PROCEEDING OF

The 51st Winter School of Theoretical Physics on Irreversible dynamics: Nonlinear, Nonlocal and Non-Markovian Manifestations, organized by the University of Wrocław and the University of Opole, was held in Lądek Zdrój, Poland, during the period 9–14 February 2015.

PREFACE

The 51st Winter School of Theoretical Physics on *Irreversible dynamics: Nonlinear, Nonlocal and Non-Markovian Manifestations*, organized by the University of Wrocław and the University of Opole, was held in Lądek Zdrój, Poland, during the period 9–14 February 2015.

The conspicuous "non" attitude in the School leading scientific thread was inspired by the continually deepening theoretical understanding of the broad field of irreversible phenomena and related dynamical processes. Presently we know that various deviations from the well-established through decades framework need to be accounted for. They no longer can be considered irrelevant. Even if we keep in mind that physics may be perceived as an art of approximate modeling, both on the experimental and theoretical levels of description of reality. We are aware of a number of major theoretical contributions to theories of nonlinear, nonlocally induced and non-Markovian stochastic processes (of purely classical and quantum origin) that were completed in the seventies and eighties of the 20th century. Those were the golden years of the more or less traditional semigroup theory as well.

A revival and new developments in that theoretical framework, in various areas of physics and mathematics, are being documented nowadays, specifically with a strong emphasis on quantum problems. A significant departure from the semigroup framework proved to be necessary in the study of open quantum systems, where various non-Markovian dynamics scenarios had to be classified and understood.

Nonetheless, a broad semigroup dynamics framework has been here considered as a conceptual basis for other extensions of the traditional formalism of the nonequilibrium statistical mechanics (and thence irreversible dynamics), like e.g. the nonlocal and nonlinear evolution scenarios. It has been also viewed as a solid departure point towards modern approaches to non-Markovian evolutions of quantum systems.

The main purpose of the School was to create a platform for an exchange of modern viewpoints/ideas on the irreversible dynamics, that are physics-inspired but whose range might extend from theoretical physics proper, through mathematical physics towards pure mathematics. Plenary lectures and likewise their audience have shared a mixed origin: theoretical physics and pure mathematics not set against each other, but regarded as a source of mutual inspiration.

School plenary lectures typically provided reviews of relevant topics. It is seldom so that original new results can emerge on their basis in a relatively short time. It is a gift from our lecturers that some of them have undertaken the serious endeavour to write a comprehensive paper that would convey the new yet unpublished message

as a direct outcome of the School activities. The present guest issue of the *Reports on Mathematical Physics* contains a distinctive sample of contributions that cover majority of central topics we wished to address as the School Organizers. We thank warmly the contributiors for their excelent job.

Last but not least we wish to acknowledge a financial support from the Polish Academy of Sciences and Polish Academy of Arts and Sciences, we have received to enhance the School activities.

Guest Editors and the School Organizers:

Lech Jakóbczyk
Wojciech Cegła
Andrzej Frydryszak
Piotr Garbaczewski (Opole)
Robert Olkiewicz

MARKOV CHAIN MONTE CARLO AND IRREVERSIBILITY

MICHELA OTTOBRE

Department of Mathematics, Heriot-Watt University, Edinburgh EH14 4AS, UK
(e-mail: m.ottobre@hw.ac.uk)

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Markov Chain Monte Carlo (MCMC) methods are statistical methods designed to sample from a given measure π by constructing a Markov chain that has π as invariant measure and that converges to π. Most MCMC algorithms make use of chains that satisfy the detailed balance condition with respect to π; such chains are therefore reversible. On the other hand, recent work [18, 21, 28, 29] has stressed several advantages of using irreversible processes for sampling. Roughly speaking, irreversible diffusions converge to equilibrium faster (and lead to smaller asymptotic variance as well). In this paper we discuss some of the recent progress in the study of nonreversible MCMC methods. In particular: i) we explain some of the difficulties that arise in the analysis of nonreversible processes and we discuss some analytical methods to approach the study of continuous-time irreversible diffusions; ii) most of the rigorous results on irreversible diffusions are available for continuous-time processes; however, for computational purposes one needs to discretize such dynamics. It is well known that the resulting discretized chain will not, in general, retain all the good properties of the process that it is obtained from. In particular, if we want to preserve the invariance of the target measure, the chain might no longer be reversible. Therefore iii) we conclude by presenting an MCMC algorithm, the SOL-HMC algorithm [23], which results from a nonreversible discretization of a nonreversible dynamics.

Keywords: Markov chain Monte Carlo, nonreversible diffusions, hypocoercivity, Hamiltonian Monte Carlo.

1. Introduction

The combined use of Bayesian statistics and Markov Chain Monte-Carlo (MCMC) sampling methods has been one of the great successes of applied mathematics and statistics in the last 60 years. While the Bayesian approach constitutes a flexible framework for inference through data assimilation, MCMC turns such a theoretical framework into practice by providing a powerful sampling mechanism to extract information from the posterior measure. For this reason, and because of the wide spectrum of problems that can be recast in Bayesian form, MCMC has been a revolution in the applied sciences. MCMC is employed in parameter estimation, model validation and, ultimately, in inference. Combined with the Bayesian inference paradigm, MCMC is of current use in finance, biology (population genetics, molecular biology), meteorology, epidemiology, optimization, cryptography, molecular dynamics, computational physics (to gain knowledge about statistical quantities of interest in

the study of large particle systems in their equilibrium state), in rare event sampling, in big data analysis and in the field of inverse problems. This list is far from exhaustive.

The increasing popularity of MCMC and the need to tackle problems of growing complexity have brought higher demands on the efficiency of such algorithms, which are often undeniably costly. The answer to such demands has produced both a higher level of sophistication in the design of MCMC algorithms and the introduction of a plethora of different approaches. We would however be very unfair to MCMC if we described it as a mere algorithmic tool: the study of MCMC has in fact opened (or it is related to) a range of beautiful questions in an unimmaginable wide range of areas of mathematics, from pure probability to analysis, all the way to number theory [11, 36].

The purpose of MCMC is to sample from a given target distribution π or, more commonly, to calculate expectations with respect to π, i.e. integrals of the form

$$\int_{\chi} f(x)d\pi(x), \tag{1.1}$$

when analytic (or deterministic) methods are not feasible. Here π and f are a measure and a function, respectively, both defined on the state space χ. Broadly speaking, the calculation of integrals (1.1) is of interest in the applied sciences for several reasons: i) for different choices of the function f, such integrals represent various statistical properties of a system in equilibrium (with stationary measure π) or properties of the posterior measure, π, in a Bayesian context; ii) if X_t is the solution at time t of a given stochastic differential equation (SDE), then the expectation

$$\mathbb{E}[f(X_t)] \tag{1.2}$$

can be recast in the form (1.1); iii) thanks to the Feynman–Kac formula, integrals of type (1.1) are representations of the solution of a large class of PDEs, as well.

Roughly speaking (we will be more precise in Section 4), the basic prescription behind MCMC can be explained as follows: construct a Markov chain $\{x_n\}_{n\in\mathbb{N}}$ that converges to our target distribution π. In this way, if we run the chain "long enough", as $n \to \infty$ we will effectively be extracting samples from π. Also, if the chain we constructed enjoys good ergodic properties, the ergodic theorem can be employed, thereby providing an approximation for the quantity (1.1)

$$\lim_{n\to\infty} \frac{1}{n} \sum_{k=0}^{n-1} f(x_k) = \mathbb{E}_{\pi}(f) := \int_{\chi} f(x)d\pi(x). \tag{1.3}$$

In order for this process to work efficiently, the constructed chain should: i) converge to equilibirum as fast as possible (all the samples out of equilibrium are not needed); ii) once equilibrium is reached, explore the state space as quickly and thoroughly as possible. This paper intends to comment on some aspects related to point i). Regarding i): the classical MCMC framework—and in particular the popular Metropolis–Hastings (M–H) technique (see Section 4.1)—typically makes

use of *reversible chains*, i.e. chains which satisfy the *detailed balance condition* with respect to π. However, it is a well documented principle that, loosely speaking, nonreversible chains might converge to equilibrium faster than reversible ones. We will be more clear on this matter in Section 3. For the moment let us just say that this observation has started to produce a stream of literature aimed at improving the speed of convergence to equilibrium of MCMC methods by designing algorithms that produce nonreversible chains. In this spirit, we will present an algorithm, recently introduced in [23], which does not belong to the M–H framework, as it produces a Markov chain which does not satisfy detailed balance with respect to the target measure. This is the SOL-HMC algorithm (Second Order Langevin–Hybrid Monte Carlo), presented in Section 5. In the present paper we will mostly be concerned with irreversibility and therefore we will only tangentially comment on another important aspect related to the SOL–HMC algorithm: SOL–HMC does not suffer from the so-called *curse of dimensionality*. That is, the cost of the algorithm does not increase when the dimension of the space in which it is implemented increases. We will be more precise on this point in Section 4.2.

The remainder of the paper is organized as follows: in Section 2 we recall some basic definitions, mostly with the purpose of fixing the notation for the rest of the paper (references are given for those not familiar with the topic). Section 3 is devoted to the study of exponentially fast convergence to equilibrium for irreversible dynamics. The Markov dynamics presented here, central to the development of the SOL–HMC algorithm, are hypoelliptic and irreversible; i.e. their generator is nonelliptic and not self-adjoint, so classical techniques do not apply; in order to study these degenerate dynamics the *Hypocoercivity Theory* has been recently introduced in [38]. Section 3 contains a short account of such an approach. Section 4 is devoted to an elementary introduction to MCMC, including the popular Random Walk Metropolis (RWM), Metropolis Adjusted Langevin Algorithm (MALA) and Hybrid (or Hamiltonian) Monte Carlo (HMC). The last section, Section 5, contains an example of an irreversible MCMC algorithm, the so-called SOL–HMC (Second-Order Langevin–Hamiltonian Monte Carlo), introduced in [23]. In this context we will explain how irreversibility can be obtained from the composition of Markov transition probabilities that do satisfy detailed balance.

2. Preliminaries and notation

In this section we briefly recall some basic facts that will be used in the following. More details about the basic formalism introduced here can be found in [3, 25, 15, 12]. Consider an ordinary stochastic differential equation in $\mathbb{R}^d$ of the form[1]

$$dx(t) = b(x_t)dt + \sigma(x_t)dW_t, \tag{2.1}$$

where W_t is a d-dimensional standard Brownian motion and the drift and diffusion coefficients ($b : \mathbb{R}^d \to \mathbb{R}^d$ and $\sigma : \mathbb{R}^d \to \mathbb{R}^{d\times d}$, respectively) are globally Lipshitz. It

[1]For any time-dependent process or function, we will use the notations h_t and $h(t)$ interchangeably.

is a standard fact that under these assumptions there exists a unique strong solution to the SDE (2.1). The solution $x(t)$ is a Markov diffusion process. Because b and σ are time-independent, $x(t)$ is a time-homogeneous Markov process.

To the process x_t we can associate a Markov semigroup as follows. For any function $f : \mathbb{R}^d \to \mathbb{R}$, say[2] $f \in \mathcal{B}_m$, and any point $x \in \mathbb{R}^d$, we can define

$$f(x,t) := \mathbb{E}\left[f(x_t)|x_0 = x\right],$$

where $\mathbb{E}$ denotes expected value (with respect to the noise W_t). Notice that the function f is a deterministic function. By using the Itô formula, one can immediately see that $f(x,t)$ solves the Cauchy problem

$$\begin{aligned} \partial_t f(x,t) &= \mathcal{L} f(x,t), \\ f(x,0) &= f(x), \qquad x \in \mathbb{R}^d, \end{aligned} \tag{2.2}$$

where $\mathcal{L}$ is the second-order differential operator defined on smooth functions as

$$\mathcal{L} = \sum_{i=1}^{d} b^i(x)\partial_{x_i} + \frac{1}{2}\sum_{i,j=1}^{d} \Sigma_{ij}(x)\partial^2_{x_i x_j}, \qquad \Sigma(x) := \sigma(x)\sigma^T(x),$$

having denoted by σ^T the transpose of the matrix σ. The operator $\mathcal{L}$ is (under the assumptions of the Hille–Yoshida theorem) the *generator* of the Markov semigroup $\mathcal{P}_t$ associated with the PDE (2.2); i.e. formally

$$f(x,t) = e^{t\mathcal{L}} f(x) = (\mathcal{P}_t f)(x).$$

With abuse of nomenclature, we will often refer to $\mathcal{L}$ as to the generator of the diffusion process (2.1). The standard example belonging to this framework is the heat semigroup: in this case the process $x(t)$ is simply Brownian motion (i.e. in (2.1) $b = 0$ and σ is the identity matrix) and the (formal) generator of the semigroup is the Laplacian operator.

We recall that a probability measure μ on $\mathbb{R}^d$ is *invariant* for the Markov semigroup $\mathcal{P}_t$ if, for every $h \in \mathcal{B}_m$,

$$\int_{\mathbb{R}^d} (\mathcal{P}_t h)(x)\mu(dx) = \int_{\mathbb{R}^d} h(x)\mu(dx).$$

Using the dual semigroup $\mathcal{P}'_t$, acting on measures, this can also be rewritten as $\mathcal{P}'_t\mu = \mu$ or $\mathcal{L}'\mu = 0$, where $\mathcal{L}'$ denotes the L^2-adjoint of $\mathcal{L}$.[3]

In view of the link between the Markov process x_t solution of the SDE (2.1) and the semigroup $\mathcal{P}_t$, every attribute of the semigroup will also hold for the process and vice versa, unless otherwise stated. So e.g. we say that the measure μ is invariant for the process $x(t)$ if it is invariant for the semigroup associated to $x(t)$. The measure μ is called invariant because if $x(0)$ is distributed according

[2] $\mathcal{B}_m := \{\text{bounded and measurable functions on } \mathbb{R}^d\}$.

[3] $\mathcal{L}$ is the generator of the dynamics and the associated evolution equation, equation (2.2), governs the evolution of the observables. $\mathcal{L}'$ is often refereed to as the *Fokker–Planck* operator; $\mathcal{L}'$ describes the evolution of the law of the process.

to μ, $x(0) \sim \mu$, then $x(t) \sim \mu$ for every $t \geq 0$. The process x_t is *ergodic* if it admits a unique invariant measure. In this case the only invariant measure is called the ergodic measure of the process and it represents the equilibrium state (in law) of the system.

Central to our discussion will be the definition of reversibility.

DEFINITION 2.1. A Markov semigroup $\mathcal{P}_t$ is *reversible* with respect to a probability measure μ (or, equivalently, the probability measure μ is reversible for the Markov semigroup $\mathcal{P}_t$) if for any $f, g \in \mathcal{B}_m$

$$\int (\mathcal{P}_t f) g \, d\mu(x) = \int f (\mathcal{P}_t g) \, d\mu(x). \tag{2.3}$$

In this case it is also customary to say that $\mathcal{P}_t$ satisfies the *detailed balance condition* with respect to μ.

Notice that if μ is reversible then it is invariant as well. If x_t is reversible with respect to μ and $x(0) \sim \mu$ then for any $T > 0$ and any $0 \leq t_1 \leq \ldots \leq t_k < T$, the law of $(x_0, x_{t_1}, \ldots, x_{t_k}, x_T)$ is the same as the law of $(x_T, x_{T-t_1}, \ldots, x_{T-t_k}, x_0)$. In other words, the forward and the time-reversed process have the same law (on this matter see e.g. [25, Section 4.6]). It is easy to show that $\mathcal{P}_t$ is reversible with respect to μ if and only if the generator $\mathcal{L}$ is symmetric in L^2_μ, where

$$L^2_\mu := \left\{ \text{functions } f : \mathbb{R}^d \to \mathbb{C} \text{ such that } \int_{\mathbb{R}^d} f^2 d\mu < \infty \right\}.$$

Because we will be using discrete-time as well as continuous-time Markov processes, we mention here that for a given Markov chain x_n, $n \in \mathbb{N}$, on a state space S (tipically S will be a finite or countable set, $\mathbb{R}^d$ or a separable Hilbert space $\mathcal{H}$), we will denote by $p(x, A), x \in S, A \subset S$, the transition probabilities of the chain (and by $p^n(x, A)$ the n-step transition probabilities). If S is finite or countable the transition probabilities are specified by $\{p(x, y)\}_{x,y \in S}$. In this case the detailed balance condition with respect to a measure π on S can be rewritten as follows

$$\pi(x) p(x, y) = \pi(y) p(y, x), \qquad \forall x, y \in S. \tag{2.4}$$

If the above holds, we say that x_n is reversible with respect to π.

Finally, for a measure μ on $\mathbb{R}^d$, we will use the same Greek letter to denote both the measure and its density (when such a density exists), i.e. we will write $\mu(dx) = \mu(x)dx$; $\mathcal{Z}$ will always denote a generic normalizing constant and for a differential operator A, $\mathcal{D}(A)$ will indicate the domain of A.

3. Irreversibility

In this section we will be concerned with the study of exponentially fast convergence to equilibrium for irreversible Markov dynamics, i.e. dynamics generated by nonsymmetric operators. As a term of comparison, let us start from the reversible case.

The theory concerning reversible Markov processes has been much more developed than the theory for nonreversible ones. This is mostly due to the fact that the generator of a reversible Markov process is a symmetric and, under some assumptions, self-adjoint operator; self-adjoint operators enjoy good spectral properties [27], which makes the study of convergence to equilibrium more accessible than in the non self-adjoint, irreversible case.

The study of exponentially fast convergence to equilibrium for reversible processes has been tackled using both probabilistic and analytic techniques. The most comprehensive reference on the analytic approach is [3]. While we do not intend to review the existing methods, we would like to recall some basic results. This is mainly to point out, by comparison, what are some of the difficulties in studying the problem of exponentially fast convergence to equilibrium in the irreversible case. Before stating the next definition we recall the following nomenclature: let $\mathcal{T}$ be a second-order differential operator; suppose that the spectrum of $\mathcal{T}$, $\sigma(\mathcal{T})$, is only made of simple isolated eigenvalues, that all such eigenvalues have positive (negative, respectively) real part and assume $0 \in \sigma(\mathcal{T})$. Then the *spectral gap* of $\mathcal{T}$, $\mathfrak{S}(\mathcal{T})$, is the smallest (biggest, respectively) real part of the nonzero eigenvalues of $\mathcal{T}$. Notice that if $\mathcal{T}$ is the generator of a strongly continuous ergodic Markov semigroup then $0 \in \mathfrak{S}(\mathcal{T})$, by the Koopman–Von Neumann theorem (see [7, Theorem 1.2.1]).

DEFINITION 3.1. Given a Markov semigroup $\mathcal{P}_t$ with generator $\mathcal{L}$, we say that a measure π which is reversible for $\mathcal{P}_t$ satisfies a *spectral gap inequality* if there exists a constant $\alpha > 0$ such that

$$\alpha \int_{\mathbb{R}} \left[f - \int_{\mathbb{R}} f \, d\pi \right]^2 d\pi \leq -\langle \mathcal{L} f, f \rangle_\pi, \qquad \text{for every } f \in L^2_\pi \cap \mathcal{D}(\mathcal{L}). \tag{3.1}$$

The largest positive number α such that (3.1) is satisfied is the *spectral gap* of the self-adjoint operator $\mathcal{L}$.

The term on the RHS of (3.1) is called the *Dirichlet form* of the operator $\mathcal{L}$.

REMARK 3.1. If $\mathcal{L}$ is a self-adjoint operator then the form $\langle \mathcal{L} f, f \rangle_\pi$ is real-valued. In particular the spectrum of $\mathcal{L}$ is real. If $\mathcal{L}$ is the generator of a strongly continuous Markov semigroup and the semigroup is ergodic then we already know that 0 is a simple eigenvalue of $\mathcal{L}$. If (3.1) holds, then $\langle \mathcal{L} f, f \rangle_\pi \leq 0$ for every f, therefore the self-adjoint operator $-\mathcal{L}$ is *positive* and all the eigenvalues of $-\mathcal{L}$ will be positive. The biggest positive α such that (3.1) holds is the smallest nonzero eigenvalue of $-\mathcal{L}$, i.e. α is the spectral gap.[4] The next proposition clarifies why spectral gap inequalities are so important. Notice however that, at least on a formal level, it makes sense to talk about spectral gap inequalities if one can guarantee that the quantity $\langle \mathcal{L} f, f \rangle_\pi$ is at least real. This cannot be guaranteed in general if $\mathcal{L}$ is not self-adjoint. □

[4]This reasoning might appear more transparent if we take mean zero functions, that is f such that $\int f \, d\pi = 0$.

PROPOSITION 3.1. *A measure π reversible with respect to the Markov semigroup $\mathcal{P}_t$ satisfies a spectral gap inequality (with constant α) if and only if*

$$\int_{\mathbb{R}} \left(\mathcal{P}_t f - \int_{\mathbb{R}} f d\pi \right)^2 d\pi \leq e^{-2\alpha t} \int_{\mathbb{R}} \left(f - \int_{\mathbb{R}} f d\pi \right)^2 d\pi, \tag{3.2}$$

for all $t \geq 0$ and $f \in L^2_\pi$.

A proof of the above proposition can be found in [15, Chapter 2]. The spectral gap inequality formalism is one of the most established techniques to study exponential convergence for reversible diffusions. However this cannot be used—at least not as it is—in the irreversible case (on this point we also mention the related interesting paper [19]).

If irreversible diffusions are harder to study than reversible ones, it is natural to wonder why one would want to employ them in the study of MCMC. The reason is readily explained: plenty of numerical evidence—although not as many theoretical results—shows that irreversible processes converge to equilibrium faster than reversible dynamics. We illustrate this idea with an example (to the best of our knowledge this is one of the very few examples where rigorous results are available). Consider the Ornstein–Uhlenbeck process (OU)

$$dY_t = -Y_t dt + \sqrt{2} dW_t, \qquad Y_t \in \mathbb{R}^d. \tag{3.3}$$

Y_t is ergodic with unique invariant measure $\pi(y) = e^{-|y|^2/2}/\mathcal{Z}$. Y_t is also reversible with respect to π. Now consider the process Z_t obtained from Y_t by adding a nonreversible perturbation to the drift, i.e. modify the OU process in such a way that the invariant measure of the new process is still π but Z_t is no longer reversible with respect to π,

$$dZ_t = (-Z_t + \gamma(Z_t))dt + \sqrt{2} dW_t, \qquad \text{with } \nabla \cdot (\gamma(z) e^{-V(z)}) = 0.$$

The condition $\nabla \cdot (\gamma(z) e^{-V(z)}) = 0$ is added in order to preserve the invariance of π. It can be shown (see [21, 18, 24]) that $\mathfrak{S}(Z) \leq \mathfrak{S}(Y)$ and that the process Z_t converges faster than Y_t.

One of the most popular approaches to study exponential convergence to equilibium in the nonreversible case is given by the *hypocoercivity theory*, which we briefly review below.

3.1. Hypocoercivity theory and second-order Langevin equation

Let us start by introducing the Second-Order Langevin (SOL) equation, which is possibly the simplest example of dynamics that retains all the properties that we are interested in. Also, it is the dynamics that we will use to construct the SOL–HMC algorithm in Section 5. By SOL we mean the following SDE (or slight variations):

$$\begin{aligned} dq &= p dt \\ dp &= -\partial_q V(q) dt - p dt + \sqrt{2} dW_t, \end{aligned} \tag{3.4}$$

where $(q, p) \in \mathbb{R}^2$, $V(q) \in \mathcal{C}^\infty$ is a confinig potential (i.e. $V(q) \to \infty$ as $|q| \to \infty$ and $V(q)$ grows at least quadratically at infinity[5]) and W_t is a one-dimensional standard Brownian motion. The generator of (3.4) is

$$\mathcal{L} = p\partial_q - \partial_q V(q)\partial_p - p\partial_p + \partial_p^2 \tag{3.5}$$

and the corresponding Fokker–Planck operator is

$$\mathcal{L}' = -p\partial_q + \partial_q V(q)\partial_p + \partial_p(p\cdot) + \partial_p^2. \tag{3.6}$$

Notice that $\mathcal{L}'$ is nonuniformly elliptic. In particular, it is *hypoelliptic*. We will not linger on this fact here and refer the reader to [39] for a concise and clear introduction to the hypoellipticity theory. We just observe that the fact that $\partial_t - \mathcal{L}'$ is hypoelliptic on $\mathbb{R}_+ \times \mathbb{R}^2$ implies that the law of the process (3.5) has a density for every $t > 0$. The dynamics generated by the operator (3.5) is ergodic as well and the density of the unique invariant measure of such a dynamics is

$$\rho(q, p) = \frac{e^{-(V(q)+p^2/2)}}{\mathcal{Z}}. \tag{3.7}$$

The dynamics described by (3.4) can be thought of as split into a Hamiltonian component,

$$\begin{aligned} \dot{q} &= p, \\ \dot{p} &= -\partial_q V(q), \end{aligned} \tag{3.8}$$

plus an OU process (in the p variable, see (3.3)):

$$\begin{aligned} dq &= pdt, \\ dp &= -\partial_q V(q)dt \underbrace{-pdt + \sqrt{2}dW_t}_{\text{OU process}}. \end{aligned}$$

Indeed, Eqs. (3.8) are the equations of motion of a Hamiltonian system with Hamiltonian

$$H(q, p) = V(q) + \frac{p^2}{2}.$$

At the level of the generator this is all very clear: we can write the operator $\mathcal{L}$ as

$$\mathcal{L} = \mathcal{L}_H + \mathcal{L}_{OU},$$

where

$$\mathcal{L}_H := p\partial_q - \partial_q V(q)\partial_p \tag{3.9}$$

is the Liouville operator of classical Hamiltonian mechanics and

$$\mathcal{L}_{OU} := -p\partial_p + \partial_p^2$$

[5]Under this assumption strong uniqueness and nonexplosivity are guaranteed, see e.g. [35, Chapter 10].

is the generator of an OU process in the p variable. By the point of view of our formalism, the Hamiltonian dynamics (3.8) admits infinitely many invariant measures, indeed

$$-\mathcal{L}'_H f(H(q,p)) = \mathcal{L}_H f(H(q,p)) = 0 \qquad \text{for every } f \text{ (smooth enough)}.$$

So any integrable and normalized function of the Hamiltonian is an invariant probability measure for (3.8). Adding the OU process amounts to selecting one equilibrum.

To distinguish between the flat L^2 adjoint of an operator T and the adjoint in the weighted L^2_ρ, we shall denote the first by T' and the latter by T^*. The scalar product and norm of L^2_ρ will be denoted by $\langle\cdot,\cdot\rangle_\rho$ and $\|\cdot\|_\rho$, respectively. Notice now that the generator $\mathcal{L}_H$ of the Hamiltonian part of the Langevin equation is antisymmetric both in L^2 and in L^2_ρ. It is indeed straightforward to see that

$$\mathcal{L}_H = -\mathcal{L}'_H.$$

Also, $\langle \mathcal{L}_H f, g\rangle_\rho = -\langle f, \mathcal{L}_H g\rangle_\rho$ for every f, g say in $L^2_\rho \cap \mathcal{D}(\mathcal{L}_H)$,

$$\begin{aligned}\langle \mathcal{L}_H f, g\rangle_\rho &= \int_{\mathbb{R}}\int_{\mathbb{R}} \left(p\partial_q f - q\partial_p f\right) g\rho\, dpdq \\ &= -\int_{\mathbb{R}}\int_{\mathbb{R}} fp\partial_q(g\rho)\, dpdq + \int_{\mathbb{R}}\int_{\mathbb{R}} fq\partial_p(g\rho)\, dpdq \\ &= -\int_{\mathbb{R}}\int_{\mathbb{R}} fp(\partial_q g)\rho + \int_{\mathbb{R}}\int_{\mathbb{R}} qf(\partial_p g)\rho = -\langle f, \mathcal{L}_H g\rangle_\rho.\end{aligned}$$

The generator of the OU process is instead symmetric in $\mathcal{L}^2_\rho$ and, in particular,

$$\mathcal{L}_{OU} = -T^*T,$$

where

$$T = \partial_p, \qquad \text{so that} \qquad T^* = -\partial_p + p.$$

In conclusion, the generator of the Langevin equation decomposes into a symmetric and antisymmetric part. Moreover, the antisymmetric part comes from the Hamiltonian deterministic component of the dynamics, the symmetric part comes from the stochastic component.

Using Stone's theorem (see e.g. [27]) we also know that the semigroup generated by $\mathcal{L}_H$ is norm-preserving, while it is easy to see that the semigroup generated by $\mathcal{L}_{OU}$ is dissipative, indeed

$$\begin{aligned}\frac{d}{dt}\|e^{t\mathcal{L}_{OU}}h\|^2_\rho &= 2\langle \mathcal{L}_{OU}e^{t\mathcal{L}_{OU}}h, e^{t\mathcal{L}_{OU}}h\rangle_\rho \\ &= -2\langle T^*Th_t, h_t\rangle_\rho = -2\|Th_t\|^2_\rho < 0,\end{aligned}$$

where we used the notation $h_t(x) = e^{t\mathcal{L}_{OU}}h(x)$. In conclusion, so far we have the following picture:

$$\mathcal{L} = \underbrace{\mathcal{L}_H}_{\substack{\text{skew}\\ \text{symmetric}\\ \downarrow\\ \text{deterministic}\\ \text{conservative}}} - \underbrace{T^*T}_{\substack{\text{symmetric}\\ \downarrow\\ \text{stochastic}\\ \text{dissipative}}}$$

This is precisely the setting of the hypocoercivity theory. The hypocoercivity theory, subject of [38], is concerned with the problem of exponential convergence to equilibrium for evolution equations of the form[6]

$$\partial_t h + \left(A^*A - B\right) h = 0, \tag{3.10}$$

where B is an antisymmetric operator [7]. We shall briefly present some of the basic elements of such a theory and then see what are the outcomes of such a technique when we apply it to the Langevin equation (3.4).

We first introduce the necessary notation. Let $\mathcal{H}$ be a Hilbert space, *real* and separable, $\|\cdot\|$ and $(\cdot,\cdot)$ the norm and scalar product of $\mathcal{H}$, respectively. Let A and B be unbounded operators with domains $\mathcal{D}(A)$ and $\mathcal{D}(B)$ respectively, and assume that B is antisymmetric, i.e. $B^* = -B$, where * denotes adjoint in $\mathcal{H}$. We shall also assume that there exists a vector space $\mathcal{S} \subset \mathcal{H}$, dense in $\mathcal{H}$, where all the operations that we will perform involving A and B are well defined.

Writing the involved operator in the form $\mathcal{T} = A^*A - B$ has several advantages. Some of them are purely computational. For example, for operators of this form checking the contractivity of the semigroup associated with the dynamics (3.10) becomes trivial. Indeed, the antisymmetry of B implies

$$(Bx, x) = -(x, Bx) \qquad \Longrightarrow \qquad (Bx, x) = 0. \tag{3.11}$$

This fact, together with $(A^*Ax, x) = \|Ax\|^2 \geq 0$, immediately gives

$$\frac{1}{2}\frac{d}{dt}\|e^{-t\mathcal{T}}h\|^2 \overset{(3.11)}{=} -\|Ah_t\|^2 \leq 0.$$

On the other hand, conceptually, the decomposition $A^*A - B$ is physically meaningful as the symmetric part of the operator, A^*A, corresponds to the stochastic (dissipative) part of the dynamics, whereas the antisymmetric part corresponds to the deterministic (conservative) component.

DEFINITION 3.2. We say that an unbounded linear operator $\mathcal{T}$ on $\mathcal{H}$ is *relatively bounded* with respect to the linear operators $T_1, ..., T_n$ if the domain of $\mathcal{T}$, $\mathcal{D}(\mathcal{T})$, is contained in the intersection $\cap\mathcal{D}(T_j)$ and there exists a constant $\alpha > 0$ s.t.

$$\forall h \in \mathcal{D}(\mathcal{T}), \qquad \|\mathcal{T}h\| \leq \alpha(\|T_1h\| + ... + \|T_nh\|).$$

[6]Generalizations to the form $\partial_t h + \left(\sum_{i=1}^m {A_i}^*A_i - B\right) h = 0$ as well as further generalizations are presented in [38]. We refer the reader to such a monograph for these cases.

[7]Notice that, for less than regularity issues, any second-order differential operator $\mathcal{L}$ can be written in the form $A^*A - B$.

DEFINITION 3.3 (Coercivity). Let $\mathcal{T}$ be an unbounded operator on a Hilbert space $\mathcal{H}$, denote its kernel by $\mathcal{K}$ and assume there exists another Hilbert space $\tilde{\mathcal{H}}$ continuously and densely embedded in $\mathcal{K}^\perp$. If $\|\cdot\|_{\tilde{\mathcal{H}}}$ and $(\cdot,\cdot)_{\tilde{\mathcal{H}}}$ are the norm and scalar product on $\tilde{\mathcal{H}}$, respectively, then the operator $\mathcal{T}$ is said to be λ-*coercive on* $\tilde{\mathcal{H}}$ if

$$(\mathcal{T}h, h)_{\tilde{\mathcal{H}}} \geq \lambda \|h\|^2_{\tilde{\mathcal{H}}}, \qquad \forall h \in \mathcal{K}^\perp \cap D(\mathcal{T}),$$

where $D(\mathcal{T})$ is the domain of $\mathcal{T}$ in $\tilde{\mathcal{H}}$.

Notice the parallel with (3.1). Notice also that, from the above discussion, for every $h \in \mathcal{D}(\mathcal{T})$, the number $(\mathcal{T}h, h)$ is always real. Not surprisingly, the following proposition gives an equivalent definition of coercivity (cf. Proposition 3.1).

PROPOSITION 3.2. *With the same notation as in Definition* 3.3, $\mathcal{T}$ *is* λ-*coercive on* $\tilde{\mathcal{H}}$ *iff*

$$\| e^{-\mathcal{T}t} h \|_{\tilde{\mathcal{H}}} \leq e^{-\lambda t} \| h \|_{\tilde{\mathcal{H}}}, \qquad \forall h \in \tilde{\mathcal{H}} \text{ and } t \geq 0.$$

DEFINITION 3.4 (Hypocoercivity). With the same notation of Definition 3.3, assume $\mathcal{T}$ generates a continuous semigroup. Then $\mathcal{T}$ is said to be λ-*hypocoercive on* $\tilde{\mathcal{H}}$ if there exists a constant $\kappa > 0$ such that

$$\| e^{-\mathcal{T}t} h \|_{\tilde{\mathcal{H}}} \leq \kappa e^{-\lambda t} \| h \|_{\tilde{\mathcal{H}}}, \qquad \forall h \in \tilde{\mathcal{H}} \text{ and } t \geq 0. \tag{3.12}$$

REMARK 3.2. We remark that the only difference between Definition 3.3 and Definition 3.4 is in the constant κ on the right-hand side of (3.12), when $\kappa > 1$. Thanks to this constant, the notion of hypocoercivity is invariant under a change of equivalent norm, as opposed to the definition of coercivity which relies on the choice of the Hilbert norm. Hence the basic idea employed in the proof of exponentially fast convergence to equilibrium for degenerate diffusions generated by operators in the form (3.10), is to appropriately construct a norm on $\tilde{\mathcal{H}}$, equivalent to the existing one, and such that in this norm the operator is coercive. □

We will state in the following the basic theorem in the theory of hypocoercivity. Generalizations can be found in [38].

THEOREM 3.1. *With the notation introduced so far, let* $\mathcal{T}$ *be an operator of the form* $\mathcal{T} = A^*A - B$, *with* $B^* = -B$. *Let* $\mathcal{K} = \operatorname{Ker}\mathcal{T}$, *define* $C := [A, B]$, [8] *and consider the norm*

$$\|h\|^2_{\mathcal{H}^1} := \|h\|^2 + \|Ah\|^2 + \|Ch\|^2$$

on $\mathcal{K}^\perp$ [9]. *Suppose the following holds:*

(1) A *and* A^* *commute with* C,
(2) $[A, A^*]$ *is relatively bounded with respect to* I *and* A,
(3) $[B, C]$ *is relatively bounded with respect to* A, A^2, C *and* AC,

[8] Given two differential operators X and Y we denote by $[X, Y] = XY - YX$ the commutator between X and Y.

[9] One can prove that space $\mathcal{K}^\perp$ is the same irrespective of whether we consider the scalar product $\langle\cdot,\cdot\rangle$ of $\mathcal{H}$ or the scalar product $\langle\cdot,\cdot\rangle_{\mathcal{H}^1}$ associated with the norm $\|\cdot\|_{\mathcal{H}^1}$.

then there exists a scalar product $((\cdot,\cdot))$ *on* $\mathcal{H}^1/\mathcal{K}$ *defining a norm equivalent to the* $\mathcal{H}^1$ *norm such that*

$$((h,\mathcal{T}h)) \geq k(\|Ah\|^2 + \|Ch\|^2), \qquad \forall h \in \mathcal{H}^1/\mathcal{K}, \tag{3.13}$$

for some constant $k > 0$. *If, in addition to the above assumptions, we have*

$$A^*A + C^*C \text{ is } \kappa\text{-coercive for some } \kappa > 0, \tag{3.14}$$

then $\mathcal{T}$ *is hypocoercive in* $\mathcal{H}^1/\mathcal{K}$: *there exist constants* $c, \lambda > 0$ *such that*

$$\|e^{-t\mathcal{L}}\|_{\mathcal{H}^1/\mathcal{K}\to\mathcal{H}^1/\mathcal{K}} \leq ce^{-\lambda t}.$$

REMARK 3.3. Let $\mathcal{K}$ be the kernel of $\mathcal{T}$ and notice that $\mathrm{Ker}(A^*A) = \mathrm{Ker}(A)$ and $\mathcal{K} = \mathrm{Ker}(A) \cap \mathrm{Ker}(B)$. Suppose $\mathrm{Ker}\, A \subset \mathrm{Ker}\, B$; then $\mathrm{Ker}\,\mathcal{T} = \mathrm{Ker}\, A$. In this case the coercivity of $\mathcal{T}$ is equivalent to the coercivity of A^*A. So the case we are interested in is the case in which A^*A is coercive and $\mathcal{T}$ is not. In order for this to happen A^*A and B cannot commute; if they did, then $e^{-t\mathcal{T}} = e^{-tA^*A}e^{tB}$. Therefore, since e^{tB} is norm preserving, we would have $\|e^{-t\mathcal{T}}\| = \|e^{-tA^*A}\|$. This is the intuitive reason why commutators (especially of the form $[A, B]$) appear in Theorem 3.1.

