of all authors, the corresponding author states that there is no conflict of interest.

Chapter 3

Thermodynamic formalism for continuous-time quantum Markov semigroups: the detailed balance condition, entropy, and equilibrium quantum Markov processes

Abstract

This chapter is part of the work [BKL22]. Let $M_n(\mathbb{C})$ denote the set of n by n complex matrices. Consider continuous time quantum semigroups $\mathcal{P}_t = e^{t\,\mathcal{L}}$, $t \geq 0$, where $\mathcal{L} : M_n(\mathbb{C}) \to M_n(\mathbb{C})$ is the infinitesimal generator. If we assume that $\mathcal{L}(I) = 0$, we will call $e^{t\,\mathcal{L}}$, $t \geq 0$ a quantum Markov semigroup. Given a stationary density matrix $\rho = \rho_{\mathcal{L}}$, for the quantum Markov semigroup $\mathcal{P}_t$, $t \geq 0$, we can define a continuous time stationary quantum Markov process, denoted by X_t, $t \geq 0$. Given an *a priori* Laplacian operator $\mathcal{L}_0 : M_n(\mathbb{C}) \to M_n(\mathbb{C})$, we will present a natural concept of entropy for a class of density matrices on $M_n(\mathbb{C})$. Given a Hermitian operator $A : \mathbb{C}^n \to \mathbb{C}^n$ (which plays the role of a Hamiltonian), we will study a version of the variational principle of pressure for A. A density matrix ρ_A maximizing pressure will be called an equilibrium density matrix. From ρ_A we will derive a new infinitesimal generator $\mathcal{L}_A$. Finally, the continuous time quantum Markov process defined by the semigroup $\mathcal{P}_t = e^{t\,\mathcal{L}_A}$, $t \geq 0$, and an initial stationary density matrix, will be called the continuous time equilibrium quantum Markov process for the Hamiltonian A. It corresponds to the quantum ther-

modynamical equilibrium for the action of the Hamiltonian A.

3.1 Introduction

We are interested in continuous time stationary quantum Markov process which corresponds to equilibrium for a quantum bath (interacting with a quantum system) under the action of a certain given Hamiltonian. Therefore, our results concern continuous-time quantum channels.

In [CM17] the authors present a detailed study of a nice version of the detailed balance condition for a continuous-time quantum Markov semigroup on $M_n(\mathbb{C})$, $n \in \mathbb{N}$. In Theorem 4.2 in [CM17] it is explained that the detailed balance condition for a classical continuous-time Markov Chain, with values on a finite state space, corresponds to the commutative part of the dynamical evolution of the continuous-time quantum Markov semigroup. Results of [CM17] are used here in an essential way.

On page 75 in Section 9 in [Kač80], and also on page 114 in Section 5 in [Str84], for a classical continuous-time Markov Chain satisfying the detailed balance condition, a deviation function (which is a form of entropy) is introduced and a variational principle (in some sense a form of maximizing pressure) is considered (see expression 9.18 in page 76 in [Kač80]). We would like to extend the results obtained for the classical commutative setting to the non-commutative setting of quantum Markov semigroups satisfying the detailed balance condition as described in [CM17].

We will present a natural concept of entropy for a class of density matrices (see Section 3.3). We point out that the dynamics of the flow in the set of matrices is encapsulated on the infinitesimal generator and the entropy we consider here is at the level of this linear operator. In this sense, this concept of entropy has no *direct* dynamical content. Our setting is the quantum channel version of the classical ones considered in [Kač80] and [Str84].

After introducing entropy we will study a version of the variational principle of pressure and its relation to an eigenvalue problem for a certain type of transfer operator (see Section 3.5 and expression (3.34) in Section 3.6). In classical Thermodynamic Formalism, the Ruelle operator plays this role. The Ruelle Theorem describes a relation of equilibrium states with a corresponding eigenvalue problem (see [PP90]). The Ruelle operator is an infinite-dimensional version of the Perron-Frobenius operator. The transfer operator we consider here is not exactly an extension of the concept of Ruelle operator. A density matrix maximizing pressure will be called an equilibrium density matrix. We will provide examples in Section 3.5.

Our results are in some sense the quantum analogous of the reasoning delineated in [BEL08] and [LNT13], which considered the dynamics of continuous-time dynamics (a flow) in the Skorokhod space.

Our definition of entropy is also different from the ones in [BKL21b] and [BKL21a] which considered quantum channels in discrete-time dynamics.

Taking into account the concept and the notation described in section 5 in [CM17] we will denote by $\mathcal{L}_0$ (the Laplacian) the generator of the heat semigroup. We will choose a special $\mathcal{L}_0$ (see Definition 7) which will play the role of the *a priori* Laplacian. Our particular choice of $\mathcal{L}_0$ is analogous to taking the normalized counting probability as the *a priori* probability in the classical definition of Kolmogorov-Shannon entropy (see discussion in [LMMS15]).

From this $\mathcal{L}_0$ (which is fixed from now on) we will be able to define the detailed balanced condition (as described in [CM17]) and the Laplacian-entropy.

Definition 4. *Given a density operator ρ define the Laplacian-entropy by*

$$h(\rho) = \; Tr[\, \rho^{1/2} \mathcal{L}_0^{\dagger}(\rho^{1/2})\,], \tag{3.1}$$

where we set $\mathcal{L}_0$ by Definition 7, and $\mathcal{L}_0^{\dagger}$ is the dual operator with respect to the GNS inner product in $M_n(\mathbb{C})$: $\langle A, B\rangle = Tr(A^* B)$.

Our source of inspiration for the definition of entropy was the classical setting of continuous-time Markov chains as described by M. Kač in Section 9 in [Kač80] and by D. W. Stroock in Section 5 in [Str84].

Expression (5.12) in [Str84] defines the so-called *rate function* I in the setting of classical continuous-time Markov Processes taking values on the compact metric space E. If L is the infinitesimal generator, then (5.12) means

$$I(\nu) = - \inf_{u>0,\, u\in C(E)} \int \frac{Lu}{u} d\nu,$$

where $C(E)$ is the set of real continuous functions defined on E.

Later, for reversible processes, the above formula simplifies to expression (5.18) in [Str84], which claims

$$I(\nu) = - \int \phi^{1/2} L \phi^{1/2} d\mu, \quad \phi = \frac{d\nu}{d\mu}.$$

In [Str84] it is used the term symmetric operator but in other contexts, this would correspond to conditions like reversibility or the detailed balanced condition.

Under the detailed balanced condition, in the quantum channel context, one should replace the role of L by the generator of a QMS, which is usually denoted by $\mathcal{L}$ (the Lindbladian). Probabilities are replaced by densities ρ (states). In this case, (5.12) in [Str84] corresponds here to

$$I(\rho) = - \inf_{U>0} \mathrm{Tr}\,(\rho\, U^{-1}\, \mathcal{L}_0\, U),$$

where the infimum is taken over the positive matrices $U \in M_n$.

In [Str84] (see also [Kač80]) the variational principle is taken as

$$\lambda(V) = \sup_{\text{prob } \nu} \left(\int V d\nu - I(\nu) \right),$$

where $\lambda(V)$ is the main eigenvalue of a certain operator.

Denote $D_n = \{\rho \geq 0 : \mathrm{Tr}(\rho) = 1\}$, the set of density matrices.

In section 3.5 we consider an analogous problem: given an Hermitian operator $A : \mathbb{C}^n \to \mathbb{C}^n$, we consider the variational problem:

$$P_A = \sup_{\rho \in D_n} \{ h(\rho) + \mathrm{Tr}(A\rho) \}. \tag{3.2}$$

A matrix ρ_A maximizing P_A will be called an equilibrium density for the operator A.

A connection of P_A of expression (3.2) with the eigenvalue of a certain linear operator is described in expression (3.34) in Section 3.6 (see also (3.35)). In this way, we get all elements for establishing a continuous time quantum channel version of the classical Ruelle operator (see [PP90], [LMMS15], [BEL08], [LNT13]).

Our entropy has a difference of sign when compared with the setting of [Str84], so we wonder if there exists a connection between $h(\rho)$ and $-I(\rho)$. In section 3.7 we will show this connection in the special case of the heat-semigroup with the *a priori* generator $\mathcal{L}_0$ defined in section 3.3. We will show that:

Theorem 5. *Given the density matrix ρ, then*

$$h(\rho) = \inf_{A>0} Tr\,(\rho\, A^{-1}\, \mathcal{L}_0(A)).$$

Following [CM17], we will present in Section 3.8 the classical Markov Chain associated with a continuous-time quantum channel and we will provide examples.

3.2 An outline of the main prerequisites

Given a linear operator $A : \mathbb{C} \to \mathbb{C}$, its dual (with respect to the canonical inner product), is denoted by $A^* : \mathbb{C} \to \mathbb{C}$.

Denote by $M_n(\mathbb{C}) = M_n$ the set of n by n complex matrices with the GNS inner product $\langle A, B\rangle = \mathrm{Tr}\,(A^*\, B)$. Given a linear operator $T : M_n \to M_n$, its dual with respect to this inner product is denoted by $T^\dagger : M_n \to M_n$. That is, for all matrices A, B we get

$$\langle T(A), B\rangle = \langle A, T^\dagger(B)\rangle.$$

We denote by $\mathbf{1}$ the diagonal matrix with entries $\frac{1}{n}$. Then, $\mathbf{1}$ is a density matrix and also the unity of the C^*-algebra $M_n(\mathbb{C})$. We denote by $\mathfrak{G}_+$ the set of invertible density matrices (operators) $\rho : M_n \to M_n$. Recall that a density matrix is a positive semi-definite, Hermitian operator of trace one.

We will consider **continuous time quantum semigroups** (QS) the ones given by $\mathcal{P}_t = e^{t\,\mathcal{L}}$, $t \geq 0$, where $\mathcal{L} : M_n(\mathbb{C}) \to M_n(\mathbb{C})$ is the infinitesimal generator (see Definition 5.5.1 and also Section 9.3.2 in [Cha15]). The linear operator $\mathcal{L}$ should satisfy the conditional complete positivity property (see section 5 in [Cha15] or section 6 in [Wol12]). We assume that $\mathcal{L}(A^*) = (\mathcal{L}(A))^*$, for all $A \in M_n(\mathbb{C})$. Given a selfadjoint matrix $A \in M_n(\mathbb{C})$, the dynamical evolution $t \to e^{t\mathcal{L}}(A)$ is called the Heisenberg dynamical evolution. Given a density matrix $\rho \in M_n(\mathbb{C})$, the dynamical evolution $t \to e^{t\mathcal{L}^\dagger}(\rho)$ is called the Schrödinger dynamical evolution.

If we assume that $\mathcal{L}(I) = 0$, we will call $\mathcal{P}_t = e^{t\,\mathcal{L}}$, $t \geq 0$, the continuous time **quantum Markov semigroup** (QMS) associated to $\mathcal{L}$ (see Definition 5.5.2 and also section 7 in [Cha15]). It is known that in this case $e^{t\,\mathcal{L}}(\mathbf{1}) = \mathbf{1}$, for all $t \geq 0$. Continuous time quantum Markov semigroups provide a convenient mathematical description of the irreversible dynamics of an open quantum system.

If $\rho = \rho_{\mathcal{L}}$ is such that $\mathcal{L}^\dagger(\rho) = 0$, then for all $t \geq 0$, we get $e^{t\,\mathcal{L}^\dagger}(\rho) = \rho$ and we say that ρ is the **stationary density matrix for the continuous time quantum Markov semigroup** with infinitesimal generator $\mathcal{L}$. Section 9.4 in [Cha15] presents a discussion on the uniqueness of the stationary matrix ρ.

We call X_t, $t \geq 0$, the **continuous time quantum Markov process** (QMP) associated to the infinitesimal generator $\mathcal{L}$, the process associated to the pair $(e^{t\,\mathcal{L}},\, \rho_{\mathcal{L}})$, $t \geq 0$. We can ask questions about ergodicity for such a process (see Section 11 in [Cha15]).

Given the (QMP) associated to $\mathcal{L}$ and the stationary density operator ρ, take an observable (a self-adjoint matrix) $A \in M_n$. Then, we get that

$$t \to \mathrm{Tr}(\rho\, e^{t\mathcal{L}}(A))$$

describes the time evolution of the expected value of the observable A.

We say that $\mathcal{L}$ is irreducible if for every non-zero matrix $A \geq 0$, and every strictly positive $t > 0$, we have $e^{t\,\mathcal{L}}(A) > 0$. We will also assume that $\mathcal{L}$ is irreducible (see Sections 10 and 11 in [Cha15]).

Given $\sigma \in \mathfrak{G}_+$, consider the inner product $\langle\, ,\, \rangle_\sigma$ in the set of matrices in M_n given by $\langle A, B\rangle_\sigma = \mathrm{Tr}\,(A^* B\sigma) = \langle A, B\sigma\rangle$.

Definition 6. *Given $\sigma \in \mathfrak{G}_+$, we say that the QMS $e^{t\mathcal{L}}, t \geq 0$, satisfies the σ-detailed balance condition if $\mathcal{L}$ is symmetric with respect to $\langle\, ,\, \rangle_\sigma$. That is, for all matrices $A, B \in M_n$ we get*

$$\langle \mathcal{L}(A), B\rangle_\sigma = \langle A, \mathcal{L}(B)\rangle_\sigma.$$

Given $\sigma \in \mathfrak{G}_+$, if the QMS $e^{t\mathcal{L}}, t \geq 0$, satisfies the σ-detailed balance condition, then, σ is stationary for the evolution of the semigroup $e^{t\mathcal{L}^\dagger}, t \geq 0$ (see Lemma 13).

The explicit form of the infinitesimal generator of a continuous-time quantum Markov semigroups satisfying the detailed balance condition is described by expression (3.4) in [CM17] (see our expression (3.14)).

Definition 7. *We denote $\mathcal{L}_0$ the infinitesimal generator satisfying d.b.c. where we take $\sigma = \mathbb{1}$. $\mathcal{L}_0$ will be called the Laplacian (see Section 3 in [CM17]).*

The semigroup $\mathcal{P}_t = e^{t\,\mathcal{L}_0}$, $t \geq 0$, describes the unperturbed continuous time quantum channel.

Given the *a priori* Laplacian operator $\mathcal{L}_0 : M_n(\mathbb{C}) \to M_n(\mathbb{C})$, we will present a natural concept of entropy for a class of density matrices ρ on $M_n(\mathbb{C})$ (see Definition 8).

Given a Hermitian operator $A : \mathbb{C}^n \to \mathbb{C}^n$ (which plays the role of minus the Hamiltonian), we will consider in Section 3.5 a variational principle of pressure for A, which is given by Definition 15.

A density matrix ρ_A maximizing pressure will be called an equilibrium density matrix for A. This matrix (in fact $\rho_A^{1/2}$) will satisfy an eigenvalue property for a certain linear operator $\mathfrak{L}_A$ to be described in Section 3.6. From ρ_A we will derive a new infinitesimal generator $\mathcal{L}_A$. Finally, the continuous-time quantum Markov Process X_t, $t \geq 0$, associated to $\mathcal{P}_t = e^{t\,\mathcal{L}_A}$, $t \geq 0$, and ρ_A, will be called the continuous-time equilibrium quantum Markov semigroup for the Hamiltonian A. This new process describes a continuous-time quantum channel after the perturbation by the selfadjoint operator A.

3.3 The heat semigroup and entropy of density operators

In this section the inner product in M_n is $\langle A, B\rangle = \mathrm{Tr}(A^* B)$.

Denote by e_j, $j = 1, ..., n$, the canonical base in $\mathbb{C}^n$, and by

$$\mathfrak{I}_{i,j} = |\, e_i \,\rangle\langle\, e_j \,| : \mathbb{C}^n \to \mathbb{C}^n,$$

where $i, j = 1, ..., n$. Note that $\mathfrak{I}^*_{i,j} = |\, e_j \,\rangle\langle\, e_i \,|$.

We denote by $\mathfrak{I}_{i,j}$ the matrix which is zero in all entries, up to the entry i, j, where it has the value 1.

We denote by $\mathtt{1}$ the operator identity I times $\frac{1}{n}$. The matrix $\mathtt{1}$ describes an invertible density operator.

$\mathcal{L}_0$ denotes the infinitesimal generator satisfying d.b.c. for $\sigma = \mathtt{1}$.

One can show that $\mathfrak{I}_{i,j}$, $i, j = 1, ..., n$, is an orthonormal basis for $\mathcal{L}_0$ associated to the eigenvalue 0.

Following section 5 in [CM17] we call $\mathcal{L}_0$ (the Laplacian) the generator of the heat semigroup (the Laplacian)

$$A \to \mathcal{L}_0(A) = \sum_{i,j=1}^{n} (V^*_{i,j}\, [A, V_{i,j}] + \, [V_{i,j}, A]\, V^*_{i,j}), \tag{3.3}$$

where $V_{i,j} = |\, \eta_i \,\rangle\langle\, \eta_j \,|$ and η_i, $i \in \{1, 2, ..., n\}$, is a orthonormal basis of $\mathbb{C}^n$. Consequently, $V^*_{i,j} = |\, \eta_j \,\rangle\langle\, \eta_i \,|$.

This operator is negative-semi definite. (see page 1827 in [CM17] and also (3.14) and (3.16) of next section. Notice that

$$\begin{aligned}
\mathcal{L}_0(A) &= \sum_{i,j=1}^{n} \Big(V^*_{i,j}\, [A, V_{i,j}] + \, [V_{i,j}, A]\, V^*_{i,j}\Big) \\
&= \sum_{i,j=1}^{n} \Big(|\, \eta_j \,\rangle\langle\, \eta_i \,|\, A \,|\, \eta_i \,\rangle\langle\, \eta_j \,| - |\, \eta_j \,\rangle\langle\, \eta_i \,||\, \eta_i \,\rangle\langle\, \eta_j \,|\, A \\
&\qquad + \, |\, \eta_i \,\rangle\langle\, \eta_j \,| A \,|\, \eta_j \,\rangle\langle\, \eta_i \,| - A \,|\, \eta_i \,\rangle\langle\, \eta_j \,|\,|\, \eta_j \,\rangle\langle\, \eta_i \,|\Big) \\
&= \sum_{i,j=1}^{n} \Big(a_{ii} \,|\, \eta_j \,\rangle\langle\, \eta_j \,| - |\, \eta_j \,\rangle\langle\, \eta_j \,|\, A + \, a_{jj} \,|\, \eta_i \,\rangle\langle\, \eta_i \,| - A \,|\, \eta_i \,\rangle\langle\, \eta_i \,|\Big) \\
&= 2\, \mathrm{Tr}(A) I - 2nA,
\end{aligned} \tag{3.4}$$

since $\sum_i |\, \eta_i \,\rangle\langle\, \eta_i \,| = I$. Note that $\mathcal{L}_0(I) = 2nI - 2nI = 0$.

Note that

$$\mathcal{L}_0^\dagger(\rho) = \sum_{i,j=1}^{n} ([V_{i,j}\,\rho, V_{i,j}^*] + [V_{i,j}, \rho\, V_{i,j}^*]\,). \tag{3.5}$$

One can show that $\mathcal{L}_0^\dagger = \mathcal{L}_0$ and Tr $(\imath\, \mathcal{L}_0(A)) = 0$, for all $A \in M_n$.

$\sigma = \imath$ is invariant for the flow $e^{t\mathcal{L}_0^\dagger}$.

Definition 8. *Given a density operator ρ define the Laplacian-entropy*

$$h(\rho) = \; Tr\,[\,\rho^{1/2}\mathcal{L}_0^\dagger(\rho^{1/2})\,] \tag{3.6}$$

This definition is consistent with expression (5.18) on page 113 in [Str84].

Our main result in this section is the explicit expression for entropy to be described by Proposition 10.

First, we want to show the following Lemma:

Lemma 9. $h(\imath) = 0$.