COMMENT [On the Proof of Theorem 3.1]. We will not write a proof of this theorem but we will explain how it works. The idea is the same that we have explained in Remark 3.2. Consider the norm

$$((h,h)) := \|h\|^2 + a\ \|Ah\|^2 + c\|Ch\|^2 + 2b(Ah, Ch),$$

where a, b and c are three strictly positive constants to be chosen. Assumptions (1), (2) and (3) are needed to ensure that this norm is equivalent to the $\mathcal{H}^1$ norm, i.e. that there exist constants $c_1, c_2 > 0$ such that

$$c_1\|h\|_{\mathcal{H}^1} \leq ((h,h)) \leq c_2\|h\|_{\mathcal{H}^1}.$$

If we can prove that $\mathcal{T}$ is coercive in this norm, then by Proposition 3.2 and Remark 3.2 we have also shown exponential convergence to equilibrium in the $\mathcal{H}^1$ norm, i.e. hypocoercivity. So the whole point is proving that

$$((\mathcal{T}h,h)) \geq K((h,h)),$$

for some $K > 0$. If (1), (2) and (3) of Theorem 3.1 hold, then (with a few lengthy but surprisingly not at all complicated calculations) (3.13) follows. From now on $K > 0$ will denote a generic constant which might not be the same from line to line. The coercivity of $A^*A + C^*C$ means that we can write

$$\begin{aligned}\|Ah\|^2 + \|Ch\|^2 &= \frac{1}{2}(\|Ah\|^2 + \|Ch\|^2) + \frac{1}{2}(\|Ah\|^2 + \|Ch\|^2)\\ &\geq \frac{1}{2}(\|Ah\|^2 + \|Ch\|^2) + \frac{K}{2}\|h\|^2\\ &\geq K\|h\|_{\mathcal{H}^1}.\end{aligned}$$

Combining this with (3.13), we obtain

$$((h, \mathcal{T}h)) \geq k(\|Ah\|^2 + \|Ch\|^2) \geq K\|h\|_{\mathcal{H}^1} \geq K((h,h)).$$

This concludes the sketch of the proof. Another important observation is that, in practice, the coercivity of $A^*A + C^*C$ boils down to a Poincaré inequality. This will be clear when we apply this machinery to the Langevin equation, see proof of Theorem 3.2. □

We now use Theorem 3.1 to prove exponentially fast convergence to equilibrium for the Langevin dynamics. We shall apply such a theorem to the operator $\mathcal{L}$ defined in (3.5) on the space $\mathcal{H} = L^2_\rho$, where ρ is the equilibrium distribution (3.5). (The space $\mathcal{S}$ can be taken to be the space of Schwartz functions.) The operators A and B are then

$$A = \partial_p \qquad \text{and} \qquad B = p\partial_q - \partial_q V \partial_p,$$

so that

$$C := [A, B] = AB - BA = \partial_q.$$

The kernel $\mathcal{K}$ of the operator $\mathcal{L}$ is made of constants and in this case the norm $\mathcal{H}^1$ will be the Sobolev norm of the weighted $H^1(\rho)$,

$$\|f\|^2_{H^1_\rho} := \|f\|^2_\rho + \|\partial_q f\|^2_\rho + \|\partial_p f\|^2_\rho.$$

Let us first calculate the commutators needed to check the assumptions of Theorem 3.1.

$$[A, C] = [A^*, C] = 0, \qquad [A, A^*] = \mathrm{Id}, \tag{3.15}$$

and

$$[B, C] = -\partial_q^2 V(q)\partial_p. \tag{3.16}$$

THEOREM 3.2. *Let $V(q)$ be a smooth potential such that*

$$|\partial_q^2 V| \leq \alpha\big(1 + |\partial_q V|\big), \qquad \textit{for some constant } \alpha > 0. \tag{3.17}$$

Also, assume that $V(q)$ is such that the measure $e^{-V(q)}$ satisfies a Poincaré inequality[10]*. Then, there exist constants $C, \lambda > 0$ such that for all $h_0 \in H^1(\rho)$,*

$$\left\| e^{-t\mathcal{L}} h_0 - \int h_0 \, d\rho \right\|_{H^1(\rho)} \leq C e^{-\lambda t} \|h_0\|_{H^1(\rho)}, \tag{3.18}$$

where we recall that here $\mathcal{L}$ is the operator (3.5) .

Proof: We will use Theorem 3.1. Conditions (1) and (2) are satisfied, due to (3.15). In [38, page 56 and Lemma A.19] it is shown that condition (3) holds under the assumption (3.17) on the potential V. Now we turn to condition (3.14). Let us first write the operator $\widehat{\mathcal{L}} = A^*A + C^*C$ (notice that $\widehat{\mathcal{L}}$ is elliptic),

$$\widehat{\mathcal{L}} = p\partial_p - \partial_p^2 + \partial_q V \partial_q - \partial_q^2.$$

[10]Theorem A.1 in [38] gives some sufficient conditions in order for e^{-V} to satisfy such an inequality.

The operator $\widehat{\mathcal{L}}$ is coercive if

$$\int \left(\left| \partial_q h \right|^2 + \left| \partial_p h \right|^2 \right) d\rho \geq \kappa \|h\|_\rho^2.$$

The above is a Poincaré inequality for the measure ρ (as we have already observed, the kernel of $\mathcal{T}$ is the set of constant functions, so it suffices to write the Poincaré inequality for mean zero functions, as we have done in the above). Therefore, in order for $\widehat{\mathcal{L}}$ to be coercive, it is sufficient for the measure $\rho = e^{-V(q)} e^{-p^2/2}$ to satisfy a Poincaré inequality. This probability measure is the product of a Gaussian measure (in p) which satisfies a Poincaré inequality, and of the probability measure $e^{-V(q)}$. In order to conclude the proof it is sufficient, therefore, to use the assumption that $e^{-V(q)}$ satisfies a Poincaré inequality. □

More details about the above proof can also be found in [25].

We mention that while the hypocoercivity theory has rapidly become one of the most popular techniques to study return to equilibrium for hypoelliptic-irreversible processes, other avenues have recently been opened [24], based on spectral theory and semiclassical analysis (in this context, we would also point out the paper [13]). While the first approach mostly provides qualitative results, the latter allows a more quantitative study. In other words, through the hypocoercivity techniques we only know that some $\lambda > 0$ exists, such that (3.18) holds; the spectral approach [24] gives instead the exact rate of exponential convergence, i.e. it determines λ. However, in comparison to the hypocoercivity framework, spectral techniques only apply to a more restricted class of hypoelliptic diffusions. Quantitative information for the Ornstein–Uhlenbeck process has been obtained also by using the hypocoercivity-type techniques [1].

4. Markov chain Monte Carlo

A standard and practical reference on MCMC is the book [30]. A rigorous approach to the theory of Markov chains and some theoretical results about MCMC are contained in [22]. The case for using MCMC is passionately argued in [11].

As we have already mentioned in Introduction, MCMC algorithms can be employed for two purposes: i) sampling from a given target distribution $\pi(x)$ which is known only up to its normalizing constant or ii) approximate statistical quantities of π, that is, calculate integrals of the form (1.1). In order to achieve either i) or ii), the MCMC approach consists in building a Markov chain x_n that has π as (unique) invariant measure. Then, for example under an assumption of positive recurrence, the ergodic theorem holds (e.g. for all $f \in L^1_\pi$), and the average on the left-hand side of (1.3) is, for n large enough, a good approximation of the integral on the right-hand side. We will not discuss here the very important practical issue of how big n should be and other related issues.

In algorithmical practice, it is a standard procedure to start by building a chain which admits the target measure π as unique invariant measure. This obviously does not ensure that the chain will converge to π (in whichever sense, see Example 4.1

below) and therefore a significant amount of literature has been devoted to the study of convergence criteria applicable to MCMC chains. Reviewing these criteria is beyond the scope of the present paper and we refer the reader to [14, 22, 34] and references therein. However, for Markov chains as well as for continuous time Markov processes, it is still the case that the great majority of the convergence results concern reversible processes. This is mostly due to the popularity of the Metropolis–Hastings algorithm, which we introduce in Section 4.1. Before presenting the general algorithm, we start with a simple example (see [2]).

EXAMPLE 4.1. Suppose we want to sample from a measure π defined on a finite state space S. In order to do so, we shall construct a Markov chain x_n that converges to π, in the sense that if $p(x, y)$ are the transition probabilities of the Markov chain x_n, then we want

$$\lim_{n\to\infty} p^n(x, y) = \pi(y). \tag{4.1}$$

With the intent of constructing x_n (or, equivalently, $p(x, y)$) we can proceed as follows. Let $q(x, y)$ be an arbitrary transition probability on S. Suppose the transition matrix $Q = (q(x, y))_{(x,y)\in S}$ is symmetric and irreducible. Given such a Q (usually called *proposal* transition matrix) and a probability distribution $\pi(x)$ on S such that $\pi(x) > 0$ for all $x \in S$, let us now construct a new transition matrix $P = (p(x, y))$ as follows:

$$p(x, y) = \begin{cases} q(x, y) & \text{if } \pi(y) \geq \pi(x) \text{ and } x \neq y, \\ q(x, y)\dfrac{\pi(y)}{\pi(x)} & \text{if } \pi(y) < \pi(x) \text{ and } x \neq y, \\ 1 - \sum_{x\neq y} p(x, y) & \text{otherwise.} \end{cases} \tag{4.2}$$

It is easy to check that the matrix $P = (p(x, y))$ constructed in this way is an irreducible transition matrix[11]. Being the state space finite, this also implies that P is recurrent and that there exists a unique stationary distribution. We can easily show that such an invariant distribution is exactly π as P is reversible with respect to π in the sense (2.4). (2.4) is obviously true when $x = y$. So suppose that $x \neq y$ and $\pi(y) \geq \pi(x)$. Then, by construction, $\pi(x)p(x, y) = \pi(x)q(x, y)$ but also $\pi(y)p(y, x) = q(y, x)[\pi(x)/\pi(y)]\pi(y)$ so that using the symmetry of q we get $\pi(y)p(y, x) = q(x, y)\pi(x)$ and we are done. If $\pi(y) < \pi(x)$ we can repeat the above with roles of x and y reversed. We are left with proving that the chain x_n with transition matrix P converges to π. We show in Appendix that convergence (in the sense (4.1)) happens for any proposal Q unless π is the uniform distribution on S (see Lemma A.1). This is just to highlight, on a simple example where calculations can be easily made by hand, that the convergence of the scheme can depend on the target measure and not only on Q. More complex (and meaningful) examples on this point can be found in [33]. □

[11] Meaning that the whole state space is irreducible under P; this implies that the state space is also closed under P (here we mean *closed* in the sense of Markov chains; that is, we say that a set A of the state space is closed if whenever $x \in A$ and y is accessible from x then also y belongs to A. For a precise definition see [10, page 246])

The procedure (4.2) can be expressed as follows: given $X_n = x_n$,
(1) generate $y_{n+1} \sim q(x_n, \cdot)$;
(2) calculate

$$\alpha(x_n, y_{n+1}) := \min\left\{1, \frac{\pi(y_{n+1})}{\pi(x_n)}\right\} \tag{4.3}$$

(3) set $X_{n+1} = \begin{cases} y_{n+1} & \text{with probability } \alpha(x_n, y_{n+1}) \\ x_n & \text{otherwise.} \end{cases}$

In practice, if $\mathcal{U}[0, 1]$ is the uniform distribution on $[0, 1]$, the algorithm that realizes the above is as follows.

ALGORITHM 4.1. Given $X_n = x_n$,
(1) generate $y_{n+1} \sim q(x_n, \cdot)$;
(2) generate $u \sim \mathcal{U}[0, 1]$;
(3) if $u < \pi(y_{n+1})/\pi(x_n)$ then $X_{n+1} = y_{n+1}$; otherwise $X_{n+1} = x_n$.

In words, given the state of the chain at time n, we pick the *proposal* $y_{n+1} \sim q(x_n, \cdot)$. Then the proposed move is accepted with probability α (4.3). If it is rejected, the chain remains where it was. For this reason $\alpha(x, y)$ is called the *acceptance probability*.

Algorithm 4.1 is a first example of a *Metropolis–Hastings algorithm*. Intuitively, it is clear why we always accept moves towards points with higher probability. We anyway make the obvious remark that if we want to construct an ergodic chain (in the sense (1.3)) with invariant probability π then the time spent by the chain in each point y of S needs to equal, in the long run, the probability assigned by π to y, i.e. $\pi(y)$. So we have to accept more frequently points with higher probability.

4.1. Metropolis–Hastings algorithm

Throughout this section our state space is $\mathbb{R}^N$. For simplicity we will assume that all the measures we use have a density with respect to the Lebesgue measure, so $\pi(x)$ will be the density of π and e.g. $q(x, y)$ will denote the density of the proposal $q(x, \cdot)$. A very nice presentation of the theory underlying the M–H algorithm in general state space can be found in [37].

A Metropolis–Hastings (M–H) algorithm is a method of constructing a time-homogeneous Markov chain or, equivalently, a transition kernel $p(x, y)$, that is reversible with respect to a given target distribution $\pi(x)$. To construct the π-invariant chain X_n we make use of a proposal kernel $q(x, y)$ which we know how to sample from and of an accept/reject mechanism with the acceptance probability

$$\alpha(x, y) = \min\left\{1, \frac{\pi(y)q(y, x)}{\pi(x)q(x, y)}\right\}. \tag{4.4}$$

For simplicity we require that $\pi(y)q(y, x) > 0$ and $\pi(x)q(x, y) > 0$. The M–H algorithm consists of two steps.

ALGORITHM 4.2 (Metropolis–Hastings algorithm). Given $X_n = x_n$,
(1) generate $y_{n+1} \sim q(x_n, \cdot)$;
(2) calculate $\alpha(x_n, y_{n+1})$ according to the prescription (4.4),
(3) set $X_{n+1} = \begin{cases} y_{n+1} & \text{with probability } \alpha(x_n, y_{n+1}), \\ x_n & \text{otherwise.} \end{cases}$

LEMMA 4.1. *If α is the acceptance probability* (4.4)*,(and assuming $\pi(y)q(y, x) > 0$ and $\pi(x)q(x, y) > 0$) the Metropolis–Hastings algorithm, Algorithm* 4.2*, produces a π-invariant time-homogeneous Markov chain*[12].

Proof: A proof of this fact can be found in [37]. □

REMARK 4.1. In order to implement Algorithm 4.2 we do not need to know the normalizing constant for π, as it gets canceled in the ratio (4.4). However, as observed in [30], we do need to know the normalizing constant for q: q is a transition probability so by definition for every fixed x the function $y \to q(x, y)$ is a probability density, i.e. it integrates to one. However, the normalizing constant of $q(x, \cdot)$ can, and in general will, depend on x. In other words, $q(x, y)$ will in general be of the form $q(x, y) = \mathcal{Z}_x^{-1}\tilde{q}(x, y)$, with $\int dy\, \tilde{q}(x, y) = \mathcal{Z}_x$ so that the ratio in the acceptance probability (4.4) can be more explicitly written as

$$\alpha(x, y) = \min\left\{1, \frac{\pi(y)\mathcal{Z}_x\tilde{q}(y, x)}{\pi(x)\mathcal{Z}_y\tilde{q}(x, y)}\right\}.$$

Clearly, if the proposal kernel is symmetric, $q(x, y) = q(y, x)$, then there is no need to know the normalizing constant for q, as the above expression for α reduces to (4.3). This is a big appeal of algorithms with symmetric proposals, such as Random Walk Metropolis, which we introduce below. □

REMARK 4.2. Let us repeat that M–H is a method to generate a π-reversible time-homogeneous Markov chain. As we have already noticed, the fact that the chain is π-reversible does not imply that π is the only invariant distribution for the chain or even less that the chain converges to π. The matter of convergence of the chain constructed via M–H is probably better studied case by case (i.e. depending on the proposal we decide to use and on the target measure that we are trying to sample from). Some results concerning convergence of the chain can be found in [22, Chapter 20] and references therein or in [32, 33]. □

4.1.1. Random Walk Metropolis (RWM)

A very popular M–H method is the so called *Random Walk Metropolis*, where the proposal y_{n+1} is of the form

$$y_{n+1} = x_n + \sigma\xi_{n+1}, \qquad \sigma > 0;$$

[12]Lemma 4.1 can be made a bit more general, see [37].

for the algorithm that is most commonly referred to as RWM, the noise ξ is Gaussian, i.e. $\xi \sim \mathcal{N}(0, \sigma^2)$ so that $q(x, y) \sim \mathcal{N}(x, \sigma^2)$[13]. Therefore the acceptance probability reduces to $\alpha = \min\{1, \pi(y)/\pi(x)\}$. The case in which the noise ξ is Gaussian has been extensively studied in the literature, for target measures defined on $\mathbb{R}^N$. We stress that the variables $\xi_1, \dots, \xi_n, \dots$ are i.i.d. random variables, independent of the current state of the chain x_n. Therefore the proposal move does not take into account any information about the current state of the chain or about the target measure. This is in contrast with the MALA algorithm, Section 4.1.2 below, where the proposal move incorporates information about the target. This makes RMW a more naive algorithm than MALA.

Moreover, RWM is not immune to the *curse of dimensionality*: the cost of the algorithm increases with the dimension N of the state space in which it is implemented. Simply put: sampling from a measure that is defined on $\mathbb{R}^N$ is more expensive than sampling from a measure defined on $\mathbb{R}^{N-1}$. Here by cost of the algorithm we mean the number of MCMC steps needed in order to explore the state space in stationarity. In order to ameliorate this problem, it is crucial to choose the proposal variance appropriately. In $\mathbb{R}^N$ it is customary to consider $\sigma^2 = cN^{-\gamma}$, where $c, \gamma > 0$ are two parameters to be appropriately tuned, the most interesting of the two being γ. If γ is too large then σ^2 is too small, so the proposed moves tend to stay close to the current value of the chain and the state space is explored very slowly. If instead γ is too small, more precisely smaller than a critical value γ_c, the average acceptance rate decreases very rapidly to zero as N tends to infinity. This means that the algorithm will reject more and more as N increases. It was shown in the seminal paper [31] that the choice $\gamma = 1$ is the one that optimally compromises between the need of moving far enough away from the current position and the need of accepting frequently enough.

4.1.2. Metropolis Adjusted Langevin Algorithm (MALA)

Consider the first order Langevin equation

$$dX_t = -\nabla V(X_t)dt + \sqrt{2\beta^{-1}}dW_t, \tag{4.5}$$

where $X_t \in \mathbb{R}^d$, $V(x)$ is a confining potential and W_t is a d-dimensional standard Brownian motion. $\beta > 0$ is a parameter (typically β^{-1} is the temperature) which from now on we fix to be equal to one, $\beta = 1$. This dynamics is ergodic; the (unique) invariant measure has a density $\rho(x)$ explicitly given by

$$\rho(x) = \frac{e^{-V(x)}}{\mathcal{Z}}, \tag{4.6}$$

where $\mathcal{Z}$ is the normalizing constant. Moreover, under the stated assumptions on the potential, X_t converges exponentially fast to the equilibrium ρ. If we want to sample from measures of the form (4.6), it is a natural idea to construct a Markov chain that

[13] In principle ξ could be chosen to be any noise with density $g(x)$ symmetric with respect to the origin, $g(x) = g(|x|)$.

converges to ρ by discretizing the continuous-time dynamics (4.5). Unfortunately one can readily see that naive discretizations can completely destroy the good properties of the dynamics (4.5). Indeed, as pointed out in [32], suppose we discretize (4.5) by using the Euler scheme with step h; that is, suppose we create a chain according to

$$X_{n+1} \sim \mathcal{N}(X_n - h\nabla V(X_n), 2hI_d), \qquad I_d = d\text{-dimensional identity matrix.}$$

Suppose your target distribution is Gaussian with zero mean and unit variance (corresponding to $V(x) = |x|^2/2$) and choose $h = 1$. Then $X_n \sim \mathcal{N}(0, 2)$ for every n. So clearly the chain converges immediately, but to the wrong invariant measure. This is the most drastic example of what can go wrong. In general when discretizing, the invariance of the target measure is only approximately preserved. To correct for the bias introduced by the discretization one can make use of the M–H accept-reject mechanism, which guarantees that the resulting chain will be reversible with respect to the target measure; in this way we can guarantee that, if the chain converges, it can only converge to the correct measure. To summarize, the MALA algorithm is as follows: suppose at step n we are in X_n. From X_n we propose to move to Y_{n+1},

$$Y_{n+1} := X_n - h\nabla V(X_n) + \sqrt{2h}\,\xi_{n+1}, \qquad \xi_{n+1} \sim \mathcal{N}(0, 1).$$

Using (4.4)[14] we then accept or reject the move to Y_{n+1}. If Y_{n+1} is accepted we set $X_{n+1} = Y_{n+1}$, otherwise $X_{n+1} = X_n$.

We stress again that in the context of the MALA algorithm the accept-reject mechanism can be seen as a way of properly discretizing the first order Langevin dynamics. The resulting chain is reversible with respect to the target distribution. Finally, also the MALA algorithm sufferes from the curse of dimensionality.

4.2. Sampling measures defined on infinite-dimensional spaces

As in Section 3.1, let $\mathcal{H}$ be a separable Hilbert space. Throughout the remainder of the paper we assume that C is a bounded, positive and symmetric operator on $\mathcal{H}$ with associated eigenvalues $\{\lambda_j^2\}_{j\in\mathbb{N}}$ and orthonormal eigenvectors $\{\varphi_j\}_{j\in\mathbb{N}}$, that is

$$C\varphi_j = \lambda_j^2 \varphi_j.$$

We will also assume that C is trace class[15] and that for some $\kappa > 1/2$ we have[16]

$$\lambda_j \asymp j^{-\kappa}.$$

The next two algorithms that we present are aimed at sampling from measures on

[14] In this case $q(x, \cdot) \sim \mathcal{N}(x - h\nabla V(x), 2hI_d)$

[15] We recall that a bounded, positive and symmetric operator on a Hilbert space is *trace class.* if $\sum_{k=1}^{\infty} \langle C\varphi_k, \varphi_k\rangle < \infty$.

[16] The notation $\asymp$ means: there esist two positive constants $c_1, c_2 > 0$ such that $c_1 j^{-\kappa} \le \lambda_j \le c_2 j^{-\kappa}$.

the space $\mathcal{H}$, in particular from measures of the form[17]

$$d\pi(q) \propto e^{-\Phi(q)} d\pi_0(q), \qquad \pi_0 \sim \mathcal{N}(0, C),\ q \in \mathcal{H}. \tag{4.7}$$

That is, the measure π that we want to sample from is a change of measure from the underlying Gaussian π_0. By the Bayesian point of view, (4.7) can be interpreted to be a posterior measure, given prior π_0 and likelyhood Φ. More details on the functional setting and in general on the material of this section can be found e.g. in [4, 36]. For background reading on Gaussian measures on infinite-dimensional spaces see [7]. It is natural to wonder why we would want to sample from a measure that is defined on an infinite dimensional space. We explain this fact with an example.

EXAMPLE 4.2 (Conditioned diffusions). Consider the Langevin equation (4.5) in a double well potential. That is, $V(x)$ is confining and has two minima, say x^- and x^+. Suppose we are interested only in the paths X_t that satisfy (4.5), together with $X(0) = x^-$ and $X(1) = x^+$. It is well known that, at least for low temperatures, if we start the path in x^-, the jump to the other potential well is a rare event, so just simulating (4.5) subject to the initial condition $X(0) = x^-$ does not sound like a good idea. The approach that we want to present here is the following: one can prove that the measure on path space (i.e. on $L^2[0, 1]$) induced by the diffusion (4.5), with $X(0) = x^-$ and $X(1) = x^+$, is indeed of the form (4.7) [36, Section 3.8 and references therein]. Sampling from such a measure means extracting information from the desired paths. □

If we want to sample from π by using the MCMC approach, then we need to construct a chain x_n, defined on $\mathcal{H}$, $\{x_n\} \subset \mathcal{H}$, such that π is the only invariant measure of x_n and x_n converges to π as well. In other words, we need to construct an algorithm that is well defined on the infinite-dimensional space $\mathcal{H}$. Assume we have been able to find such an algorithm. It is clear that in computational practice we cannot use the infinite-dimensional algorithm directly. So instead of using the chain x_n, we will use the chain x_n^N, which is obtained by projecting each element of x_n on the space $\mathcal{H}^N := \text{span}\{\varphi_1, \ldots, \varphi_N\}$. Therefore $\{x_n^N\} \subset \mathbb{R}^N$. One can prove that the chain obtained in this way, as projection of an infinite-dimensional algorithm, *does not* suffer from the curse of dimensionality. For example, the RWM algorithm suffers from the curse of dimensionality (and it is in fact not well defined in infinite dimension). However, it can be modified in such a way that the resulting algorithm is well defined in $\mathcal{H}$; such a modification is the *pre-conditioned Crank–Nicolson* (pCN) algorithm (see [36]). It is also possible to prove that while the spectral gap of the RWM chain tends to 0 as $N \to \infty$, the spectral gap of pCN does not, see [16].

4.3. Hybrid Monte Carlo

In view of the previous section, we will describe a version of the HMC algorithm which is adapted to sampling from measures of the form (4.7) and is well defined

[17] We use the symbol "$\propto$" to mean "proportional to", i.e. the LHS is equal to the RHS for less than a multiplicative constant.

in infinite dimension [5]. A very nice introduction to HMC can be found in [26]. The basic principle behind HMC is relatively simple: in order to sample from the measure π defined on $\mathcal{H}$ we will create a Markov chain $(q_k, v_k) \in \mathcal{H} \times \mathcal{H}$ that samples from the measure Π, on $\mathcal{H} \times \mathcal{H}$, defined as follows

$$d\Pi(q, v) \propto d\pi(q) d\pi_0(v), \qquad \pi_0 \sim \mathcal{N}(0, C).$$

Notice that the measure Π is the product of our target measure with a Gaussian measure (in the v component). So effectively, in the long run, the only component of the chain that we will be interested in is the first one, which is the one that will be converging to π. The measure Π can be more explicitly written as

$$d\Pi(q, v) \propto e^{-\Phi(q)} d\pi_0(q) d\pi_0(v), \qquad \pi_0 \sim \mathcal{N}(0, C).$$

If we introduce the Hamiltonian

$$H(q, v) = \frac{1}{2}\langle v, C^{-1} v\rangle + \frac{1}{2}\langle q, C^{-1} q\rangle + \Phi(q), \tag{4.8}$$

then one has

$$d\Pi(q, v) \propto e^{-H(q,v)}.$$

The Hamiltonian flow associated with the Hamiltonian function (4.8) can be written as

$$\mathcal{F}^t : \begin{cases} \dot{q} = v, \\ \dot{v} = -q - C\nabla\Phi(q). \end{cases}$$

The Hamiltonian flow $\mathcal{F}^t$ preserves functions of the Hamiltonian and, at least in finite dimensions, the volume element $dqdv$. It therefore preserves the measure Π. For this reason it is a natural idea to think of using a time-step discretization of the Hamiltonian flow as a proposal move to create the chain (q_k, v_k). However, like in the MALA case, we still need to discretize the flow $\mathcal{F}^t$. We discretize the Hamiltonian flow by "splitting" it into its linear and nonlinear part, i.e. by using the Verlet integrator. The Verlet integrator is defined as follows: let R^t and Θ^t be the flows associated with the following ODEs:

$$R^t : \begin{cases} \dot{q} = v, \\ \dot{v} = -q, \end{cases} \qquad \Theta^t : \begin{cases} \dot{q} = 0, \\ \dot{v} = -C\nabla\Phi(q), \end{cases} \tag{4.9}$$

and let

$$\chi_\tau := \Theta^{\tau/2} \circ R^\tau \circ \Theta^{\tau/2}. \tag{4.10}$$

A time step discretization (of size h) of the flow $\mathcal{F}^t$ is then given by

$$\chi_\tau^h = \chi_\tau \circ \cdots \circ \chi_\tau \qquad \left[\frac{h}{\tau}\right] \text{ times.} \tag{4.11}$$

We now have all the notation in place to introduce the HMC algorithm. Suppose at time k the first component of the chain is in q_k. Then

(1) pick $v_k \sim \mathcal{N}(0, C)$;
(2) compute
$$(q^*_{k+1}, v^*_{k+1}) = \chi^t_\tau(q_k, v_k),$$
and propose q^*_{k+1} as next move;
(3) calculate the acceptance probability α_k, according to
$$\alpha_k = 1 \wedge e^{-(H(\chi^t_\tau(q_k,v_k))-H(q_k,v_k))}; \tag{4.12}$$
(4) set $q_{k+1} = q^*_{k+1}$ with probability α. Otherwise $q_{k+1} = q_k$.

REMARK 4.3. Some comments are in order:
- Notice that at each step the component v_k is sampled independently from q_k. If the velocity variable was not resampled, the algorithm would be stuck in areas with approximately the same probability.
- If $\mathcal{H}$ is infinite-dimensional, the Hamiltonian function (4.8) is almost surely infinite. However in order for the algorithm to be well defined, all we need is for the difference $(H(\chi^t_\tau(q_k, v_k)) - H(q_k, v_k)$ appearing in (4.12) to be finite. This is indeed the case (and the choice of integrator was in fact driven by the need to satisfy this requirement [5]).
- The generated chain is reversible with respect to the target density function.
- The above algorithm is well posed in infinite dimension i.e. for $(q, v) \in \mathcal{H} \times \mathcal{H}$.

□

5. An irreversible MCMC algorithm: the SOL–HMC

We now want to construct an MCMC algorithm which results from appropriately discretizing the second-order Langevin equation. The algorithm that we will present has been introduced in [23] and can be understood as a generalization of [17]. In order to carry out such a discretization we will make use of a modification of the HMC algorithm which we have just presented. Again, we want to sample from a measure π of the form (4.7). First of all, let us rewrite the SOL equation in a way adapted to our context,

$$\begin{aligned} dq &= v\,dt, \\ dv &= [-q - C\,\nabla\Phi(q)]\,dt - v\,dt + \sqrt{2C}dW_t. \end{aligned} \tag{5.1}$$

Eq. (5.1) is well-posed in an infinite-dimensional context [23], it is ergodic and it admits our target π as unique invariant measure. Again, like for the MALA algorithm, if we discretize the equation naively we risk to destroy all the good properties of the dynamics. In particular, if we were to discretize and then use the Metropolis–Hastings accept-reject mechanism, we would end up with a chain that does sample from the correct measure, but such a chain would be reversible. What we want to do here instead is to discretize the irreversible Markov dynamics (5.1) in such a way to produce an irreversible chain. It is clear that in order to do so we will have to leave the comfort of the Metropolis–Hastings setting.

In order to present the SOL–HMC algorithm, we first need to introduce the numerical integrator that we will use. To integrate (5.1) numerically, we construct an integrator which takes advantage of the structure of the equation highlighted in Section 3.1. Namely, we look again at the splitting "Hamiltonian + OU process". Recall the definition of the flows R^t, Θ^t, Eq. (4.9), and define $\mathcal{O}^t$ to be the map that gives the solution at time t of the system

$$\mathcal{O}^t : \begin{cases} \dot{q} = 0, \\ \dot{v} = -v\,dt + \sqrt{2C}\,dW_t. \end{cases}$$

Let χ_τ and χ_τ^h be defined as in (4.10) and (4.11), respectively. For given positive parameters h and δ (to be appropriately tuned), the proposal move and acceptance probability of the SOL–HMC algorithm are then given by

$$(q^*, v^*) = (\chi_\tau^h \circ \mathcal{O}^\delta)(q, v) \tag{5.2}$$

and

$$\alpha = 1 \wedge e^{-[H(q^*,v^*) - H(\mathcal{O}^\delta(q,v))]}, \tag{5.3}$$

respectively. With this notation in place, the SOL–HMC algorithm proceeds as follows:

(1) given (q_k, v_k), let

$$(q_k', v_k') = \mathcal{O}^\delta(q_k, v_k)$$

and propose

$$(q_{k+1}^*, v_{k+1}^*) = (\chi_\tau^u)(q_k', v_k');$$

(2) calculate the acceptance probability α_k, according to (5.3);

(3) set

$$(q_{k+1}, v_{k+1}) = \begin{cases} (q_{k+1}^*, v_{k+1}^*) & \text{with probability } \alpha, \\ \mathcal{O}^\delta(q_k, -v_k) & \text{with probability } 1-\alpha. \end{cases}$$

In words: if at step k we are in (q_k, v_k), we first calculate (q_k', v_k') (notice that $q_k' = q_k$). Then we propose a move to (q_{k+1}^*, v_{k+1}^*). If the move is accepted then $(q_{k+1}, v_{k+1}) = (q_{k+1}^*, v_{k+1}^*)$. Otherwise we change the sign of the velocity, i.e. we consider $(q_k, -v_k)$ and evolve for time δ according to $\mathcal{O}^\delta$, so that $(q_{k+1}, v_{k+1}) = \mathcal{O}^\delta(q_k, -v_k)$. Notice that in case of rejection of the proposal (q_{k+1}^*, v_{k+1}^*) we do not stay where we started from, i.e. in (q_k, v_k), but we move to $\mathcal{O}^\delta(q_k, -v_k)$.

REMARK 5.1. Again, let us make a few observations about the algorithm.

- The relevant energy difference here is $H(q', v') - H(q^*, v^*)$ (rather than $H(q, v) - H(q^*, v^*)$); indeed the first step in the definition of the proposal (q^*, v^*), namely the OU process $\mathcal{O}^\delta(q, v)$, is based on an exact integration and preserves the desired invariant measure. Therefore the accept-reject mechanism (which is here only to account for the numerical error made by the integrator χ_τ^h) doesn't need to include also the energy difference $H(q, v) - H(q', v')$.

- The flip of the sign of the velocity in case of rejection of (q^*, v^*) is there to guarantee that the overall proposal moves are symmetric. This is done in order to ensure that the acceptance probability can be defined only in terms of the ratio $\Pi(q^*, v^*)/\Pi(q', v')$, i.e. in terms of the energy difference $H(q', v') - H(q^*, v^*)$. An interesting discussion on the matter can be found in [20, Chapter 2].
- The algorithm is well posed in finite as well as in infinite dimension.
- Most importantly, the algorithm produces an irreversible chain. How did we lose reversibility? The important observation that this algorithm is based on is the following [26]: detailed balance is not preserved under composition. That is, if we consider a Markov transition kernel, say r, resulting from the composition of transition kernels, each of them satisfying detailed balance, r does not, in general, satisfy detailed balance as well. In the same way, *each step of the SOL–HMC algorithm satisfies detailed balance; however their composition does not.* □

Beyond [17, 23] the only other MCMC irreversible algorithms that we know of are [6, 8] (see also references therein). The advantages of irreversibility by the point of view of asymptotic variance have also been investigated in [9, 28, 29].

Appendix

LEMMA A.1. *With the setting and assumptions of Example* 4.1*, if* π *is not the uniform distribution then the chain* x_n *with transition probabilities* $p(x, y)$ *defined in* (4.2) *converges in the sense* (4.1) *to the target distribution* π *for any choice of the (irreversible and symmetric) proposal matrix* Q*. If* π *is the uniform distribution then convergence may happen or not, depending on* Q*.*

Proof: (See [2] for more details on this proof) The proof is quite simple so we only sketch it. A time-homogeneous Markov chain (MC) on a finite state space S is said to be *regular* if there exists a positive integer $k > 0$ such that $p^k(x, y) > 0$ for all $x, y \in S$. Clearly a regular MC is irreducible. It is easy to prove the following: if for any x and y in S there exists an integer $n > 0$ such that $p^n(x, y) > 0$ and there exists $a \in S$ such that $p(a, a) > 0$ then the chain is regular. (Notice that k is independent of x and y whereas $n = n(x, y)$, i.e. it depends on the choice of x and y.) A standard result in the basic theory of MCs states that if x_n is a regular chain on a finite state space then the chain has exactly one stationary distribution π, and

$$\lim_{n\to\infty} p^n(x, y) = \pi(y), \qquad \text{for all } x \text{ and } y \in S. \tag{A.1}$$

With these premises, and assuming that π is not the uniform distribution on S, we want to show that the chain with transition matrix P is regular. Recall that Q is irreducible, hence P is irreducible as well, therefore it is true that for all x, y there exists $n = n(x, y) > 0$ such that $p^{n(x,y)}(x, y) > 0$. Therefore we only need to find a state $a \in S$ such that $p(a, a) > 0$. Let M be the set $M = \{x \in S : \pi(x) = \max_{y\in S} \pi(y)\}$. Because Q is irreducible there exist $a \in M$ and $b \in M^c$ such that $q(a, b) > 0$ and clearly by construction $\pi(a) > \pi(b)$. Notice also

that from the definition of P, $p(x, y) \leq q(x, y)$ for all $x \neq y$. Then

$$\begin{aligned} p(a,a) &= 1 - \sum_{x \neq a} p(a,x) = 1 - \sum_{x \neq a,b} p(a,x) - p(a,b) \\ &\geq 1 - \sum_{x \neq a,b} q(a,x) - q(a,b)\pi(b)/\pi(a) \\ &= 1 - \sum_{x \neq a} q(a,x) + q(a,b)\,[1 - \pi(b)/\pi(a)] \\ &= q(a,a) + q(a,b)\,[1 - \pi(b)/\pi(a)] \geq q(a,b)\,[1 - \pi(b)/\pi(a)] > 0. \end{aligned}$$

On the other hand if $\pi(x)$ is the uniform distribution on S then $p(x, y) = q(x, y)$ so, because $q(x, y)$ is symmetric, detailed balance is still satisfied so π is still invariant[18]. However, if $q(x, y)$ is periodic then convergence in the sense (A.1) does not take place. (However, ergodic averages will still converge). □

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[18]Notice that, in the setting of this lemma, if $q(x, y)$ is not symmetric then the uniform distribution might not be an invariant measure.