Proof. Notice $\imath^{1/2} = \sqrt{\frac{1}{n}}\, I$. It follows that

$$\mathcal{L}_0^\dagger(\imath^{1/2}) = \sqrt{\frac{1}{n}}\,\mathcal{L}_0^\dagger(\delta) = 0.$$

Thus, $h(\imath) = 0$. □

Consider now a general density operator $\rho \in \mathfrak{S}_+$. We want to estimate $h(\rho)$. From expression (3.4),

$$\begin{aligned} h(\rho) &= \mathrm{Tr}\Big[\,\rho^{1/2}\mathcal{L}_0^\dagger(\rho^{1/2})\,\Big] \\ &= \mathrm{Tr}\Big[\,\rho^{1/2}\Big(2\,\mathrm{Tr}(\rho^{1/2})I - 2n\rho^{1/2}\Big)\,\Big] \\ &= 2\,\mathrm{Tr}(\rho^{1/2})\mathrm{Tr}(\rho^{1/2}) - 2n\mathrm{Tr}(\rho) \\ &= 2\,\mathrm{Tr}(\rho^{1/2})^2 - 2n. \end{aligned}$$

If λ_j, $j = 1, ..., d$, are the eigenvalues of ρ, we have

$$h(\rho) = 2\left(\sum_{j=1}^{n}\sqrt{\lambda_i}\right)^2 - 2n.$$

Note that $\sup(\sum_{j=1}^n \sqrt{\lambda_j})^2 = n$ and $\inf(\sum_{j=1}^n \sqrt{\lambda_j})^2 = 1$.

Therefore, for fixed n and a given ρ, $h(\rho) \leq 0$.

Note $h(\rho)$ can be very negative if n is large. We get the following proposition by looking at this last inequality:

Proposition 10. *The entropy h depends only on $\{\lambda_i\}$ the eigenvalues of ρ and*

$$h(\rho) = 2\,Tr\,(\rho^{1/2})^2 - 2n = 2\left(\sum_{j=1}^{n}\sqrt{\lambda_i}\right)^2 - 2n \le 0.$$

Note that as $\sum_{j=1}^n \lambda_j = 1$, the maximal value of $h(\rho)$ is zero, and this happens when all eigenvalues $\lambda_j = 1$ are equal to $\frac{1}{n}$. Thus, the maximal value of entropy is attained by the density matrix $\imath$.

Remark 1. *For fixed A we denote $\partial_{i,j}(A) = [V_{i,j}, A]$ and $\partial_{i,j}^\dagger(A) = [V_{i,j}^*, A]$.*

$\partial_{i,j}$ is a version of the momentum operator $\frac{1}{i}\frac{\partial}{\partial x}$ acting on the set L^2 of functions for the Lebesgue probability on the circle. Indeed, denote by D the operator $g \to D(g) = \frac{1}{i}g'$. For fixed $a : [0,1) \to \mathbb{R}$, take the multiplication operator $g \to a\,g$ acting on functions g. Then, the operator

$$g \to D(ag) - aD(g) = \frac{1}{i}a'\,g,$$

describes multiplication by $\frac{1}{i}a' = \frac{1}{i}\frac{\partial\, a}{\partial x}$.

We point out that $\sum_{i,j}\partial_{i,j}\partial_{i,j}^\dagger$ corresponds to second derivative (Laplacian). On the other hand, $\sum_{i,j}\partial_{i,j}\partial_{i,j}$ corresponds to minus second derivative (minus Laplacian).

3.4 The general setting for detailed balanced condition

Before we begin the study of the quantum case we will state the results for the detailed balanced condition when the continuous time Markov Chain takes values on $\{1, 2.., k\}$. Denote by $\mathfrak{s} = (\mathfrak{s}_1, ..., \mathfrak{s}_k)$ the initial invariant probability for the zero row sum matrix $W = (W_{i,j})_{i,j=1,...,k}$.

The detailed balance condition for W is: for all $i, j = 1, ..., k$

$$\mathfrak{s}_i W_{i,j} = \mathfrak{s}_j W_{j,i}.$$

Consider the inner product in $\mathbb{R}^k$

$$\langle x, y\rangle_{\mathfrak{s}} = \sum_{j=1}^{k} \mathfrak{s}_j x_j y_j.$$

It is easy to see that W satisfies the detailed balance condition, if and only if, W is self-adjoint for the inner product $\langle ., .\rangle_{\mathfrak{s}}$.

The above is the classical (commutative) setting for presenting the detailed balance condition. We are interested in presenting the non-commutative version of the concept.

We will be interested here in the C^*-Algebra $\mathcal{A} = M_n$ of complex n by n matrices. The inner product in M_n is $\langle A, B\rangle = \mathrm{Tr}\,[A^*\,B]$. Following the notation of [CM17] the associated Hilbert space will be denoted by $\mathfrak{h}_{\mathcal{A}}$.

We will fix from now on an element $\sigma : \mathbb{C}^n \to \mathbb{C}^n$ in $\mathfrak{S}_+$. A hypothesis that can be helpful for ergodic properties is to assume that all eigenvalues of σ are simple.

Now, we present some preliminary definitions and properties taken from [CM17].

Once we fix the Hamiltonian H we fix the density state σ via $\sigma = e^{-h}$ (in some sense we are considering a "normalized" Hamiltonian). In fact, $\sigma = \frac{e^{-H}}{Tr(e^{-H})}$ and $h = H + \log Tr(e^{-H})$.

Assume that the linear transformation, $\Delta_\sigma : M_n \to M_n$, is given by $A \to \Delta_\sigma(A) = \sigma\,A\,\sigma^{-1}$. Note that $\Delta_\sigma(\sigma) = \sigma$ and $\Delta_\sigma(\mathbf{1}) = \mathbf{1}$.

Assume each eigenvalue of σ is simple.

$\Delta_\sigma^{-1} : M_n \to M_n$, is given by $B \to \Delta_\sigma(B) = \sigma^{-1}\,B\,\sigma$.

Note that $(\Delta_\sigma(A))^* = \Delta_\sigma^{-1}(A^*)$.

$\mathcal{K} : M_n \to M_n$ is positive preserving, if $\mathcal{K}(A) \geq 0$, in the case $A \geq 0$.

Δ_σ is positive but not positive preserving.

We say that $\mathcal{K} : M_n \to M_n$ is self-adjointness preserving, if $(\mathcal{K}(A))^* = \mathcal{K}(A^*)$.

Remember that by definition $\mathcal{K}^\dagger : M_n \to M_n$ is the one such that for all A, B

$$\mathrm{Tr}[A^*\mathcal{K}(B)] = \langle A, \mathcal{K}(B)\rangle = \langle \mathcal{K}^\dagger(A), B\rangle = \mathrm{Tr}[(\mathcal{K}^\dagger(A))^*\,B].$$

$\mathcal{K} : M_n \to M_n$ is self-adjoint if $\mathcal{K} = \mathcal{K}^\dagger$.

Δ_σ is self-adjoint.

Note that if $\Delta_\sigma(E) = e^{-w}E$, then $\Delta_\sigma(E^*) = e^{w}E^*$.

Assume that $\eta_j \in \mathbb{C}^n$, $j = 1, 2, ..., n$, is an orthonormal basis for $h = -\log\sigma$,

$$h(\eta_j) = \lambda_j \eta_j, \ \ \forall j. \tag{3.7}$$

Then, $\eta_j \in \mathbb{C}^n$, $j = 1, 2, ..., n$, is also an orthonormal basis for σ.

$h = -\log\sigma$ plays the role of the Hamiltonian.

Then, we get that $\eta_j \in \mathbb{C}^n$, $j = 1, 2, ..., n$, is an orthonormal basis for σ,

$$\sigma(\eta_j) = e^{-\lambda_j}\eta_j, \ \ \forall j. \tag{3.8}$$

As $\sigma : \mathbb{C}^n \to \mathbb{C}^n$ is in $\mathfrak{S}_+$, we get that

$$\sum_{j=1}^{n} e^{-\lambda_j} = 1. \tag{3.9}$$

For $\alpha = (\alpha_1, \alpha_2)$, where $\alpha_1, \alpha_2 \in \{1, 2, ..., n\}$, denote

$$w_{\alpha_1,\alpha_2} = w_\alpha = \lambda_{\alpha_1} - \lambda_{\alpha_2}. \tag{3.10}$$

If $\sigma = \mathbf{1}$, then, all $w_{\alpha_1,\alpha_2} = 0$.

For each pair $\alpha \in \{1, 2, ..., n\}^2$, denote

$$F_\alpha = |\, \eta_{\alpha_1} \rangle \langle \eta_{\alpha_2} \,|.$$

Note that

$$F^*_{(\alpha_1,\alpha_2)} = F_{(\alpha_2,\alpha_1)}. \tag{3.11}$$

Moreover,

$$\Delta_\sigma(F_\alpha) = e^{-\lambda_{\alpha_1} + \lambda_{\alpha_2}} \, F_\alpha. \tag{3.12}$$

Indeed,

$$\Delta_\sigma(F_\alpha) = \sigma \,|\, \eta_{\alpha_1} \rangle \langle \eta_{\alpha_2} \,|\, \sigma^{-1} = e^{-\lambda_{\alpha_1}} \,|\, \eta_{\alpha_1} \rangle \langle \eta_{\alpha_2} \,|\, \sigma^{-1} =$$

$$e^{-\lambda_{\alpha_1} + \lambda_{\alpha_2}} \,|\, \eta_{\alpha_1} \rangle \langle \eta_{\alpha_2} \,| = e^{-\lambda_{\alpha_1} + \lambda_{\alpha_2}} \, F_\alpha.$$

This shows that:

Lemma 11. *The operators $F_\alpha = |\, \eta_{\alpha_1} \rangle \langle \eta_{\alpha_2} \,|$, $\alpha_1, \alpha_2 \in \{1, 2, ..., n\}$, describe a natural orthonormal basis of Δ_σ. The corresponding eigenvalues are $e^{-\lambda_{\alpha_1} + \lambda_{\alpha_2}}$.*

Note that if $\alpha = (\alpha_1, \alpha_2)$ is such that $\alpha_1 \neq \alpha_2$, then,

$$\mathrm{Tr}(F_\alpha) = 0$$

and, for $\alpha, \tilde{\alpha} \in \{1, 2, ..., n\}^2$

$$\mathrm{Tr}(F^*_\alpha \, F_{\tilde{\alpha}}) = \delta_{\alpha,\tilde{\alpha}} := \delta_{\alpha_1,\tilde{\alpha}_1} \delta_{\alpha_2,\tilde{\alpha}_2}.$$

Now we denote the different F_α, $\alpha \in \{1, 2, ..., n\}^2$, by V_k, $k = 1, ..., n^2$ (in order to use the same notation as in [CM17]). In this identification, we also denote for each $k = 1, ..., n^2$, the value $w_k = \lambda_{\alpha_1} - \lambda_{\alpha_2}$, for the corresponding $\alpha = (\lambda_{\alpha_2}, \lambda_{\alpha_1})$.

Then, the family $V_1, ..., V_{n^2}$ represent the different eigenmatrices (an orthonormal basis) for Δ_σ associated to the eigenvalues $e^{-w_1}, ..., e^{-w_{n^2}}$, where $w_k \in \mathbb{R}$, $k = 1, ..., n^2$. $\mathbf{1}$ and σ are eigenmatrices associated to the eigenvalue 1. The matrices V_k do not have to be self-adjoint, but from (3.11) we get

$$\{V_1, ..., V_{n^2}\} = \{V_1^*, ..., V_{n^2}^*\}.$$

Therefore, if w_k is in the above list, there exists a j such that $w_j = -w_k$.

Given the Hamiltonian $h = -\log \sigma$, the modular automorphism $\alpha_t : M_n \to M_n$, $t \geq 0$, is defined by

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

This is the Heisenberg point of view.

A Quantum Markov Semigroup (QMS) is a continuous one-parameter semigroup of linear transformations $\mathcal{P}_t : M_n \to M_n$, $t \geq 0$, such that for each $t \geq 0$, $\mathcal{P}_t$ is completely positive and $\mathcal{P}_t(\mathbf{1}) = \mathbf{1}$.

It is natural to focus on quantum Markov semigroups that commute with the modular operator Δ_σ associated to their invariant states σ.

Consider a QMS $\mathcal{P}_t : M_n \to M_n$, $t \geq 0$, of the form

$$\mathcal{P}_t = e^{t\mathcal{L}},$$

for some linear operator $\mathcal{L} : M_n \to M_n$.

The operator $\mathcal{L}$ acts on observables (self-adjoint matrices). Note that $\mathcal{L}(\mathbf{1}) = 0$. The dual operator $\mathcal{L}^\dagger$ acts on density matrices.

A state σ (density) is invariant if $\mathrm{Tr}[\sigma \, \mathcal{L}(A)] = 0$, for all $A \in M_n$. In other words, $\mathcal{L}^\dagger(A) = 0$.

In terms of the possible inner products described in Definition 2.2 in [CM17], we will choose $s = 1$.

Remember that given σ we consider the inner product $\langle \, , \rangle_\sigma = \langle \, , \rangle_1$ in M_n, where

$$\langle A, B \rangle_\sigma = \mathrm{Tr}\, [\sigma A^* B].$$

From [CM17] we get:

Proposition 12. *Given the density operator σ, the the QMS $\mathcal{P}_t : M_n \to M_n$, $t \geq 0$, of the form $\mathcal{P}_t = e^{t\mathcal{L}}$, satisfies the σ- detailed balance condition, if and only if,*

$$\mathcal{L} \circ \Delta_\sigma = \Delta_\sigma \circ \mathcal{L}. \tag{3.13}$$

If $\mathcal{P}_t = e^{t\mathcal{L}}$, satisfies the σ-detailed balanced condition, then, for all $t \geq 0$,

$$\mathcal{P}_t \circ \Delta_\sigma = \Delta_\sigma \circ \mathcal{P}_t.$$

Moreover, for any t, t' and matrix A we get that

$$(\alpha_{t'} \circ \mathcal{P}_t)(A) = (\mathcal{P}_t \circ \alpha_{t'})(A).$$

It follows from (3.13) that $V_1, ..., V_{n^2}$ is an orthonormal basis for $\mathcal{L}$ associated to the eigenvalues $e^{-v_1}, ..., e^{-v_{n^2}}$, where $v_j \in \mathbb{R}$, $j = 1, ..., n^2$.

Lemma 13. *σ is a stationary density matrix for the semigroup with infinitesimal generator $\mathcal{L}$.*

Proof. Note that

$$\begin{aligned}
[V_{i,j}\,\sigma, V_{i,j}^*] &= |\,\eta_i\,\rangle\langle\,\eta_j\,|\sigma|\,\eta_j\,\rangle\langle\,\eta_i\,| - |\,\eta_j\,\rangle\langle\,\eta_i\,||\,\eta_i\,\rangle\langle\,\eta_j\,|\sigma \\
&= e^{-\lambda_j}|\,\eta_i\,\rangle\langle\,\eta_i\,| - e^{\lambda_j}|\,\eta_j\,\rangle\langle\,\eta_j\,| \\
&= e^{-\lambda_j}\left(|\,\eta_i\,\rangle\langle\,\eta_i\,| - |\,\eta_j\,\rangle\langle\,\eta_j\,|\right)
\end{aligned}$$

and

$$\begin{aligned}
[V_{i,j}, \sigma\, V_{i,j}^*] &= |\,\eta_i\,\rangle\langle\,\eta_j\,|\sigma|\,\eta_j\,\rangle\langle\,\eta_i\,| - \sigma|\,\eta_j\,\rangle\langle\,\eta_i\,||\,\eta_i\,\rangle\langle\,\eta_j\,| \\
&= e^{-\lambda_j}|\,\eta_i\,\rangle\langle\,\eta_i\,| - e^{\lambda_j}|\,\eta_j\,\rangle\langle\,\eta_j\,| \\
&= e^{-\lambda_j}\left(|\,\eta_i\,\rangle\langle\,\eta_i\,| - |\,\eta_j\,\rangle\langle\,\eta_j\,|\right).
\end{aligned}$$

Using expression (3.16) we get

$$\begin{aligned}
\mathcal{L}^\dagger(\sigma) &= 2\sum_{i,j} e^{(\lambda_j-\lambda_i)/2} e^{-\lambda_j}\left(|\,\eta_i\,\rangle\langle\,\eta_i\,| - |\,\eta_j\,\rangle\langle\,\eta_j\,|\right) \\
&= 2\left[\sum_j e^{-\lambda_j/2}\sum_i e^{-\lambda_i/2}|\,\eta_i\,\rangle\langle\,\eta_i\,| - \sum_i e^{-\lambda_i/2}\sum_j e^{-\lambda_j/2}|\,\eta_j\,\rangle\langle\,\eta_j\,|\right] \\
&= 0.
\end{aligned}$$

□

Remember that for each pair $i, j \in \{1, 2, ..., n\}$, we denote

$$V_{i,j} = |\,\eta_i\,\rangle\langle\,\eta_j\,|,$$

where η_i, $i \in \{1, 2, ..., n\}$, is the orthonormal basis of eigenvectors for $h = -\log\sigma$ associated to the eigenvalues λ_j (according to (3.7)). As we mention before $w_{i,j} = \lambda_i - \lambda_j$, $i, j \in \{1, 2, ..., n\}$.

Theorem 14. *If $\mathcal{P}_t = e^{t\mathcal{L}}$, satisfies the σ-detailed balanced condition, then $\mathcal{L}$ is of the form*

$$A \to \mathcal{L}(A) = \sum_{i,j=1}^{n} e^{-w_{i,j}/2} \,(V_{i,j}^{*}\,[A, V_{i,j}] + \,[V_{i,j}^{*}, A]\, V_{i,j}), \tag{3.14}$$

where $V_{i,j} = |\,\eta_i\,\rangle\langle\,\eta_j\,|$ and $w_{i,j} = \lambda_i - \lambda_j$, $i, j \in \{1, 2, ..., n\}$, are real numbers such that (3.8), (3.9) *and* (3.10) *are true (which also means $\Delta_\sigma(V_{i,j}) = e^{-\lambda_i+\lambda_j}\, V_{i,j}$).*

Note that given $\sigma \in \mathfrak{G}_+$, the eigenvetors $|\,\eta_i\,\rangle$ and eigenvalues λ_j, $j \in \{1, 2, ..., n\}$, are determined. Therefore, if $\mathcal{P}_t = e^{t\mathcal{L}}$ satisfies the σ-detailed balanced condition, then, $\mathcal{L}$ is uniquely determined.

Remark 2. *Conversely, given σ in $\mathfrak{G}_+$ and V_j, $j = 1, 2, ..., n^2$, such that,*
1. $\Delta_\sigma V_j = e^{-w_j} V_j$,
2. $\{V_j, j = 1, 2, ..., n^2\} = \{V_j^{*}, j = 1, 2, ..., n^2\}$,
then,

$$A \to \mathcal{L}(A) = \sum_{j=1}^{n^2} e^{-w_j/2} \,(V_j^{*}\,[A, V_j] + \,[V_j^{*}, A]\, V_j), \tag{3.15}$$

is the infinitesimal generator of a QMS $e^{t\mathcal{L}}$, $t \geq 0$, which satisfies d.b.c. for the given σ. Therefore, σ is stationary (invariant) for $e^{t\mathcal{L}^\dagger}$, $t \geq 0$.

The dual operator $\mathcal{L}^\dagger$ satisfies

$$\rho \to \mathcal{L}^\dagger(\rho) = \sum_{i,j=1}^{n} e^{-w_{i,j}/2} \,([V_{i,j}\,\rho, V_{i,j}^{*}] + \,[V_{i,j}, \rho\, V_{i,j}^{*}]\,) \tag{3.16}$$

Remark 3. *If $\mathcal{P}_t = e^{t\mathcal{L}}$, satisfies the detailed balanced condition for the $\sigma = \mathbb{1}$, then from* (3.13) *we get that $V_{i,j} = \mathfrak{I}_{i,j}$, $i, j = 1, ..., n$. This is the case when $\mathcal{L} = \mathcal{L}_0$.*

3.5 The Pressure problem

Definition 15. *Given an Hermitian operator $A : \mathbb{C}^n \to \mathbb{C}^n$, $D_n = \{\rho \geq 0 : Tr(\rho) = 1\}$, consider*

$$P_A(\rho) = h(\rho) + Tr(A\rho) \tag{3.17}$$

and

$$P_A = \sup_{\rho \in D_n} P_A(\rho). \tag{3.18}$$

A matrix ρ_A maximizing P_A is called an equilibrium density operator for A.