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IRREDUCIBLE DECOMPOSITIONS AND STATIONARY STATES OF QUANTUM CHANNELS

RAFFAELLA CARBONE

Dipartimento di Matematica dell'Universitá di Pavia,
via Ferrata, 1, 27100 Pavia, Italy
(e-mail: raffaella.carbone@unipv.it)

and

YAN PAUTRAT

Laboratoire de Mathématiques d'Orsay, Univ. Paris-Sud,
CNRS, Université Paris-Saclay, 91405 Orsay, France
(e-mail: yan.pautrat@math.u-psud.fr)

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For a quantum channel (completely positive, trace-preserving map), we prove a generalization to the infinite-dimensional case of a result by Baumgartner and Narnhofer [3]: this result is, in a probabilistic language, a decomposition of a general quantum channel into its irreducible recurrent components. More precisely, we prove that the positive recurrent subspace (i.e. the space supporting the invariant states) can be decomposed as the direct sum of supports of extremal invariant states; this decomposition is not unique, in general, but we can determine all the possible decompositions. This allows us to describe the full structure of invariant states.

Keywords: quantum channel, (extremal) invariant state, enclosure.

1. Introduction

The time evolution of states of a closed quantum system is usually described as the conjugation by a group of unitary operators on the Hilbert space representing the state space of the system. When the system is open, that is, interacts with its surroundings, the situation is more complicated and rigorous treatment usually requires approximations. The most standard approach was put on solid mathematical ground by Davies in the seventies (in [12], see also [13]), and leads to describe the system's evolution by a semigroup $(\Phi_t)_{t\in\mathbb{R}_+}$ of linear maps on the set of states (i.e. positive, normalized functionals acting on the set of operators on the Hilbert space) with specific algebraic properties (see Section 2). Many features of these continuous parameter semigroups are already contained in the case of discrete semigroups $(\Phi^n)_{n\in\mathbb{N}}$. In addition, the interest in the discrete case was renewed by quantum computation theory (where the maps Φ model quantum gates, see [21]) and by quantum repeated interaction systems, see [7]. We therefore restrict ourselves

to the discrete case, and focus on the study of $\Phi = \Phi^1$, a linear map which is completely positive and trace-preserving. Such a map is called a quantum channel.

The study of ergodic properties of an open quantum system is related to the study of invariants of Φ, and of the associated spectrum. Analogies with operators associated with Markov chains (see Example 2.1) inspired the development of a notion of irreducible quantum channel by various authors in the seventies and eighties (see [1,15,16,19]), with different (and sometimes conflicting) definitions and implications. Associated with this notion is the possibility to decompose a reducible quantum channel into a sum of irreducible ones. A vision of this decomposition as related to an intuitive notion of trajectories (as for Markov chains), however, was not developed explicitly before the work of Baumgartner and Narnhofer in [3], where it is done in the case of a finite-dimensional Hilbert space.

In [11], we studied open quantum random walks, a special class of evolutions belonging to the above case. This led us to restate and extend the results of [3] to the case of open quantum random walks, which required in particular an extension to the infinite-dimensional case. Our proofs, however, apply to a wider class of evolutions than just quantum random walks. We therefore describe our results in full generality here. Even if the statements of the results remain the same, we underline that the infinite-dimensional context forces to have various modifications with respect to the original proofs presented in [3]: the existence of a null recurrent subspace has to be considered here and this affects the ergodic properties of the process (see e.g. Theorem 2.1 in [18]); also compactness arguments and spectral properties need a little more attention; the characterization of minimal enclosures (Proposition 5.3), for instance, requires completely new elements here.

The structure of this article is as follows. In Section 2, we describe our framework and in particular the evolutions Φ of interest, the so-called quantum channels. In Section 3, we recall the different notions of irreducibility. In Section 4, we define enclosures, our key tool, which originated in [3]. In Section 5, we describe the relation between enclosures and supports of invariant states. In Section 6 we discuss the structure of invariant states of a simple reducible evolution. In Section 7, we state our general decomposition theorem, that describes irreducible decompositions of evolutions and the general structure of the set of invariant states. In Section 8, we apply these results to a number of examples.

2. States and quantum channels

In this section we give a short summary of the theory of quantum channels, i.e. completely positive, trace-preserving maps on an ideal of trace-class operators. We fix a separable Hilbert space $\mathcal{H}$, which is supposed to play the role of a state space for a quantum system. We denote by $\mathcal{I}_1(\mathcal{H})$ the set of trace-class operators on $\mathcal{H}$ (see [22]), and equip it with the topology induced by the trace norm. We recall that the topological dual $\mathcal{I}_1(\mathcal{H})^*$ can be identified with the algebra $\mathcal{B}(\mathcal{H})$ of bounded linear operators through the Schatten duality $(\rho, X) \mapsto \mathrm{Tr}(\rho X)$. Therefore, the topology of $\mathcal{I}_1(\mathcal{H})$ is the same as the weak topology induced by $\mathcal{B}(\mathcal{H})$. We

also recall that an operator X on $\mathcal{H}$ is called nonnegative (respectively positive or positive-definite), denoted $X \geq 0$ (resp. $X > 0$), if for $\varphi \in \mathcal{H} \setminus \{0\}$, one has $\langle \varphi, X\varphi \rangle \geq 0$ (resp. $\langle \varphi, X\varphi \rangle > 0$).

The states of a system will be represented by an operator belonging to a specific class:

DEFINITION 2.1. An operator ρ is called a *state* if it is self-adjoint (i.e. $\rho = \rho^*$), nonnegative, and is trace-class with trace one. We denote by $\mathcal{S}(\mathcal{H})$ the set of states on $\mathcal{H}$. A state is called *faithful* if it is positive definite.

REMARK 2.1. In the literature, a state is sometimes defined as a positive linear form on $\mathcal{B}(\mathcal{H})$ mapping Id to 1, i.e. as an element of the set

$$\mathcal{B}(\mathcal{H})^*_{+,1} = \{\eta \in B(\mathcal{H})^* \text{ s.t. } \eta(X) \geq 0 \text{ for } X \geq 0 \text{ and } \eta(\mathrm{Id}) = 1\}$$

equipped with the weak-* topology. The objects defined in Definition 2.1 are then called normal states. Obviously $\mathcal{S}(\mathcal{H})$ is homeomorphic to a subset of $\mathcal{B}(\mathcal{H})^*_{+,1}$.

Consider now a linear map Φ on $\mathcal{I}_1(\mathcal{H})$. We say that this map is positive if it maps nonnegative elements of $\mathcal{I}_1(\mathcal{H})$ to nonnegative elements of $\mathcal{I}_1(\mathcal{H})$. We say that it is n-positive, for $n \in \mathbb{N}$, if the map $\Phi \otimes \mathrm{Id}_{\mathcal{M}_n(\mathbb{C})}$ is positive as a map on $\mathcal{I}_1(\mathcal{H} \otimes \mathbb{C}^n)$; and completely positive if it is n-positive for any n in $\mathbb{N}$. We say that it is trace-preserving if, for any $\rho \in \mathcal{I}_1(\mathcal{H})$, one has $\mathrm{Tr}(\Phi(\rho)) = \mathrm{Tr}(\rho)$; in particular a positive trace-preserving map induces a map on $\mathcal{S}(\mathcal{H})$. Our main objects of interest will be maps that are completely positive and trace-preserving.

DEFINITION 2.2. A completely positive, trace-preserving map on a space $\mathcal{I}_1(\mathcal{H})$ is called *a quantum channel on* $\mathcal{H}$.

REMARK 2.2. A positive linear map on $\mathcal{I}_1(\mathcal{H})$ is automatically bounded (see Lemma 2.2 in [24]), so that it is weak-continuous.

The following theorem states a well-known fact about quantum channels (see [20, 21]).

THEOREM 2.1. *A linear map Φ on $\mathcal{I}_1(\mathcal{H})$ is completely positive if and only if there exists a family $(V_i)_{i\in I}$ of operators on $\mathcal{H}$ such that for any ρ in $\mathcal{I}_1(\mathcal{H})$,*

$$\Phi(\rho) = \sum_{i\in I} V_i \rho V_i^*. \tag{2.1}$$

If in addition Φ is trace-preserving, then the operators V_i satisfy the relation

$$\sum_{i\in I} V_i^* V_i = \mathrm{Id}_{\mathcal{H}}.$$

The decomposition (2.1) is called the Kraus form of Φ, and the family $(V_i)_{i\in I}$ an unravelling. Note that an unravelling of Φ is not unique (see [21] for more details).

We have mentioned that a source of inspiration is the analogy between quantum channels and Markov chains. In the following example we point out that Markov

chains are a special case of quantum channels. Note that, for any two vectors x and y in a Hilbert space $\mathcal{H}$ with scalar product $\langle \cdot, \cdot \rangle$ (which we assume is antilinear in the left variable), we denote by $|x\rangle\langle y|$ the map $z \mapsto \langle y, z\rangle\ x$.

EXAMPLE 2.1. Consider a Markov chain $(X_n)_n$ on a countable set E with transitions $p_{i,j} = \mathbb{P}(X_{n+1} = i \mid X_n = j)$. If we let $\mathcal{H}$ be $\ell^2(E)$, the set of (complex-valued) square-summable sequences indexed by E, denote by $(e_i)_{i\in E}$ the canonical orthonormal basis, and consider $V_{i,j} = \sqrt{p_{i,j}}\,|e_i\rangle\langle e_j|$ for i, j in E, then (2.1) defines a quantum channel which maps $\sum_{i\in E} \pi_n(i) \otimes |e_i\rangle\langle e_i|$ to $\sum_{i\in E} \pi_{n+1}(i) \otimes |e_i\rangle\langle e_i|$ where $\pi_{n+1} = p\pi_n$. In addition, any invariant state is of the form $\rho = \sum_{i\in E} \pi(i)|e_i\rangle\langle e_i|$ with $(\pi(i))_{i\in E}$ an invariant probability measure for the Markov chain.

REMARK 2.3. Trace-preservation of a map Φ is equivalent to $\Phi^*(\mathrm{Id}) = \mathrm{Id}$. The adjoint Φ^* is then a positive, unital (i.e. $\Phi^*(\mathrm{Id}) = \mathrm{Id}$) map on $\mathcal{B}(\mathcal{H})$, and by the Russo–Dye theorem [23] one has $\|\Phi^*\| = \|\Phi^*(\mathrm{Id})\|$ so that $\|\Phi\| = \|\Phi^*\| = 1$.

A quantum channel represents the (discrete) dynamics of an open quantum system in the Schrödinger picture (see [21] for more details). We denote by $\mathcal{F}(\Phi)$ the subset of $\mathcal{I}_1(\mathcal{H})$ of invariant elements of Φ and we will be specifically interested in the set $\mathcal{S}(\mathcal{H}) \cap \mathcal{F}(\Phi)$ of invariant states, i.e. elements of $\mathcal{S}(\mathcal{H})$ that are invariant by Φ.

For a state ρ we will consider its support, which is defined as the range of the projection $\mathrm{Id} - P_0(\rho)$, where

$$P_0(\rho) = \sup\{P \ \text{orthogonal projection s.t.}\ \rho(P) = 0\}.$$

The supremum taken above is considered with respect to the order induced by the relation $\geq$ for operators, and always exists in the present situation. Following [18], we denote

$$\mathcal{R} = \sup\{\mathrm{supp}\,\rho \mid \rho \ \text{an invariant state}\}$$

so that by definition, $\mathrm{supp}\,\rho \subset \mathcal{R}$ if ρ is an invariant state. This space is often called the fast recurrent space, in parallel with the classical case, where the fast recurrent configurations are the ones which support the invariant probability laws. The orthogonal complement of $\mathcal{R}$ is

$$\mathcal{D} = \{x \in \mathcal{H} \mid \langle x, \rho\, x\rangle = 0 \quad \text{for any invariant state } \rho\}.$$

REMARK 2.4. In [3], the states $\mathcal{R}$ and $\mathcal{D}$ are defined without reference to the set of invariant states as

$$\mathcal{D} = \{x \in \mathcal{H} \mid \langle x, \Phi^n(\rho)\, x\rangle \underset{n\to\infty}{\longrightarrow} 0 \ \text{for any state } \rho\}$$

and $\mathcal{R} = \mathcal{D}^\perp$. These different definitions of $\mathcal{R}$ and $\mathcal{D}$ are equivalent in finite dimension.

REMARK 2.5. The space $\mathcal{D}$ is the sum of the transient and slow recurrent subspaces, as defined in [26].

3. Irreducibility

Before we discuss decompositions of quantum channels, we need to discuss the relevant reducing components of the decomposition, i.e. irreducible quantum channels. As we will see in Proposition 3.2, irreducibility is strongly connected with the uniqueness of the invariant state.

As we already mentioned in Introduction, however, different definitions of irreducibility of quantum channels can be found in the literature. We will briefly recall them here. First we need to define some relevant concepts.

DEFINITION 3.1. Let Φ be a quantum channel on $\mathcal{S}(\mathcal{H})$. We say that an orthogonal projection P:

- *reduces* Φ if we have $\Phi\big(P\mathcal{I}_1(\mathcal{H})P\big) \subset P\mathcal{I}_1(\mathcal{H})P$,
- is *subharmonic* for Φ^* if $\Phi^*(P) \geq P$.

The complete proof of the following Proposition is given in [11].

PROPOSITION 3.1. *Let Φ be a quantum channel on $\mathcal{I}_1(\mathcal{H})$. The following properties are equivalent:*

- *Φ is Davies-irreducible: the only orthogonal projections reducing Φ are $P = 0$ and* Id*;*
- *the only orthogonal projections that are subharmonic for Φ^* are $P = 0$ and* Id*;*
- *ergodicity: for any state ρ, the operator $(\exp t\Phi)(\rho)$ is definite-positive for any $t > 0$.*

We say that Φ is irreducible if and only if any of the above properties holds.

REMARK 3.1. Regarding the above concepts and their interrelations:

- The equivalence between the first two properties follows from the simple observation that an orthogonal projection reduces Φ if and only if it is subharmonic for Φ^* (see [11, Proposition 3.3]).
- The definition of ergodicity given here originates in [24], and extends the definition given in [16] to infinite-dimensional $\mathcal{H}$.
- There exists yet another notion of irreducibility: one says that Φ is Evans-irreducible if the only orthogonal projections that are harmonic for Φ, i.e. such that $\Phi^*(P) = P$, are $P = 0$ and Id. Clearly Davies-irreducibility implies Evans-irreducibility, but the converse is not true in general.

In the same fashion as for Markov semigroups, there exists a Perron–Frobenius theorem related to the property of irreducibility. We state it in the next proposition, in a form essentially due to Schrader in [24].

PROPOSITION 3.2. *Let Φ be a quantum channel on $\mathcal{I}_1(\mathcal{H})$, and assume it has an eigenvalue λ of modulus* 1*, with eigenvector ρ. Then:*

- 1 *is also an eigenvalue, with eigenvector $|\rho| = (\rho^*\rho)^{1/2}$,*
- *if Φ is irreducible, then λ is a simple eigenvalue and $|\rho| > 0$.*

REMARK 3.2. Proposition 3.2 still holds if Φ is not completely positive and trace-invariant, but simply 2-positive. For this reason, the same statement holds when the map Φ on $\mathcal{I}_1(\mathcal{H})$ is replaced with the map Φ^* on $\mathcal{B}(\mathcal{H})$, and all subsequent results about quantum channels will hold for 2-positive and trace-invariant maps on $\mathcal{I}_1(\mathcal{H})$, as long as they do not involve the Kraus form or unravelling of Φ.

An immediate consequence of this proposition is that an irreducible quantum channel on $\mathcal{I}_1(\mathcal{H})$ has at most one invariant state. In Sections 6 and 7 we will study the relations between the invariant states of a reducible quantum channel and the invariant states of its irreducible components.

4. Enclosures and communicating classes

For Markov chains, it is well known that irreducibility is related with the notion of communication within the induced graph. In addition, communicating classes have an explicit description as orbits of points, and are the relevant objects to break down a reducible Markov chain into irreducible ones. In this section we introduce the notion of enclosure, that will parallel the notion of closed set for Markov chains, and allows us to study irreducible decompositions of quantum channels.

DEFINITION 4.1. Let Φ be a quantum channel. A closed subspace $\mathcal{V}$ is an *enclosure* for Φ if, for any state ρ, $\operatorname{supp}\rho \subset \mathcal{V}$ implies $\operatorname{supp}\Phi(\rho) \subset \mathcal{V}$.

We will call nontrivial any enclosure which is neither $\{0\}$ nor $\mathcal{H}$. Clearly, a subspace $\mathcal{V}$ is an enclosure if and only if it is the range of a reducing orthogonal projector. Therefore, a quantum channel Φ is irreducible if and only if it has no nontrivial enclosures. Enclosures are relevant to reducibility properties and consequently to many other features of the channel; indeed, the notion of enclosure has been used in literature with different names (see for instance [4, 5, 8]).

We now prove a simpler characterization of enclosures.

LEMMA 4.1. *A closed vector subspace $\mathcal{V}$ of $\mathcal{H}$ is an enclosure if and only if, for any x in $\mathcal{V}$ with $\|x\| = 1$, the state $\Phi(|x\rangle\langle x|)$ has support in $\mathcal{V}$.*

Proof: Let ρ be a state with support in $\mathcal{V}$. The spectral decomposition of ρ is of the form $\sum_{i\in I}\lambda_i|e_i\rangle\langle e_i|$ with $\lambda_i > 0$, $\sum_{i\in I}\lambda_i = 1$ and $e_i \in \mathcal{V}$. Therefore, $\operatorname{supp}\Phi(|e_i\rangle\langle e_i|) \subset \operatorname{supp}\Phi(\rho)$, which shows the direct implication; in addition, the support of $\Phi(\rho)$ is the supremum of the projectors on the ranges of $\Phi(|e_i\rangle\langle e_i|)$ and this shows the converse. □

This has the following useful corollary. Note that, for $(\mathcal{V}_i)_{i\in I}$ a family of closed subspaces of $\mathcal{H}$, we denote by e.g. $\mathcal{V}_1 + \mathcal{V}_2 + \ldots$ or $\sum_{i\in I}\mathcal{V}_i$ the closed vector space generated by $\bigcup_{i\in I}\mathcal{V}_i$.

COROLLARY 4.1. *Let $\mathcal{V}_1$ and $\mathcal{V}_2$ be two enclosures. The closed subspace $\mathcal{V}_1 + \mathcal{V}_2$ is also an enclosure.*

Proof: By a direct computation, $|x_1+x_2\rangle\langle x_1+x_2| \leq 2\,|x_1\rangle\langle x_1|+2\,|x_2\rangle\langle x_2|$ for x_1, x_2 in $\mathcal{V}_1, \mathcal{V}_2$ respectively. Applying Lemma 4.1 shows that $\mathcal{V}_1+\mathcal{V}_2$ is an enclosure. □

This allows us to obtain an explicit characterization of enclosures in terms of unravellings of Φ, and connect them to a notion of orbit under the action of possible transitions of Φ.

PROPOSITION 4.1. *Consider a quantum channel Φ with unravelling $(V_i)_{i\in I}$. A subspace $\mathcal{V}$ of $\mathcal{H}$ is an enclosure if and only if $V_i\,\mathcal{V} \subset \mathcal{V}$ for any i.*

Proof: The proposition follows from Lemma 4.1 and the fact that, by the trace norm continuity of Φ one has for any $x \in \mathcal{V}$,

$$\Phi(|x\rangle\langle x|) = \sum_{i\in I} |V_i x\rangle\langle V_i x|. \qquad \square \tag{4.1}$$

Our goal is to consider enclosures defined as the set of points accessible from a given initial $x \in \mathcal{H}$. Proposition 4.1 suggests a natural definition and proposition.

PROPOSITION 4.2. *Let Φ be a quantum channel on $\mathcal{I}_1(\mathcal{H})$. Let $(V_i)_{i\in I}$ be an unravelling of Φ. For x in $\mathcal{H}\setminus\{0\}$, we call enclosure generated by x the closed vector space*

$$\mathrm{Enc}(x) = \mathbb{C}x + \overline{\mathrm{span}\{V_{i_1}\cdots V_{i_n}\,x,\ |\, n\in\mathbb{N}^*,\ i_1,..i_n \in I\}}. \tag{4.2}$$

With this definition, the space $\mathrm{Enc}(x)$ is the smallest enclosure containing x.

Proof: It follows from (4.1) that Definition (4.2) also satisfies

$$\mathrm{Enc}(x) = \overline{\mathrm{span}\{\mathrm{supp}\,\Phi^n(|x\rangle\langle x|),\ n\geq 0\}}. \tag{4.3}$$

This shows that Definition (4.2) is independent of the choice of unravelling. The fact that $\mathrm{Enc}(x)$ is an enclosure then follows from Proposition 4.1. □

REMARK 4.1. This implies in particular that a quantum channel Φ is irreducible if and only if $\mathcal{H} = \mathrm{Enc}(x)$ for any x in $\mathcal{H}\setminus\{0\}$.

We can define a notion of accessibility among vectors in $\mathcal{H}$, related to the notion of enclosure, and consider an equivalence relation. We will argue, however, that this will not immediately provide us with an interesting decomposition of a quantum channel.

DEFINITION 4.2. For x, y in $\mathcal{H}$, we say that:
- y is *accessible* from x (and denote it by $x\to y$) if $y \in \mathrm{Enc}(x)$;
- y *and* x *communicate* (and denote it by $x\leftrightarrow y$) if $\mathrm{Enc}(x) = \mathrm{Enc}(y)$.

One can immediately observe that accessibility is a transitive relation, and communication is an equivalence relation. We denote by $\mathcal{C}(x)$ the equivalence class of a vector x in $\mathcal{H}$ for the relation $\leftrightarrow$,

$$\mathcal{C}(x) = \{y \in \mathrm{Enc}(x) \ \text{ s.t. } \ x \in \mathrm{Enc}(y)\}.$$

An equivalence class of a vector x by $\leftrightarrow$ is a subset of $\mathrm{Enc}(x)$ but it is not a vector space since, for $x \neq 0$, $\mathcal{C}(x)$ cannot contain 0. Even adding the point 0 may fail to make $\mathcal{C}(x)$ a vector space, as the next example shows.

EXAMPLE 4.1. Take $\mathcal{H} = \mathbb{C}^2$ and denote by e_1, e_2 its canonical basis. Consider a quantum channel Φ on $\mathcal{I}_1(\mathcal{H})$ with unravelling (V_1, V_2) given by $V_1 = \sqrt{p}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ and $V_2 = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-p} \end{pmatrix}$ for some $p \in (0,1)$ so that, for $\rho = \begin{pmatrix} \rho_{1,1} & \rho_{1,2} \\ \rho_{2,1} & \rho_{2,2} \end{pmatrix}$ in $\mathcal{I}_1(\mathcal{H})$, we have

$$\Phi(\rho) = \begin{pmatrix} p\rho_{2,2} + \rho_{1,1} & \sqrt{1-p}\,\rho_{1,2} \\ \sqrt{1-p}\,\rho_{2,1} & (1-p)\rho_{2,2} \end{pmatrix}.$$

By an immediate direct computation, the state $|e_1\rangle\langle e_1|$ is the only invariant state of this map. We want to describe the equivalence classes and the enclosures of the map Φ. We notice that, for any vector $u = {}^t(u_1, u_2)$ in $\mathbb{C}^2$,

$$|u\rangle\langle u| = \begin{pmatrix} |u_1|^2 & u_1\bar{u}_2 \\ \bar{u}_1 u_2 & |u_2|^2 \end{pmatrix} \text{ so that } \Phi(|u\rangle\langle u|) = \begin{pmatrix} p|u_2|^2 + |u_1|^2 & \sqrt{1-p}\,u_1\bar{u}_2 \\ \sqrt{1-p}\,\bar{u}_1 u_2 & (1-p)|u_2|^2 \end{pmatrix}.$$

It is immediate that $\Phi(|u\rangle\langle u|)$ is a positive-definite matrix whenever $u_2 \neq 0$, so that

- $\mathrm{supp}\,\Phi^n(|e_1\rangle\langle e_1|) = \mathbb{C}\,e_1$ for all $n \geq 0$,
- for $u_2 \neq 0$, $\mathrm{supp}\,\Phi^n(|u\rangle\langle u|) = \mathbb{C}^2$ for all $n \geq 1$.

Identity (4.3) allows us to determine all the enclosures and equivalence classes:

- $\mathrm{Enc}(0) = \mathcal{C}(0) = \{0\}$,
- $\mathrm{Enc}(e_1) = \mathbb{C}\,e_1$ and $\mathcal{C}(e_1) = \mathrm{Enc}(e_1) \setminus \{0\}$,
- for all $u \in \mathbb{C}^2 \setminus \mathbb{C}\,e_1$, $\mathrm{Enc}(u) = \mathbb{C}^2$ and $\mathcal{C}(u) = \mathbb{C}^2 \setminus \mathbb{C}\,e_1$.

Supports of invariant states, on the other hand, are always vector spaces. Therefore, the naïve approach of considering the partition of $\mathcal{H}$ induced by the relation $\leftrightarrow$ to obtain a relevant decomposition of a quantum channel into irreducible such maps fails, as it does not seem to involve the vector space structure. A natural idea, derived from the study of Markov chains, is to consider specifically minimal objects. We therefore give the following definition of a minimal enclosure:

DEFINITION 4.3. Let $\mathcal{V}$ be an enclosure. We say that $\mathcal{V}$ is a *minimal enclosure* if any enclosure $\mathcal{V}'$ satisfying $\mathcal{V}' \subset \mathcal{V}$ is either $\{0\}$ or $\mathcal{V}$. We say that $\mathcal{V}$ is a *minimal nontrivial enclosure* if in addition $\mathcal{V} \neq \{0\}$.

The following easy proposition shows that this notion is indeed relevant.

PROPOSITION 4.3. *$\mathcal{C}(x) = \mathrm{Enc}(x) \setminus \{0\}$ if and only if $\mathrm{Enc}(x)$ is a minimal nontrivial enclosure.*

Proof: If $\mathcal{C}(x) = \mathrm{Enc}(x) \setminus \{0\}$, then, for all y in $\mathrm{Enc}(x) \setminus \{0\}$, we have $\mathrm{Enc}(x) = \mathrm{Enc}(y)$ and consequently $\mathrm{Enc}(x)$ is minimal. Conversely, if $\mathcal{V} = \mathrm{Enc}(x)$ is a minimal enclosure, for any y in $\mathcal{V} \setminus \{0\}$, $\mathrm{Enc}(y)$ is a nontrivial enclosure contained in $\mathcal{V}$ so that $\mathrm{Enc}(y) = \mathcal{V}$. Therefore $x \leftrightarrow y$ and $\mathcal{V} = \mathcal{C}(x) \cup \{0\}$. □

5. Enclosures and invariant states

Baumgartner and Narnhofer in [3] studied a decomposition of a quantum channel related to the supports of extremal invariant states, in the case of a finite-dimensional space $\mathcal{H}$. In the present paper, we extend this analysis to the infinite-dimensional case. For this we will need to relate extremal invariant states to minimal enclosures. We will see that the form of invariant states for the quantum channel is dictated by the uniqueness or nonuniqueness of the decompositions into minimal enclosures and that this is related to the existence of mutually nonorthogonal minimal enclosures. The first result is as follows.

PROPOSITION 5.1. *Let Φ be a quantum channel on $\mathcal{H}$.*

1. *The support of an invariant state is an enclosure.*
2. *The fast recurrent subspace $\mathcal{R}$ is an enclosure.*

Proof: To prove the first point, fix an invariant state ρ_0, and let ρ be another state with support contained in $\operatorname{supp}\rho_0$. Fix an orthonormal family of eigenvectors for ρ_0 generating $\operatorname{supp}\rho_0$, and let X_0 be the set of finite linear combinations of these vectors. This set X_0 is dense in $\operatorname{supp}\rho_0$ and for every x in X_0 there exists λ such that $|x\rangle\langle x| \leq \lambda\rho_0$. Therefore there exists an approximation of ρ in the $\mathcal{I}_1(\mathcal{H})$ norm sense by an increasing sequence of finite-rank operators $(\rho_p)_p$ such that for every p there exists a λ_p with $\rho_p \leq \lambda_p\rho_0$, so that $\Phi(\rho_p) \leq \lambda_p\Phi(\rho_0)$ and therefore $\operatorname{supp}\Phi(\rho_p) \subset \operatorname{supp}\rho_0$. The sequence $\Phi(\rho_p)$ is increasing and weakly convergent to $\Phi(\rho)$ so that $\operatorname{supp}\Phi(\rho) \subset \operatorname{supp}\rho_0$, which proves that $\operatorname{supp}\rho_0$ is an enclosure.

To prove the second point, associate with every invariant state ρ the orthogonal projector P_ρ on its support. Then the orthogonal projector P on $\mathcal{R}$ is the supremum of the family $(P_\rho)_\rho$. For any invariant state ρ, P_ρ is subharmonic, i.e. $\Phi^*(P_\rho) \geq P_\rho$ and moreover, $\Phi^*(P) \geq \Phi^*(P_\rho) \geq P_\rho$, so that $\Phi^*(P) \geq P$ and the conclusion follows. □

REMARK 5.1. The first point of the previous proposition has already been proven in [17] and [26] in the dual setting, *i.e.* considering reducing projections for Φ^*. If $\mathcal{H}$ is separable, the second point can also be derived from a result in [26] which proves that there exists an invariant state with support equal to $\mathcal{R}$.

REMARK 5.2. The converse of point 1 of Proposition 5.1 is not true. Consider Example 2.1 associated with the symmetric random walk on $\mathbb{Z}$. Then $\mathcal{H} = \ell^2(\mathbb{Z})$ is an enclosure but the quantum channel Φ has no invariant state.

PROPOSITION 5.2. *Let $\mathcal{V}$ be an enclosure, $\mathcal{W}$ be a subspace of $\mathcal{H}$ which is in direct sum with $\mathcal{V}$, and $P_\mathcal{V}$ and $P_\mathcal{W}$ be the projections associated with the decomposition $\mathcal{V} \oplus \mathcal{W}$. Consider a state ρ with support in $\mathcal{V} \oplus \mathcal{W}$ and denote*

$$\rho_\mathcal{V} = P_\mathcal{V}\,\rho\,P_\mathcal{V}, \qquad \rho_\mathcal{W} = P_\mathcal{W}\,\rho\,P_\mathcal{W}, \qquad \rho_\mathcal{C} = P_\mathcal{V}\,\rho\,P_\mathcal{W}, \qquad \rho'_\mathcal{C} = P_\mathcal{W}\,\rho\,P_\mathcal{V}.$$

Similarly, decompose $\Phi(\rho)$ into $\Phi(\rho)_\mathcal{V} + \Phi(\rho)_\mathcal{W} + \Phi(\rho)_\mathcal{C} + \Phi(\rho)'_\mathcal{C}$. Then

1. $P_{\mathcal{W}}\,(\Phi(\rho_{\mathcal{C}}) + \Phi(\rho'_{\mathcal{C}}))\,P_{\mathcal{W}} = 0$,
2. *if* $\mathcal{Z}$ *is another enclosure with* $\mathcal{V} \subset \mathcal{Z} \subset \mathcal{R}$, *then* $\mathcal{Z} \cap \mathcal{V}^{\perp}$ *is an enclosure,*
3. *if* $\mathcal{W}$ *is also an enclosure, then*

$$\Phi(\rho)_{\mathcal{V}} = \Phi(\rho_{\mathcal{V}}), \qquad \Phi(\rho)_{\mathcal{W}} = \Phi(\rho_{\mathcal{W}}), \qquad \Phi(\rho)_{\mathcal{C}} = \Phi(\rho_{\mathcal{C}}), \qquad \Phi(\rho)'_{\mathcal{C}} = \Phi(\rho'_{\mathcal{C}}).$$

Proof:

1. Let $\kappa_{\pm\varepsilon} = \frac{1}{\varepsilon}\,\rho_{\mathcal{V}} \pm (\rho_{\mathcal{C}} + \rho_{\mathcal{C}'}) + \varepsilon\,\rho_{\mathcal{W}}$. We have $\kappa_{\pm\varepsilon} \geq 0$ (as can be checked from $\langle u, \kappa_{\pm\varepsilon}\,u\rangle = \langle u_{\pm\sqrt{\varepsilon}}, \kappa\,u_{\pm\sqrt{\varepsilon}}\rangle$, where $u_{\pm\sqrt{\varepsilon}} = \frac{1}{\sqrt{\varepsilon}}\,P_{\mathcal{V}}u \pm \sqrt{\varepsilon}\,P_{\mathcal{W}}u$), so that $\Phi(\kappa_{\pm\varepsilon}) \geq 0$, and, because $\mathcal{V}$ is an enclosure, the support of $\Phi(\rho_{\mathcal{V}})$ is contained in $\mathcal{V}$, so that

$$P_{\mathcal{W}}\,\Phi(\kappa_{\pm\varepsilon})\,P_{\mathcal{W}} = \pm P_{\mathcal{W}}\big(\Phi(\rho_{\mathcal{C}}) + \Phi(\rho'_{\mathcal{C}})\big)P_{\mathcal{W}} + \varepsilon\,P_{\mathcal{W}}\,\Phi(\rho_{\mathcal{W}})\,P_{\mathcal{W}} \geq 0,$$

   and by necessity $P_{\mathcal{W}}\,(\Phi(\rho_{\mathcal{C}}) + \Phi(\rho'_{\mathcal{C}}))\,P_{\mathcal{W}} = 0$.

2. Consider $\mathcal{W} = \mathcal{Z} \cap \mathcal{V}^{\perp}$ and ρ any invariant state; then

$$\rho_{\mathcal{V}} + \rho_{\mathcal{W}} + \rho_{\mathcal{C}} + \rho'_{\mathcal{C}} = \Phi(\rho_{\mathcal{V}}) + \Phi(\rho_{\mathcal{W}}) + \Phi(\rho_{\mathcal{C}}) + \Phi(\rho'_{\mathcal{C}}).$$

   Considering $P_{\mathcal{W}} \cdot P_{\mathcal{W}}$ this yields $\rho_{\mathcal{W}} = P_{\mathcal{W}}\Phi(\rho_{\mathcal{W}})P_{\mathcal{W}}$, so that $P_{\mathcal{V}}\,\Phi(\rho_{\mathcal{W}})\,P_{\mathcal{V}}$ is positive with zero trace. Therefore $P_{\mathcal{V}}\,\Phi(\rho_{\mathcal{W}})\,P_{\mathcal{V}} = 0$ which implies $P_{\mathcal{V}}\,\Phi(\rho_{\mathcal{W}}) = \Phi(\rho_{\mathcal{W}})\,P_{\mathcal{V}} = 0$ and so $\rho_{\mathcal{W}} = \Phi(\rho_{\mathcal{W}})$. As the support of a stationary state, $\operatorname{supp}\rho_{\mathcal{W}} = \operatorname{supp}\rho \cap \mathcal{Z} \cap \mathcal{V}^{\perp}$ is an enclosure. By the same argument used to prove point 2 of Proposition 5.1, the supremum of $\operatorname{supp}\rho \cap \mathcal{Z} \cap \mathcal{V}^{\perp}$ over all possible invariant states ρ is still an enclosure, and this is $\mathcal{Z} \cap \mathcal{V}^{\perp}$.

3. If $\mathcal{V}$ and $\mathcal{W}$ are enclosures, then by definition $\operatorname{supp}\Phi(\rho_{\mathcal{V}}) \subset \mathcal{V}$ and $\operatorname{supp}\Phi(\rho_{\mathcal{W}}) \subset \mathcal{W}$. The equality

$$\Phi(\rho_{\mathcal{V}}) + \Phi(\rho_{\mathcal{W}}) + \Phi(\rho_{\mathcal{C}}) + \Phi(\rho'_{\mathcal{C}}) = \Phi(\rho)_{\mathcal{V}} + \Phi(\rho)_{\mathcal{W}} + \Phi(\rho)_{\mathcal{C}} + \Phi(\rho)'_{\mathcal{C}}$$

   implies $\Phi(\rho_{\mathcal{V}}) = \Phi(\rho)_{\mathcal{V}}$ and $\Phi(\rho_{\mathcal{W}}) = \Phi(\rho)_{\mathcal{W}}$. We then have $\Phi(\rho)_{\mathcal{C}} + \Phi(\rho)'_{\mathcal{C}} = \Phi(\rho_{\mathcal{C}}) + \Phi(\rho'_{\mathcal{C}})$. Since $\operatorname{Ran}\rho_{\mathcal{C}} \subset \mathcal{V} \subset \operatorname{Ker}\rho_{\mathcal{C}}$ and $V_i\mathcal{V} \subset \mathcal{V}$ for all i by Proposition 4.1, one has $\operatorname{Ran}\Phi(\rho_{\mathcal{C}}) \subset \mathcal{V} \subset \operatorname{Ker}\Phi(\rho_{\mathcal{C}})$ and therefore $P_{\mathcal{W}}\Phi(\rho_{\mathcal{C}})P_{\mathcal{V}} = 0$. This implies $\Phi(\rho'_{\mathcal{C}}) = \Phi(\rho)'_{\mathcal{C}}$ and similarly $\Phi(\rho_{\mathcal{C}}) = \Phi(\rho)_{\mathcal{C}}$. □

COROLLARY 5.1. *For any enclosure* $\mathcal{V}$ *contained in* $\mathcal{R}$, *there exists an invariant state* ρ *such that* $\operatorname{supp}\rho \subset \mathcal{V}$.

Proof: By definition of $\mathcal{R}$, there exists an invariant state ρ with $\operatorname{supp}\rho \cap \mathcal{V} \neq \{0\}$. By Proposition 5.2, $P_{\mathcal{V}}\,\rho\,P_{\mathcal{V}}$ is (up to normalization) an invariant state with support in $\mathcal{V}$. □

We will now discuss the connection between minimal enclosures and extremal invariant states, i.e. states ρ such that $\rho = t\,\rho_1 + (1-t)\,\rho_2$, with ρ_1, ρ_2 in $\mathcal{S}(\mathcal{H}) \cap \mathcal{F}(\Phi)$ and $t \in (0, 1)$, implies $\rho_1 = \rho_2 = \rho$.

REMARK 5.3. The distinction between states and normal states mentioned in Remark 2.1 does not lead to an ambiguity: by Example 4.1.35 in [6], the set $\mathcal{S}(\mathcal{H})$,

when viewed as a subspace of $\mathcal{B}(\mathcal{H})^*_{+,1}$, is a face, so that $\rho \in \mathcal{S}(\mathcal{H})$ is extremal regarding convex decompositions in $\mathcal{S}(\mathcal{H}) \cap \mathcal{F}(\Phi)$ if and only if it is extremal regarding convex decompositions in $\mathcal{B}(\mathcal{H})^*_{+,1} \cap \mathcal{F}(\Phi)$.

The following proposition is the main result in this section.

PROPOSITION 5.3. *A subspace of $\mathcal{R}$ is a minimal enclosure if and only if it is the support of an extremal invariant state. Moreover, any enclosure included in $\mathcal{R}$ contains a (nontrivial) minimal enclosure. Equivalently, for any invariant state ρ, there exists an extremal invariant state ρ_{ex} with* $\operatorname{supp}\rho_{\mathrm{ex}} \subset \operatorname{supp}\rho$.

Proof: If $\mathcal{V}$ is a minimal enclosure contained in $\mathcal{R}$, then by Corollary 5.1, there exists a Φ-invariant state $\rho_{\mathcal{V}}$ with support in $\mathcal{V}$. By the discussion following Definition 4.1, the restriction of Φ to $\mathcal{I}_1(\mathcal{V})$ is irreducible. Proposition 3.2 shows that $\rho_{\mathcal{V}}$ is the unique Φ-invariant state with support in $\mathcal{V}$, and $\operatorname{supp}\rho_{\mathcal{V}} = \mathcal{V}$. This $\rho_{\mathcal{V}}$ must be extremal since $\rho_{\mathcal{V}} = t\,\rho_1 + (1-t)\,\rho_2$ with ρ_1, ρ_2 invariant states and $t \in (0,1)$ would imply that ρ_1, ρ_2 are invariant states with support in $\mathcal{V}$ but then by uniqueness, $\rho_{\mathcal{V}} = \rho_1 = \rho_2$.

Conversely, if $\mathcal{V} = \operatorname{supp}\rho$ with ρ an extremal invariant state, then by Proposition 5.1, $\mathcal{V}$ is an enclosure. If we suppose, by contradiction, that it is not minimal, then there exists an enclosure $\mathcal{W}$ with $\mathcal{W} \subsetneq \mathcal{V} \subset \mathcal{R}$ and, by Corollary 5.1, an invariant state ρ' with $\operatorname{supp}\rho' \subset \mathcal{W}$. Since ρ is faithful on $\mathcal{V}$, by the same argument as in the proof of Proposition 5.1, we can approximate ρ' in the $\mathcal{I}_1(\mathcal{V})$ norm sense by a sequence $(\rho'_p)_p$ of finite-dimensional operators such that for every p, there exists λ_p with $\rho'_p \leq \lambda_p \rho$. If we let $\Psi_n = \frac{1}{n}\sum_{k=0}^{n-1}\Phi^k$ then by a standard compactness argument, $(\Psi_n(\rho'_p))_n$ converges weakly to a Φ-invariant nonnegative trace-class operator ρ_p^{inv} which therefore satisfies $\rho_p^{\mathrm{inv}} \leq \lambda_p\,\rho$. The extremality of ρ implies that ρ_p^{inv} is proportional to ρ. This in turn implies that $(\Psi_n(\rho'))_n$ converges weakly to ρ, but $\Psi_n(\rho') = \rho'$ by the Φ-invariance of ρ'. Therefore, $\rho' = \rho$, a contradiction.

By Proposition 5.1 and Corollary 5.1, the second and third claims are equivalent. To prove the second one, consider the maps $\Phi^*_{\mathcal{R}}$ on the set $\mathcal{B}(\mathcal{R})$ of bounded operators acting on $\mathcal{R}$ defined by

$$\Phi^*_{\mathcal{R}}(P_{\mathcal{R}}\,x\,P_{\mathcal{R}}) = P_{\mathcal{R}}\,\Phi^*(x)\,P_{\mathcal{R}},$$

and denote by $\mathcal{F}(\Phi^*_{\mathcal{R}})$ the vector space of the fixed points for $\Phi^*_{\mathcal{R}}$, i.e. $\mathcal{F}(\Phi^*_{\mathcal{R}}) = \{X \in P_{\mathcal{R}}\mathcal{B}(\mathcal{H})P_{\mathcal{R}} : \Phi^*_{\mathcal{R}}(X) = X\}$. We know that $\mathcal{F}(\Phi^*_{\mathcal{R}})$ is the image of a normal conditional expectation by Theorem 2.1 of [18]. The proof of Theorem 5 of [25] shows then that $\mathcal{F}(\Phi^*_{\mathcal{R}})$ is an atomic subalgebra. It is trivial to verify that the projections contained in $\mathcal{F}(\Phi^*_{\mathcal{R}})$ are exactly the projections on enclosures contained in $\mathcal{R}$. So, for any enclosure $\mathcal{V}$, we consider the corresponding projection $P_{\mathcal{V}} \in \mathcal{F}(\Phi^*_{\mathcal{R}})$; but since $\mathcal{F}(\Phi^*_{\mathcal{R}})$ is atomic, it contains a minimal projection $P' \leq P$ and the range of P' is then a minimal enclosure contained in $\mathcal{V}$. □

REMARK 5.4. The proof of point 3 of Proposition 5.3 can be given in a more constructive way: consider an invariant state ρ, which by restriction one can assume is faithful, i.e. with support $\mathcal{H}$. By the Banach–Alaoglu theorem, the set $\mathcal{B}(\mathcal{H})^*_{+,1} \cap \mathcal{F}(\Phi)$ is a compact, convex, metrizable subset of the locally convex space $\mathcal{B}(\mathcal{H})^*$ equipped with the weak-* topology. By Theorem 4.1.11 and Proposition 4.1.3 in [6], and the fact that affine maps on $\mathcal{B}(\mathcal{H})^*$ are exactly the maps $\eta \mapsto \eta(X)$ for $X \in \mathcal{B}(\mathcal{H})$, there exists a Borel probability measure μ in $\mathcal{B}(\mathcal{H})^*$, such that $\rho(X) = \int \eta(X) \mathrm{d}\mu(\eta)$ for any X, and μ has support in the set of extremal states of $\mathcal{B}(\mathcal{H})^*_{+,1} \cap \mathcal{F}(\Phi)$. Since in addition the set $\mathcal{S}(\mathcal{H}) \cap \mathcal{F}(\Phi)$ is a face, μ has support in the set of extremal states of $\mathcal{S}(\mathcal{H}) \cap \mathcal{F}(\Phi)$. For any Borel set B of $\mathcal{B}(\mathcal{H})^*$ with $\mu(B) > 0$ one can define $\rho_B = \frac{1}{\mu(B)} \int_B \eta(X) \mathrm{d}\mu(\eta)$. This ρ_B is a state with $\operatorname{supp} \rho_B \subset \operatorname{supp} \rho$. By considering a sequence of Borel sets that are balls $B(\rho_0, \frac{1}{n})$ for the metric compatible with the weak-* topology restricted to the unit sphere of $\mathcal{B}(\mathcal{H})^*$, one has for μ-almost all ρ_0 that $\rho_{B(\rho_0, \frac{1}{n})} \to \rho_0$ in the topology of $\mathcal{S}(\mathcal{H})$, so that $\operatorname{supp} \rho_0 \subset \operatorname{supp} \rho$.

For any quantum channel Φ, point 2 of Proposition 5.2, together with Proposition 5.3, will allow us to decompose the space $\mathcal{R}$ associated with Φ into a direct sum of minimal enclosures, and each of them is the support of an extremal invariant state. We give the following sequel to the two results quoted above, that essentially shows that the procedure of taking orthogonal complements is efficient in terms of decomposition into minimal enclosures.

LEMMA 5.1. *Let $\mathcal{V} = \mathcal{V}_1 + \cdots + \mathcal{V}_n + \mathcal{V}_{n+1}$, where the $\mathcal{V}_i$, $i = 1, \ldots, n+1$, are distinct minimal enclosures contained in $\mathcal{R}$, and $\mathcal{V}_i \perp \mathcal{V}_j$ for $i \neq j$ in $1, \ldots, n$. Then there exists a minimal enclosure $\mathcal{V}'_{n+1}$, orthogonal to $\mathcal{V}_1, \ldots, \mathcal{V}_n$ and such that $\mathcal{V} = \mathcal{V}_1 + \ldots + \mathcal{V}_n + \mathcal{V}'_{n+1}$. If $n = 1$ then one can take $\mathcal{V}'_2 = \mathcal{V} \cap \mathcal{V}_1^\perp$. In particular, if a subspace of $\mathcal{R}$ can be written as a sum of minimal enclosures, then it can be written as a sum of mutually orthogonal minimal enclosures.*

Proof: Let us first prove the claim for $n = 1$. We know that $\mathcal{V}$ is an enclosure as direct sum of two enclosures and so by Proposition 5.2, $\mathcal{V}'_2$ is an enclosure. If $\mathcal{V}_2 \perp \mathcal{V}_1$ then $\mathcal{V}'_2 = \mathcal{V}_2$ and there is nothing to prove. Assume therefore that $\mathcal{V}_2 \not\perp \mathcal{V}_1$. Proposition 5.3 provides us with a nontrivial minimal enclosure $\mathcal{W} \subseteq \mathcal{V}'_2$. Then $\mathcal{W} \not\subset \mathcal{V}_2$ for otherwise $\mathcal{W} = \mathcal{V}_2 \subset \mathcal{V}'_2$ and $\mathcal{V}_2 \perp \mathcal{V}_1$, a contradiction. Since $\mathcal{W} \subset \mathcal{V}_1 + \mathcal{V}_2$, there exists $w = v_1 + v_2$ in $\mathcal{W}$ with $v_i \in \mathcal{V}_i$ and $v_i \neq 0$ for $i = 1, 2$. Then $0 \neq v_2 = w - v_1 \in \mathcal{V}_2 \cap (\mathcal{W} + \mathcal{V}_1)$. Since $\mathcal{V}_2$ is a minimal enclosure one must have $\mathcal{V}_2 \subset \mathcal{W} + \mathcal{V}_1$ so that $\mathcal{V}_1 + \mathcal{V}_2 = \mathcal{V}_1 + \mathcal{W}$ and necessarily $\mathcal{W} = \mathcal{V}'_2$. This proves the minimality of $\mathcal{V}'_2$.

Now if $n > 1$, define $\mathcal{V}'_{n+1,1} = (\mathcal{V}_1 + \mathcal{V}_{n+1}) \cap \mathcal{V}_1^\perp$. By the preceding discussion, $\mathcal{V}'_{n+1,1}$ is orthogonal to $\mathcal{V}_1$ and $\mathcal{V}_1 + \mathcal{V}_{n+1} = \mathcal{V}_1 + \mathcal{V}'_{n+1,1}$. Then define $\mathcal{V}'_{n+1,2} = (\mathcal{V}_2 + \mathcal{V}'_{n+1,1}) \cap \mathcal{V}_2^\perp$. This $\mathcal{V}'_{n+1,2}$ is now orthogonal to $\mathcal{V}_1$ and $\mathcal{V}_2$ and $\mathcal{V}_2 + \mathcal{V}'_{n+1,1} = \mathcal{V}_2 + \mathcal{V}'_{n+1,2}$ so that $\mathcal{V}_1 + \mathcal{V}_2 + \mathcal{V}_{n+1} = \mathcal{V}_1 + \mathcal{V}_2 + \mathcal{V}'_{n+1,2}$. Iterating this process gives the desired $\mathcal{V}'_{n+1}$ in the form of $\mathcal{V}'_{n+1,n}$. □

We therefore have our main tool for decompositions of quantum channels into irreducible ones. We wish to relate these decompositions to the structure of invariant states of Φ. In the case of Markov chains, it is well known that these are all convex combinations of the extremal invariant states associated with irreducible parts in the decomposition. We will see in the next section, however, that this is not the case for general quantum channels.

6. Invariant states of nonirreducible quantum channels

In this section we study the last ingredient of our decomposition, that is, how the invariant states of a quantum channel on a sum $\mathcal{V}_1 + \mathcal{V}_2$ of two minimal enclosures relate to the extremal invariant states associated with these two minimal enclosures. We will see that this relation will depend on the uniqueness of the decomposition $\mathcal{V}_1 + \mathcal{V}_2$.

Let us define what we mean by this uniqueness. We say that the decomposition of a subspace $\mathcal{Z}$ of $\mathcal{R}$ in a direct sum of minimal enclosures is unique, if, whenever $(\mathcal{V}_\alpha)_{\alpha\in A}$ and $(\mathcal{W}_\beta)_{\beta\in B}$ are two families of minimal enclosures with

$$\mathcal{V}_\alpha \cap \mathcal{V}_{\alpha'} = \{0\} \text{ for any } \alpha \neq \alpha', \qquad \mathcal{W}_\beta \cap \mathcal{W}_{\beta'} = \{0\} \quad \text{for any } \beta \neq \beta',$$

and $\mathcal{Z} = \sum_{\alpha\in A} \mathcal{V}_\alpha = \sum_{\beta\in B} \mathcal{W}_\beta$, then the sets $\{\mathcal{V}_\alpha, \alpha \in A\}$ and $\{\mathcal{W}_\beta, \beta \in B\}$ coincide, and in particular A and B have the same cardinality.

The following lemma characterizes the situations when the decomposition of a subspace as the direct sum of two enclosures is unique. First remark that, by point 2 in Proposition 5.2, if x and y are in $\mathcal{R}$ then

- either $\mathrm{Enc}(x) \perp \mathrm{Enc}(y)$,
- or $x \notin \mathrm{Enc}(y)^\perp$ and $y \notin \mathrm{Enc}(x)^\perp$.

Indeed, if $y \in \mathrm{Enc}(x)^\perp \cap \mathcal{R}$ then $\mathrm{Enc}(y) \perp \mathrm{Enc}(x)$.

LEMMA 6.1. *Let $\mathcal{V} = \mathcal{V}_1 + \mathcal{V}_2$, where $\mathcal{V}_1$ and $\mathcal{V}_2$ are minimal enclosures contained in $\mathcal{R}$. The decomposition of $\mathcal{V}$ in a direct sum of minimal enclosures is unique if and only if any enclosure $\mathcal{W}$ such that $\mathcal{W} \not\perp \mathcal{V}_1$ and $\mathcal{W} \not\perp \mathcal{V}_2$ satisfies $\mathcal{W} \cap \mathcal{V} = \{0\}$. If the latter statement holds, then the two enclosures are orthogonal.*

Proof: Assume the decomposition of $\mathcal{V}$ as a direct sum of minimal enclosures is unique. Then $\mathcal{V}_1 \perp \mathcal{V}_2$, otherwise by Proposition 5.2, $\mathcal{V} \cap \mathcal{V}_1^\perp$ would be an enclosure that does not contain $\mathcal{V}_2$, leading to a different decomposition of $\mathcal{V}$. Now consider a minimal enclosure $\mathcal{W}$ with $\mathcal{W} \not\perp \mathcal{V}_1$ and $\mathcal{W} \not\perp \mathcal{V}_2$. This implies $\mathcal{W} \neq \mathcal{V}_1$ so that $\mathcal{W} \cap \mathcal{V}_1 = \{0\}$. If $\mathcal{W} \cap \mathcal{V} \neq \{0\}$ then it is an enclosure in $\mathcal{W}$ so by minimality, $\mathcal{W} \subset \mathcal{V}$. Then $\mathcal{W} \oplus \mathcal{V}_1$ is a direct sum of minimal enclosures contained in $\mathcal{V}$, so, by Proposition 5.3, one can complete this as a decomposition of $\mathcal{V}$ into a direct sum of minimal enclosures. This is a contradiction, leading to $\mathcal{W} \cap \mathcal{V} = \{0\}$.

Now assume that any enclosure $\mathcal{W}$ such that $\mathcal{W} \not\perp \mathcal{V}_1$ and $\mathcal{W} \not\perp \mathcal{V}_2$ satisfies $\mathcal{W} \cap \mathcal{V} = \{0\}$. Taking first $\mathcal{W} = \mathcal{V}_2$, which obviously has a nontrivial intersection with $\mathcal{V}$, we obtain that $\mathcal{V}_1 \perp \mathcal{V}_2$. Now consider some minimal enclosure $\mathcal{V}_3$ contained

in $\mathcal{V}$. Then, by assumption, one has e.g. $\mathcal{V}_3 \perp \mathcal{V}_1$ and $\mathcal{V}_3 \not\perp \mathcal{V}_2$ and so $\mathcal{V}_3 \subset \mathcal{V}_1^{\perp} \cap \mathcal{V}$, which, as proved above, is $\mathcal{V}_2$. This proves the uniqueness of the decomposition. □

Next we need to strengthen Proposition 5.2 to distinguish between the situations where the decomposition into minimal enclosures is unique or not. The first result treats the situation where the decomposition is unique. To simplify the notation, from now on, when $\mathcal{V}$ is an enclosure, we will denote by $\Phi_{|\mathcal{V}}$ (instead of $\Phi_{|\mathcal{I}_1(\mathcal{V})}$) the restriction of Φ to $\mathcal{I}_1(\mathcal{V})$.

PROPOSITION 6.1. *If ρ is Φ-invariant and $\mathcal{V}$ and $\mathcal{W}$ are two minimal enclosures contained in $\mathcal{R}$, such that the decomposition of $\mathcal{V}+\mathcal{W}$ into a sum of minimal enclosures is unique, then $P_{\mathcal{V}}\,\rho\,P_{\mathcal{W}} = P_{\mathcal{W}}\,\rho\,P_{\mathcal{V}} = 0$, i.e. with the notation of Proposition 5.2 one has $\rho_{\mathcal{C}} = \rho'_{\mathcal{C}} = 0$.*

Proof: If $\mathcal{V}$ and $\mathcal{W}$ are minimal enclosures in $\mathcal{R}$, then, by Proposition 5.3, they are the supports of extremal invariant states $\rho_{\mathcal{V}}$ and $\rho_{\mathcal{W}}$. Because the decomposition of $\mathcal{V}+\mathcal{W}$ into minimal enclosures is unique, $\rho_{\mathcal{V}}$ and $\rho_{\mathcal{W}}$ are the unique extremal invariant states of $\Phi_{|(\mathcal{V}+\mathcal{W})}$. Since the set of invariant states is convex, then by the Krein–Milman theorem, ρ is a convex combination of $\rho_{\mathcal{V}}$ and $\rho_{\mathcal{W}}$, so $\rho_{\mathcal{C}}$ and $\rho'_{\mathcal{C}}$ must be zero. □

REMARK 6.1. Consider the quantum channel Φ associated with a Markov chain as in Example 2.1. It is a simple observation that a minimal enclosure for Φ is necessarily of the form $\mathcal{V} = \ell^2(C)$ for C a minimal communication class for the Markov chain (where $\ell^2(C)$ is viewed as a subspace of $\ell^2(E)$). Therefore, two distinct minimal enclosures $\mathcal{V}_1$ and $\mathcal{V}_2$ are necessarily orthogonal, decompositions into sums of minimal enclosures are unique, and any invariant state on $\mathcal{H} = \ell^2(V_1 + V_2)$ is a convex combination of the extremal invariant states ρ_1, ρ_2 with supports $\ell^2(V_1)$, $\ell^2(V_2)$, respectively.

A second result will allow us to describe more explicitly the situation where the decomposition into minimal enclosures is not unique, and describe the associated invariant states.

PROPOSITION 6.2. *Let $\mathcal{V}_1$ and $\mathcal{V}_2$ be two minimal enclosures contained in $\mathcal{R}$. Assume that the decomposition of $\mathcal{V} = \mathcal{V}_1 + \mathcal{V}_2$ in a direct sum of minimal enclosures is not unique. Then* $\dim \mathcal{V}_1 = \dim \mathcal{V}_2$. *If, in addition, $\mathcal{V}_1 \perp \mathcal{V}_2$ (as can be chosen by Lemma* 5.1) *then there exists a partial isometry Q from $\mathcal{V}_1$ to $\mathcal{V}_2$ satisfying*

$$Q^*Q = \mathrm{Id}_{|\mathcal{V}_1}, \qquad Q\,Q^* = \mathrm{Id}_{|\mathcal{V}_2}, \tag{6.1}$$

and for any ρ in $\mathcal{I}_1(\mathcal{H})$, and $R = Q P_{\mathcal{V}_1} + Q^* P_{\mathcal{V}_2}$,

$$R\,\Phi(\rho)\,P_{\mathcal{V}_i} + P_{\mathcal{V}_i}\,\Phi(\rho)\,R = \Phi\big(R\,\rho\,P_{\mathcal{V}_i} + P_{\mathcal{V}_i}\,\rho\,R\big) \qquad \text{for } i = 1, 2. \tag{6.2}$$

Proof: By Lemma 6.1, there exists a minimal enclosure $\mathcal{W}$ in $\mathcal{V}_1 + \mathcal{V}_2$ such that $\mathcal{W} \not\perp \mathcal{V}_i$, $i = 1, 2$. If $\mathcal{V}_1 \cap \mathcal{W}^{\perp} = \{0\}$ then by minimality of $\mathcal{V}_1$, we have $\mathcal{V}_1 \subset \mathcal{W}^{\perp}$,

a contradiction. Therefore $\mathcal{V}_1 \subset \mathcal{W}$, and $\dim \mathcal{V}_1 \leq \dim \mathcal{W}$; by symmetry one has $\dim \mathcal{V}_1 = \dim \mathcal{W}$.

Assume now that $\mathcal{V}_1 \perp \mathcal{V}_2$. Define the map $\Phi^*_{\mathcal{R}}$ as in the proof of Proposition 5.3. By Remark 3.2, if $E = \mathcal{V}_1$, $\mathcal{V}_2$ or $\mathcal{W}$, then P_E is (up to multiplication) the unique invariant of the restriction Φ^*_E of $\Phi^*_{\mathcal{R}}$ to $\mathcal{B}(E)$. Consider the decomposition of $P_{\mathcal{W}} = \left(\begin{smallmatrix} A & B^* \\ B & C \end{smallmatrix}\right)$ in the splitting $\mathcal{V} = \mathcal{V}_1 \oplus \mathcal{V}_2$, where necessarily $B \neq 0$. A simple consequence of Proposition 5.2 is that in the same decomposition, $\Phi^*_{\mathcal{R}}(P_{\mathcal{W}}) = \left(\begin{smallmatrix} \Phi^*_{\mathcal{R}}(A) & \Phi^*_{\mathcal{R}}(B)^* \\ \Phi^*_{\mathcal{R}}(B) & \Phi^*_{\mathcal{R}}(C) \end{smallmatrix}\right)$. Therefore A is proportional to $P_{\mathcal{V}_1}$ and C to $P_{\mathcal{V}_2}$. Writing relations $P = P^* = P^2$ satisfied by $P_{\mathcal{W}}$, one sees that B must be proportional to an operator Q satisfying relations (6.1). Fix Q; for $\theta \in [0, \pi]$, the operator defined by

$$P_\theta = \begin{pmatrix} \cos^2\theta & \sin\theta\cos\theta\, Q^* \\ \sin\theta\cos\theta\, Q & \sin^2\theta \end{pmatrix}$$

is an orthogonal projection preserved by the map $\Phi^*_{\mathcal{R}}$. So its range is an enclosure and, by point 3 of Proposition 5.2, P_θ will satisfy the relation

$$\Phi(P_\theta\, \rho\, P_\theta) = P_\theta\, \Phi(\rho)\, P_\theta,$$

for any ρ in $\mathcal{I}_1(\mathcal{H})$. Differentiating this relation with respect to θ, we have

$$\Phi\left(\frac{\mathrm{d}P_\theta}{\mathrm{d}\theta}\, \rho\, P_\theta + P_\theta\, \rho\, \frac{\mathrm{d}P_\theta}{\mathrm{d}\theta}\right) = \frac{\mathrm{d}P_\theta}{\mathrm{d}\theta}\, \Phi(\rho)\, P_\theta + P_\theta\, \Phi(\rho)\, \frac{\mathrm{d}P_\theta}{\mathrm{d}\theta}.$$

Computing the derivatives at $\theta = 0$ and $\theta = \pi/2$, we obtain relations (6.2). □

COROLLARY 6.1. *Assume that $\mathcal{V} = \mathcal{V}_1 + \mathcal{V}_2$ where $\mathcal{V}_1$ and $\mathcal{V}_2$ are mutually orthogonal minimal enclosures, contained in $\mathcal{R}$, but that the decomposition of $\mathcal{V}$ into a direct sum of minimal enclosures is nonunique. For $i = 1, 2$ let ρ_i^{inv} be the unique invariant state with support in $\mathcal{V}_i$. Consider Q the partial isometry defined in Proposition* 6.2. *Then $\rho_2^{\mathrm{inv}} = Q\, \rho_1^{\mathrm{inv}}\, Q^*$.*

If ρ is an invariant state with support in $\mathcal{V}$, then:

- *$P_{\mathcal{V}_1}\, \rho\, P_{\mathcal{V}_1}$ is proportional to ρ_1^{inv},*
- *$P_{\mathcal{V}_2}\, \rho\, P_{\mathcal{V}_2}$ is proportional to ρ_2^{inv},*
- *$P_{\mathcal{V}_1}\, \rho\, P_{\mathcal{V}_2}$ is proportional to $\rho_1^{\mathrm{inv}}\, Q^* = Q^* \rho_2^{\mathrm{inv}}$,*
- *$P_{\mathcal{V}_2}\, \rho\, P_{\mathcal{V}_1}$ is proportional to $\rho_2^{\mathrm{inv}}\, Q = Q \rho_1^{\mathrm{inv}}$.*

Proof: The first identity is obtained by applying relation (6.2) to $\rho = \rho_1^{\mathrm{inv}}$ with P_1, then applying it again to the resulting relation, this time with P_2.

That each $\rho_{i,j} = P_{\mathcal{V}_i} \rho P_{\mathcal{V}_j}$ is an invariant is an immediate consequence of Proposition 5.2. The relation satisfied by $\rho_{1,2}$ and $\rho_{2,1}$ is then obtained by applying relation (6.2) to e.g. $\rho_{1,2}$, with P_1 or P_2. □

7. Irreducible decompositions of quantum channels and invariant states

We are now in a position to state the relevant decomposition associated with Φ.

PROPOSITION 7.1. *Let Φ be a quantum channel on a separable Hilbert space $\mathcal{H}$. There exists a decomposition of $\mathcal{H}$ in the form*

$$\mathcal{H} = \mathcal{D} + \sum_{\alpha\in A} \mathcal{V}_\alpha + \sum_{\beta\in B}\sum_{\gamma\in C_\beta} \mathcal{V}_{\beta,\gamma}, \tag{7.1}$$

where any set A, B, C_β is at most countable, any C_β has cardinality at least two, and:

- *every $\mathcal{V}_\alpha$ or $\mathcal{V}_{\beta,\gamma}$ in this decomposition is a minimal enclosure,*
- *for β in B, any minimal enclosure that is not orthogonal to $\sum_{\gamma\in C_\beta}\mathcal{V}_{\beta,\gamma}$ is contained in $\sum_{\gamma\in C_\beta}\mathcal{V}_{\beta,\gamma}$,*
- *any two distinct subspaces $\mathcal{D}$, $\mathcal{V}_\alpha$, $\mathcal{V}_{\beta,\gamma}$ are mutually orthogonal.*

Notice that the sets A and B above can be empty, but they are simultaneously empty only when Φ does not admit any invariant state.

Proof: We start with the orthogonal decomposition $\mathcal{H} = \mathcal{D} + \mathcal{R}$, and proceed to decompose $\mathcal{R}$, when it is not trivial. Consider the set of all minimal enclosures $\mathcal{V}$ with the property that any minimal enclosure different from $\mathcal{V}$ is orthogonal to $\mathcal{V}$. By separability, this set is at most countable. Then we can denote all such minimal enclosures by $\mathcal{V}_\alpha$, with α in a (countable) set of indices A. Let $\mathcal{O}$ be the direct sum of all these enclosures, $\mathcal{O} = \sum_{\alpha\in A}\mathcal{V}_\alpha$. Then $\mathcal{O}$ is an enclosure, and, by point 2 of Proposition 5.2, $\mathcal{R}\cap\mathcal{O}^\perp$ is also an enclosure.

Assume that $\mathcal{R}\cap\mathcal{O}^\perp$ is nontrivial; we proceed to decompose it. Let $\beta(1) = 1$ and consider a minimal enclosure $\mathcal{V}_{\beta(1),1} \subset \mathcal{R}\cap\mathcal{O}^\perp$. By the definition of $\mathcal{O}$, there exists a minimal enclosure $\mathcal{V}_2$ in $\mathcal{R}\cap\mathcal{O}^\perp$, and by Lemma 5.1 we can choose $\mathcal{V}_{\beta(1),2}$ minimal, orthogonal to $\mathcal{V}_1$, and such that $\mathcal{V}_{\beta(1),1} + \mathcal{V}_{\beta(1),2} = \mathcal{V}_{\beta(1),1} + \mathcal{V}_2$. If all minimal enclosures are either included in $\mathcal{V}_{\beta(1),1} + \mathcal{V}_{\beta(1),2}$ or orthogonal to $\mathcal{V}_{\beta(1),1} + \mathcal{V}_{\beta(1),2}$, we set $C_{\beta(1)} = \{1, 2\}$. Otherwise, we call $\mathcal{V}_3$ a minimal enclosure not included in and not orthogonal to $\mathcal{V}_{\beta(1),1}+\mathcal{V}_{\beta(1),2}$. By Lemma 5.1 we can choose $\mathcal{V}_{\beta(1),3}$ minimal, orthogonal to $\mathcal{V}_{\beta(1),1} + \mathcal{V}_{\beta(1),2}$ and such that

$$\mathcal{V}_{\beta(1),1} + \mathcal{V}_{\beta(1),2} + \mathcal{V}_{\beta(1),3} = \mathcal{V}_{\beta(1),1} + \mathcal{V}_{\beta(1),2} + \mathcal{V}_3,$$

and we proceed again with the same method for a denumerable number of steps so that we construct $C_{\beta(1)}$. If $\mathcal{R}\cap\mathcal{O}^\perp\cap\big(\sum_{\gamma\in C_{\beta(1)}} E_{\beta(1),\gamma}\big)^\perp \neq \{0\}$, we can iterate the procedure. □

Before we state our next result, let us give some notation. We fix a decomposition (7.1) as considered in Proposition 7.1. We define

$$P_0 = P_{\mathcal{R}^\perp}, \qquad P_i = P_{\mathcal{V}_i} \quad \text{for } i \in A \text{ or } i \in \textstyle\bigcup_{\beta\in B}\{\beta\}\times C_\beta,$$

and, for a state ρ, and i, j taking the values 0, $\alpha \in A$ or $(\beta,\gamma) \in \bigcup_{\beta\in B}\{\beta\}\times C_\beta$,

$$\rho_i = P_i\,\rho\,P_i, \qquad \rho_{i,j} = P_i\,\rho\,P_j. \tag{7.2}$$

As before, we denote by ρ_i^{inv} the unique invariant state of $\Phi_{|\mathcal{V}_i}$.

We can now state the following result.

THEOREM 7.1. *Let ρ be a Φ-invariant state and consider a related orthogonal decomposition of the form* (7.1)*. With the notation* (7.2)*, we have*

1. $\rho_0 = 0$,
2. *every ρ_i is proportional to ρ_i^{inv}, for all indices $i \in A \cup \bigcup_{\beta\in B}\{\beta\} \times C_\beta$,*
3. *for $\gamma \neq \gamma'$ in C_β, the off-diagonal term $\rho_{((\beta,\gamma),(\beta,\gamma'))}$, which we simply denote by $\rho_{(\beta,\gamma,\gamma')}$, may be nonzero, and is Φ-invariant. In addition, there exists a partial isometry $Q_{(\beta,\gamma,\gamma')}$ from $\mathcal{V}_{\beta,\gamma}$ to $\mathcal{V}_{\beta,\gamma'}$ such that:*
   - $\rho^{\mathrm{inv}}_{(\beta,\gamma')} = Q_{(\beta,\gamma,\gamma')}\, \rho^{\mathrm{inv}}_{(\beta,\gamma)}\, Q^*_{(\beta,\gamma,\gamma')}$,
   - $\rho_{(\beta,\gamma,\gamma')}$ *is proportional to* $Q^*_{(\beta,\gamma,\gamma')}\, \rho^{\mathrm{inv}}_{(\beta,\gamma')} = \rho^{\mathrm{inv}}_{(\beta,\gamma)}\, Q^*_{(\beta,\gamma,\gamma')}$,
4. *all other $\rho_{i,j}$ (for i, j taking all possible values in $\{0\} \cup A \cup \bigcup_{\beta\in B}\{\beta\} \times C_\beta$) are zero.*

Proof: This follows from a repeated application of Propositions 5.2 and 7.1, and Corollary 6.1. □

REMARK 7.1. The decomposition of an invariant state ρ given by Theorem 7.1 can be rewritten in the same form as in formula (12) of Theorem 7 in [3], or as in Theorem 22 of [14], by simple algebraic manipulations. The key object is an isomorphism between $\mathcal{V}_{\beta,1} \otimes \mathbb{C}^{C_\beta}$ and $\sum_{\gamma\in C_\beta} \mathcal{V}_{\beta,\gamma}$ for each β, given by

$$\mathcal{E}(u \otimes x) = \sum_{\gamma\in C_\beta} u_\gamma\, Q_{(\beta,1,\gamma)}x \quad \text{for} \quad u = (u_\gamma)_{\gamma\in C_\beta}.$$

REMARK 7.2. The representation of invariant states appearing in Theorem 7.1 has recently been studied in [14], where an analogous result is proven in infinite dimension (and in the continuous time setting, but this point is not crucial). Our techniques and starting points are completely different and essentially replicate the approach used in [3] and [11]. Concerning the orthogonal decomposition and the representation of invariant states, however, our result is more general than the one in [14, Theorem 2.1], since we do not need to assume the atomicity of the decoherence free algebra (notice that the existence of a faithful normal invariant state assumed in [14] is not a restriction, since our decomposition is anyway only for the fast recurrent subspace $\mathcal{R}$, and by Remark 5.1, the restriction of Φ to $\mathcal{R}$ has a faithful invariant state). The key step which allows us to avoid this additional assumption is that we can prove that the fixed point algebra $\mathcal{F}(\Phi^*_{\mathcal{R}})$ is atomic. When there exists a faithful invariant state, this means that $\mathcal{F}(\Phi^*)$ is atomic. However, we do not know whether the decoherence free algebra (see [14]), usually denoted by $\mathcal{N}(\Phi^*)$, is atomic, neither can we so far deduce other generalizations of the results on the structure of this algebra studied in [14].

8. Examples

Even though our proofs do carry over to infinite dimension, the mechanisms behind the decompositions of quantum channels are the same for finite- and infinite-dimensional systems. Due to the lack of space, we consider mostly finite-dimensional examples.