Question: Is there $\mathcal{L}$ such that ρ_A is stationary for $\mathcal{L}$? The converse in Theorem 3.1 in [CM17] may be useful.

The expression of entropy we found in Proposition 10 suggests we look at the matrices of the form $\xi = \rho^{1/2}$, where ρ is a density. In order to study the problem of who maximizes P_A, we then define

$$\Xi_n = \{\xi \geq 0 : \xi^2 \in D_n\}, \tag{3.19}$$

the set of square roots of density operators and

$$\mathrm{p}_A(\xi) = h_{1/2}(\xi) + \mathrm{Tr}(A\xi^2), \tag{3.20}$$

where $h_{1/2}(\xi) := 2\mathrm{Tr}(\xi)^2 - 2n = h(\xi^2)$ by Proposition 10. Notice that $\mathrm{p}_A(\xi) = P_A(\xi^2)$.

Proposition 16. *If ξ maximizes the functional p_A, then there exists a κ satisfying*

$$2\kappa\xi = 4\,Tr(\xi)I + A\xi + \xi A. \tag{3.21}$$

Proof. We will use Lagrange Multipliers. Let $g : M_n(\mathbb{C}) \to \mathbb{R}$, $g(\zeta) = \mathrm{Tr}(\zeta^2) - 1$. We have $Dg(\zeta)(\cdot) = 2\mathrm{Tr}(\zeta\,\cdot)$, which means $Dg(\zeta)$ is not identically 0 unless $\zeta = 0$, and $g(0) = -1$. This way, 0 is a regular value of g. We are good since we are looking for a maximal ξ in $\Xi_n \subset g^{-1}(0)$.

Remark 4. *Although Ξ_n is not the whole level set $g^{-1}(0)$, it will contain a maximizer for p_A. This is justified as follows: if $\xi \in \Xi$ and $\eta \in g^{-1}(0) \setminus \Xi_n$ have the same square $\xi^2 = \eta^2$, then $\mathrm{p}_A(\xi) \geq \mathrm{p}_A(\eta)$, since $Tr(\xi)^2 \geq Tr(\eta)^2$. To illustrate that, consider*

$$\xi = \begin{pmatrix} \frac{3}{5} & 0 \\ 0 & \frac{4}{5} \end{pmatrix}, \eta_1 = \begin{pmatrix} -\frac{3}{5} & 0 \\ 0 & -\frac{4}{5} \end{pmatrix} \text{ and } \eta_2 = \begin{pmatrix} -\frac{3}{5} & 0 \\ 0 & \frac{4}{5} \end{pmatrix}.$$

All of the above are in $g^{-1}(0)$, with only $\xi \in \Xi_2$. We have $Tr(\xi)^2 = Tr(\eta_1)^2 > Tr(\eta_2)^2$, and thus $\mathrm{p}_A(\xi) = \mathrm{p}_A(\eta_1) > \mathrm{p}_A(\eta_2)$.

A maximal element ξ then satisfies, for all $h \in M_n(\mathbb{C})$ and some $\kappa \in \mathbb{R}$,

$$\begin{cases} D\mathrm{p}_A(\xi)(h) = \kappa Dg(\xi)(h) \\ g(\xi) = 0, \end{cases} \tag{3.22}$$

with $Dp_A(\xi)(h) = 4\mathrm{Tr}(\xi)\mathrm{Tr}(h) + \mathrm{Tr}(A\{\xi, h\})$ and $Dg(\xi)(h) = 2\mathrm{Tr}(h\xi)$.

Taking $h = |\, e_j \,\rangle\langle\, e_i \,|$ we have

$$2\kappa\xi_{ij} = 4\mathrm{Tr}(\xi)\delta_{i,j} + \{A, \xi\}_{ij}.$$

Since the above is true for every i, j, it corresponds to the coordinate equations of the matrix equation

$$2\kappa\xi = 4\mathrm{Tr}(\xi)I + A\xi + \xi A. \tag{3.23}$$

□

Note that if $\xi = \rho_A^{1/2}$, then it follows from (3.23)

$$\kappa\rho_A \;=\; 2\mathrm{Tr}(\rho_A^{1/2})\,\rho_A^{1/2} + \frac{1}{2}\,(A\,\rho_A + \rho_A^{1/2}A\rho_A^{1/2}). \tag{3.24}$$

Indeed,

$$2\kappa\rho_A = (2\kappa\xi)\xi = 4\mathrm{Tr}(\xi)\,\xi + A\xi\xi + \xi A\xi = 4\mathrm{Tr}(\xi)\,\xi + A\rho_A + \xi A\xi. \tag{3.25}$$

Moreover, by doing the product by the other side, we get

$$2\kappa\rho_A = \xi(2\kappa\xi) = \xi\,4\mathrm{Tr}(\xi) + \xi\,A\xi + \xi\,\xi A = 4\mathrm{Tr}(\xi)\,\xi + \xi A\xi + \rho_A A, \tag{3.26}$$

revealing that $\boldsymbol{A\rho_A = \rho_A A}$. In particular, A and ρ_A are simultaneously diagonalizable.

Proposition 17. *If ξ maximizes p_A, then the following statements are true*

1. *$Tr(A\xi) = (\kappa - 2n)\,Tr(\xi)$;*
2. *$P_A(\rho_A) = P_A(\xi^2) = p_A(\xi) = \kappa - 2n$;*

Proof. In (3.22) take $h = I$ and $h = \xi$, respectively. □

Remark 5. *The problem of finding the maximizing density $\rho = \xi^2$ for a general Hermitian A can be reduced to the study of the diagonal case. Since A is hermitian, it is diagonalizable. We have $UAU^* = \Lambda$, the latter a diagonal matrix, for some unitary matrix U. Multiplying on the left by U and on the right by U^* in the above matrix equation (3.23) gives us*

$$2\kappa\; U\xi U^* = 4\,Tr(\xi)UU^* + UAU^*\; U\xi U^* + U\xi U^*\; UAU^*$$

$$\iff\; 2\kappa\eta = 4\,Tr(\eta) + \Lambda\eta + \eta\Lambda,$$

where $\eta := U\xi U^*$. We arrive at a particular version of (3.23) on which the matrix is diagonal.

Theorem 18. *If $A = Diag(a_1, \dots, a_n)$, there is a* unique *element $\xi \in \Xi$ which maximizes p_A. Furthermore, ξ is also diagonal, with*

$$\xi_{ii} = \frac{c}{\kappa - a_i},$$

where κ is given implicitly on the data $a_1, ..., a_n$ and c is such that $Tr(\xi^2) = 1$. Consequently, the density that maximizes the pressure P_A is

$$\rho_A = \frac{1}{Tr\left(\rho_A\right)} \begin{pmatrix} \frac{1}{(\kappa-a_1)^2} & & & \\ & \frac{1}{(\kappa-a_2)^2} & & \\ & & \ddots & \\ & & & \frac{1}{(\kappa-a_n)^2} \end{pmatrix}.$$

Proof. For A diagonal, the expression (3.23) becomes

$$2\kappa\xi_{ij} = 4\mathrm{Tr}(\xi)\delta_{i,j} + \xi_{ij}(a_i + a_j). \tag{3.27}$$

If we take $i = j$ in the expression above,

$$\kappa\xi_{ii} = 2\mathrm{Tr}(\xi) + \xi_{ii}a_i \iff (\kappa - a_i)\xi_{ii} = 2\mathrm{Tr}(\xi). \tag{3.28}$$

We know that $\mathrm{Tr}(\xi) > 0$, because $\mathrm{Tr}(\xi) = 0$ leads to $\xi = 0$. Then $\xi_{ii} \neq 0$ and $\kappa > a_i$ for all i. So,

$$\frac{1}{\kappa - a_i} = \frac{\xi_{ii}}{2\mathrm{Tr}(\xi)} \tag{3.29}$$

and

$$\sum_{i=1}^{n} \frac{1}{\kappa - a_i} = \frac{1}{2}. \tag{3.30}$$

We need to find κ to completely characterize the maximal ξ. Suppose that $a_1 = \max_i a_i$. Notice that $f(x) = \sum_{i=1}^{n} \frac{1}{x-a_i}$, for $x \neq a_i$ has a vertical asymptote at a_1, $\lim_{x\to a_1^+} f(x) = \infty$, and it decreases to $\lim_{x\to\infty} f(x) = 0$. By the intermediate value theorem, we have a $\kappa > a_1$ s.t. $f(\kappa) = 1/2$.

Alternatively, one can find it as one of the roots of the following polynomial, which is the expression (3.29) rewritten.

$$\frac{1}{2}\det(\kappa I - A) - \sum_{i=1}^{n} \det\Big(\kappa I - A + (a_i - \kappa + 1)|\, e_i\, \rangle\langle\, e_i\,|\Big) = 0. \tag{3.31}$$

There is just one root that is bigger than all a_i, therefore it is κ.

Claim: ξ is diagonal. Let's prove that the other entries, outside the diagonal, are null. For $i \neq j$, the expression (3.23) gives us $2\kappa\xi_{ij} = \xi_{ij}(a_i+a_j)$, or equivalently,

$$\xi_{ij}(2\kappa - (a_i + a_j)) = 0.$$

We know that $\kappa > a_i, \forall i$. Thus $2\kappa > a_i + a_j$. This leaves us with $\xi_{ij} = 0$.