EXAMPLE 8.1 (classical Markov chains). Consider as in Example 2.1 a Markov chain on a countable set E. Denote by $(C_\alpha)_{\alpha\in A}$ the family of minimal communication classes C_α such that the Markov chain has an invariant probability $\pi^{(\alpha)}$ with support C_α, by $R = \cup_{\alpha\in A} C_\alpha$ the (disjoint) union of these classes, and by D the complement $D = E \setminus R$. Then, according to the discussion in Remark 6.1, the decomposition (7.1) of $\mathcal{H} = \ell^2(E)$ is given by

$$\mathcal{H} = \mathcal{D} + \sum_{\alpha\in A} \mathcal{V}_\alpha \qquad \text{where } \mathcal{D} = \ell^2(D),\ \ \mathcal{V}_\alpha = \ell^2(C_\alpha)$$

and any invariant state on $\mathcal{H}$ is a convex combination of the extremal states, which are of the form $\sum_{i\in C_\alpha} \pi_i^{(\alpha)} |e_i\rangle\langle e_i|$.

EXAMPLE 8.2. Consider the quantum channel defined in Example 4.1. From the computations in Example 4.1, one has $\mathcal{R} = \mathbb{C}\, e_1$ and therefore $\mathcal{D} = \mathbb{C}\, e_2$.

EXAMPLE 8.3 (2×2 matrices). Consider $\mathcal{H} = \mathbb{C}^2$ and Φ a positive quantum map on the algebra $\mathcal{B}(\mathbb{C}^2)$, which we identify with the set $M_2(\mathbb{C})$ of 2×2 matrices and equiped with the scalar product $\langle x, y\rangle_{M_2} = \mathrm{tr}(x^* y)$. The Pauli matrices

$$\sigma_0 = \frac{1}{\sqrt{2}}\,\mathrm{Id}_{\mathbb{C}^2}, \quad \sigma_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

form an orthonormal basis of $M_2(\mathbb{C})$ and satisfy

$$\sigma_k^2 = \sigma_0^2, \qquad \sigma_k\sigma_j = -\sigma_j\sigma_k, \qquad \sigma_j\sigma_k = i\sigma_\ell,$$

if $(j, k, \ell) \in \{(1, 2, 3), (2, 3, 1), (3, 1, 2)\}$.

It is easy to see that, since Φ is trace preserving and positive, its matrix in the basis $\{\sigma_0, \sigma_1, \sigma_2, \sigma_3\}$ is of the form

$$\Phi = \begin{pmatrix} 1 & {}^t 0 \\ b & A \end{pmatrix} \tag{8.1}$$

where $b \in \mathbb{R}^3$, ${}^t 0 = (0, 0, 0)$, A is a 3×3 matrix with real coefficients. The map Φ is positive if and only if $\|b + Ax\| \le 1$ for all x such that $\|x\| \le 1$ (see [9] for more details, even if in the continuous time setting).

It is well known that states on $\mathbb{C}^2$ are all operators of the form $\rho = \sigma_0 + u\cdot\sigma$ with u in $\mathbb{R}^3$, $\|u\| \le 1$ (here we use the standard notation $u\cdot\sigma = \sum_{i=1,2,3} u_i\,\sigma_i$). This is called the Bloch sphere representation. In addition, it is easy to see that a state $\rho = \sigma_0 + u\cdot\sigma$ is invariant for Φ if and only if $b + Au - u = 0$.

Essentially, the problem of decomposing $\mathcal{R}$ into minimal enclosures is reduced to solving the linear system $b + Au - u = 0$, and then considering if there exist solutions with $\|u\| = 1$ and how many they are. However, by the Markov–Kakutani theorem (see [22]), an invariant state always exists. For the decomposition of the fast recurrent space $\mathcal{R}$, only 3 different cases are possible.

- There exists a unique invariant state ρ. Then the only minimal enclosure in $\mathcal{R}$ is $\mathcal{R}$ itself and it has dimension 2 when ρ is faithful and 1 otherwise.
- There exist infinitely many invariant states, and they are given by all convex combinations of two extremal invariant states ρ_1 and ρ_2. Then $\mathcal{R}$ can be written in a unique way as the direct sum of two minimal enclosures, which are the supports of ρ_1 and ρ_2.
- There exist infinitely many extremal invariant states. Then any state is invariant, any one dimensional subspace is an enclosure, and $\mathcal{R}$ can be written as $\mathcal{R} = \mathbb{C}\, e_1 \oplus \mathbb{C}\, e_2$, for any two linearly independent vectors e_1, e_2 in $\mathbb{C}^2$. This third case is possible if and only if Φ is the identity operator.

EXAMPLE 8.4. Define $V = \mathbb{N} \cup \{0\}$, $\mathfrak{h} = \mathbb{C}^3$, $\mathcal{H} = \mathfrak{h} \otimes \ell^2(V)$ and fix a canonical basis $(e_k)_{k=1,2,3}$ of $\mathfrak{h}$ so that we represent matrices and vectors in this basis. Choose $p, q > 0$ such that $p < 1/2$, $p + q < 1$ and a family of operators $(L_{i,j})_{i,j\in V}$ on $\mathfrak{h}$ such that $L_{ij} = 0$ when $|i - j| \geq 2$, $L_{00} = \sqrt{1-p}\,\mathrm{Id}_{\mathfrak{h}}$, $L_{j+1,j} = \sqrt{p}\,\mathrm{Id}_{\mathfrak{h}}$ for $j \geq 0$ and

$$L_{j-1,j} = \begin{pmatrix} \sqrt{1-p} & 0 & 0 \\ 0 & \sqrt{1-p} & 0 \\ 0 & 0 & \sqrt{q} \end{pmatrix} \qquad \text{for } j \geq 1,$$

$$L_{j,j} = \sqrt{\frac{(1-p-q)}{2}} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} \qquad \text{for } j \geq 1.$$

We have $\sum_{i\in V} L_{i,j}^* L_{ij} = \mathrm{Id}$ for all j in V, so that the map Φ acting on $\mathcal{I}_1(\mathcal{H})$ defined by

$$\Phi(\rho) = \sum_{i,j\in V} (L_{i,j} \otimes |i\rangle\langle j|)\, \rho\, (L_{i,j}^* \otimes |j\rangle\langle i|),$$

is a quantum channel. This map Φ is an open quantum random walk with transition operators $(L_{i,j})_{i,j\in V}$ as defined in [2]. Denote by $(|j\rangle)_{j\in V}$ the canonical basis of $\ell^2(V)$. It was proved in [11] that minimal enclosures for open quantum random walks are generated by vectors of the form $u \otimes |i\rangle$. Consider therefore $u = {}^t(u_1, u_2, u_3)$ in $\mathfrak{h}$, then

$$\mathrm{Enc}(u \otimes |i\rangle) = \begin{cases} \mathrm{span}\{u \otimes |j\rangle,\ j \geq 0\}, & \text{if } u_3 = 0, \\ \mathrm{span}\{e_3 \otimes |j\rangle,\ (e_1 + e_2) \otimes |j\rangle,\ j \geq 0\}, & \text{if } u_3 \neq 0, u_1 = u_2 \\ \mathcal{H}, & \text{if } u_3 \neq 0, u_1 \neq u_2. \end{cases}$$

The enclosures described in the first case ($u_3 = 0$) are the minimal ones and so they support the extremal invariant states of the evolution. Using finite difference equations as for similar classical Markov chains, one can compute these extremal invariant states,

$$\rho(u) = c \sum_{j\geq 0} \left(\frac{p}{1-p}\right)^j |u\rangle\langle u| \otimes |j\rangle\langle j|,$$

for $u = {}^t(u_1, u_2, 0) \neq 0$ and a normalizing constant c.

Then we have $\mathcal{R} = \text{span}\,\{e_1, e_2\} \otimes \ell^2(V)$, $\mathcal{D} = \text{span}\,\{e_3\} \otimes \ell^2(V)$ and the decomposition (7.1) can be written with A empty, B consisting of only one element β, $C_\beta = \{1, 2\}$,

$$\mathcal{V}_{\beta,1} = \text{span}\{v^1 \otimes |j\rangle,\, j \geq 0\}, \qquad \mathcal{V}_{\beta,2} = \text{span}\{v^2 \otimes |j\rangle,\, j \geq 0\},$$

for any linearly independent vectors v^1 and v^2 orthogonal to e_3. We observe that $\rho^{\text{inv}}_{\beta,1} = \rho(e_1)$ is the only invariant state with support $E = \text{span}\{e_1 \otimes |j\rangle,\, j \geq 0\}$ and, defining Q as $|e_2\rangle\langle e_1|$, that any invariant state has a decomposition

$$\rho = \begin{pmatrix} t\,\rho(e_1) & \lambda\,\rho(e_1)Q^* \\ \bar{\lambda}\,Q\rho(e_1) & (1-t)\,Q\rho(e_1)Q^* \end{pmatrix} \qquad \text{with } t \in [0, 1].$$

Using the previous expressions for enclosures, one can also deduce the communication classes, in particular for the vectors of the form $u \otimes |j\rangle$, which are the most interesting in the special case of open quantum random walks.

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QUANTUM STOCHASTIC EQUATIONS FOR AN OPTO-MECHANICAL OSCILLATOR WITH RADIATION PRESSURE INTERACTION AND NON-MARKOVIAN EFFECTS

ALBERTO BARCHIELLI*

Politecnico di Milano, Dipartimento di Matematica,
piazza Leonardo da Vinci 32, 20133 Milano, Italy
(e-mail: alberto.barchielli@polimi.it)

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The quantum stochastic Schrödinger equation or Hudson–Parthasarathy (HP) equation is a powerful tool to construct unitary dilations of quantum dynamical semigroups and to develop the theory of measurements in continuous time via the construction of output fields. An important feature of such an equation is that it allows to treat not only absorption and emission of quanta, but also scattering processes, which however had very few applications in physical modelling. Moreover, recent developments have shown that also some non-Markovian dynamics can be generated by suitable choices of the state of the quantum noises involved in the HP-equation. This paper is devoted to an application involving these two features, non-Markovianity and scattering process. We consider a micro-mirror mounted on a vibrating structure and reflecting a laser beam, a process giving rise to a radiation-pressure force on the mirror. We show that this process needs the scattering part of the HP-equation to be described. On the other side, non-Markovianity is introduced by the dissipation due to the interaction with some thermal environment which we represent by a phonon field, with a nearly arbitrary excitation spectrum, and by the introduction of phase noise in the laser beam. Finally, we study the full power spectrum of the reflected light and we show how the laser beam can be used as a temperature probe.

Keywords: quantum optomechanics, quantum stochastic differential equations, radiation pressure interaction, quantum Langevin equations, heterodyne detection.

1. Introduction

Quantum optomechanical systems represent an active field of research, very important both from the theoretical and experimental point of views, with applications in quantum optics and quantum information [1–6]. A great interest is due to the possibility of seeing quantum effects in a macroscopic mechanical resonator, say a mirror mounted on a vibrating structure and coupled to optical elements by radiation pressure. Typically, the theoretical description of such a kind of systems is based on the *quantum Langevin equations* [7, 8], a flexible approach allowing also

*Also: Istituto Nazionale di Fisica Nucleare (INFN), Sezione di Milano, and Istituto Nazionale di Alta Matematica (INDAM-GNAMPA).

for the introduction of non-Markovian effects. Recently, some experimental evidence of non-Markovian effects in an optomechanical system has been reported [9].

To get mathematically consistent quantum Langevin equations one has to use the *quantum stochastic calculus* and the *quantum stochastic Schrödinger equation*, or Hudson–Parthasarathy equation (HP-equation) [10, 11]. In this mathematical context the quantum Langevin equations appear under the name of *Evans-Hudson flows* or *quantum flows* [11–13]. In [14] a description of a dissipative mechanical oscillator has been obtained in terms of quantum stochastic differential equations; this description is fully consistent and valid at any temperature and it respects some symmetry requirements and physical constraints such as a weak form of equipartition at equilibrium and the translation invariance of the dissipative part of the dynamics. Non-Markovian effects have been introduced by a suitable choice of the state of the *quantum noises* appearing in the HP-equation. In Section 2 the quantum stochastic model of a dissipative mechanical oscillator is presented. An equation of Hudson–Parthasarathy type gives the unitary dynamics of the oscillator interacting with a Bose field (here representing the phonon field). The evolution equations for the system operators in the Heisenberg picture are the quantum Langevin equations and a suitable choice of the state of the field (based on a field analog of the P-representation in the case of discrete modes) allows for the introduction of thermal, non-Markovian effects.

Usual quantum Langevin equations allow to describe absorption and emission of energy quanta by the main system, not scattering processes. As a matter of fact it seems that the existing literature takes into account the mirror/light radiation pressure interaction only if mediated by cavity modes; indeed the subject is often called *cavity optmechanics* [4, 6]. This is due to the fact that some interesting physical phenomena as laser cooling appear when a cavity mode is involved [3–6, 14], but also to the fact that a way to describe at a quantum level the direct scattering of laser light by a vibrating mirror is lacking. In this respect, another advantage of the HP-equation is that it allows also for the description of scattering processes [15, 16]. Section 3 introduces, into the HP-equation describing the mechanical oscillator, the radiation pressure interaction due to a laser directly illuminating the mirror. Finally, in Section 4, we show how to describe the heterodyne detection of the reflected light and we study the properties of the resulting power spectrum; this last step involves also the theory of measurements in continuous time [17–22]. In particular we show that, for a weak probe laser, the model produces explicit expressions for the spectrum due to elastic scattering of the photons and for the *side-bands* due to *Stokes and anti-Stokes scattering*.

We end this introduction by recalling the HP-equation and some related notions. We give a short, heuristic presentation; a mathematically rigourous formulation of quantum stochastic calculus, HP-equations and related notions can be found in [11, 12, 19, 21, 23]. Firstly, we introduce the formal fields $b_k(t)$, $b_k^\dagger(t)$, $t \in \mathbb{R}$, $k = 1 \dots d$, satisfying the canonical commutation rules (CCRs)

$$\left[b_i(s), b_k^\dagger(t)\right] = \delta_{ik}\delta(t-s), \qquad [b_i(s), b_k(t)] = 0. \tag{1}$$

In this paper we consider only the representation of the CCRs (1) on the Fock space, the one characterized by the existence of the vacuum state. For quantum stochastic calculus involving non-Fock representations see, for instance, [24]. Let us introduce the Hilbert space $L^2(\mathbb{R})\otimes\mathbb{C}^d = L^2(\mathbb{R};\mathbb{C}^d)$ (the one-particle space) and its symmetrized powers $L^2(\mathbb{R};\mathbb{C}^d)^{\otimes_s n}$ (the n-particle space). We denote by $\Gamma \equiv \Gamma\big(L^2(\mathbb{R};\mathbb{C}^d)\big)$ the *symmetric Fock space* over $L^2(\mathbb{R};\mathbb{C}^d)$, i.e. $\Gamma = \mathbb{C}\oplus\sum_{n=1}^{\infty} L^2(\mathbb{R};\mathbb{C}^d)^{\otimes_s n}$, and by $\psi(f)$, $f \in L^2(\mathbb{R};\mathbb{C}^d)$, the *coherent vectors,* whose components in the $0, 1, \ldots, n, \ldots$ particle spaces are

$$\psi(f) := e^{-\frac{1}{2}\|f\|^2}\left(1, f, (2!)^{-1/2} f\otimes f, \ldots, (n!)^{-1/2} f^{\otimes n}, \ldots\right). \tag{2}$$

Note that $\psi(0)$ represents the vacuum state and that

$$\langle\psi(g)|\psi(f)\rangle = \exp\left\{-\frac{1}{2}\|f\|^2 - \frac{1}{2}\|g\|^2 + \langle g|f\rangle\right\}.$$

Let $\{z_k,\ k \geq 1\}$ be the canonical basis in $\mathbb{C}^d$ and for any $f \in L^2(\mathbb{R};\mathbb{C}^d)$ let us set $f_k(t) := \langle z_k|f(t)\rangle_{\mathbb{C}^d}$. Then we have $b_k(t)\,\psi(f) = f_k(t)\,\psi(f)$. By formally writing

$$B_k(t) = \int_0^t b_k(s)ds, \qquad B_k^\dagger(t) = \int_0^t b_k^\dagger(s)ds, \tag{3}$$

we get the *annihilation* and *creation processes*, families of mutually adjoint operators, whose actions on the coherent vectors are given by

$$B_k(t)\,\psi(f) = \int_0^t f_k(s)\,ds\,\psi(f), \qquad \langle\psi(g)|B_k^\dagger(t)\psi(f)\rangle = \int_0^t \overline{g_k(s)}\,ds\,\langle\psi(g)|\psi(f)\rangle;$$

the overline denotes the complex conjugation. By a property of Fock spaces, the action on the coherent vectors uniquely determines a densely defined linear operator. In terms of the integrated processes the CCRs (1) become

$$[B_k(t), B_l^\dagger(s)] = \delta_{kl}\min\{t, s\}, \qquad [B_k^\dagger(t), B_l^\dagger(s)] = [B_k(t), B_l(s)] = 0. \tag{4}$$

We introduce also the *gauge processes*

$$\Lambda_{kl}(t) = \int_0^t b_k^\dagger(s)b_l(s)ds, \qquad \langle\psi(g)|\Lambda_{kl}(t)\psi(f)\rangle = \int_0^t \overline{g_k(s)}\,f_l(s)ds\,\langle\psi(g)|\psi(f)\rangle. \tag{5}$$

The operator $\Lambda_{kk}(t)$ turns out to be a number operator and it counts the quanta present in the field k in the time interval $(0, t)$. Quantum stochastic calculus is an Itô type calculus with respect to the integrators dt, $dB_k(t)$, $dB_k^\dagger(t)$, $d\Lambda_{kl}(t)$ satisfying the Itô product rules

$$\begin{aligned} dB_k(t)dB_l^\dagger(t) &= \delta_{kl}dt, & dB_i(t)d\Lambda_{kl}(t) &= \delta_{ik}dB_l(t), \\ d\Lambda_{kl}(t)dB_i^\dagger(t) &= \delta_{li}dB_k^\dagger(t), & d\Lambda_{kl}(t)d\Lambda_{ij}(t) &= \delta_{li}d\Lambda_{kj}(t); \end{aligned} \tag{6}$$

all the other possible products vanish. We shall need also the *generalized Weyl operators* $\mathcal{W}(g; V)$, where $g \in L^2(\mathbb{R};\mathbb{C}^d)$ and V is a unitary operator on $L^2(\mathbb{R};\mathbb{C}^d)$; these are unitary operators defined by

$$\mathcal{W}(g;V)\,\psi(f)=\exp\{i\,\mathrm{Im}\langle Vf|g\rangle\}\,\psi(Vf+g),\qquad \forall f\in L^2(\mathbb{R};\mathbb{C}^d). \tag{7}$$

From the definition one obtains the composition law

$$\mathcal{W}(h;V)\,\mathcal{W}(g;U)=\exp\{-i\,\mathrm{Im}\langle h|Vg\rangle\}\,\mathcal{W}(h+Vg;VU). \tag{8}$$

In the case $V=\mathbb{1}$, it is possible to show that

$$\mathcal{W}(g;\mathbb{1})=\exp\left\{\sum_{k=1}^{d}\left(\int_{-\infty}^{+\infty}g_k(t)dB_k^\dagger(t)-\text{h.c.}\right)\right\},$$

where h.c. means Hermitian conjugate, and from (7) one sees that $\mathcal{W}(g;\mathbb{1})$ is the field analogue of what is called a displacement operator in quantum optics [22]. Instead, in the case $g=0$ in (7), we get that $\mathcal{W}(0;V)$ is the *second quantization* of the one-particle unitary operator V [11, p. 136].

Let us introduce now a quantum system with separable Hilbert space $\mathcal{H}$; let H, R_k, S_{kl} be the system operators with H self-adjoint and the operator matrix (S_{kl}) defining a unitary operator S on $\mathcal{H}\otimes\mathbb{C}^d$. Then, we consider the system/field evolution equation given by the HP-equation

$$\begin{aligned}dU(t)=\Bigg\{&\sum_k R_k\,dB_k^\dagger(t)+\sum_{kl}(S_{kl}-\delta_{kl})\,d\Lambda_{kl}(t)\\&-\sum_{kl}R_k^\dagger S_{kl}\,dB_l(t)-\left(\frac{1}{2}\sum_k R_k^\dagger R_k+iH\right)dt\Bigg\}U(t),\end{aligned} \tag{9}$$

with the initial condition $U(0)=\mathbb{1}$. When H and R_k are bounded operators there is a unique solution, which is unitary and strongly continuous in t [11]. When these operators are unbounded some restrictions are needed in order to control the domains; then, the existence, uniqueness, unitarity can be proved [12, 23]. The solution $U(t)$ gives the evolution in the interaction picture with respect to the free evolution of the field, which is modelled by the so-called left time shift $\Theta(t)$ in the Fock space; indeed, $\hat{U}(t)=\Theta(t)U(t)$, $t\geq 0$, and $\hat{U}(t)=U(-t)^\dagger\Theta(-t)^\dagger$, $t<0$, defines a strongly continuous unitary group, whose Hamiltonian has been characterized in [25].

If we now consider a generic system operator X, its evolution in the Heisenberg description is given by $X(t)=U(t)^\dagger XU(t)$. By differentiating this product according to the rules of quantum stochastic calculus, summarized by (6), and taking into account that $U(t)$ is a unitary operator, we get the *quantum Langevin equations*

$$\begin{aligned}dX(t)=&\left(i[H(t),X(t)]-\frac{1}{2}\sum_k\big(R_k(t)^\dagger[R_k(t),X(t)]+[X(t),R_k(t)^\dagger]R_k(t)\big)\right)dt\\&+\sum_{kl}S_{lk}(t)^\dagger[X(t),R_l(t)]dB_k^\dagger(t)-\sum_{kl}[X(t),R_l(t)^\dagger]S_{lk}(t)dB_k(t)\\&+\sum_{kl}\left(\sum_j S_{jk}(t)^\dagger X(t)S_{jl}(t)-\delta_{kl}\right)d\Lambda_{kl}(t).\end{aligned} \tag{10}$$

If ρ_0 is a generic statistical operator for the system and σ a field state, we can consider the reduced state of the system $\rho(t) = \mathrm{Tr}_\Gamma \left\{ U(t)\,(\rho_0 \otimes \sigma)\, U(t)^\dagger \right\}$. When σ is the vacuum state or, more generally, a coherent vector, then the reduced system state $\rho(t)$ satisfies a Markovian master equation [11, 19] with a Lindblad type generator [26]. If a more general state is taken for σ, non-Markov effects enter into play and a simple closed evolution equation for the reduced dynamics could even not exist [18, 19, 27].

Also the fields in the Heisenberg picture can be introduced [28]; these are the *output fields*

$$\begin{aligned} B_k^{\mathrm{out}}(t) =& U(t)^\dagger B_k(t) U(t), \qquad B_k^{\mathrm{out}\,\dagger}(t) = U(t)^\dagger B_k^\dagger(t) U(t), \\ & \Lambda_{kl}^{\mathrm{out}}(t) = U(t)^\dagger \Lambda_{kl}(t) U(t). \end{aligned} \tag{11}$$

The outputs fields represent the fields after the interaction with the system, while $B_k(t)$, $B_k^\dagger(t)$, $\Lambda_{kl}(t)$ are the fields before the interaction and, so, they are called *input fields*. By differentiating the products defining the output fields and using (9) and (6), we get the input/output relations [19]

$$dB_k^{\mathrm{out}}(t) = \sum_l S_{kl}(t)\, dB_k(t) + R_k(t)\, dt, \tag{12}$$

$$\begin{aligned} d\Lambda_{kl}^{\mathrm{out}}(t) = & \sum_{ij} S_{ki}(t)^\dagger S_{lj}(t)\, d\Lambda_{ij}(t) + \sum_i S_{ki}(t)^\dagger R_l(t)\, dB_i^\dagger(t) \\ & + \sum_i R_k(t)^\dagger S_{li}(t)\, dB_i(t) + R_k(t)^\dagger R_l(t)\, dt. \end{aligned} \tag{13}$$

By the properties of $U(t)$ we get $U(T)^\dagger B_k(t) U(T) = U(t)^\dagger B_k(t) U(t)$, $\forall T \geq t$, and similar equations for the other fields. This implies that the output fields satisfy the same CCRs as the input fields. Self-adjoint combinations of the output fields commuting for different times represent field observables which can be measured with continuity in time and this is the key ingredient for a quantum theory of measurements in continuous time [17, 19, 21].

2. Langevin equations for a mechanical oscillator in a thermal bath

In this section we present the description of a quantum dissipative mechanical oscillator obtained in [14, Sections 2, 3]. The Hilbert space of the system is $\mathcal{H} = L^2(\mathbb{R})$ and q and p denote the usual position and momentum operators in dimensionless units, satisfying the commutation relations $[q, p] = i$. We denote by $\Omega_{\mathrm{m}} > 0$ the bare frequency of the mechanical oscillator and by $\gamma_{\mathrm{m}} > 0$ its damping rate; we consider only the underdamped case: $\Omega_{\mathrm{m}} > \gamma_{\mathrm{m}}/2$. Then, we introduce the damped frequency ω_{m} and the phase factor τ by

$$\omega_{\mathrm{m}} = \sqrt{\Omega_{\mathrm{m}}^2 - \frac{\gamma_{\mathrm{m}}^2}{4}}, \qquad \tau = \frac{\omega_{\mathrm{m}}}{\Omega_{\mathrm{m}}} - \frac{i}{2}\frac{\gamma_{\mathrm{m}}}{\Omega_{\mathrm{m}}}. \tag{14}$$

We define now the mode operator

$$a_{\mathrm{m}} = \sqrt{\frac{\Omega_{\mathrm{m}}}{2\omega_{\mathrm{m}}}}\,(q + i\tau\, p) = \frac{1}{\sqrt{2\omega_{\mathrm{m}}\Omega_{\mathrm{m}}}}\left(\Omega_{\mathrm{m}} q + \frac{\gamma_{\mathrm{m}}}{2}\, p + i\omega_{\mathrm{m}} p\right), \tag{15}$$

satisfying the commutation rules $[a_{\mathrm{m}}, a_{\mathrm{m}}^{\dagger}] = 1$. The inverse transformation turns out to be

$$q = \sqrt{\frac{\Omega_{\mathrm{m}}}{2\omega_{\mathrm{m}}}}\left(\overline{\tau}\, a_{\mathrm{m}} + \tau a_{\mathrm{m}}^{\dagger}\right), \qquad p = i\sqrt{\frac{\Omega_{\mathrm{m}}}{2\omega_{\mathrm{m}}}}\left(a_{\mathrm{m}}^{\dagger} - a_{\mathrm{m}}\right). \tag{16}$$

We need also the self-adjoint operator

$$H_{\mathrm{m}} = \frac{\hbar\Omega_{\mathrm{m}}}{2}\left(p^2 + q^2\right) + \frac{\hbar\gamma_{\mathrm{m}}}{4}\{q, p\} = \hbar\omega_{\mathrm{m}}\left(a_{\mathrm{m}}^{\dagger} a_{\mathrm{m}} + \frac{1}{2}\right). \tag{17}$$

We introduce now the HP-equation for a mechanical oscillator in a thermal bath by taking in (9) a single field $B_1(t) \equiv B_{\mathrm{th}}(t)$ and $H = H_{\mathrm{m}}$, $R_1 = \sqrt{\gamma_{\mathrm{m}}}\, a_{\mathrm{m}}$, $S = \mathbb{1}$. By (10) the quantum Langevin equations for a_{m}, q, p turn out to be

$$da_{\mathrm{m}}(t) = -\left(i\omega_{\mathrm{m}} + \frac{\gamma_{\mathrm{m}}}{2}\right) a_{\mathrm{m}}(t)dt - \sqrt{\gamma_{\mathrm{m}}}\, dB_{\mathrm{th}}(t), \tag{18}$$

$$dq(t) = \Omega_{\mathrm{m}} p(t)dt + dC_q(t), \tag{19a}$$

$$dp(t) = -\big(\Omega_{\mathrm{m}} q(t) + \gamma_{\mathrm{m}} p(t)\big)dt + dC_p(t), \tag{19b}$$

in which we have introduced the Hermitian quantum noises

$$C_q(t) = -\sqrt{\frac{\gamma_{\mathrm{m}}\Omega_{\mathrm{m}}}{2\omega_{\mathrm{m}}}}\left(\overline{\tau}\, B_{\mathrm{th}}(t) + \tau B_{\mathrm{th}}^{\dagger}(t)\right), \quad C_p(t) = i\sqrt{\frac{\gamma_{\mathrm{m}}\Omega_{\mathrm{m}}}{2\omega_{\mathrm{m}}}}\left(B_{\mathrm{th}}(t) - B_{\mathrm{th}}^{\dagger}(t)\right). \tag{20}$$

By (4) the new noises obey the commutation rules

$$\big[C_q(t), C_p(s)\big] = i\gamma_{\mathrm{m}} \min\{t, s\}, \qquad \big[C_q(t), C_q(s)\big] = \big[C_p(t), C_p(s)\big] = 0. \tag{21}$$

Obviously, from (15), (16) we have that Eq. (18) for a_{m} is equivalent to the system (19) for q and p. By construction, due to the unitarity of $U(t)$, the commutation relations for the system operators are preserved; also a direct verification is possible by showing that the quantum stochastic differential of $[q(t), p(t)]$ vanishes due to (21). Our choice of the field state will be such that the mean values of the noises $C_q(t)$, $C_p(t)$ are vanishing and this gives that the evolution equations for the mean values of q and p coming from (19) are exactly the classical equations for an underdamped oscillator. This fact is a first justification of the choice (17) for the Hamiltonian and of the unusual connection (16) of position and momentum with the mode operator.

2.1. The field state

As field state we take the mixture of coherent states

$$\sigma_{\mathrm{th}}^{T} = \mathbb{E}[|\psi(f_T)\rangle\langle\psi(f_T)|], \qquad f_T(s) = 1_{(0,T)}(s) f(s), \tag{22}$$

where f is a complex stochastic process with locally square integrable trajectories and $\mathbb{E}$ denotes the expectation with respect to the probability law of the process f. In the argument of a coherent vector only square integrable functions are allowed, while the trajectories of the process f are only locally square integrable. So, we have introduced the cutoff T, representing a large time, which we will let tend to infinity in the final formulae describing the quantities of direct physical interest. As explained in [14, Section 3.2.1] this is a field analog of the regular P-representation for the case of discrete modes [7]. In quantum optics, mixtures of coherent vectors with respect to probability measures are interpreted as classical states. For nonclassical states signed measures are needed.

To represent the phonon bath [14] we take f to be a complex Gaussian stationary stochastic process with vanishing mean, $\mathbb{E}[f(t)] = 0$, and correlation functions

$$\mathbb{E}[f(t)\, f(s)] = 0, \qquad \mathbb{E}[\overline{f(t)}\, f(s)] =: F(t-s). \tag{23}$$

Thanks to stationarity, the function $F(t)$ is positive definite, so that according to Bochner's theorem its Fourier transform

$$N(\nu) = \int_{-\infty}^{+\infty} e^{-i\nu t} F(t)\, dt \tag{24}$$

is a positive function, which we assume to be absolutely integrable, thus implying a finite power spectral density for the process. The function $N(\nu)$ will play the role of thermal noise spectrum.

By this choice of the state we get that the noises (20) have vanishing means and symmetrized quantum correlations given by

$$\frac{\partial^2}{\partial t\, \partial s} \langle \{C_q(t), C_q(s)\} \rangle = \frac{\partial^2}{\partial t\, \partial s} \langle \{C_p(t), C_p(s)\} \rangle = \gamma_{\mathrm{m}} \frac{\Omega_{\mathrm{m}}}{\omega_{\mathrm{m}}} \left[\delta(t-s) + 2\,\mathrm{Re}\, F(t-s) \right], \tag{25}$$

$$\frac{\partial^2}{\partial t\, \partial s} \langle \{C_q(t), C_p(s)\} \rangle = 2\gamma_{\mathrm{m}}\, \mathrm{Im}\, F(t-s) - \frac{\gamma_{\mathrm{m}}^2}{2\omega_{\mathrm{m}}} \left[\delta(t-s) + 2\,\mathrm{Re}\, F(t-s) \right], \tag{26}$$

where $\langle \{C_i(t), C_j(s)\} \rangle := \lim_{T \to +\infty} \mathrm{Tr}_\Gamma(\{C_i(t), C_j(s)\} \sigma_{\mathrm{th}}^T)$. Let us stress that the noises appearing in the system (19) cannot be arbitrary. First of all the quantum Langevin equations are Heisenberg equations of motion for a unitary dynamics (even if an approximated dynamics) and unitarity implies the conservation of all commutation relations. So, the noises in (19) have to guarantee the preservation of the commutation relations $[q(t), p(t)] = i$, $\forall t \geq 0$, [7, Chapters 1, 3] by satisfying themselves suitable commutations relations (Eqs. (21) in our case). Moreover, their symmetrized correlations must be compatible with their commutators; indeed, by identifying the index q with 1 and p with 2, we must have the positivity condition

$$\sum_{i,j=1}^{2} \int_0^T dt \int_0^T ds\, \overline{h_i(t)}\, h_j(s)\, \frac{\partial^2}{\partial t\, \partial s} \langle \{C_i(t), C_j(s)\} + [C_i(t), C_j(s)] \rangle \geq 0, \qquad \forall T > 0,$$

for all choices of the test functions $h_i(t)$. Also this property is true in our case

because our noises and their correlations are an exact consequence of a unitary model and of the choice of a well defined state. This is not true in other proposals, where the positivity property above is not satisfied or divergences are introduced by ill-defined approximations; see the discussion in [14, Section 3.3].

2.2. The reduced state of the mechanical oscillator

Let ρ_0 be the initial state of the oscillator. It is easy to see that the random reduced state $\mathrm{Tr}_\Gamma\{U(t)\,(\rho_0 \otimes |\psi(f_T)\rangle\langle\psi(f_T)|)\,U(t)^\dagger\}$ satisfies an usual quantum master equation with random coefficients. But this is not true for its mean, the reduced state

$$\rho(t) = \mathrm{Tr}_\Gamma\{U(t)\rho_0 \otimes \sigma_{\mathrm{th}}^T U(t)^\dagger\}, \qquad 0 \le t < T.$$

By the properties of HP-equation there is no dependence on T as long as $T \ge t$. In any case it is possible to characterize the equilibrium state of the system by solving the linear quantum Langevin equations (19) and computing the first two moments of $q(t)$ and $p(t)$ for $t \to +\infty$. The reduced equilibrium state

$$\rho_{\mathrm{eq}} = \lim_{t\to+\infty} \lim_{T\to+\infty} \mathrm{Tr}_\Gamma \left\{U(t)\left(\rho_0 \otimes \sigma_{\mathrm{th}}^T\right) U(t)^\dagger\right\}$$

turns out [14] to be a Gaussian state with $\langle q\rangle_{\mathrm{eq}} = \langle p\rangle_{\mathrm{eq}} = 0$ and

$$\langle q^2\rangle_{\mathrm{eq}} = \langle p^2\rangle_{\mathrm{eq}} = \frac{\Omega_{\mathrm{m}}}{\omega_{\mathrm{m}}}\left(N_{\mathrm{eff}} + \frac{1}{2}\right), \qquad \langle\{q,\,p\}\rangle_{\mathrm{eq}} = -\frac{\gamma_{\mathrm{m}}}{\omega_{\mathrm{m}}}\left(N_{\mathrm{eff}} + \frac{1}{2}\right), \tag{27}$$

where

$$N_{\mathrm{eff}} := \frac{\gamma_{\mathrm{m}}}{2\pi}\int_{\mathbb{R}} \frac{N(\nu)}{\frac{\gamma_{\mathrm{m}}^2}{4} + (\omega_{\mathrm{m}} - \nu)^2}\,d\nu. \tag{28}$$

An important property of our model is that the energy equipartition in the mean holds: $\frac{\hbar\Omega_{\mathrm{m}}}{2}\langle q^2\rangle_{\mathrm{eq}} = \frac{\hbar\Omega_{\mathrm{m}}}{2}\langle p^2\rangle_{\mathrm{eq}}$. Moreover, the mean of the Hamiltonian (17) turns out to be

$$\langle H_{\mathrm{m}}\rangle_{\mathrm{eq}} = \hbar\omega_{\mathrm{m}}\left(N_{\mathrm{eff}} + \frac{1}{2}\right).$$

3. Radiation pressure interaction

We consider now the case of a mirror mounted on a vibrating structure and directly illuminated by a laser, so that it is subject to a radiation pressure force. One has to add a further interaction term into the HP-equation suitable to produce a force proportional to the photon flux in equation (19b) for p. If we consider a well-collimated laser beam and a perfect mirror, it is possible to represent the light by a single ray impinging on the mirror and reflected according to the laws of geometrical optics. So, we take $d = 2$ and $B_1(t) \equiv B_{\mathrm{th}}(t)$, $H = H_{\mathrm{m}}$, $R_1 = \sqrt{\gamma_{\mathrm{m}}}\,a_{\mathrm{m}}$, $S_{11} = 1$ as before; moreover, we add a further field $B_2(t) \equiv B_{\mathrm{em}}(t)$, representing the electromagnetic field, and we write $\Lambda_{\mathrm{em}}(t) = \Lambda_{22}(t)$. A force proportional to the rate of photon arrivals means to have a term $v\,d\Lambda_{\mathrm{em}}(t)$ in (19b); v is a coupling constant depending on the mirror/light coupling and the incidence angle. By comparing this expression

with (10) with $X = p$, one sees that we need $S_{22} \equiv S = e^{i\phi}e^{ivq}$ and $S_{12} = S_{21} = 0$, $R_2 = 0$; ϕ is a phase shift introduced by the mirror. So, the final HP-equation is

$$dU(t) = \left\{ -\frac{i}{\hbar} H_{\rm m} dt + \sqrt{\gamma_{\rm m}} \left(a_{\rm m} dB^{\dagger}_{\rm th}(t) - a^{\dagger}_{\rm m} dB_{\rm th}(t) \right) \right. \\ \left. + (S-1)\, d\Lambda_{\rm em}(t) - \frac{\gamma_{\rm m}}{2}\, a^{\dagger}_{\rm m} a_{\rm m} dt \right\} U(t), \qquad (29)$$

$$S = e^{i\phi}e^{ivq}, \quad v \in \mathbb{R}, \quad \phi \in [0, 2\pi), \qquad U(0) = \mathbb{1}.$$

From (10) one gets the relevant quantum Langevin equations

$$da_{\rm m}(t) = -\left(i\omega_{\rm m} + \frac{\gamma_{\rm m}}{2} \right) a_{\rm m}(t) dt - \sqrt{\gamma_{\rm m}}\, dB_{\rm th}(t) + i\tau v \sqrt{\frac{\Omega_{\rm m}}{2\omega_{\rm m}}}\, d\Lambda_{\rm em}(t), \qquad (30)$$

or, equivalently,

$$dq(t) = \Omega_{\rm m} p(t) dt + dC_q(t), \qquad (31a)$$

$$dp(t) = -\left(\Omega_{\rm m} q(t) + \gamma_{\rm m} p(t) \right) dt + dC_p(t) + v d\Lambda_{\rm em}(t). \qquad (31b)$$

The quantum noises $C_q(t)$ and $C_p(t)$ are given by (20). The linearity of such equations allows for an explicit solution

$$a_{\rm m}(t) = e^{-\left(i\omega_{\rm m} + \frac{\gamma_{\rm m}}{2}\right)t} a_{\rm m} - \sqrt{\gamma_{\rm m}} \int_0^t e^{-\left(i\omega_{\rm m} + \frac{\gamma_{\rm m}}{2}\right)(t-s)} dB_{\rm th}(s) \\ + i\tau v \sqrt{\frac{\Omega_{\rm m}}{2\omega_{\rm m}}} \int_0^t e^{-\left(i\omega_{\rm m} + \frac{\gamma_{\rm m}}{2}\right)(t-s)} d\Lambda_{\rm em}(s), \qquad (32)$$

leading for the position and momentum Heisenberg operators to

$$q(t) = e^{-\gamma_{\rm m} t/2} \left(q \cos \omega_{\rm m} t + \frac{\gamma_{\rm m} q + 2\Omega_{\rm m} p}{2\omega_{\rm m}} \sin \omega_{\rm m} t \right) \\ - \sqrt{\frac{\Omega_{\rm m}\gamma_{\rm m}}{2\omega_{\rm m}}} \left\{ \overline{\tau} \int_0^t e^{-\left(i\omega_{\rm m} + \frac{\gamma_{\rm m}}{2}\right)(t-s)} dB_{\rm th}(s) + \text{h.c.} \right\} \\ + \frac{\Omega_{\rm m} v}{\omega_{\rm m}} \int_0^t e^{-\frac{\gamma_{\rm m}}{2}(t-s)} \sin \omega_{\rm m} (t-s)\, d\Lambda_{\rm em}(s), \qquad (33)$$

$$p(t) = e^{-\gamma_{\rm m} t/2} \left(p \cos \omega_{\rm m} t - \frac{2\Omega_{\rm m} q + \gamma_{\rm m} p}{2\omega_{\rm m}} \sin \omega_{\rm m} t \right) \\ + \sqrt{\frac{\Omega_{\rm m}\gamma_{\rm m}}{2\omega_{\rm m}}} \left\{ i \int_0^t e^{-\left(i\omega_{\rm m} + \frac{\gamma_{\rm m}}{2}\right)(t-s)} dB_{\rm th}(s) + \text{h.c.} \right\} \\ + v \int_0^t e^{-\frac{\gamma_{\rm m}}{2}(t-s)} \left(\cos \omega_{\rm m} (t-s) - \frac{\gamma_{\rm m}}{2\omega_{\rm m}} \sin \omega_{\rm m} (t-s) \right) d\Lambda_{\rm em}(s). \qquad (34)$$

3.1. Input-output relations

We now consider the Heisenberg picture for the electromagnetic component of the field:

$$B_{\rm em}^{\rm out}(t) = U(t)^\dagger B_{\rm em}(t) U(t), \qquad \Lambda_{\rm em}^{\rm out}(t) = U(t)^\dagger \Lambda_{\rm em}(t) U(t). \tag{35}$$

By (12), (13) we get the input-output relations

$$dB_{\rm em}^{\rm out}(t) = S(t) dB_{\rm em}(t) = e^{ivq(t)+i\phi} dB_{\rm em}(t), \tag{36}$$

$$d\Lambda_{\rm em}^{\rm out}(t) = S(t)^\dagger S(t) d\Lambda_{\rm em}(t) = d\Lambda_{\rm em}(t). \tag{37}$$

Note that the number operator for the photons is not changed by the interaction with the mirror.

By using (33) the scattering operator can be decomposed as the product

$$S(t) = e^{ivq(t)+i\phi} = S_0(t) \mathcal{W}_{\rm th}(\ell_t; \mathbb{1}) \mathcal{W}_{\rm em}(0; V(t)), \tag{38}$$

where a system operator and two generalized Weyl operators appear:

$$S_0(t) = e^{i\phi} \exp\left\{ iv e^{-\gamma_{\rm m} t/2} \left(q \cos \omega_{\rm m} t + \frac{\gamma_{\rm m} q + 2\Omega_{\rm m} p}{2\omega_{\rm m}} \sin \omega_{\rm m} t \right) \right\} \overset{t\to+\infty}{\longrightarrow} e^{i\phi}, \tag{39}$$

$$\mathcal{W}_{\rm th}(\ell_t; \mathbb{1}) = \exp\left\{ \int_0^{+\infty} \ell_t(s) dB_{\rm th}^\dagger(s) - \text{h.c.} \right\}, \tag{40}$$

$$\mathcal{W}_{\rm em}(0; V(t)) = \exp\left\{ i \frac{\Omega_{\rm m} v^2}{\omega_{\rm m}} \int_0^t e^{-\frac{\gamma_{\rm m}}{2}(t-s)} \sin \omega_{\rm m} (t-s)\, d\Lambda_{\rm em}(s) \right\}, \tag{41}$$

with

$$\ell_t(\bullet) = -iv\tau \sqrt{\frac{\Omega_{\rm m}\gamma_{\rm m}}{2\omega_{\rm m}}}\, 1_{(0,t)}(\bullet) e^{(i\omega_{\rm m} - \frac{\gamma_{\rm m}}{2})(t-\bullet)}, \tag{42}$$

$$\begin{aligned} \big(V(t)u\big)(s) &= V(s;t)u(s), \qquad \forall u \in L^2(\mathbb{R}), \\ V(s;t) &= \exp\left\{ iv^2 h(t-s) 1_{(0,t)}(s) \right\}, \qquad h(r) = \frac{\Omega_{\rm m}}{\omega_{\rm m}} e^{-\frac{\gamma_{\rm m}}{2} r} \sin \omega_{\rm m} r. \end{aligned} \tag{43}$$

The Weyl operator $\mathcal{W}_{\rm th}(\ell_t; \mathbb{1})$ (40) is a displacement operator with function ℓ_t (42) acting on the thermal component, while $\mathcal{W}_{\rm em}(0; V(t))$ (41) is the second quantization of the unitary operator $V(t)$ (43) and it acts only on the electromagnetic component.

3.2. The field state

Now the environment is described by a two-component field and its state must describe the phonon bath and the laser light. As the field state we take the mixture of coherent states

$$\sigma_{\rm env}^T = \mathbb{E}[|\psi(u_T)\rangle\langle\psi(u_T)|], \qquad u_T(s) = 1_{(0,T)}(s) u(s), \qquad u(s) = \begin{pmatrix} f(s) \\ g(s) \end{pmatrix}, \tag{44}$$

where f is the stochastic process described in Section 2.1 and g describes a phase-

diffusion model of a laser [18], namely

$$g(t) = \lambda e^{-i\left(\omega_0 t + \sqrt{L_p}\, W(t)\right)}, \qquad \lambda \in \mathbb{C}, \quad \omega_0 > 0, \quad L_p > 0;$$

$W(t)$ is a standard Wiener process independent from the process f. It is easy to see that

$$\lim_{T\to+\infty}\left[\left|\frac{1}{\sqrt{T}}\int_0^T e^{i\mu t} g(t)dt\right|^2\right] = \frac{|\lambda|^2 L_p}{\frac{L_p^2}{4} + (\mu-\omega_0)^2};$$

so, the laser light has carrier frequency ω_0 and Lorentzian spectrum of width L_p. A possible generalization would be to replace the constant λ by a further stochastic process $\lambda(t)$. This would allow to describe also amplitude fluctuations.

With this choice of the state, for the thermal noises C_q and C_p we have vanishing means and symmetrized correlations (25), (26), while for the electromagnetic field we get

$$\mathrm{Tr}\left\{dB_{\mathrm{em}}(t)\sigma_{\mathrm{env}}^T\right\} = \lambda e^{-\left(i\omega_0+\frac{L_p}{2}\right)t}dt, \qquad \mathrm{Tr}\left\{d\Lambda_{\mathrm{em}}(t)\sigma_{\mathrm{env}}^T\right\} = |\lambda|^2\, dt, \tag{45}$$

$$\mathrm{Tr}\left\{dB_{\mathrm{em}}^\dagger(s) dB_{\mathrm{em}}(t)\sigma_{\mathrm{env}}^T\right\} = |\lambda|^2\, e^{-i\omega_0(t-s)-\frac{L_p}{2}|t-s|}dt\, ds, \tag{46}$$

$$\mathrm{Tr}\left\{d\Lambda_{\mathrm{em}}(s)\, d\Lambda_{\mathrm{em}}(t)\sigma_{\mathrm{env}}^T\right\} = \left[\delta(t-s) + |\lambda|^2\right]|\lambda|^2\, dtds. \tag{47}$$

3.3. The equilibrium state of the mechanical oscillator

Again, we can introduce the reduced state of the mechanical oscillator

$$\rho(t) = \mathrm{Tr}_\Gamma\{U(t)\left(\rho_0\otimes\sigma_{\mathrm{env}}^T\right)U(t)^\dagger\}, \qquad 0 \le t < T,$$

and the reduced equilibrium state

$$\rho_{\mathrm{eq}} = \lim_{t\to+\infty}\lim_{T\to+\infty}\mathrm{Tr}_\Gamma\left\{U(t)\left(\rho_0\otimes\sigma_{\mathrm{env}}^T\right)U(t)^\dagger\right\}.$$

By working in the Heisenberg picture, from (32)–(34) and the moments of the fields we get easily

$$\langle p\rangle_{\mathrm{eq}} = 0, \qquad \langle q\rangle_{\mathrm{eq}} = \frac{v\,|\lambda|^2}{\Omega_{\mathrm{m}}} =: q_\infty, \qquad \langle\{q,p\}\rangle_{\mathrm{eq}} = -\frac{\gamma_{\mathrm{m}}}{\omega_{\mathrm{m}}}\left(N_{\mathrm{eff}}+\frac{1}{2}\right), \tag{48}$$

$$\langle q^2\rangle_{\mathrm{eq}} - q_\infty^2 = \langle p^2\rangle_{\mathrm{eq}} = \frac{\Omega_{\mathrm{m}}}{\omega_{\mathrm{m}}}\left(N_{\mathrm{eff}}+\frac{1}{2}\right) + \frac{|\lambda|^2 v^2}{2\gamma_{\mathrm{m}}}, \tag{49}$$

where N_{eff} is given by (28). By (49) the energy equipartition in mean holds again for the fluctuation part. Moreover, the mechanical mode occupancy is given by

$$\langle a_{\mathrm{m}}^\dagger a_{\mathrm{m}}\rangle_{\mathrm{eq}} - \frac{\Omega_{\mathrm{m}} q_\infty^2}{2\omega_{\mathrm{m}}} = N_{\mathrm{eff}} + \frac{\Omega_{\mathrm{m}} v^2\,|\lambda|^2}{2\omega_{\mathrm{m}}\gamma_{\mathrm{m}}};$$

we have also

$$\langle a_{\mathrm{m}}^2\rangle_{\mathrm{eq}} - \frac{\Omega_{\mathrm{m}} q_\infty^2}{2\omega_{\mathrm{m}}} = \frac{|\lambda|^2 v^2}{4\omega_{\mathrm{m}}\Omega_{\mathrm{m}}}\left(\frac{\gamma_{\mathrm{m}}}{2}+i\omega_{\mathrm{m}}\right) = i\tau\,\frac{|\lambda|^2 v^2}{4\omega_{\mathrm{m}}}.$$

Finally, it is possible to show that in the limiting case of constant phonon spectrum, i.e. $N(\nu) \to N_{\text{eff}}$, and no phase diffusion, i.e. $L_p \downarrow 0$, the reduced system state satisfies a Markovian master equation with the Liouville operator

$$\mathcal{L}[\rho] = -\frac{i}{\hbar}\,[H_{\text{m}},\,\rho] + \gamma_{\text{m}}\,(N_{\text{eff}}+1)\left(a_{\text{m}}\rho a_{\text{m}}^{\dagger} - \frac{1}{2}\left\{a_{\text{m}}^{\dagger}a_{\text{m}},\,\rho\right\}\right) + \gamma_{\text{m}}N_{\text{eff}}\left(a_{\text{m}}^{\dagger}\rho a_{\text{m}} - \frac{1}{2}\left\{a_{\text{m}}a_{\text{m}}^{\dagger},\,\rho\right\}\right) + |\lambda|^2\left(e^{ivq}\rho e^{-ivq} - \rho\right).$$

The last term is new and describes the momentum kicks due to the scattering of photons. The other terms of the Liouville operator have the appearance of an usual generator for the dynamics of a mode in a thermal bath; however, the important point is that the link of the mode operator with the position and momentum is not the usual one, but it is given by (15), (16) [14, Section 2.2].

4. Heterodyne detection

To get information on the mechanical oscillator we can detect in various ways and analyse the light reflected by the vibrating mirror. In the balanced heterodyne detection scheme the light coming from our system is made to beat with a strong laser field (the local oscillator). The light impinging on the mirror and the local oscillator are produced by different laser sources; the stimulating laser frequency ω_0 and the local oscillator frequency, say μ, are in general different. Moreover, the phase difference cannot be maintained stable and this erases some interference terms. It can be shown [19, Section 3.5] that the balanced heterodyne detection scheme corresponds to the measurement in continuous time of the observables

$$I(\mu;\,t) = \int_0^t \sqrt{\varkappa}\,e^{-\varkappa(t-s)/2}\,e^{i\mu s + i\alpha}\,dB_{\text{em}}(s) + \text{h.c.}, \tag{50}$$

where α is a phase depending on the optical paths and $\sqrt{\varkappa}\,e^{-\varkappa t/2}$, $\varkappa > 0$, represents the detector response function. In the Heisenberg description the observables become the "output current"

$$I_{\text{out}}(\mu;\,t) = U(t)^{\dagger} I(\mu;\,t) U(t). \tag{51}$$

By using (36) we obtain the explicit expression

$$I_{\text{out}}(\mu;\,t) = J(t) + \text{h.c.}, \qquad J(t) = \sqrt{\varkappa}\,e^{i(\alpha+\phi)}\int_0^t e^{-\frac{\varkappa}{2}(t-s)+i\mu s}e^{ivq(s)}dB_{\text{em}}(s). \tag{52}$$

By the definition of $I(\mu;\,t)$ and the properties of $U(t)$ (see the discussion at the end of Section 1) we get $[I(\mu;\,t),\,I(\mu;\,s)] = [I_{\text{out}}(\mu;\,t),\,I_{\text{out}}(\mu;\,s)] = 0$, which says that the output current at time t and the current at time s are compatible observables. Note that to change μ means to change the frequency of the local oscillator, that is to change the measuring apparatus. In general $I_{\text{out}}(\mu;\,t)$ and $I_{\text{out}}(\mu';\,s)$ do not commute, even for $t = s$.

By the rules of quantum mechanics, once one has the commuting observables $I_{\text{out}}(\mu;\,t)$, $t \geq 0$, and the system/field state $\rho_0 \otimes \sigma_{\text{env}}^{T}$, the probability law of the

stochastic process representing the output of the detection apparatus is obtained [17,19]. By taking the second moment of the output current the mean output power is obtained [14,19], and at large times it turns out to be proportional to

$$P(\mu) = \lim_{T\to+\infty} \frac{1}{T} \int_0^T \langle I_{\rm out}(\mu;t)^2\rangle_T dt, \qquad \langle\bullet\rangle_T := {\rm Tr}\left\{\bullet\ \rho_0 \otimes \sigma_{\rm env}^T\right\}; \tag{53}$$

the limit is in the sense of the distributions in μ. As a function of μ, $P(\mu)$ is known as *power spectrum*.

By using directly (53), (51), (50), (37), without computing the explicit expression of $P(\mu)$, one gets easily the "total output power"

$$\frac{1}{2\pi}\int_{\mathbb{R}} d\mu\,[P(\mu)-1] = 2\,|\lambda|^2\,. \tag{54}$$

For the sake of comparison it is interesting to have also the power spectrum of the input light,

$$P_{\rm in}(\mu) = \lim_{T\to+\infty} \frac{1}{T} \int_0^T \langle I(\mu;t)^2\rangle_T dt = 1 + \frac{2\,|\lambda|^2\,\kappa}{\frac{\kappa^2}{4} + (\mu-\omega_0)^2}, \qquad \kappa := \varkappa + L_p; \tag{55}$$

the final explicit expression in (55) is easily computed by using (46) and the CCRs. Moreover, we have immediately

$$\frac{1}{2\pi}\int_{\mathbb{R}} d\mu\,[P_{\rm in}(\mu)-1] = 2\,|\lambda|^2\,. \tag{56}$$

Let us stress that the equality of the total input and output powers is essentially due to (37).

4.1. Exact results

The explicit expression of the power spectrum can be computed, as we shall show below. Firstly, (53) reduces to

$$P(\mu) = 1 + 2 \lim_{T\to+\infty} \frac{1}{T} \int_0^T \langle J(t)^\dagger J(t)\rangle_T dt; \tag{57}$$

then, we obtain

$$\begin{aligned} P(\mu) = 1 + 4\,|\lambda|^2 \exp\left\{2\,|\lambda|^2\,{\rm Re}\int_0^{+\infty} du\left(e^{iv^2h(u)}-1\right) - \frac{\left(N_{\rm eff}+\frac{1}{2}\right)\Omega_{\rm m}}{\omega_{\rm m}}\,v^2\right\} \\ \times\,{\rm Re}\int_0^{+\infty} dt\,e^{\left(i(\mu-\omega_0)-\frac{\kappa}{2}\right)t} \exp\left\{|\lambda|^2\int_0^{+\infty} ds\left[e^{iv^2h(t+s)}-1\right]\left[e^{-iv^2h(s)}-1\right]\right. \\ \left. + \int_{\mathbb{R}} dv\,\frac{\Omega_{\rm m}\gamma_{\rm m}v^2\left[(N(v)+1)\,e^{ivt}+N(v)e^{-ivt}\right]}{4\pi\,\omega_{\rm m}\left(\frac{\gamma_{\rm m}^2}{4}+(v-\omega_{\rm m})^2\right)}\right\}, \end{aligned} \tag{58}$$

where $h(t)$ is given in (43) and $\kappa = \varkappa + L_p$. Let us stress that this is an exact result obtained from a unitary quantum evolution and the monitoring in continuous time of commuting observables. Note that in this expression the thermal contributions (the terms containing $N(\nu)$), and the electromagnetic contributions (the terms containing the function h), are completely interlaced.

4.1.1. Proof of Eqs. (57) **and** (58)

Let us sketch now the proof of the previous formulae. By (52) we have

$$\langle I_{\text{out}}(\mu;t)^2\rangle_T = 2\,\text{Re}\langle J(t)^2\rangle_T + \langle J(t)J(t)^\dagger\rangle_T + \langle J(t)^\dagger J(t)\rangle_T.$$

By the presence of the limit in (53), these terms contribute to $P(\mu)$ only with their large time behaviour. By using (36), (38)–(43), (46) we get

$$\begin{aligned}
\langle J(t)^2\rangle_T &\simeq \varkappa\lambda^2 e^{2i(\alpha+\phi)} \int_0^t ds \int_0^t dr\, e^{-\varkappa\left(t-\frac{s+r}{2}\right)+i\left(\mu-\omega_0\right)(s+r)-\frac{L_p}{2}|s-r|-2L_p(s\wedge r)} \\
&\qquad \times V(s;r)\langle \mathcal{W}_{\text{th}}(\ell_s;\mathbb{1})\mathcal{W}_{\text{th}}(\ell_r;\mathbb{1})\rangle_T \langle \mathcal{W}_{\text{em}}\big(0;V(s)\big)\mathcal{W}_{\text{em}}\big(0;V(r)\big)\rangle_T, \\
\langle J(t)^\dagger J(t)\rangle_T &\simeq 2\varkappa\,|\lambda|^2\,\text{Re}\int_0^t ds \int_0^s dr\, e^{-\varkappa\left(t-\frac{s+r}{2}\right)+i\left(\mu-\omega_0\right)(s-r)-\frac{L_p}{2}(s-r)} \\
&\qquad \times \langle \mathcal{W}_{\text{th}}(\ell_r;\mathbb{1})^\dagger \mathcal{W}_{\text{th}}(\ell_s;\mathbb{1})\rangle_T \langle \mathcal{W}_{\text{em}}\big(0;V(r)\big)^\dagger \mathcal{W}_{\text{em}}\big(0;V(s)\big)\rangle_T, \qquad (59) \\
\langle J(t)J(t)^\dagger\rangle_T - 1 &\simeq 2\varkappa\,|\lambda|^2\,\text{Re}\int_0^t ds \int_0^s dr\, V(r;s) e^{-\varkappa\left(t-\frac{s+r}{2}\right)+i\left(\mu-\omega_0\right)(s-r)-\frac{L_p}{2}(s-r)} \\
&\qquad \times \langle \mathcal{W}_{\text{th}}(\ell_s;\mathbb{1})\mathcal{W}_{\text{th}}(\ell_r;\mathbb{1})^\dagger\rangle \langle \mathcal{W}_{\text{em}}\big(0;V(s)\big)\mathcal{W}_{\text{em}}\big(0;V(r)\big)^\dagger\rangle_T.
\end{aligned}$$

Then, one can check that $\lim_{t\to+\infty}\lim_{T\to+\infty}\langle J(t)^2\rangle_T = 0$. Moreover, by using the composition law (8) for generalized Weyl operators and (42), (43), we get

$$\mathcal{W}_{\text{em}}\big(0;V(s)\big)\mathcal{W}_{\text{em}}\big(0;V(r)\big)^\dagger = \mathcal{W}_{\text{em}}\big(0;V(r)\big)^\dagger \mathcal{W}_{\text{em}}\big(0;V(s)\big)$$

and, for s, r large and $s > r$,

$$\begin{aligned}
V(r;s)\mathcal{W}_{\text{th}}(\ell_s;\mathbb{1})\mathcal{W}_{\text{th}}(\ell_r;\mathbb{1})^\dagger &= V(r;s)\mathcal{W}_{\text{th}}(\ell_r;\mathbb{1})^\dagger \mathcal{W}_{\text{th}}(\ell_s;\mathbb{1}) \exp\{2i\,\text{Im}\langle\ell_s|\ell_r\rangle\} \\
&\simeq \mathcal{W}_{\text{th}}(\ell_r;\mathbb{1})^\dagger \mathcal{W}_{\text{th}}(\ell_s;\mathbb{1}).
\end{aligned}$$

This gives $\langle J(t)J(t)^\dagger\rangle_T \simeq 1 + \langle J(t)^\dagger J(t)\rangle_T$ and, so, (57) is proved.

Let us consider now (59); recall that $h(u)$ and $V(s,t)$ are given in (43) and $\ell_t(s)$ in (42). Firstly, the electromagnetic contribution gives, for $s > r$,

$$\begin{aligned}
\langle \mathcal{W}_{\text{em}}\big(0;V(r)\big)^\dagger \mathcal{W}_{\text{em}}\big(0;V(s)\big)\rangle_T &= \exp\left\{\int_0^s \left(\overline{V(u;r)}\,V(u;s) - 1\right)|\lambda|^2\,du\right\} \\
&= a(s)\,\overline{a(r)}\,\exp\left\{|\lambda|^2\int_0^r du\left[e^{iv^2h(s-u)}-1\right]\left[e^{-iv^2h(r-u)}-1\right]\right\} \\
&\simeq |a(\infty)|^2 \exp\left\{|\lambda|^2\int_0^r du\left[e^{iv^2h(s-u)}-1\right]\left[e^{-iv^2h(r-u)}-1\right]\right\},
\end{aligned}$$

with

$$a(s) = \exp\left\{|\lambda|^2 \int_0^s du \left(e^{iv^2 h(u)} - 1\right)\right\}.$$

Then, again for $s > r$ and both large, the thermal contribution gives

$$\begin{aligned}
\langle \mathcal{W}_{\rm th}(\ell_r; \mathbb{1})^\dagger \mathcal{W}_{\rm th}(\ell_s; \mathbb{1})\rangle_T &= \mathbb{E}\left[\exp\left\{2i\,\mathrm{Im}\langle f|\ell_s - \ell_r\rangle + \langle \ell_r|\ell_s\rangle - \frac{\|\ell_s\|^2 + \|\ell_r\|^2}{2}\right\}\right] \\
&= \exp\left\{-\frac{1}{2}\left(\int_0^s |\ell_s(u)|^2\,du + \int_0^r |\ell_r(u)|^2\,du\right) + \int_0^r \overline{\ell_r(u)}\,\ell_s(u)du \right. \\
&\quad \left. - \frac{1}{2\pi}\int_{\mathbb{R}} d\nu\, N(\nu)\left|\int_0^s du\, e^{iu\nu}\big(\ell_s(u) - \ell_r(u)\big)\right|^2\right\} \simeq \exp\left\{-\frac{(2N_{\rm eff}+1)\,\Omega_{\rm m} v^2}{2\omega_{\rm m}}\right. \\
&\quad \left. + \frac{\Omega_{\rm m} v^2}{2\omega_{\rm m}} e^{(i\omega_{\rm m} - \frac{\gamma_{\rm m}}{2})(s-r)} + \int_{\mathbb{R}} d\nu\, \frac{\Omega_{\rm m}\gamma_{\rm m} N(\nu) v^2 \cos\nu(s-r)}{2\pi\omega_{\rm m}\left(\frac{\gamma_{\rm m}^2}{4} + (\omega_{\rm m} - \nu)^2\right)}\right\} \\
&= \exp\left\{-\frac{(2N_{\rm eff}+1)\,\Omega_{\rm m} v^2}{2\omega_{\rm m}} + \int_{\mathbb{R}} d\nu\, \frac{\Omega_{\rm m}\gamma_{\rm m} v^2\left[(N(\nu)+1)\,e^{i\nu(s-r)} + N(\nu)e^{-i\nu(s-r)}\right]}{4\pi\omega_{\rm m}\left(\frac{\gamma_{\rm m}^2}{4} + (\omega_{\rm m} - \nu)^2\right)}\right\}.
\end{aligned}$$

By inserting these results into (59) and the expression found into (57), we get the final result (58).

4.2. Linear response

When the laser light is used as a probe to get information on the dissipative oscillator, the beam can be taken to be weak, which means $|\lambda|^2$ is small. In this case only the linear response is important and we can simplify (58) by considering only the "optical susceptibility"

$$\Sigma(\mu) := \lim_{|\lambda|\downarrow 0} \frac{P(\mu) - 1}{|\lambda|^2}.$$

By (58) the weak probe limit gives immediately

$$\begin{aligned}
\Sigma(\mu) = 4\exp\left\{-\frac{\left(N_{\rm eff} + \frac{1}{2}\right)\Omega_{\rm m}}{\omega_{\rm m}}\, v^2\right\} \mathrm{Re}\int_0^{+\infty} dt\, e^{(i(\mu-\omega_0) - \frac{\kappa}{2})t} \\
\times \exp\left\{\int_{\mathbb{R}} d\nu\, \frac{\Omega_{\rm m}\gamma_{\rm m} v^2\left[(N(\nu)+1)\,e^{i\nu t} + N(\nu)e^{-i\nu t}\right]}{4\pi\omega_{\rm m}\left(\frac{\gamma_{\rm m}^2}{4} + (\nu - \omega_{\rm m})^2\right)}\right\}. \qquad (60)
\end{aligned}$$

Now, the power spectrum is

$$P(\mu) \simeq 1 + |\lambda|^2\,\Sigma(\mu) \qquad (61)$$

and we see that in this limit the thermal contribution is completely unaffected by the electromagnetic one. So, we can use the optical probe as a mean to gain information on the mechanical occupancy spectrum $N(\nu)$.

To compute the time integral in (60) one needs to develop the last exponential in a power series. The result is much more clear when $N(\nu)$ is slowly varying in a neighbourhood of ω_{m} of width γ_{m}. In this case we can make the approximation $N(\nu) \simeq N(\omega_{\mathrm{m}})$ in the last line of (60); by (28) we have also $N_{\mathrm{eff}} \simeq N(\omega_{\mathrm{m}})$. By power expansion we get

$$\begin{aligned}\Sigma(\mu) &\simeq 4\exp\left\{-\frac{\left(N(\omega_{\mathrm{m}})+\frac{1}{2}\right)\Omega_{\mathrm{m}}}{\omega_{\mathrm{m}}}\,v^2\right\}\mathrm{Re}\int_0^{+\infty} dt\, e^{(i(\mu-\omega_0)-\frac{\kappa}{2})t} \\ &\quad\times\exp\left\{\frac{\Omega_{\mathrm{m}}v^2}{2\omega_{\mathrm{m}}}\left[(N(\omega_{\mathrm{m}})+1)\,e^{(i\omega_{\mathrm{m}}-\frac{\gamma_{\mathrm{m}}}{2})t}+N(\omega_{\mathrm{m}})e^{-(i\omega_{\mathrm{m}}+\frac{\gamma_{\mathrm{m}}}{2})t}\right]\right\} \\ &= 2\exp\left\{-\frac{\left(N(\omega_{\mathrm{m}})+\frac{1}{2}\right)\Omega_{\mathrm{m}}}{\omega_{\mathrm{m}}}\,v^2\right\} \\ &\quad\times\sum_{m=0}^{\infty}\sum_{j=0}^{m}\frac{\Omega_{\mathrm{m}}^m v^{2m}}{j!(m-j)!2^m\omega_{\mathrm{m}}^m}\,\frac{\left(N(\omega_{\mathrm{m}})+1\right)^j N(\omega_{\mathrm{m}})^{m-j}\,(\kappa+m\gamma_{\mathrm{m}})}{\frac{(\kappa+m\gamma_{\mathrm{m}})^2}{4}+[\mu-\omega_0-(m-2j)\,\omega_{\mathrm{m}}]^2}. \end{aligned} \tag{62}$$

So, $\Sigma(\mu)$ appears to be a series of peaks centred on $\omega_0 \pm n\omega_{\mathrm{m}}$ and we write

$$\Sigma(\mu) \simeq 2\exp\left\{-\frac{\left(N(\omega_{\mathrm{m}})+\frac{1}{2}\right)\Omega_{\mathrm{m}}}{\omega_{\mathrm{m}}}\,v^2\right\}\sum_{n\in\mathbb{Z}}\Pi_n(\mu). \tag{63}$$

By reorganizing the sums we get the expressions of the various peaks and by integration their weights.

- The peak centred in ω_0,

$$\Pi_0(\mu) = \sum_{j=0}^{\infty}\frac{\Omega_{\mathrm{m}}^{2j}v^{4j}\left(N(\omega_{\mathrm{m}})+1\right)^j N(\omega_{\mathrm{m}})^j\,(\kappa+2j\gamma_{\mathrm{m}})}{(j!)^2\,4^j\omega_{\mathrm{m}}^{2j}\left[\frac{(\kappa+2j\gamma_{\mathrm{m}})^2}{4}+(\mu-\omega_0)^2\right]}; \tag{64}$$

here the term with $j=0$ represents the elastic scattering of photons, while a term with $j>0$ represents the scattering of a photon with exchange with the mechanical oscillator of j energy quanta ω_{m}. The weight of the peak is

$$\frac{1}{2\pi}\int_{\mathbb{R}}\Pi_0(\mu)d\mu = \sum_{j=0}^{\infty}\frac{1}{(j!)^2}\left(\frac{\Omega_{\mathrm{m}}^2v^4\left(N(\omega_{\mathrm{m}})+1\right)N(\omega_{\mathrm{m}})}{4\omega_{\mathrm{m}}^2}\right)^j. \tag{65}$$

For $N(\omega_{\mathrm{m}})=0$ the previous formulae reduce to

$$\Pi_0(\mu) = \frac{\kappa}{\frac{\kappa^2}{4}+(\mu-\omega_0)^2}, \qquad \frac{1}{2\pi}\int_{\mathbb{R}}\Pi_0(\mu)d\mu = 1. \tag{66}$$

- The peaks centred in $\omega_0 - n\omega_{\rm m}$, $n = 1, 2, \ldots$, (Stokes scattering),

$$\Pi_{-n}(\mu) = \sum_{j=0}^{\infty} \frac{\Omega_{\rm m}^{2j+n} v^{4j+2n} \big(N(\omega_{\rm m}) + 1\big)^{j+n} N(\omega_{\rm m})^j \big(\kappa + (2j+n)\,\gamma_{\rm m}\big)}{j!(j+n)!2^{2j+n}\omega_{\rm m}^{2j+n}\left[\frac{(\kappa+(2j+n)\gamma_{\rm m})^2}{4} + (\mu - \omega_0 + n\omega_{\rm m})^2\right]}\,; \quad (67)$$

here the term with $j = 0$ represents the cession of a quantum $\omega_{\rm m}$ from the photon to the mechanical oscillator, while a term with $j > 0$ represents the same process plus the exchange of other j quanta. The weight is

$$\frac{1}{2\pi}\int_{\mathbb{R}} \Pi_{-n}(\mu)d\mu = \big(N(\omega_{\rm m}) + 1\big)^n \sum_{j=0}^{\infty} \frac{\Omega_{\rm m}^{2j+n} v^{4j+2n} \big(N(\omega_{\rm m}) + 1\big)^j N(\omega_{\rm m})^j}{j!(j+n)!2^{2j+n}\omega_{\rm m}^{2j+n}}\,. \quad (68)$$

For $N(\omega_{\rm m}) = 0$ we get

$$\Pi_{-n}(\mu) = \frac{\Omega_{\rm m}^n v^{2n} \big(\kappa + n\gamma_{\rm m}\big)}{n!2^n\omega_{\rm m}^n\left[\frac{(\kappa+n\gamma_{\rm m})^2}{4} + (\mu - \omega_0 + n\omega_{\rm m})^2\right]}\,, \quad (69)$$

$$\frac{1}{2\pi}\int_{\mathbb{R}} \Pi_{-n}(\mu)d\mu = \frac{\Omega_{\rm m}^n v^{2n}}{n!2^n\omega_{\rm m}^n}. \quad (70)$$

- The peaks centred in $\omega_0 + n\omega_{\rm m}$, $n = 1, 2, \ldots$, (anti-Stokes scattering),

$$\Pi_{n}(\mu) = \sum_{j=0}^{\infty} \frac{\Omega_{\rm m}^{2j+n} v^{4j+2n} \big(N(\omega_{\rm m}) + 1\big)^{j} N(\omega_{\rm m})^{j+n} \big(\kappa + (2j+n)\,\gamma_{\rm m}\big)}{j!(j+n)!2^{2j+n}\omega_{\rm m}^{2j+n}\left[\frac{(\kappa+(2j+n)\gamma_{\rm m})^2}{4} + (\mu - \omega_0 - n\omega_{\rm m})^2\right]}\,, \quad (71)$$

here the term with $j = 0$ represents the cession of a quantum $\omega_{\rm m}$ from the mechanical oscillator to the photon, while a term with $j > 0$ represents the same process plus the exchange of other j quanta. Note that the weight turns out to be

$$\frac{1}{2\pi}\int_{\mathbb{R}} \Pi_{n}(\mu)d\mu = \left(\frac{N(\omega_{\rm m})}{N(\omega_{\rm m}) + 1}\right)^n \frac{1}{2\pi}\int_{\mathbb{R}} \Pi_{-n}(\mu)d\mu. \quad (72)$$

For $N(\omega_{\rm m}) = 0$ we get $\Pi_n(\mu) = 0$.

The asymmetry between Stokes and anti-Stokes scattering is the base for using the optical probe as a device for thermometry at low temperatures. Indeed, we have

$$N(\omega_{\rm m}) = \frac{\int_{\mathbb{R}} \Pi_1(\mu)d\mu}{\int_{\mathbb{R}} \Pi_{-1}(\mu)d\mu - \int_{\mathbb{R}} \Pi_1(\mu)d\mu} \quad (73)$$

and this quantity can be estimated by the area under the curve of the experimental data when the peaks in $\omega_0 \pm \omega_{\rm m}$ are well separated from the elastic peak in ω_0, which means that the widths $\gamma_{\rm m}$ and $\kappa = \varkappa + L_p$ are sufficiently small. The *resolved-sideband thermometry* is a technique already used in somewhat similar situations [4, 6].