To conclude the pressure problem, we write

$$\xi = \mathrm{Diag}(\xi_{11}, ..., \xi_{nn}), \quad \xi_{ii} = \frac{c}{\kappa - a_i}, \tag{3.32}$$

where c is the constant that makes $\mathrm{Tr}(\xi^2) = 1$, i.e.,

$$c = \left(\sum_{i=1}^{n} \frac{1}{(\kappa - a_i)^2} \right)^{-1/2}.$$

This way, given $a_1, ..., a_n$, we find κ, then c and finally ξ.

□

Corollary 19. *If A is diagonalizable, with UAU^* diagonal, then the maximizing density ρ_A for P_A is such that $U\rho_A U^*$ is diagonal.*

Proof. If A was not diagonal at first, we proceed as in Remark 5 and use the last theorem to find a maximal $\eta = U\xi U^*$ which is diagonal. Then $\eta^2 = U\xi^2 U^* = U\rho_A U^*$ is diagonal. □

Remark 6. *Using (3.29), we know that if $A = a_1 I$ then $\xi_{ii} = \xi_{11}$ for all i. Since A is diagonal and $Tr(\xi^2) = \sum_i \xi_{ii}^2 = n\xi_{11}^2 = 1$, it follows that $\xi = \frac{1}{\sqrt{n}} I$ is the only ξ that maximizes p_A.*

Example 1. *Let*

$$A = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 2 \end{pmatrix}.$$

What is the equilibrium density ρ_A, i.e., the density that maximizes P_A? Let's diagonalize A.

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix}, \quad UAU^* = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}.$$

Now we apply Theorem 18. κ satifies

$$\frac{1}{\kappa+1}+\frac{1}{\kappa-1}+\frac{1}{k-2}=\frac{1}{2},$$

and $\kappa>-1,1,2$. We get $\kappa\approx 6.902$. Thus, the maximizing density for UAU^* is

$$\rho_{UAU^*}=\frac{1}{\operatorname{Tr}\left(\rho_{UAU^*}\right)}\begin{pmatrix}\frac{1}{(6.902+1)^2}&&\\&\frac{1}{(6.902-1)^2}&\\&&\frac{1}{(6.902-2)^2}\end{pmatrix}$$
$$=\begin{pmatrix}0.186&&\\&0.332&\\&&0.482\end{pmatrix}.$$

Finally,

$$\rho_A=U^*\rho_{UAU^*}U$$
$$=\begin{pmatrix}0.259&0.073&0\\0.073&0.259&0\\0&0&0.482\end{pmatrix}.$$

Notice that

$$P(\rho_A)=h(\rho_A)+\operatorname{Tr}(A\rho_A)$$
$$=2\operatorname{Tr}(\rho_A^{1/2})^2-2n+\operatorname{Tr}(UAU^*U\rho_AU^*)$$
$$=2\operatorname{Tr}((U\rho_AU^*)^{1/2})^2-2n+\operatorname{Tr}(UAU^*U\rho_AU^*)$$
$$=2\left(\sqrt{0.186}+\sqrt{0.332}+\sqrt{0.482}\right)^2-6+(-1\cdot 0.186+1\cdot 0.332+2\cdot 0.482)$$
$$\approx 0.902\approx\kappa-6.$$

in accordance with Proposition 17.

3.6 The pressure P_A as an eigenvalue problem

Consider the linear operator $\mathfrak{L}_A$

$$\xi\to\mathfrak{L}_A(\xi)=2\operatorname{Tr}(\xi)I+\frac{1}{2}(A\xi+\xi A). \tag{3.33}$$

Suppose ρ_A is an equilibrium density operator for the selfadjoint matrix A.

From (3.21) we get that $\xi = \rho_A^{1/2}$ is an eigenmatrix for the linear operator $\mathfrak{L}_A$ associated to the eigenvalue κ, that is

$$\mathfrak{L}_A(\rho_A^{1/2}) = \kappa\, \rho_A^{1/2} \tag{3.34}$$

From item 2. in Theorem 17 we get that $P_A(\rho_A) = \kappa - 2n$.

In this way, the equilibrium density operator is related to an eigenvalue problem in a similar fashion as in classical Thermodynamic Formalism.

The equilibrium matrix ρ_A satisfies

$$\kappa\rho_A \;=\; 2\mathrm{Tr}(\rho_A^{1/2})\, \rho_A^{1/2} + \frac{1}{2}\,(A\, \rho_A + \rho_A^{1/2} A \rho_A^{1/2}), \tag{3.35}$$

but this is not exactly a linear relation.

3.7 A connection between $h(\rho)$ and $I(\nu)$

We will present a connection between the concepts of $h(\rho)$ and $-I(\rho)$.

Recall that $\mathbf{\imath} = Id/n$ satisfies the detailed balance condition, which is the quantum equivalent of reversibility.

We are going to establish a connection of the Laplacian-entropy of Definition 3.6 with the one in (5.18) of [Str84]. The notion of Radon-Nikodym derivative is not clear in the quantum setting, but we can consider a natural analogy in our reasoning and we write $\frac{d\nu}{d\mu} = A$, if

$$\mathrm{Tr}(\nu U) = \mathrm{Tr}(\mu A U).$$

This corresponds of writing A in the form $A = \mu^{-1}\nu$. When looking at (5.18), L is symmetric in $L^2(\mu)$, and our operator $\mathcal{L}_0$ satisfies d.b.c. for $\mathbf{\imath}$. Therefore, here we will address the computation of the corresponding expression $\frac{d\nu}{d\mathbf{\imath}}$. Then, it is natural to consider $A = \mathbf{\imath}^{-1}\nu = n\nu$. Therefore, (5.18) in our setting corresponds to

$$I(\nu) = -\int (n\nu)^{1/2} \mathcal{L}_0((n\nu)^{1/2})\, d\mathbf{\imath}$$

$$= -n\mathrm{Tr}(\mathbf{\imath}\, \nu^{1/2} \mathcal{L}_0(\nu^{1/2}))$$

$$= -\mathrm{Tr}(\nu^{1/2} \mathcal{L}_0(\nu^{1/2})),$$

and then, $-h(\nu)$ come up.

Remark 7. *Recall that for an* $A = \sum_{kl} a_{kl} |\, k\,\rangle\langle\, l\,|$,

$$
\begin{aligned}
\mathcal{L}_0(A) &= \sum_{i,j=1}^{n} (V_{ij}^*[A, V_{ij}] + [V_{ij}, A]V_{ij}^*), \quad \textit{for } V_{ij} = |\, i\,\rangle\langle\, j\,| \\
&= \sum_{i,j=1}^{n} V_{ji}AV_{ij} - V_{ji}V_{ij}A + V_{ij}AV_{ji} - AV_{ij}V_{ji} \\
&= 2\sum_{i,j=1}^{n} V_{ji}AV_{ij} - \sum_{i,j=1}^{n} |\, j\,\rangle\langle\, i\,||\, i\,\rangle\langle\, j\,|A - \sum_{i,j=1}^{n} A|\, i\,\rangle\langle\, j\,||\, j\,\rangle\langle\, i\,| \\
&= 2\sum_{i,j=1}^{n} V_{ji}AV_{ij} - n\sum_{j=1}^{n} |\, j\,\rangle\langle\, j\,|A - n\sum_{i=1}^{n} A|\, i\,\rangle\langle\, i\,| \\
&= 2\sum_{i,j=1}^{n} V_{ji}AV_{ij} - 2nA \\
&= 2\sum_{i,j=1}^{n} |\, j\,\rangle\langle\, i\,|A|\, i\,\rangle\langle\, j\,| - 2nA \\
&= 2\sum_{i,j,k,l=1}^{n} a_{kl}|\, j\,\rangle\langle\, i\,||\, k\,\rangle\langle\, l\,||\, i\,\rangle\langle\, j\,| - 2nA \\
&= 2\sum_{i,j=1}^{n} a_{ii}|\, j\,\rangle\langle\, j\,| - 2nA \\
&= 2\sum_{i=1}^{n} a_{ii}\sum_{j=1}^{n} |\, j\,\rangle\langle\, j\,| - 2nA \\
&= 2\,Tr(A)I - 2nA.
\end{aligned}
$$

The next step is to write the entropy as an infimum. We will show that:

Theorem 20. *Given the density matrix* ρ

$$h(\rho) = \inf_{A>0} Tr(\rho\, A^{-1}\, \mathcal{L}_0(A)).$$

For the proof, we will need the following result:

Lemma 21. *In the space* M_n *of matrices* $n \times n$*, is true that*

$$\inf_{B>0} Tr(BU)\; Tr(UB^{-1}) = Tr(U)^2.$$

Proof. Let $B > 0$ be a general positive matrix. Let $|\, i\,\rangle$ be the orthonormal basis of eigenvectors of B. Then, we can write $B = \sum_{i=1}^{n} b_i \,|\, i\,\rangle\langle\, i\,|$, and in this basis, U can be written as $U = \sum_{j,k=1}^{n} u_{jk} \,|\, j\,\rangle\langle\, k\,|$. Thus,

$$BU = \sum_{ijk} b_i u_{jk} \,|\, i\,\rangle\langle\, i\,||\, j\,\rangle\langle\, k\,| = \sum_{ik} b_i u_{ik} \,|\, i\,\rangle\langle\, k\,|$$

$$\Longrightarrow \operatorname{Tr}(BU) = \sum_{i=1}^{n} b_i u_{ii}.$$

$$UB^{-1} = \sum_{ijk} \frac{u_{jk}}{b_i} \,|\, j\,\rangle\langle\, k\,||\, i\,\rangle\langle\, i\,| = \sum_{ij} \frac{u_{ji}}{b_i} \,|\, j\,\rangle\langle\, i\,|$$

$$\Longrightarrow \operatorname{Tr}(UB^{-1}) = \sum_{i=1}^{n} \frac{u_{ii}}{b_i}.$$

Therefore,

$$\operatorname{Tr}(UB)\operatorname{Tr}(BU^{-1}) = \sum_{i,j=1}^{n} \frac{b_j}{b_i} u_{ii}u_{jj} = \frac{1}{2}\sum_{i,j=1}^{n} \left(\frac{b_j}{b_i} + \frac{b_i}{b_j}\right) u_{ii}u_{jj}$$

$$\geq \sum_{i,j=1}^{n} u_{ii}u_{jj} = \left(\sum_{i=1}^{n} u_{ii}\right)^2 = \operatorname{Tr}(U)^2.$$

Notice that we used the fact that $x + 1/x \geq 2$, for all $x > 0$. By now, we have the lower bound $\operatorname{Tr}(U)^2$. To finish, notice that $B = Id$ achieves this bound, so we conclude that

$$\inf_{B>0} \operatorname{Tr}(BU)\operatorname{Tr}(UB^{-1}) = \operatorname{Tr}(U)^2.$$

□

Now we proceed to prove the theorem.

Proof. Using Remark 7, we have

$$A^{-1}\mathcal{L}_0(A) = 2A^{-1}\operatorname{Tr}(A) - 2nI$$

$$\Rightarrow \operatorname{Tr}(\rho A^{-1}\mathcal{L}_0(A)) = 2\operatorname{Tr}(\rho A^{-1}).\operatorname{Tr}(A) - 2n\operatorname{Tr}(\rho)$$
$$= 2\operatorname{Tr}(\rho A^{-1})\operatorname{Tr}(A) - 2n.$$

Writing A in the form $A = B\rho^{1/2}$ will not change the infimum, which will be now taken over $B > 0$. This means

$$\begin{aligned}
\inf_{A>0} 2\,\mathrm{Tr}(\rho A^{-1})\mathrm{Tr}(A) - 2n &= 2 \inf_{B>0} \mathrm{Tr}(\rho^{1/2}B^{-1})\mathrm{Tr}(B\rho^{1/2}) - 2n \\
&= 2\,\mathrm{Tr}(\rho^{1/2})^2 - 2n \\
&= h(\rho).
\end{aligned}$$

As the infimum was computed by Lemma 21 we proved the claim. $\square$

3.8 From quantum to classical

Definition 22. *Given σ and an infinitesimal generator $\mathcal{L}$ of the form* (3.14)*, we say that the matrix Q is the matrix associated to $\mathcal{L}$, if Q is $n \times n$ real matrix with entries $Q_{i,j} = Tr[F_{i,i}\mathcal{L}F_{j,j}]$, where $F_{i,i} = |\,\eta_i\,\rangle\langle\,\eta_i\,|$.*

This matrix is line sum zero with positive values outside the diagonal (see [CM17]). The matrix $Q^{\dagger}$, the transpose of Q, has a stationary eigenvector probability $\overrightarrow{\sigma} \in (0,1)^n$ associated to the eigenvalue 0.

Lemma 23. *Given l, k, the entry $Q_{l,k} = Tr[F_{l,l}\,\mathcal{L}F_{k,k}]$ is given by*

$$Q_{l,k} = 2\,e^{-w_{k,l}/2} - 2\delta_{l,k}\sum_{i=1}^{n} e^{-w_{i,l}/2}. \tag{3.36}$$

Proof. Indeed, when, $A = V_{k,k} = |\,\eta_k\,\rangle\langle\,\eta_k\,|$ we get

$$\begin{aligned}
V_{i,j}^{*}[A, V_{i,j}] &= |\,\eta_j\,\rangle\langle\,\eta_i\,|\,\big[\,A\,,|\,\eta_i\,\rangle\langle\,\eta_j\,|\,\big] \\
&= |\,\eta_j\,\rangle\langle\,\eta_i\,|\,\big(\,|\,\eta_k\,\rangle\langle\,\eta_k\,|\,|\,\eta_i\,\rangle\langle\,\eta_j\,| - |\,\eta_i\,\rangle\langle\,\eta_j\,|\,|\,\eta_k\,\rangle\langle\,\eta_k\,|\big) \\
&= \delta_{i,k}\,|\,\eta_j\,\rangle\langle\,\eta_j\,| - \delta_{j,k}\,|\,\eta_j\,\rangle\langle\,\eta_k\,|
\end{aligned}$$

Moreover, when $A = V_{k,k} = |\,\eta_k\,\rangle\langle\,\eta_k\,|$

$$\begin{aligned}
[V_{i,j}^{*}, A]\,V_{i,j} &= \big[\,|\,\eta_j\,\rangle\langle\,\eta_i\,|,\,A\,\big]\;|\,\eta_i\,\rangle\langle\,\eta_j\,| \\
&= \big(\,|\,\eta_j\,\rangle\langle\,\eta_i\,|\,|\,\eta_k\,\rangle\langle\,\eta_k\,| - \,|\,\eta_k\,\rangle\langle\,\eta_k\,|\,|\,\eta_j\,\rangle\langle\,\eta_i\,|\big)\;|\,\eta_i\,\rangle\langle\,\eta_j\,| \\
&= \delta_{i,k}\,|\,\eta_j\,\rangle\langle\,\eta_j\,| - \delta_{j,k}\,|\,\eta_k\,\rangle\langle\,\eta_j\,|.
\end{aligned}$$

Then, when $A = V_{k,k} = |\,\eta_k\,\rangle\langle\,\eta_k\,|$

$$\begin{aligned}
&e^{-w_{i,j}/2}\left(V_{i,j}^{*}[A, V_{i,j}] + [V_{i,j}^{*}, A]\,V_{i,j}\right) \\
&= e^{-w_{i,j}/2}\left(\,2\delta_{i,k}|\,\eta_j\,\rangle\langle\,\eta_j\,| - \delta_{j,k}\,|\,\eta_j\,\rangle\langle\,\eta_k\,| - \delta_{j,k}\,|\,\eta_k\,\rangle\langle\,\eta_j\,|\,\right)
\end{aligned}$$

$$= e^{-w_{i,j}/2} \left(2\delta_{i,k} | \, \eta_j \,\rangle\langle\, \eta_j \,| - 2\delta_{j,k} \,| \, \eta_k \,\rangle\langle\, \eta_k \,| \right),$$

and finally

$$\begin{aligned}
\mathcal{L}(A) &= \sum_{i,j=1}^{n} e^{-w_{i,j}/2} \, (V_{i,j}^{*}[A, V_{i,j}] + [V_{i,j}^{*}, A] \, V_{i,j}) \\
&= \sum_{i=1}^{n} \sum_{j=1}^{n} e^{-w_{i,j}/2} \, (\, 2\delta_{i,k} | \, \eta_j \,\rangle\langle\, \eta_j \,| - 2\delta_{j,k} \,| \, \eta_k \,\rangle\langle\, \eta_k \,| \,) \\
&= 2 \sum_{j=1}^{n} e^{-w_{k,j}/2} \,| \, \eta_j \,\rangle\langle\, \eta_j \,| - 2 \sum_{i=1}^{n} e^{-w_{i,k}/2} \,| \, \eta_k \,\rangle\langle\, \eta_k \,|
\end{aligned}$$

Therefore, when $A = V_{k,k} = | \, \eta_k \,\rangle\langle\, \eta_k \,|$, given l

$$\begin{aligned}
&| \, \eta_l \,\rangle\langle\, \eta_l \,| \; \mathcal{L}(A) \\
&= 2 \,| \, \eta_l \,\rangle\langle\, \eta_l \,| \sum_{j=1}^{n} e^{-w_{k,j}/2} \,| \, \eta_j \,\rangle\langle\, \eta_j \,| - 2 \,| \, \eta_l \,\rangle\langle\, \eta_l \,| \sum_{i=1}^{n} e^{-w_{i,k}/2} \,| \, \eta_k \,\rangle\langle\, \eta_k \,| \\
&= 2 \sum_{j=1}^{n} e^{-w_{k,j}/2} | \, \eta_l \,\rangle\langle\, \eta_l \,| | \, \eta_j \,\rangle\langle\, \eta_j \,| - 2 \sum_{i=1}^{n} e^{-w_{i,k}/2} | \, \eta_l \,\rangle\langle\, \eta_l \,| | \, \eta_k \,\rangle\langle\, \eta_k \,| \\
&= 2 \, e^{-w_{k,l}/2} | \, \eta_l \,\rangle\langle\, \eta_l \,| - 2\delta_{l,k} \sum_{i=1}^{n} e^{-w_{i,l}/2} | \, \eta_l \,\rangle\langle\, \eta_l \,|.
\end{aligned}$$

From this,

$$Q_{lk} = 2 \, e^{-w_{k,l}/2} - 2\delta_{l,k} \sum_{i=1}^{n} e^{-w_{i,l}/2} \tag{3.37}$$

$$= \begin{cases} 2 \, e^{-w_{k,l}/2} = 2 \, e^{(\lambda_l - \lambda_k)/2} & \text{if } l \neq k \\[2ex] 2 \, e^{-w_{l,l}/2} - 2 \sum_{i=1}^{n} e^{-w_{i,l}/2} = 2 - 2 \sum_{i=1}^{n} e^{(\lambda_l - \lambda_i)/2} & \text{if } l = k \end{cases}$$

□

Notice that:

$$
\begin{aligned}
\sum_{k=1}^{n} Q_{lk} &= Q_{ll} + \sum_{k:\, k\neq l} Q_{lk} \\
&= 2\, e^{-w_{l,l}/2} - 2 \sum_{i=1}^{n} e^{-w_{i,l}/2} + 2 \sum_{k:\, k\neq l} e^{-w_{k,l}/2} \\
&= -2 \sum_{i=1}^{n} e^{-w_{i,l}/2} + 2 \sum_{k=1}^{n} e^{-w_{k,l}/2} \\
&= 0.
\end{aligned}
$$

Note that the expression (3.36) for the matrix Q depends on the eigenvalues $e^{-\lambda_i}$, $i \in \{1, 2.., n\}$, and not the specific eigenfunctions η_i, $i \in \{1, 2.., n\}$, of σ. This means that many density matrices σ can determine the same matrix Q.