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ENTROPIC FLUCTUATIONS IN GAUSSIAN DYNAMICAL SYSTEMS

V. JAKŠIĆ

Department of Mathematics and Statistics, McGill University,
805 Sherbrooke Street West, Montreal, QC, H3A 2K6, Canada
(e-mail: jaksic@math.mcgill.ca)

C.-A. PILLET

Aix-Marseille Université, CNRS UMR 7332, CPT, 13288 Marseille, France
Université de Toulon, CNRS UMR 7332, CPT, 83957 La Garde, France
(e-mail: pillet@univ-tln.fr)

and

A. SHIRIKYAN

Department of Mathematics, University of Cergy–Pontoise,
CNRS UMR 8088, 2 avenue Adolphe Chauvin, 95302 Cergy–Pontoise, France
(e-mail: Armen.Shirikyan@u-cergy.fr)

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We study nonequilibrium statistical mechanics of a Gaussian dynamical system and compute in closed form the large deviation functionals describing the fluctuations of the entropy production observable with respect to the reference state and the nonequilibrium steady state. The entropy production observable of this model is an unbounded function on the phase space, and its large deviation functionals have a surprisingly rich structure. We explore this structure in some detail.

Keywords: nonequilibrium statistical mechanics, entropy production, Gallavotti–Cohen symmetry, fluctuation relations, large deviations.

1. Introduction

In this paper, we prove and elaborate the results announced in Section 9 of [23]. We consider a dynamical system described by a real separable Hilbert space $\mathcal{K}$ and the equation of motion

$$\frac{d}{dt}x_t = \mathcal{L}x_t, \qquad x_0 \in \mathcal{K}, \tag{1}$$

where $\mathcal{L}$ is a bounded linear operator on $\mathcal{K}$. Let D be a strictly positive bounded symmetric operator on $\mathcal{K}$ and $(\mathfrak{X}, \omega_D)$ the Gaussian random field over $\mathcal{K}$ with zero mean value and covariance D. Eq. (1) induces a flow $\phi_{\mathcal{L}} = \{\phi^t_{\mathcal{L}}\}$ on $\mathfrak{X}$, and our

starting point is the dynamical system $(\mathfrak{X}, \phi_{\mathcal{L}}, \omega_D)$ (its detailed construction is given in Section 2.1). We compute in closed form and under minimal regularity assumptions the nonequilibrium characteristics of this model by exploiting its Gaussian nature. In particular, we discuss the existence of a nonequilibrium steady state (NESS), compute the steady state entropy production, and study the large deviations of the entropy production observable w.r.t. both the reference state ω_D and the NESS. To emphasize the minimal mathematical structure behind the results, in the main body of the paper we have adopted an abstract axiomatic presentation. In Section 3, the results are illustrated on the example of the one-dimensional harmonic crystal. For additional information and a pedagogical introduction to the theory of entropic fluctuations in classical nonequilibrium statistical mechanics, we refer the reader to the reviews [23, 27].

There are very few models for which the large deviation functionals of the entropy production observable can be computed in a closed form, and we hope that our results may serve as a guide for future studies. In addition, an important characteristic of a Gaussian dynamical system is that its entropy production observable is an unbounded function on the phase space. This unboundedness has dramatic effects on the form and regularity properties of the large deviation functionals that require modifications of the celebrated fluctuation relations [12, 13, 15, 16]. Although this topic has received a considerable attention in the physics literature [1, 2, 6, 14, 19, 30–32], to the best of our knowledge, it has not been studied in the mathematically rigorous literature on the subject. Thus, another goal of this paper is to initiate a research program dealing with mathematical theory of extended fluctuation relations in nonequilibrium statistical mechanics, which emerge when some of the usual regularity assumptions (such as compactness of the phase space, boundedness of the entropy production observable, smoothness of the time reversal map) are not satisfied.

The paper is organized as follows. In Section 2.1 we introduce Gaussian dynamical systems. In Section 2.2 we define the entropy production observable and describe its basic properties. In Section 2.3 we introduce the NESS. Our main results are stated in Sections 2.4 and 2.5. The entropy production observable is defined as the phase space contraction rate of the reference measure ω_D under the flow $\phi_{\mathcal{L}}$, and in Section 2.6 we examine the effects of a perturbation of the reference measure on the large deviation theory. In Section 3 we illustrate our results on two classes of examples, toy models and harmonic chains. The proofs are given in Section 4.

The focus of this paper is the mathematics of the large deviation theory of the entropy production observable. The physical implications of our results will be discussed in the continuation of this paper [24].

2. The model and results

2.1. Gaussian dynamical systems

In order to setup our notation, we start with some basic facts about classical Gaussian dynamical systems. We refer the reader to [9] for a more detailed introduction to this subject.

Let Γ be a countably infinite set and

$$\mathfrak{X} = \{x = (x_n)_{n\in\Gamma} \mid x_n \in \mathbb{R}\} = \mathbb{R}^\Gamma.$$

For $x \in \mathfrak{X}$ and $I \subset \Gamma$, we denote $x_I = (x_i)_{i\in I} \in \mathbb{R}^I$. Let $l = (l_n)_{n\in\Gamma}$ be a given sequence of strictly positive numbers such that $\sum_{n\in\Gamma} l_n = 1$ (we shall call such a sequence a *weight*). Then

$$d(x, y) = \sum_{n\in\Gamma} l_n \frac{|x_n - y_n|}{1 + |x_n - y_n|}$$

is a metric on $\mathfrak{X}$ and $(\mathfrak{X}, d)$ is a complete separable metric space. Its Borel σ-algebra $\mathcal{F}$ is generated by the set of all cylinders

$$C_I(B) = \{x \in \mathfrak{X} \mid x_I \in B\},$$

where $I \subset \Gamma$ is finite and $B \subset \mathbb{R}^I$ is a Borel set.

Let ν and ω be two Borel probability measures on $\mathfrak{X}$. We shall write $\nu \ll \omega$ when ν is absolutely continuous w.r.t. ω. The corresponding Radon–Nikodym derivative is denoted by

$$\Delta_{\nu|\omega} = \frac{d\nu}{d\omega}.$$

We will also use the notation[1]

$$\ell_{\nu|\omega} = \log \Delta_{\nu|\omega}.$$

The two measures ν and ω are called equivalent, denoted $\nu \simeq \omega$, if they are mutually absolutely continuous, i.e. $\omega \ll \nu$ and $\nu \ll \omega$. We adopt the shorthand $\nu(f) = \int_{\mathfrak{X}} f d\nu$. The relative entropy of ν w.r.t. ω is defined as

$$\mathrm{Ent}(\nu|\omega) = \begin{cases} -\nu(\ell_{\nu|\omega}) & \text{if } \nu \ll \omega, \\ -\infty & \text{otherwise.} \end{cases} \tag{2}$$

We recall that $\mathrm{Ent}(\nu|\omega) \le 0$, with equality iff $\nu = \omega$. For $\alpha \in \mathbb{R}$, the relative Rényi α-entropy of ν w.r.t. ω is defined as

$$\mathrm{Ent}_\alpha(\nu|\omega) = \begin{cases} \log \omega\left(e^{\alpha \ell_{\nu|\omega}}\right) & \text{if } \nu \ll \omega, \\ -\infty & \text{otherwise.} \end{cases}$$

We denote by $\mathcal{K} \subset \mathfrak{X}$ the real Hilbert space with inner product

$$(x, y) = \sum_{n\in\Gamma} x_n y_n, \tag{3}$$

i.e. $\mathcal{K} = \ell^2_{\mathbb{R}}(\Gamma)$. The matrix elements of a linear operator A on $\ell^2_{\mathbb{R}}(\Gamma)$ w.r.t. its standard basis are denoted by A_{nm}.

[1] Throughout the paper we adopt the convention $\log x = -\infty$ for $x \le 0$.

Let $\mathfrak{X}_l, \mathfrak{X}_l^* \subset \mathfrak{X}$ be real Hilbert spaces with respective inner products

$$(x, y)_l = \sum_{n\in\Gamma} l_n x_n y_n, \qquad (x, y)_{l^*} = \sum_{n\in\Gamma} l_n^{-1} x_n y_n,$$

($\mathfrak{X}_l^*$ is the dual of $\mathfrak{X}_l$ w.r.t. the duality (3)). Clearly,

$$\mathfrak{X}_l^* \subset \mathcal{K} \subset \mathfrak{X}_l \subset \mathfrak{X},$$

with continuous and dense inclusions. All the measures on $(\mathfrak{X}, \mathcal{F})$ we will consider here will be concentrated on $\mathfrak{X}_l$.

Let D be a bounded, strictly positive operator on $\mathcal{K}$. The centered Gaussian measure of covariance D on $(\mathfrak{X}, \mathcal{F})$ is the unique Borel probability measure ω_D specified by its value on cylinders

$$\omega_D(C_I(B)) = \frac{1}{\sqrt{\det(2\pi D_I)}} \int_B e^{-\frac{1}{2}(x, D_I^{-1}x)} dx,$$

where $D_I = [D_{ij}]_{i,j\in I}$. The measure ω_D is also uniquely specified by its characteristic function

$$\mathfrak{X}_l^* \ni y \mapsto \chi(y) = \int_{\mathfrak{X}} e^{i(y,x)}\, d\omega_D(x) = e^{-(y,Dy)/2}.$$

The bound

$$\int_{\mathfrak{X}} \|x\|_l^2 d\omega_D(x) = \int_{\mathfrak{X}} \sum_{n\in\Gamma} l_n x_n^2\, d\omega_D(x) = \sum_{n\in\Gamma} l_n D_{nn} \le \|D\|, \tag{4}$$

implies that $\omega_D(\mathfrak{X} \setminus \mathfrak{X}_l) = 0$, *i.e.*, that ω_D is concentrated on $\mathfrak{X}_l$.

Let $\mathcal{T}$ be the real vector space of all trace class operators on $\mathcal{K}$ and $\|T\|_1 = \mathrm{tr}((T^*T)^{1/2})$ the trace norm on $\mathcal{T}$. The pair $(\mathcal{T}, \|\cdot\|_1)$ is a real Banach space. By the Feldman–Hajek–Shale theorem, two Gaussian measures ω_{D_1} and ω_{D_2} on $(\mathfrak{X}, \mathcal{F})$ are equivalent iff $T = D_2^{-1} - D_1^{-1} \in \mathcal{T}$. In this case, one has

$$\Delta_{\omega_{D_2}|\omega_{D_1}}(x) = \sqrt{\det(I + D_1 T)}\, e^{-(x,Tx)/2}, \tag{5}$$

$$\mathrm{Ent}(\omega_{D_2}|\omega_{D_1}) = \frac{1}{2}\mathrm{tr}\left(D_1 T (I + D_1 T)^{-1}\right) - \frac{1}{2}\log\det(I + D_1 T).$$

Note that $\det(I + D_1 T) = \det\left(I + D_1^{1/2} T D_1^{1/2}\right) = \det(D_1^{1/2} D_2^{-1} D_1^{1/2}) > 0$.

Let $\mathcal{L}$ be a bounded linear operator on $\mathcal{K}$ such that $\mathcal{L}^*\mathfrak{X}_l^* \subset \mathfrak{X}_l^*$. It follows that $\mathcal{L}$ has a continuous extension to $\mathfrak{X}_l$ which we also denote by $\mathcal{L}$. For $x \in \mathfrak{X}$ and $t \in \mathbb{R}$ we set

$$\phi_{\mathcal{L}}^t(x) = \begin{cases} e^{t\mathcal{L}}x & \text{if } x \in \mathfrak{X}_l, \\ x & \text{if } x \notin \mathfrak{X}_l. \end{cases} \tag{6}$$

The map $(t, x) \mapsto \phi_{\mathcal{L}}^t(x)$ is measurable and $\phi_{\mathcal{L}} = \{\phi_{\mathcal{L}}^t\}_{t\in\mathbb{R}}$ is a group of automorphisms of the measurable space $(\mathfrak{X}, \mathcal{F})$ describing the time evolution. We shall call $\phi_{\mathcal{L}}$ the

dynamics generated by $\mathcal{L}$ and $(\mathfrak{X}, \phi_{\mathcal{L}}, \omega_D)$ a Gaussian dynamical system. Note that for ω_D-almost all $x \in \mathfrak{X}$, $\phi_{\mathcal{L}}^t(x) = e^{t\mathcal{L}}x$ for all $t \in \mathbb{R}$.

We end this section with a simple example of a physical system fitting this abstract framework. We follow [22] and consider a one-dimensional harmonic crystal. We shall complete the analysis of this example in Section 3.2.

EXAMPLE 2.1. $\Lambda \subset \mathbb{Z}$, the crystal lattice, is a finite or infinite set of consecutive integers. The phase space and Hamiltonian of the harmonic crystal are

$$\mathbb{R}^\Lambda \oplus \mathbb{R}^\Lambda = \{(p,q) = (\{p_n\}_{n\in\Lambda}, \{q_n\}_{n\in\Lambda}) \mid p_n, q_n \in \mathbb{R}\},$$
$$H_\Lambda(p,q) = \sum_{n\in\Lambda}\left(\frac{p_n^2}{2} + \frac{q_n^2}{2} + \frac{(q_n - q_{n-1})^2}{2}\right),$$

where we set $q_n = 0$ for $n \notin \Lambda$ (Dirichlet boundary conditions). The Hamilton equations of motion are

$$\begin{pmatrix}\dot{p}\\ \dot{q}\end{pmatrix} = \mathcal{L}_\Lambda \begin{pmatrix}p\\ q\end{pmatrix},$$

where

$$\mathcal{L}_\Lambda = \begin{pmatrix}0 & -j_\Lambda\\ 1_\Lambda & 0\end{pmatrix},$$

j_Λ being the restriction of the finite difference operator

$$(jq)_n = 3q_n - q_{n+1} - q_{n-1} \tag{7}$$

to $\mathbb{R}^\Lambda$ with Dirichlet boundary condition, and 1_Λ the identity on $\mathbb{R}^\Lambda$ (which we shall later identify with the projection $\mathbb{R}^\mathbb{Z} \to \mathbb{R}^\Lambda$). Clearly, for all Λ, j_Λ is a bounded self-adjoint operator on $\ell^2_\mathbb{R}(\Lambda)$ satisfying $1 \le j_\Lambda \le 5$.

To fit this model into our abstract framework, we assume that Λ is infinite and set $\Gamma_\Lambda = \Lambda \times \mathbb{Z}_2$, $\mathfrak{X}_\Lambda = \mathbb{R}^{\Gamma_\Lambda} = \mathbb{R}^\Lambda \oplus \mathbb{R}^\Lambda$ with the weight sequence $l = (l_{n,i})_{(n,i)\in\Gamma_\Lambda}$, where $l_{n,i} = c_\Lambda(1+n^2)^{-1}$ and c_Λ is a normalization constant. One easily verifies that $\mathcal{L}_\Lambda^* \mathfrak{X}_{\Lambda l}^* \subset \mathfrak{X}_{\Lambda l}^*$ and that the dynamics of the harmonic crystal is described by the group $e^{t\mathcal{L}_\Lambda}$. Let h_Λ be the self-adjoint operator on $\mathcal{K}_\Lambda = \ell^2_\mathbb{R}(\Lambda) \oplus \ell^2_\mathbb{R}(\Lambda)$ associated to the quadratic form $2H_\Lambda$. Energy conservation implies $\mathcal{L}_\Lambda^* h_\Lambda + h_\Lambda \mathcal{L}_\Lambda = 0$. Equivalently, the operator L_Λ defined by

$$L_\Lambda = h_\Lambda^{1/2} \mathcal{L}_\Lambda h_\Lambda^{-1/2} = \begin{pmatrix}0 & -j_\Lambda^{1/2}\\ j_\Lambda^{1/2} & 0\end{pmatrix},$$

is skew-adjoint. Since $1 \le h_\Lambda \le 5$, this implies in particular that the group $e^{t\mathcal{L}_\Lambda}$ is uniformly bounded on $\mathcal{K}_\Lambda$.

2.2. Entropy production observable

Our starting point is the dynamical system $(\mathfrak{X}, \phi, \omega)$, where ϕ is the dynamics on $\mathfrak{X}$ generated by $\mathcal{L}$ and ω is the centered Gaussian measure with covariance D (from now on, $\mathcal{L}$ and D are fixed, and we shall omit explicit reference to them).

The measure ω is sometimes called the initial or the reference state of the system. Observables are measurable functions $f : \mathfrak{X} \to \mathbb{C}$. They evolve according to

$$f_t(x) = f \circ \phi^t(x).$$

The expectation of an observable f at time $t \in \mathbb{R}$ is given by

$$\omega_t(f) = \omega(f_t) = \int f_t(x) d\omega(x),$$

where $\omega_t = \omega \circ \phi^{-t}$ is the centered Gaussian measure on $(\mathfrak{X}, \mathcal{F})$ with covariance

$$D_t = e^{t\mathcal{L}} D e^{t\mathcal{L}^*}.$$

D_t is a bounded strictly positive operator on $\ell^2_{\mathbb{R}}(\Gamma)$ and $\omega_t(\mathfrak{X}_l) = 1$ for all t. By the Feldman–Hajek–Shale theorem, the two measures ω_t and ω are equivalent iff $T_t := D_t^{-1} - D^{-1} \in \mathcal{T}$. We shall assume more.

(G1) The map $\mathbb{R} \ni t \mapsto T_t \in \mathcal{T}$ is differentiable at $t = 0$.

As will be seen later, this condition implies that the function $t \mapsto T_t$ is differentiable for all t. The *entropy production observable* (or *phase space contraction rate*) for $(\mathfrak{X}, \phi, \omega)$ is defined by

$$\sigma(x) = \frac{d}{dt} \ell_{\omega_t|\omega}(x)\Big|_{t=0}, \qquad x \in \mathcal{K}.$$

A simple computation shows that (cf. (37))

$$\sigma(x) = (x, \varsigma x) - \operatorname{tr}(D\varsigma), \tag{8}$$

where

$$\varsigma = -\frac{1}{2} \frac{dT_t}{dt}\Big|_{t=0}, \tag{9}$$

and the derivative is understood in the sense of $\mathcal{T}$ (in particular, $\varsigma \in \mathcal{T}$). Since $\mathcal{T}$ is continuously embedded in the Banach space of all bounded operators on $\mathcal{K}$, we have

$$\varsigma = \frac{1}{2}(\mathcal{L}^* D^{-1} + D^{-1}\mathcal{L}).$$

REMARK. If A is a self-adjoint element of $\mathcal{T}$, then the quadratic form (x, Ax) has a unique extension from $\mathcal{K}$ to an element of $L^1(\mathfrak{X}, d\omega)$. With a slight abuse of notation, we shall also denote this extension by (x, Ax) (see Lemma 4.1 below for a more precise statement). Thus, the entropy production observable (8) is a continuous function on $\mathcal{K}$ and an integrable function on $\mathfrak{X}$ w.r.t. the measure ω.

PROPOSITION 2.1. *Suppose that* (G1) *holds. Then:*

(1) *The function* $\mathbb{R} \ni t \mapsto \sigma_t \in L^1(\mathfrak{X}, d\omega)$ *is continuous.*

(2) $\ell_{\omega_t|\omega} = \int_0^t \sigma_{-s}\, ds$ *holds as the Riemann integral of a continuous* $L^1(\mathfrak{X}, d\omega)$*-valued function. It also holds for* ω*-almost every* $x \in \mathfrak{X}$ *as the Lebesgue integral of a real-valued function.*

(3) *The function* $\mathbb{R} \ni t \mapsto e^{\ell_{\omega_t|\omega}} \in L^1(\mathfrak{X}, d\omega)$ *is* C^1 *and*

$$\frac{d}{dt} e^{\ell_{\omega_t|\omega}} = e^{\ell_{\omega_t|\omega}} \sigma_{-t}. \tag{10}$$

(4) $\omega_t(\sigma) = \mathrm{tr}(\varsigma(D_t - D))$ *and in particular* $\omega(\sigma) = 0$.
(5) $\mathrm{Ent}(\omega_t|\omega) = -\int_0^t \omega_s(\sigma) ds$.

In specific examples, it may happen that only finitely many matrix elements ς_{nm} are nonzero, and in this case the map $x \mapsto \sigma(x)$ is continuous on $\mathfrak{X}$. The function σ is bounded only in the trivial case $\sigma = 0$. Note that $\sigma = 0$ iff $\omega_t = \omega$ for all t; this follows, for instance, from the cocycle property (38).

2.3. Nonequilibrium steady state

Our next assumptions are:

(G2) There are some numbers $0 < m < M < \infty$ such that $m \leq D_t \leq M$ for all $t \in \mathbb{R}$.

(G3) The following strong limits exist:

$$\mathrm{s}\text{-}\lim_{t \to \pm\infty} D_t = D_\pm.$$

It is clear that $m \leq D_\pm \leq M$, and $\mathcal{L} D_\pm + D_\pm \mathcal{L}^* = 0$. In what follows, we set

$$\delta = \frac{m}{M - m}. \tag{11}$$

REMARK. The verification of Assumptions (G2) and (G3) in concrete models generally rests on spectral and scattering theoretic arguments. The reader is referred to [22, Section 1.9] for an example. Note in particular that if Γ is a finite set, then (G2) and (G3) cannot be both satisfied. Indeed, either the spectrum of the generator $\mathcal{L}$ is purely imaginary, or it contains an eigenvalue with nonzero real part. In the first case, there exists a nonzero $u \in \mathcal{K}$ such that the function $(u, D_t u) = (e^{t\mathcal{L}^*} u, D e^{t\mathcal{L}^*} u)$ is periodic. In the second case, Assumption (G2) implies that for some nonzero $u \in \mathcal{K}$ and $t \to \infty$

$$(u, (D_t + D_{-t})u) \geq m \left(\|e^{-t\mathcal{L}^*} u\|^2 + \|e^{t\mathcal{L}^*} u\|^2 \right) \to \infty.$$

In both cases we have a contradiction to Assumption (G3).

Let $\omega_\pm$ be the centered Gaussian measure on $(\mathfrak{X}, \mathcal{F})$ with covariance $D_\pm$.

PROPOSITION 2.2. *Suppose that* (G1)–(G3) *hold. Then:*
(1) *For any bounded continuous function* $f : \mathfrak{X} \to \mathbb{R}$,

$$\lim_{t \to \pm\infty} \omega_t(f) = \omega_\pm(f).$$

(2) $\sigma \in L^1(\mathfrak{X}, d\omega_\pm)$ *and*

$$\omega_\pm(\sigma) = \lim_{t\to\pm\infty} \omega_t(\sigma) = \mathrm{tr}(\varsigma(D_\pm - D)).$$

Note that

$$\omega_+(\sigma) = \lim_{t\to\infty} \frac{1}{t}\int_0^t \omega_s(\sigma)ds = -\lim_{t\to\infty}\frac{1}{t}\mathrm{Ent}(\omega_t|\omega).$$

We shall call ω_+ the NESS and the nonnegative number $\omega_+(\sigma)$ the entropy production of $(\mathfrak{X}, \phi, \omega)$.

2.4. Entropic fluctuations with respect to the reference state

Time reversal invariance plays an important role in nonequilibrium statistical mechanics, and in particular in formulation of the fluctuation relations. Hence, we shall also consider the following hypothesis.

(G4) There exists a unitary involution $\vartheta : \mathcal{K} \to \mathcal{K}$ such that $\vartheta(\mathfrak{X}_l) \subset \mathfrak{X}_l$, $\vartheta\mathcal{L} = -\mathcal{L}\vartheta$, and $\vartheta D = D\vartheta$.

This assumption implies that $D_{-t} = \vartheta D_t \vartheta$ for all $t \in \mathbb{R}$, and thus $D_- = \vartheta D_+ \vartheta$ and $\omega_+ = \omega_- \circ \vartheta$. Moreover, it follows from definition (9) that $\vartheta\varsigma = -\varsigma\vartheta$. This in turn implies that $\mathrm{tr}(D\varsigma) = 0$ and

$$\sigma(x) = (x, \varsigma x), \qquad \omega_+(\sigma) = -\omega_-(\sigma). \tag{12}$$

For simplicity of notation and exposition, we shall state and prove our main results under the time reversal invariance assumption, which covers the cases of physical interest. With a minor modifications of the statements and the proofs, most of our results hold without this assumption. We leave these generalizations to the interested reader.

The relative Rényi entropy functional, which is defined by

$$e_t(\alpha) = \mathrm{Ent}_\alpha(\omega_t|\omega) = \log\omega(e^{\alpha\ell_{\omega_t|\omega}}), \tag{13}$$

is a priori finite only for $\alpha \in [0, 1]$. To describe its properties, we introduce the sets

$$J_t = \left\{\alpha \in \mathbb{R} \mid D^{-1} + \alpha T_t > 0\right\}, \qquad t \in \mathbb{R},$$

and denote by $\mathbb{C}_\pm$ the open upper/lower half-plane.

PROPOSITION 2.3. *Suppose that* (G1), (G2) *and* (G4) *hold. Then:*

(1) $J_t = (-\delta_t, 1 + \delta_t)$ *for some* $\delta_t \geq \delta$ *and* $J_{-t} = J_t$.

(2) *The function* $\alpha \mapsto e_t(\alpha)$ *is finite on the interval* J_t *and is equal to* $+\infty$ *for* $\alpha \notin J_t$. *Moreover, this function is convex, extends to an analytic function on the cut plane* $\mathbb{C}_+ \cup \mathbb{C}_- \cup J_t$, *and satisfies*

$$e_t(0) = e_t(1) = 0, \qquad e_t'(0) \leq 0, \qquad e_t'(1) \geq 0. \tag{14}$$

In particular, $e_t(\alpha) \leq 0$ *for* $\alpha \in [0, 1]$ *and* $e_t(\alpha) \geq 0$ *otherwise.*

(3) *The finite time Evans–Searles symmetry* $e_t(\alpha) = e_t(1-\alpha)$ *holds for all* t *and* α.

REMARK. Proposition 2.3 also holds for finite-dimensional Gaussian dynamical systems (i.e. in cases where the set Γ is finite). In particular, the finite time Evans–Searles symmetry holds for such systems. It is not hard to see that in such cases Assumption (G2) requires the spectrum of $\mathcal{L}$ to be purely imaginary and semi-simple. Assumption (G3) and the necessity of an infinite-dimensional phase space only becomes apparent when considering the large-time behaviour of the system.

We now study the statistical properties of trajectories as $t \to +\infty$. The intervals J_t do not necessarily form a monotone family, and we define the minimal interval

$$\underline{J} = \liminf_{t\to\infty} J_t = \bigcup_{T>0} \bigcap_{t>T} J_t.$$

Clearly, one has $\underline{J} = (-\underline{\delta}, 1+\underline{\delta})$, where $\underline{\delta} = \liminf_{t\to\infty} \delta_t \geq \delta$.

THEOREM 2.1. *Suppose that* (G1)–(G4) *hold.*

(1) *The limit*

$$e(\alpha) := \lim_{t\to+\infty} \frac{1}{t} e_t(\alpha) \tag{15}$$

exists for $\alpha \in \underline{J}$. *Moreover, the function* $e(\alpha)$ *is convex on the interval* $\underline{J}$ *and satisfies the relations*

$$\begin{aligned} &e(0) = e(1) = 0, && e'(0) = -\omega_+(\sigma) \leq 0, \\ &e'(1) = \omega_+(\sigma) \geq 0, && e(1-\alpha) = e(\alpha). \end{aligned} \tag{16}$$

(2) *The function* $e(\alpha)$ *extends to an analytic function on the cut plane* $\mathbb{C}_+ \cup \mathbb{C}_- \cup \underline{J}$, *and there is a unique signed Borel measure* ν *with support contained in* $\mathbb{R} \setminus \underline{J}$ *such that* $\int |r|^{-1} d|\nu|(r) < \infty$ *and*

$$e(\alpha) = -\int_{\mathbb{R}} \log\left(1 - \frac{\alpha}{r}\right) d\nu(r). \tag{17}$$

(3) *The Large Deviation Principle holds in the following form. The function*

$$I(s) = \sup_{-\alpha\in\underline{J}} \big(\alpha s - e(-\alpha)\big)$$

is convex, takes values in $[0,\infty]$, *vanishes only at* $s = \omega_+(\sigma)$, *and satisfies the Evans–Searles symmetry relation*

$$I(-s) = I(s) + s \qquad \text{for } s \in \mathbb{R}. \tag{18}$$

Moreover, there is $\varepsilon > 0$ *such that, for any open set* $\mathcal{J} \subset (-\omega_+(\sigma)-\varepsilon, \omega_+(\sigma)+\varepsilon)$, *we have*

$$\lim_{t\to\infty} \frac{1}{t} \log \omega\left(\left\{x \in \mathfrak{X} \;\middle|\; \frac{1}{t}\int_0^t \sigma_s(x)\, ds \in \mathcal{J}\right\}\right) = -\inf_{s\in\mathcal{J}} I(s). \tag{19}$$

(4) *The Central Limit Theorem holds. That is, for any Borel set* $B \subset \mathbb{R}$, *we have*

$$\lim_{t\to\infty} \omega\left(\left\{x \in \mathfrak{X} \;\middle|\; \frac{1}{\sqrt{t}} \int_0^t (\sigma_s(x) - \omega_+(\sigma))\, ds \in B\right\}\right) = \int_B e^{-x^2/2a} \frac{dx}{\sqrt{2\pi a}},$$

where $a = e''(1)$.

(5) *The strong law of large numbers holds. That is, for* ω*-a.e.* $x \in \mathfrak{X}$, *we have*

$$\lim_{t\to\infty} \frac{1}{t} \int_0^t \sigma_s(x)\, ds = \omega_+(\sigma). \tag{20}$$

REMARK 1. In general, the two limiting measures ω_- and ω_+ are distinct. This property is closely related to the strict positivity of entropy production. In fact, it follows from the second relation in (12) that if $\omega_- = \omega_+$, then $\omega_+(\sigma) = 0$ as well as $\omega_-(\sigma) = 0$, while any of these two conditions imply that the function $e(\alpha)$ vanishes on $[0, 1]$ and, hence, identically in view of analyticity.

REMARK 2. The representation of $e(\alpha)$ as a logarithmic potential of a signed measure is somewhat surprising, and its mathematical and physical significance remains to be studied in the future. The measure ν is related to the spectral measure of the operator Q (see the proof of Theorem 2.1 for more details).

Now let $\{t_n\} \subset \mathbb{R}_+$ be a sequence such that $\delta_{t_n} \to \hat{\delta}$. We define $\hat{J} = (-\hat{\delta}, 1 + \hat{\delta})$. Note that, by Proposition 2.3 (1), we have $\hat{\delta} \geq \delta$. In the case when $\hat{\delta}$ coincides with $\overline{\delta} = \limsup_{t\to\infty} \delta_t$, we write $\overline{J}$ instead of $\hat{J}$.

THEOREM 2.2. *Suppose that* (G1)–(G4) *hold and* $\{t_n\} \subset \mathbb{R}_+$ *is a sequence satisfying the above hypothesis.*

(1) *Let* $Q = D_-^{1/2}(D_-^{-1} - D_+^{-1})D_-^{1/2}$. *Then*

$$-\frac{1}{\overline{\delta}} \leq Q \leq \frac{1}{1 + \overline{\delta}}. \tag{21}$$

Furthermore, since the function $g(z) = z^{-1}\log(1 - z)$ *is analytic in the cut plane* $\mathbb{C} \setminus [1, \infty)$, *the operator-valued function*

$$E(\alpha) = -\alpha D_-^{1/2} g(\alpha Q) D_-^{1/2}, \tag{22}$$

is analytic in the cut plane $\mathbb{C}_+ \cup \mathbb{C}_- \cup \overline{J}$.

(2) *For* $\alpha \in \hat{J}$, *the following relation holds,*

$$\hat{e}(\alpha) := \lim_{n\to\infty} \frac{1}{t_n} e_{t_n}(\alpha) = \operatorname{tr}(E(\alpha)\varsigma), \tag{23}$$

and if $\alpha \in \mathbb{R}$ *is not in the closure of* $\hat{J}$, *then*

$$\limsup_{n\to\infty} \frac{1}{t_n} e_{t_n}(\alpha) = \infty. \tag{24}$$

Moreover, the function $\hat{e}(\alpha)$ *is convex on the interval* $\hat{J}$ *and satisfies relations* (16).

(3) *The Large Deviation Principle holds in the following form. The function*

$$\hat{I}(s) = \sup_{-\alpha \in \hat{J}} (\alpha s - \hat{e}(-\alpha)) \tag{25}$$

is convex, takes values in $[0, \infty]$*, vanishes only at* $s = \omega_+(\sigma)$*, and satisfies the Evans–Searles symmetry relation* (18)*. Moreover, for any open interval* $\mathcal{J} \subset \mathbb{R}$*, we have*

$$\lim_{n\to\infty} \frac{1}{t_n} \log \omega \left(\left\{ x \in \mathfrak{X} \;\middle|\; \frac{1}{t_n} \int_0^{t_n} \sigma_s(x)\, ds \in \mathcal{J} \right\} \right) = - \inf_{s \in \mathcal{J}} \hat{I}(s). \tag{26}$$

REMARK 1. The functions $\hat{e}(\alpha)$ constructed in Theorem 2.2 coincide with $e(\alpha)$ on the minimal interval $\underline{J}$. Moreover, by Part (2) of Theorem 2.2, the functions $\hat{e}$ constructed for different sequences $\{t_n\}$ must coincide on the common domain of definition.

REMARK 2. If $\overline{\delta} = \infty$, then $\hat{e}(\alpha) = e(\alpha) = 0$ for $\alpha \in \mathbb{R}$.

REMARK 3. The local Large Deviation Principle described in Part (3) of Theorem 2.1 is an immediate consequence of the local Gärtner-Ellis theorem (see Appendix A.2 in [22]). The global Large Deviation Principle described in Part (3) of Theorem 2.2 cannot be deduced from the Gärtner-Ellis theorem. Our proof of the LDP exploits heavily the Gaussian structure of the model and is motivated by Exercise 2.3.24 in [10], see also [3, 4, 8] for related results.

2.5. Entropic fluctuations with respect to the NESS

We now turn to the statistical properties of the dynamics under the limiting measures $\omega_\pm$. In view of the time-reversal invariance (G4), it suffices to study the case of one of these measures, and we shall restrict ourselves to ω_+. Let us set (cf. Part (2) of Proposition 2.1)

$$e_{t+}(\alpha) = \log \omega_+(e^{-\alpha \ell_{\omega_t|\omega}}) = \log \omega_+\big(e^{-\alpha \int_0^t \sigma_{-s}\, ds}\big) = \log \omega_+\big(e^{-\alpha \int_0^t \sigma_s\, ds}\big),$$

where the last relation follows from the invariance of ω_+ under the flow ϕ^t. Note that, *a priori*, $e_{t+}(\alpha)$ might not be finite for any $\alpha \neq 0$.

THEOREM 2.3. *Suppose that* (G1)–(G4) *hold. Then:*

(1) *For any* $t \in \mathbb{R}$*, the function* $\mathbb{R} \ni \alpha \mapsto e_{t+}(\alpha) \in (-\infty, +\infty]$ *is convex.*

(2) *The set*

$$J_t^+ = \big\{ \alpha \in \mathbb{R} \mid D_+^{-1} - \alpha T_t > 0 \big\} \tag{27}$$

is an open interval containing $(-\delta, \delta)$*, and the function* $e_{t+}(\alpha)$ *is real analytic on* J_t^+ *and takes value* $+\infty$ *on its complement.*

(3) *Let* $\underline{J}^+$ *be the interior of the set*

$$\liminf_{t\to\infty} J_t^+ = \bigcup_{T>0} \bigcap_{t>T} J_t^+.$$

Then $\underline{J}^+$ *is an open interval containing* $(-\delta, \delta)$. *Moreover, for* $\alpha \in \underline{J}^+$, *the limit*

$$e_+(\alpha) = \lim_{t\to\infty} \frac{1}{t} e_{t+}(\alpha) \tag{28}$$

exists and defines a real-analytic function on $\underline{J}^+$. *Finally, if* α *is not in the closure of* $\underline{J}^+$, *then*

$$\limsup_{t\to\infty} \frac{1}{t} e_{t+}(\alpha) = +\infty. \tag{29}$$

(4) *The Large Deviation Principle holds in the following form. The function*

$$I^+(s) = \sup_{-\alpha\in\underline{J}^+} (\alpha s - e_+(-\alpha))$$

is convex, takes values in $[0, \infty]$, *and vanishes only at* $s = \omega_+(\sigma)$. *Moreover, there is an open interval* $\mathbb{I}^+$ *containing* $\omega_+(\sigma)$ *such that, for any open set* $\mathcal{J} \subset \mathbb{I}^+$,

$$\lim_{t\to\infty} \frac{1}{t} \log \omega_+ \left(\left\{ x \in \mathfrak{X} \;\middle|\; \frac{1}{t} \int_0^t \sigma_s(x)\, ds \in \mathcal{J} \right\} \right) = - \inf_{s\in\mathcal{J}} I^+(s).$$

(5) *The Central Limit Theorem holds. That is, for any Borel set* $B \subset \mathbb{R}$,

$$\lim_{t\to\infty} \omega_+ \left(\left\{ x \in \mathfrak{X} \;\middle|\; \frac{1}{\sqrt{t}} \int_0^t (\sigma_s(x) - \omega_+(\sigma))\, ds \in B \right\} \right) = \int_B e^{-x^2/2a_+} \frac{dx}{\sqrt{2\pi a_+}},$$

where $a_+ = e_+''(0)$.