Theorem 4.2 in [CM17] claims:

Theorem 24. *Assume that $\mathcal{L}$ is of the form* (3.14) *for σ. The matrix Q, given by $Q_{i,j} = Tr\,[F_{i,i}\mathcal{L}F_{j,j}]$ is line sum zero. The invariant probability for the classical continuous time Markov chain with infinitesimal generator Q is*

$$\overrightarrow{\sigma} = (\sigma_1, \sigma_2, ..., \sigma_n) = (Tr[\sigma F_{1,1}], Tr[\sigma F_{2,2}], ...Tr[\sigma F_{n,n}]). \tag{3.38}$$

The classical detailed balance condition

$$\sigma_i Q_{i,k} = \sigma_k Q_{k,i} \tag{3.39}$$

is satisfied.

Consider the Chapman-Kolmogorov linear differential equation on $\overrightarrow{\rho}(t) = (\rho_1(t), \rho_2(t), ..., \rho_n(t)) \in \mathbb{R}^n$,

$$\frac{d}{dt}\rho_l(t) = \sum_{k=1}^{n} (\rho_k(t) Q_{k,l} - \rho_k(t) Q_{l,k}). \tag{3.40}$$

This is equivalent to

$$\overrightarrow{\rho}(t) = e^{tQ^\dagger}(\overrightarrow{\rho}(0)). \tag{3.41}$$

The occupation time probability in $\{1, 2.., n\}$ of the continuous time Markov Chain is described by $\overrightarrow{\rho}(t)$.

$\overrightarrow{\rho}(t)$ *satisfies* (3.40), *if and only if, the quantum continuous time evolution* $\rho(t)$ *in* $\mathcal{A}$ *satisfies*

$$\rho(t) = \sum_{k=1}^{n} \frac{\rho_k(t)}{Tr(F_{k,k})}\, F_{k,k}. \tag{3.42}$$

Remember that from (3.8)

$$\sigma = \sum_{k=1}^{n} e^{-\lambda_k} |\, \eta_k \,\rangle \langle\, \eta_k \,|. \tag{3.43}$$

Then, from (3.38), given j

$$\sigma_j = \mathrm{Tr}\left[\sigma \,|\, \eta_j \,\rangle\langle\, \eta_j \,|\,\right] = \mathrm{Tr}\left[\sum_{k=1}^{n} e^{-\lambda_k} |\, \eta_k \,\rangle \langle\, \eta_k \,|\,|\, \eta_j \,\rangle\langle\, \eta_j \,|\right] = e^{-\lambda_j}. \tag{3.44}$$

Expression (3.39) means for $k \neq l$

$$e^{-\lambda_k}\, e^{\lambda_k/2 - \lambda_l/2} = e^{-\lambda_k/2 - \lambda_l/2} = e^{-\lambda_l}\, e^{\lambda_l/2 - \lambda_k/2}. \tag{3.45}$$

From (3.37) and (3.38) we get

$$\overrightarrow{\sigma} Q = (\sigma_1, \sigma_2, ..., \sigma_n) Q = (0, 0, ..., 0). \tag{3.46}$$

Example 2. *Let*

$$\sigma = \begin{pmatrix} \frac{1}{2} & & \\ & \frac{1}{3} & \\ & & \frac{1}{6} \end{pmatrix}.$$

Then

$$h = -\log \sigma = \begin{pmatrix} \log 2 & & \\ & \log 3 & \\ & & \log 6 \end{pmatrix},$$

so $\lambda_1 = \log 2$, $\lambda_2 = \log 3$ *and* $\lambda_3 = \log 6$. *The* Q *matrix given by the expression (3.36) has entries*

$$Q_{12} = 2e^{(\log 2 - \log 3)/2} = 2\left(\frac{2}{3}\right)^{1/2} = 2\frac{\sqrt{2}}{\sqrt{3}}$$

$$Q_{13} = 2e^{(\log 2 - \log 6)/2} = 2\left(\frac{2}{6}\right)^{1/2} = 2\frac{1}{\sqrt{3}}$$

$$Q_{11} = 2\left(-\frac{\sqrt{2}}{\sqrt{3}} - \frac{1}{\sqrt{3}}\right)$$

$$Q_{21} = 2e^{(\log 3 - \log 2)/2} = 2\left(\frac{3}{2}\right)^{1/2} = 2\frac{\sqrt{3}}{\sqrt{2}}$$

$$Q_{23} = 2e^{(\log 3 - \log 6)/2} = 2\left(\frac{3}{6}\right)^{1/2} = 2\frac{\sqrt{3}}{\sqrt{6}}$$

$$Q_{22} = 2(-\frac{\sqrt{3}}{\sqrt{2}} - \frac{1}{\frac{\sqrt{3}}{\sqrt{6}}})$$

$$Q_{31} = 2e^{(\log 6 - \log 2)/2} = 2\left(\frac{6}{2}\right)^{1/2} = 2\sqrt{3}$$

$$Q_{32} = 2e^{(\log 6 - \log 3)/2} = 2\left(\frac{6}{3}\right)^{1/2} = 2\sqrt{2}$$

$$Q_{33} = 2(-\sqrt{3} - \sqrt{2})$$

Thus

$$Q = 2\begin{pmatrix} -\frac{\sqrt{2}}{\sqrt{3}} - \frac{1}{\sqrt{3}} & \frac{\sqrt{2}}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ \frac{\sqrt{3}}{\sqrt{2}} & -\frac{\sqrt{3}}{\sqrt{2}} - \frac{\sqrt{3}}{\sqrt{6}} & \frac{\sqrt{3}}{\sqrt{6}} \\ \sqrt{3} & \sqrt{2} & -\sqrt{3} - \sqrt{2} \end{pmatrix}.$$

We should have that $\vec{\sigma} = (\frac{1}{2}, \frac{1}{3}, \frac{1}{6})$ is the invariant vector. In fact,

$$\begin{aligned} \frac{1}{2}(\vec{\sigma}Q)_1 &= -\frac{(\sqrt{2}+1)}{2\sqrt{3}} + \frac{\sqrt{3}}{3\sqrt{2}} + \frac{\sqrt{3}}{6} \\ &= \frac{-\sqrt{3}\sqrt{2} - \sqrt{3} + \sqrt{2}\sqrt{3} + \sqrt{3}}{6} = 0. \end{aligned}$$

$$\begin{aligned} \frac{1}{2}(\vec{\sigma}Q)_2 &= \frac{\sqrt{2}}{2\sqrt{3}} - \frac{(1+\sqrt{3})}{3\sqrt{2}} + \frac{\sqrt{2}}{6} \\ &= \frac{\sqrt{2}\sqrt{3} - \sqrt{2} - \sqrt{2}\sqrt{3} + \sqrt{2}}{6} = 0. \end{aligned}$$

$$\begin{aligned} \frac{1}{2}(\vec{\sigma}Q)_3 &= \frac{1}{2\sqrt{3}} + \frac{1}{3\sqrt{2}} - \frac{(\sqrt{2}+\sqrt{3})}{6} \\ &= \frac{\sqrt{3} + \sqrt{2} - \sqrt{2} - \sqrt{3}}{6} = 0. \end{aligned}$$

Example 3. *Let*

$$\sigma = \begin{pmatrix} \dfrac{1}{4} & 0 & \dfrac{i}{8} \\ 0 & \dfrac{1}{2} & 0 \\ -\dfrac{i}{8} & 0 & \dfrac{1}{4} \end{pmatrix}.$$

The eigenvalues of σ are $\frac{1}{8}$, $\frac{3}{8}$ and $\frac{1}{2}$. Then $h = -\log\sigma$ has eigenvalues $\lambda_1 = \log 8$, $\lambda_2 = \log\dfrac{8}{3}$ and $\lambda_3 = \log 2$. So, the Q matrix given by the expression (3.36) has entries

$$Q_{12} = 2e^{(\log 8 - \log\frac{8}{3})/2} = 2\,(3)^{1/2} = 2\sqrt{3}.$$

$$Q_{13} = 2e^{(\log 8 - \log 2)/2} = 2\left(\frac{8}{2}\right)^{1/2} = 4.$$

$$Q_{11} = -2\left(\sqrt{3} + 2\right).$$

$$Q_{21} = 2e^{(\log\frac{8}{3} - \log 8)/2} = 2\left(\frac{1}{3}\right)^{1/2} = \frac{2}{\sqrt{3}}.$$

$$Q_{23} = 2e^{(\log\frac{8}{3} - \log 2)/2} = 2\left(\frac{4}{3}\right)^{1/2} = \frac{4}{\sqrt{3}}.$$

$$Q_{22} = -\frac{6}{\sqrt{3}}.$$

$$Q_{31} = 2e^{(\log 2 - \log 8)/2} = 2\left(\frac{1}{4}\right)^{1/2} = 1.$$

$$Q_{32} = 2e^{(\log 2 - \log\frac{8}{3})/2} = 2\left(\frac{3}{4}\right)^{1/2} = \sqrt{3}.$$

$$Q_{33} = -\left(1 + \sqrt{3}\right).$$

Thus

$$Q = \begin{pmatrix} -2\left(\sqrt{3}+2\right) & 2\sqrt{3} & 4 \\ \dfrac{2}{\sqrt{3}} & -\dfrac{6}{\sqrt{3}} & \dfrac{4}{\sqrt{3}} \\ 1 & \sqrt{3} & -\left(1+\sqrt{3}\right) \end{pmatrix}.$$

We should have that $\vec{\sigma} = (\frac{1}{8}, \frac{3}{8}, \frac{1}{2})$ *is the invariant vector. In fact,*

$$\begin{aligned}(\vec{\sigma}Q)_1 &= \frac{1}{8}\left(-2\sqrt{3}-4\right) + \frac{3}{8}\frac{2}{\sqrt{3}} + \frac{1}{2} \\ &= -\frac{\sqrt{3}}{4} - \frac{1}{2} + \frac{\sqrt{3}}{4} + \frac{1}{2} = 0.\end{aligned}$$

$$(\vec{\sigma}Q)_2 = \frac{\sqrt{3}}{4} - \frac{3\sqrt{3}}{4} + \frac{2\sqrt{3}}{4} = 0.$$

$$(\vec{\sigma}Q)_3 = \frac{1}{2} + \frac{\sqrt{3}}{2} - \frac{1}{2}\left(1+\sqrt{3}\right) = 0.$$

Related results are described in (3) and (4) in [dLPP21].

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