(6) *The strong law of large numbers holds. That is, for* ω_+*-a.e.* $x \in \mathfrak{X}$, *we have*

$$\lim_{n\to\infty} \frac{1}{t} \int_0^t \sigma_s(x)\, ds = \omega_+(\sigma).$$

(7) *Let* $\underline{J}$ *be as in Theorem 2.1. Then* $e_+(\alpha) = e(\alpha)$ *for* $\alpha \in \underline{J}^+ \cap \underline{J}$. *Moreover, there is an open interval* $\mathbb{J}^+ \subset \mathbb{I}^+$ *such that* $I^+(s) = I(s)$ *for* $s \in \mathbb{J}^+$.

REMARK. This theorem is a refinement of Proposition 9.5 in [23]. We point out that parts (1) and (3) of that proposition are inaccurately formulated: in part (1), the interval $(-\delta, 1+\delta)$ has to be replaced with $(-\delta, \delta)$, while in part (3) the interval $(-\langle\sigma\rangle_+ - \varepsilon, \langle\sigma\rangle_+ + \varepsilon)$ has to be replaced with $(\langle\sigma\rangle_+ - \varepsilon, \langle\sigma\rangle_+ + \varepsilon)$.

Finally, we have the following analogue of Theorem 2.2 on statistical properties of the dynamics under the limiting measure ω_+. Let $\{t_n\} \subset \mathbb{R}_+$ be an arbitrary increasing sequence going to $+\infty$ such that the intervals $J_{t_n}^+$ defined by (27) converge to a limiting interval $\hat{J}^+$.

THEOREM 2.4. *Under the hypotheses of Theorem 2.3 the following assertions hold.*

(1) *For* $\alpha \in \hat{J}^+$, *the limit*

$$\hat{e}_+(\alpha) := \lim_{n\to\infty} \frac{1}{t_n} e_{t_n+}(\alpha) \tag{30}$$

exists and defines a real-analytic function on $\hat{J}^+$. *If* α *does not belong to the closure of* $\hat{J}^+$, *then*

$$\limsup_{n\to\infty} \frac{1}{t_n} e_{t_n+}(\alpha) = \infty.$$

Moreover, $\hat{e}_+(\alpha)$ *and* $\mathrm{tr}(E(\alpha)\varsigma)$ *coincide on their common domain of definition.*

(2) *The Large Deviation Principle holds in the following form. The function*

$$\hat{I}^+(s) = \sup_{-\alpha\in\hat{J}^+} (\alpha s - \hat{e}_+(-\alpha))$$

is convex, takes values in $[0,\infty]$ *and vanishes only at* $s = \omega_+(\sigma)$. *Moreover, for any open interval* $\mathcal{J} \subset \mathbb{R}$, *we have*

$$\lim_{n\to\infty} \frac{1}{t_n} \log \omega_+ \left(\left\{ x \in \mathfrak{X} \;\middle|\; \frac{1}{t_n} \int_0^{t_n} \sigma_s(x)\, ds \in \mathcal{J} \right\} \right) = - \inf_{s\in\mathcal{J}} \hat{I}^+(s).$$

The proof of this result is completely similar to that of Theorem 2.2, and therefore we omit it.

REMARK. Unlike in the case of the Evans–Searles symmetry, there is no a priori reason why the limiting intervals $\hat{J}^+$ should be symmetric around $\alpha = \frac{1}{2}$, and indeed in all cases we know where $\hat{J}^+$ can be computed, this property does not hold. Hence, the relation $\hat{e}_+(\alpha) = \hat{e}_+(1-\alpha)$ may fail since one side may be finite and the other infinite, leading to the failure of the Gallavotti–Cohen symmetry $\hat{I}^+(-s) = \hat{I}^+(s) + s$. The fact that for unbounded entropy production observables the Gallavotti–Cohen symmetry may fail is known in the physics literature [1, 2, 6, 14, 19, 30–32]. In some of these works one can also find various prescriptions how the entropy production observable can be modified so as to restore the Gallavotti–Cohen symmetry. We shall discuss this topic in the continuation of this paper [24].

2.6. Perturbations

We shall consider the following type of perturbation of the reference state ω. Let P be a bounded self-adjoint operator on $\mathcal{K}$ such that $D^{-1} + P > 0$. To avoid trivialities, we assume that P is not the zero operator. Let

$$D^P = (D^{-1} + P)^{-1}$$

and let ω^P be the centered Gaussian measure with covariance D^P. Obviously,

$$D_t^P = (D_t^{-1} + P_t)^{-1},$$

where $P_t = e^{-t\mathcal{L}^*} P e^{-t\mathcal{L}}$. We consider the following two cases, assuming that (G1)–(G4) hold for D.

Case 1. P is a nonnegative trace class operator such that $\vartheta P = P\vartheta$, and $\operatorname{s-lim}_{t\to\pm\infty} P_t = 0$.

In this case, ω^P and ω are equivalent and (G1)–(G4) also hold for D^P. Moreover, using the superscript P to denote the objects associated with the initial measure ω^P, we easily check that

$$D_\pm^P = D_\pm, \qquad E^P(\alpha) = E(\alpha), \qquad \varsigma^P = \varsigma + \frac{1}{2}(\mathcal{L}^* P + P\mathcal{L}), \qquad \omega_+^P(\sigma^P) = \omega_+(\sigma),$$

where we used (22) to derive the second relation. We also see that the functions $e^P(\alpha)$ and $e(\alpha)$ coincide on $\underline{J} \cap \underline{J}^P$. It is possible, however, that $\underline{J}^P \neq \underline{J}$ and $\underline{J}^{+P} \neq \underline{J}^+$, and in fact the difference could be quite dramatic. Indeed, let us fix P and consider the perturbation λP for $\lambda > 0$. Pick a unit vector φ such that $P\varphi = \kappa\varphi$ with $\kappa > 0$.

We consider first the case of $\underline{J}^{\lambda P}$. One easily sees that for any $\alpha > 1$,

$$(\varphi, ((D^{\lambda P})^{-1} + \alpha T_t^{\lambda P})\varphi) \leq \frac{\alpha}{m} - \lambda\left((\alpha - 1)\kappa - \alpha(\varphi, P_t\varphi)\right). \tag{31}$$

There exists t_0 such that for $t > t_0$, $(\alpha - 1)\kappa - \alpha(\varphi, P_t\varphi) > (\alpha - 1)\kappa/2$. Hence, for $t > t_0$ and $\lambda > 2\alpha/\kappa m(\alpha - 1)$ the right-hand side of (31) is negative which implies that $\alpha > 1 + \delta_t^{\lambda P}$. Thus

$$\underline{\delta}^{\lambda P} = \liminf_{t\to\infty} \delta_t^{\lambda P} \leq \alpha - 1$$

provided $\lambda > 2\alpha/\kappa m(\alpha - 1)$. Letting now $\alpha \downarrow 1$ we conclude that

$$\lim_{\lambda\to\infty} \underline{\delta}^{\lambda P} = 0,$$

and the intervals $\underline{J}^{\lambda P}$ collapse to $[0, 1]$ in the limit $\lambda \to \infty$.

To deal with the case of $\underline{J}^{+\lambda P}$, we set $\psi_{\alpha,t} = e^{t\mathcal{L}}\varphi$ for $\alpha > 0$ and $\psi_{\alpha,t} = \varphi$ for $\alpha < 0$. A simple analysis yields

$$(\psi_{\alpha,t}, ((D_+^{\lambda P})^{-1} - \alpha T_t^{\lambda P})\psi_{\alpha,t}) \leq \frac{1 + |\alpha|}{m}\|\psi_{\alpha,t}\|^2 - \lambda|\alpha|(\kappa - (\varphi, P_t\varphi)).$$

Repeating the previous argument, one shows that the length of the interval $\underline{J}^{+\lambda P}$ goes to zero as $\lambda \to \infty$, so that the intervals $\underline{J}^{+\lambda P}$ collapse to $\{0\}$.

Case 2. $P > 0$, $\vartheta P = P\vartheta$, and $P_t = P$ for all $t \in \mathbb{R}$.

Hypotheses (G1)–(G4) again hold for D^P, and we have

$$D_+^P = (D_+^{-1} + P)^{-1}, \qquad \varsigma^P = \varsigma, \qquad \sigma^P = \sigma.$$

Replacing P with λP, it is easy to see that $\delta^{\lambda P}$, defined by (11), satisfies $\lim_{\lambda\to\infty} \delta^{\lambda P} = \infty$. Since $(-\delta^{\lambda P}, 1 + \delta^{\lambda P}) \subset \underline{J}^{\lambda P}$ and $(-\delta^{\lambda P}, \delta^{\lambda P}) \subset \underline{J}^{+\lambda P}$, we see that the intervals $\underline{J}^{\lambda P}$ and $\underline{J}^{+\lambda P}$ extend to the whole real line in the limit $\lambda \to \infty$.

3. Examples

3.1. A toy model

Suppose that the generator $\mathcal{L}$ satisfies $\mathcal{L}^* = -\mathcal{L}$, and let $\varphi \in \mathcal{K}$ be a unit vector such that the spectral measure for $\mathcal{L}$ and φ is purely absolutely continuous. Let

$$D = I + \lambda P_\varphi,$$

where $P_\varphi = (\varphi, \cdot)\varphi$ and $\lambda > -1$. Then $D_t = I + \lambda P_{\varphi_t}$, where $\varphi_t = e^{t\mathcal{L}}\varphi$ is a continuous curve of unit vectors converging weakly to zero as $t \to +\infty$. Let $\lambda_\pm = \frac{1}{2}(|\lambda| \pm \lambda)$ denote the positive/negative part of λ. One easily verifies that (G1)–(G3) hold with $m = 1 - \lambda_-$, $M = 1 + \lambda_+$ and $D_\pm = I$, so that

$$\delta = \left|\frac{1}{2} + \frac{1}{\lambda}\right| - \frac{1}{2}.$$

Without loss of generality we may assume that (G4) holds.[2] Since $(I + \lambda P_\psi)^{-1} = I - \frac{\lambda}{1+\lambda} P_\psi$ for any unit vector ψ and any $\lambda \neq -1$, we have

$$D^{-1} + \alpha T_t = I - \frac{\lambda}{1+\lambda}\left((1-\alpha)P_\varphi + \alpha P_{\varphi_t}\right),$$
$$D_+^{-1} - \alpha T_t = I - \frac{\lambda}{1+\lambda}\alpha\left(P_\varphi - P_{\varphi_t}\right).$$

Using the simple fact that for any two linearly independent unit vectors φ, ψ and all $a, b \in \mathbb{R}$,

$$\mathrm{sp}(aP_\varphi + bP_\psi) = \{0\} \cup \left\{\frac{a+b}{2} \pm \sqrt{\left(\frac{a-b}{2}\right)^2 + ab(\psi,\varphi)^2}\right\},$$

one easily shows that

$$\delta_t = \sqrt{\frac{1}{4} + \frac{1+\lambda}{\lambda^2(1-(\varphi,\varphi_t)^2)}} - \frac{1}{2}, \qquad J_t^+ = \left\{\alpha \in \mathbb{R} \,\middle|\, |\alpha| < \frac{1+\lambda}{|\lambda|\sqrt{1-(\varphi,\varphi_t)^2}}\right\}.$$

Recalling that $(\varphi, \varphi_t) \to 0$ as $t \to +\infty$ we see that for all $\lambda > -1$, $\underline{\delta} = \overline{\delta} = \delta$ and $\underline{J}^+ = (-\delta^+, \delta^+)$ where

$$\delta^+ = \frac{1+\lambda}{|\lambda|} = \begin{cases} \delta & \text{for } \lambda \in (-1, 0], \\ 1+\delta & \text{for } \lambda \in [0, \infty). \end{cases}$$

[2] That can be always achieved by replacing $\mathcal{K}$ with $\mathcal{K} \oplus \mathcal{K}$, $\mathcal{L}$ with $\mathcal{L} \oplus \mathcal{L}^*$, φ with $\frac{1}{\sqrt{2}}\varphi \oplus \varphi$, and setting $\vartheta(\psi_1 \oplus \psi_2) = \psi_2 \oplus \psi_1$.

Furthermore, evaluating relations (46) and (86) established below, we obtain

$$e_t(\alpha) = -\tfrac{1}{2}\log\left(1 + \frac{\lambda^2}{1+\lambda}\alpha(1-\alpha)\left(1-(\varphi,\varphi_t)^2\right)\right),$$

$$e_{t+}(\alpha) = -\tfrac{1}{2}\log\left(1 - \frac{\lambda^2}{(1+\lambda)^2}\alpha^2\left(1-(\varphi,\varphi_t)^2\right)\right).$$

It follows that

$$\lim_{t\to\infty}\frac{1}{t}e_t(\alpha) = \begin{cases} 0 & \text{for } |\alpha - \tfrac{1}{2}| < \tfrac{1}{2} + \delta, \\ +\infty & \text{for } |\alpha - \tfrac{1}{2}| > \tfrac{1}{2} + \delta, \end{cases}$$

$$\lim_{t\to\infty}\frac{1}{t}e_{t+}(\alpha) = \begin{cases} 0 & \text{for } |\alpha| < \delta^+, \\ +\infty & \text{for } |\alpha| > \delta^+. \end{cases}$$

Finally, one easily computes the Legendre transforms of these limiting functions,

$$I(s) = (\tfrac{1}{2} + \delta)|s| - \tfrac{1}{2}s, \qquad I^+(s) = \delta^+|s|.$$

While the first one satisfies the fluctuation relation, i.e. $I(s) + \frac{1}{2}s$ is an even function, the second one does not.

3.2. The one-dimensional crystal

We continue the discussion of Example 2.1. Our starting point is harmonic crystal on $\Lambda = \mathbb{Z}$ and in this case we drop the subscript Λ. For our purposes we will view this crystal as consisting of three parts, the left, central, and right, specified by

$$\Lambda_\ell = (-\infty, -1], \qquad \Lambda_c = \{0\}, \qquad \Lambda_r = [1, \infty).$$

In what follows we adopt the shorthands $H_{\Lambda_\ell} = H_\ell$, $h_{\Lambda_\ell} = h_\ell$, $j_{\Lambda_\ell} = j_\ell$, etc. Clearly

$$\mathfrak{X} = \mathfrak{X}_\ell \oplus \mathfrak{X}_c \oplus \mathfrak{X}_r, \qquad \mathcal{K} = \mathcal{K}_\ell \oplus \mathcal{K}_c \oplus \mathcal{K}_r,$$

where $\mathcal{K}_s = \ell^2_{\mathbb{R}}(\Lambda_s) \oplus \ell^2_{\mathbb{R}}(\Lambda_s)$ for $s = \ell, c, r$, and

$$H = H_0 + V_\ell + V_r,$$

where

$$H_0 = H_\ell + H_c + H_r$$

and $V_\ell(p,q) = -q_0 q_{-1}$, $V_r(p,q) = -q_0 q_1$.

The reference state ω is the centered Gaussian measure with covariance

$$D = D_\ell \oplus D_c \oplus D_r,$$

where

$$D_s = T_s \begin{pmatrix} I_s & 0 \\ 0 & j_s^{-1} \end{pmatrix}, \qquad s = \ell, c, r,$$

I_s is the identity on $\ell^2_{\mathbb{R}}(\Lambda_s)$, and $T_s > 0$. Thus, initially the left/right parts of the crystal are in thermal equilibrium at temperature $T_{\ell/r}$. The Hamiltonian $V_{\ell/r}$ couples the left/right parts of the crystal to the oscillator located at the site $n = 0$ and this allows for the transfer of the energy/entropy between these two parts. The entropic fluctuation theorems for this particular Gaussian dynamical system concern statistics of the energy/entropy flow between the left and right parts of the crystal.

Hypotheses (G1)–(G4) are easily verified following the arguments of Chapter 1 in the lecture notes [22] and one finds that

$$\omega_+(\sigma) = \kappa \frac{(T_\ell - T_r)^2}{T_\ell T_r},$$

where $\kappa = (\sqrt{5} - 1)/2\pi$, and

$$e(\alpha) = -\kappa \log\left(1 + \frac{(T_\ell - T_r)^2}{T_\ell T_r}\alpha(1-\alpha)\right). \tag{32}$$

Note that $e(\alpha)$ is finite on the interval $J_o = (-\delta_o, 1 + \delta_o)$, where

$$\delta_o = \frac{\min(T_\ell, T_r)}{|T_\ell - T_r|}, \tag{33}$$

and takes the value $+\infty$ outside the interval J_o. Note also that δ_o can take any value in $(0, \infty)$ for appropriate choices of $T_\ell, T_r \in (0, \infty)$. The measure ν in Part (2) of Theorem 2.1 is

$$\nu = \kappa \mathfrak{D}_{-\delta_o} + \kappa \mathfrak{D}_{1+\delta_o},$$

where $\mathfrak{D}_a$ is the Dirac measure centered at a.

We finish this section with several remarks.

REMARK 1. The intervals $\underline{J}$, $\underline{J}^+$ can be strictly smaller then J_o. To see this, fix T_c, δ_o, $\alpha > 1$, and set $T_r = (1 + \delta_o^{-1})T_\ell$ to ensure relation (33). Let $\varphi \in \mathcal{K}$ be such that $(\varphi, h_c\varphi) = 1$. One has

$$(\varphi, (D^{-1} + \alpha T_t)\varphi) = \sum_s \frac{1}{T_s}\left((1-\alpha)(\varphi, h_s\varphi) + \alpha(\varphi_t, h_s\varphi_t)\right),$$

where $\varphi_t = e^{-t\mathcal{L}}\varphi$. Since the skew-adjoint operator L has purely absolutely continuous spectrum and h_c is compact, there exists $t_0 > 0$ such that

$$(\varphi_t, h_c\varphi_t) = (e^{-tL}h^{1/2}\varphi, h^{-1/2}h_c h^{-1/2}e^{-tL}h^{1/2}\varphi) < \frac{\alpha - 1}{2\alpha}$$

for all $t > t_0$. Moreover, since the Hamiltonian flow is uniformly bounded there exists a constant C such that

$$\frac{1}{T_{\ell/r}}\left((1-\alpha)(\varphi, h_{\ell/r}\varphi) + \alpha(\varphi_t, h_{\ell/r}\varphi_t)\right) \le C\frac{\alpha}{T_\ell}.$$

Summing up, if $T_\ell > 4CT_c\alpha/(\alpha-1)$, then

$$(\varphi, (D^{-1}+\alpha T_t)\varphi) \le \frac{1-\alpha}{2T_c} + 2C\frac{\alpha}{T_\ell} < 0,$$

for all $t > t_0$ and hence $\underline{\delta} < \alpha$. Thus, in the limit $T_\ell \to \infty$ the interval $\underline{J}$ collapses to $[0,1]$. In a similar way one can show that in the same limit the interval $\underline{J}^+$ collapses to $\{0\}$. On the other hand, arguing as in the Case 2 of Section 2.6, one can always take $T_{\ell/r}, T_c \to 0$ in such a way that in this limit the intervals $\underline{J}$, $\underline{J}^+$ extend to the whole real line.

REMARK 2. Somewhat surprisingly, even in the simplest example of the harmonic crystal discussed in this section, it appears difficult to effectively estimate the location of the intervals $\underline{J}$, $\underline{J}^+$ outside of the perturbative regimes. In particular, the subtleties regarding the location of these sets were overlooked in Sections 1.11, 1.14 and 1.15 of the lecture notes [22]. These difficulties raise many interesting questions and we leave the complete analysis of these aspects as an open problem.

REMARK 3. An interesting question is whether one can find P such that for the perturbed reference state ω^P as defined in Section 2.6 one has $\underline{J} = J_o$. That can be done as follows. Set $\beta_s = 1/T_s$, suppose that $\beta_r > \beta_\ell$ and let

$$P = \begin{pmatrix} (\beta_r - \beta_c)1_c & 0 \\ 0 & (\beta_r + 2\beta_\ell - 3\beta_c)j_c + \beta_\ell v_\ell + \beta_r v_r \end{pmatrix},$$

where $v_{\ell/r}$ denotes the self-adjoint operator associated with the quadratic form $2V_{\ell/r}$. One easily checks that

$$D^P = (\beta_r h - X h_\ell^{(N)})^{-1},$$

where $X = \beta_r - \beta_\ell > 0$,

$$h_\ell^{(N)} = \begin{pmatrix} 1_{\Lambda_\ell \cup \Lambda_c} & 0 \\ 0 & j_\ell^{(N)} \end{pmatrix},$$

and $j_\ell^{(N)}$ denotes the restriction of the operator (7) to $\mathbb{R}^{\Lambda_\ell \cup \Lambda_c}$ with Neumann boundary condition. We are concerned with the interval

$$J_t^P = \{\alpha \in \mathbb{R} \,|\, (D^P)^{-1} + \alpha T_t^P > 0\}.$$

Since

$$(D_t^P)^{-1} = \beta_r h - X e^{-t\mathcal{L}^*} h_\ell^{(N)} e^{-t\mathcal{L}} = h^{1/2}\left(\beta_r - X e^{tL} h^{-1/2} h_\ell^{(N)} h^{-1/2} e^{-tL}\right) h^{1/2},$$

a simple computation gives

$$\begin{aligned}(D^P)^{-1} + \alpha T_t^P \\ = h^{1/2}\left(\beta_r - (1-\alpha)X h^{-1/2} h_\ell^{(N)} h^{-1/2} - \alpha X e^{tL} h^{-1/2} h_\ell^{(N)} h^{-1/2} e^{-tL}\right) h^{1/2},\end{aligned}$$

and hence

$$J_t^P = \{\alpha \in \mathbb{R} \mid \beta_r/X > (1-\alpha)h^{-1/2}h_\ell^{(N)}h^{-1/2} + \alpha e^{tL}h^{-1/2}h_\ell^{(N)}h^{-1/2}e^{-tL}\}.$$

Since $\beta_r/X = 1 + \delta_o$ and

$$0 \le h_\ell^{(N)} \le h,$$

we have that for all t,

$$(-\delta_o, 1+\delta_o) \subset J_t^P.$$

Thus, $\lim_{t\to\infty} \delta_t^P = \delta_o$ and $\underline{J}^P = J_o$.

REMARK 4. In contrast to Remark 3, we do not know whether there exists P such that for the perturbed reference state ω^P one has $\underline{J}^{+P} = J_o$.

REMARK 5. In the equilibrium case $T_\ell = T_r = T$ we have $\omega_+(\sigma) = 0$, and one may naively expect that σ does not fluctuate with respect to ω and ω_+, i.e. that $e(\alpha) = e_+(\alpha) = 0$ for all α, and that $I(s) = I^+(s) = \infty$ if $s \neq 0$. If one also takes $T_c = T$ and the perturbed reference state described in Remark 3, then $\sigma = 0$, and the above expectation is obviously correct. On the other hand, for the reference state determined by D, in the high-temperature regime $T \to \infty$, T_c fixed, the interval $\underline{J}$ collapses to $[0, 1]$ while the interval $\underline{J}^+$ collapses to $\{0\}$. Hence, in this regime, the rate functions $\hat{I}(s)$ and $\hat{I}^+(s)$ are linear for $s \le 0$ and $s \ge 0$, with the slopes of the linear parts determined by the end points of the finite intervals $\hat{J}$ and $\hat{J}^+$, and the entropy production observable has nontrivial fluctuations.

REMARK 6. The scattering theory arguments of [22] that lead to the derivation of the formula (32) extend to the case of inhomogeneous one-dimensional harmonic crystal with Hamiltonian

$$H_\Lambda(p,q) = \sum_{n\in\Lambda}\left(\frac{p_n^2}{2} + \frac{\omega_n q_n^2}{2} + \frac{\kappa_n(q_n - q_{n-1})^2}{2}\right),$$

where ω_n and κ_n are positive numbers satisfying

$$C^{-1} \le \omega_n, \kappa_n \le C \qquad \text{for all } n \in \mathbb{Z},$$

and $C \ge 1$ is a constant. In this case the operator j is the Jacobi matrix

$$(jq)_n = (\omega_n + \kappa_n + \kappa_{n+1})q_n - \kappa_n q_{n-1} - \kappa_{n+1}q_{n+1}, \qquad n \in \mathbb{Z}.$$

One easily verifies that Hypotheses (G1), (G2), and (G4) hold. If j has absolutely continuous spectrum (considered as a self-adjoint operator on $\ell^2_{\mathbb{C}}(\mathbb{Z})$), then (G3) also holds. Moreover, $\omega_+(\sigma)$ and $e(\alpha)$ can be computed in closed form in terms of the scattering data of the pair (j, j_0), where $j_0 = j_\ell \oplus j_c \oplus j_r$ (for related computations in the context of open quasi-free quantum systems we refer the reader to [21, 22, 25]). The formulae for $\omega_+(\sigma)$ and $e(\alpha)$ involve the scattering matrix of the pair (j, j_0)[3] and estimating the location of the intervals $\underline{J}$, $\underline{J}^+$ is difficult.

[3]In the case of harmonic crystal considered in this section, j is a discrete Laplacian and the absolute values of the entries of the scattering matrix of the pair (j, j_0) are either 0s or 1s. For this reason the formula (32) for $e(\alpha)$ has a particularly simple form.

However, the interesting aspect of the formula for $e(\alpha)$ is that it allows to express the measure ν in Part (2) of Theorem 2.1 in terms of the scattering data. The mathematical and physical significance of this representation remain to be studied in the future. Finally, the scattering methods can be extended to treat an arbitrary number of infinite harmonic reservoirs coupled to a finite harmonic system. The discussion of such extensions is beyond the scope of this paper.

4. Proofs

4.1. An auxiliary lemma

Using the notation and conventions of Section 2.1, we have the following simple result.

LEMMA 4.1.

(1) *If* $A = A^* \in \mathcal{T}$, *then the quadratic form* $\ell^2_{\mathbb{R}}(\Gamma) \ni x \mapsto q_A(x) = (x, Ax)$ *has a unique extension to an element of* $L^1(\mathfrak{X}, d\omega_D)$ *with a norm satisfying* $\|q_A\|_1 \le \|D\|\,\|A\|_1$. *Moreover,*

$$\int q_A(x)\, d\omega_D(x) = \operatorname{tr}(DA). \tag{34}$$

(2) *Let* $\mathbb{R} \ni t \mapsto A_t = A_t^* \in \mathcal{T}$ *be differentiable at* $t = t_0$ *and let* $\dot{A}_{t_0}$ *be its derivative. Then the map* $\mathbb{R} \ni t \mapsto q_{A_t} \in L^1(\mathfrak{X}, d\omega_D)$ *is differentiable at* $t = t_0$ *and*

$$\frac{d}{dt}\, q_{A_t}\bigg|_{t=t_0} = q_{\dot{A}_{t_0}}.$$

(3) *If* 1 *does not belong to the spectrum of* A, *then the function* $\mathcal{T} \ni X \mapsto F(X) = \det(I - X)$ *is differentiable at* $X = A$ *and its derivative is given by*

$$(\mathrm{D}_A F)(X) = -F(A)\operatorname{tr}((I - A)^{-1}X). \tag{35}$$

Proof:

Part (1) By Eq. (4), the function $x \mapsto \Phi_y(x) = (y, x)$ belongs to $L^2(\mathfrak{X}, d\omega_D)$ for $y \in \mathfrak{X}_l^*$. Moreover, Fubini's theorem yields the estimate

$$\|\Phi_y\|_2^2 = \sum_{i,j\in\Gamma} y_i y_j \int x_i x_j\, d\omega_D(x) = \sum_{i,j\in\Gamma} D_{ij} y_i y_j = (y, Dy) \le \|D\|\,\|y\|^2, \tag{36}$$

which implies that the linear map $y \mapsto \Phi_y$ has a unique extension $\Phi : \ell^2_{\mathbb{R}}(\Gamma) \to L^2(\mathfrak{X}, d\omega_D)$, such that $\|\Phi\| \le \|D\|^{1/2}$.

A self-adjoint $A \in \mathcal{T}$ has a spectral representation $A = \sum_k a_k \varphi_k(\varphi_k, \cdot)$, where the a_k are the eigenvalues of A and the corresponding eigenvectors φ_k form an orthonormal basis of $\ell^2_{\mathbb{R}}(\Gamma)$. It follows that $q_A(x) = \sum_k a_k \Phi_{\varphi_k}(x)^2$ from which we conclude that q_A extends to an element of $L^1(\mathfrak{X}, d\omega_D)$ with

$$\|q_A\|_1 \le \sum_k |a_k|\,\|\Phi_{\varphi_k}\|_2^2 \le \sum_k |a_k|\,\|D\| = \|D\|\,\|A\|_1.$$

The last equality in Eq. (36) yields

$$\int q_A(x)\, d\omega_D(x) = \sum_k a_k \, \|\Phi_{\varphi_k}\|_2^2 = \sum_k a_k(\varphi_k, D\varphi_k) = \mathrm{tr}(AD),$$

which proves the identity (34).

Part (2) It follows from Part (1) that the linear map $\mathcal{T} \ni A \mapsto q_A \in L^1(\mathfrak{X}, d\omega_D)$ is bounded and hence C^1.

Part (3) Using a well-known property of the determinant (see Theorem 3.5 in [29]), we can write

$$\begin{aligned} F(A+X) = \det(I-(A+X)) &= \det((I-A)(I-(I-A)^{-1}X) \\ &= \det(I-A)\det(I-(I-A)^{-1}X) \\ &= F(A)\det(I-(I-A)^{-1}X). \end{aligned}$$

To evaluate the second factor on the right-hand side of this identity, we apply the formula

$$\det(I+Q) = 1 + \sum_{k=1}^{\infty} \mathrm{tr}(Q^{\wedge k}),$$

where $Q^{\wedge k}$ denotes the k-th antisymmetric tensor power of Q (see [29]). Since $\|Q^{\wedge k}\|_1 \leq (k!)^{-1}\|Q\|_1^k$, one has the estimate

$$|\det(I+Q) - 1 - \mathrm{tr}(Q)| \leq e^{\|Q\|_1} - 1 - \|Q\|_1 \leq \frac{e^{\|Q\|_1}}{2}\|Q\|_1^2.$$

It follows that

$$\det(I-(I-A)^{-1}X) = 1 - \mathrm{tr}((I-A)^{-1}X) + \mathcal{O}(\|X\|_1^2),$$

as $X \to 0$ in $\mathcal{T}$. Thus, we can conclude that

$$F(A+X) - F(A) = -F(A)\,\mathrm{tr}((I-A)^{-1}X) + \mathcal{O}(\|X\|_1^2),$$

and the result follows. □

4.2. Proof of Proposition 2.1

Part (1) Up to the constant $\mathrm{tr}(D\varsigma)$ (which is well defined since $\varsigma \in \mathcal{T}$), σ is given by the quadratic form q_ς which is in $L^1(\mathfrak{X}, d\omega)$ by Lemma 4.1 (1). For $x \in \mathfrak{X}_l$, i.e. ω-a.e. $x \in \mathfrak{X}$, one has

$$\sigma_t(x) - \sigma_s(x) = \frac{1}{2}\left(x, (e^{t\mathcal{L}^*}\varsigma e^{t\mathcal{L}} - e^{s\mathcal{L}^*}\varsigma e^{s\mathcal{L}})x\right),$$

whence, setting $\varsigma_t = e^{t\mathcal{L}^*}\varsigma e^{t\mathcal{L}}$ and applying again Lemma 4.1 (1), it follows that

$$\|\sigma_t - \sigma_s\|_{L^1(\mathfrak{X}, d\omega)} \leq \frac{1}{2}\|D\|\,\|\varsigma_t - \varsigma_s\|_1.$$

Thus, it suffices to show that the function $t \mapsto \varsigma_t \in \mathcal{T}$ is continuous. This immediately follows from the norm continuity of the group $e^{t\mathcal{L}}$, the fact that $\varsigma \in \mathcal{T}$, and the well-known trace inequality $\|AB\|_1 \le \|A\|\,\|B\|_1$. We note, in particular, that

$$\|\sigma_t\|_{L^1(\mathfrak{X},d\omega)} \le \|D\|\,(1 + \|e^{t\mathcal{L}}\|^2)\,\|\varsigma\|_1 \qquad \text{for } t \in \mathbb{R}.$$

Part (2) From Eq. (5), we deduce that

$$\ell_{\omega_t|\omega} = \frac{1}{2}\log\det(I + DT_t) - \frac{1}{2}q_{T_t}. \tag{37}$$

Now note that $T_t = D_t^{-1} - D^{-1}$ satisfies the cocycle relation

$$T_{t+s} = T_t + e^{-t\mathcal{L}^*}T_s e^{-t\mathcal{L}}. \tag{38}$$

It thus follows from Assumption (G1) that the function $t \mapsto T_t \in \mathcal{T}$ is everywhere differentiable and that its derivative is given by

$$\dot{T}_t = -2\varsigma_{-t}. \tag{39}$$

Lemma 4.1 (3) and the chain rule imply that the first term on the right-hand side of (37) is a differentiable function of t. Using Eq. (35), an elementary calculation shows that

$$\frac{1}{2}\frac{d}{dt}\log\det(I + DT_t)\Big|_{t=0} = -\mathrm{tr}(D\varsigma).$$

Applying Lemma 4.1 (2) to the second term on the right-hand side of Eq. (37), one further gets

$$-\frac{1}{2}\frac{d}{dt}\,q_{T_t} = q_{\varsigma_{-t}} = q_\varsigma \circ \phi^{-t}.$$

Summing up, we have shown that

$$\frac{d}{dt}\,\ell_{\omega_t|\omega} = \sigma_{-t}, \qquad t \in \mathbb{R}.$$

Since the function $t \mapsto \sigma_{-t} \in L^1(\mathfrak{X}, d\omega)$ is continuous by Lemma 4.1 (1), and $\ell_{\omega|\omega} = 0$, we can use Riemann's integral to write

$$\ell_{\omega_t|\omega} = \int_0^t \sigma_{-s}\,ds. \tag{40}$$

The fact that, for ω-almost every $x \in \mathfrak{X}$, one has

$$\ell_{\omega_t|\omega}(x) = \int_0^t \sigma_{-s}(x)\,ds, \tag{41}$$

follows from Theorem 3.4.2 in [20].

Part (3) From the cocycle relation

$$\ell_{\omega_{t+s}|\omega} = \ell_{\omega_t|\omega} + \ell_{\omega_s|\omega} \circ \phi^{-t}, \tag{42}$$

we infer

$$\xi_s = \frac{1}{s}\left(e^{\ell_{\omega_t+s|\omega}} - e^{\ell_{\omega_t|\omega}}\right) - \sigma_{-t}\, e^{\ell_{\omega_t|\omega}} = \frac{1}{s}\left(e^{\ell_{\omega_s|\omega}} - 1 - s\sigma\right)\circ\phi^{-t}\,\frac{d\omega_t}{d\omega},$$

and hence

$$\begin{aligned}\int_{\mathfrak{X}} |\xi_s|\, d\omega &= \frac{1}{|s|}\int_{\mathfrak{X}} \left|e^{\ell_{\omega_s|\omega}} - 1 - s\sigma\right|\, d\omega \\ &\leq \frac{1}{|s|}\int_{\mathfrak{X}} \left|e^{\ell_{\omega_s|\omega}} - 1 - \ell_{\omega_s|\omega}\right|\, d\omega + \frac{1}{|s|}\int_{\mathfrak{X}} \left|\ell_{\omega_s|\omega} - s\sigma\right|\, d\omega.\end{aligned}$$

To prove that relation (10) holds in $L^1(\mathfrak{X}, d\omega)$, it suffices to show that both terms on the right-hand side of this inequality vanish in the limit $s \to 0$.

To estimate the first term we note that the inequality $e^\ell - 1 - \ell \geq 0$ (which holds for $\ell \in \mathbb{R}$) combined with Eq. (34) and (37) implies

$$\begin{aligned}\frac{1}{|s|}\int_{\mathfrak{X}} \left|e^{\ell_{\omega_s|\omega}} - 1 - \ell_{\omega_s|\omega}\right|\, d\omega &= \frac{1}{|s|}\left(\omega(e^{\ell_{\omega_s|\omega}}) - 1 - \int_{\mathfrak{X}} \ell_{\omega_s|\omega}\, d\omega\right) \\ &= \frac{1}{2}\left|\frac{1}{s}\left(\operatorname{tr}(DT_s) - \log\det(I + DT_s)\right)\right|.\end{aligned}$$

By Assumption (G1), the map $s \mapsto T_s$ is differentiable in $\mathcal{T}$ at $s = 0$. Since $T_0 = 0$, we can write

$$\lim_{s\to 0}\frac{1}{|s|}\int_{\mathfrak{X}} \left|e^{\ell_{\omega_s|\omega}} - 1 - \ell_{\omega_s|\omega}\right|\, d\omega = \frac{1}{2}\left|\frac{d}{ds}\left(\operatorname{tr}(DT_s) - \log\det(I + DT_s)\right)\Big|_{s=0}\right|.$$

Using Lemma 4.1 (3) and the chain rule, we get

$$\frac{d}{ds}\left(\operatorname{tr}(DT_s) - \log\det(I + DT_s)\right)\Big|_{s=0} = \operatorname{tr}(D\dot{T}_0) - \operatorname{tr}(D\dot{T}_0) = 0.$$

To deal with the second term, we use Eq. (40), Fubini's theorem and Lemma 4.1 (1) to write

$$\begin{aligned}\frac{1}{|s|}\int_{\mathfrak{X}} \left|\ell_{\omega_s|\omega} - s\sigma\right|\, d\omega = \int_{\mathfrak{X}} \left|\int_0^1 (\sigma_{-su} - \sigma)\, du\right| &\leq \int_0^1\int_{\mathfrak{X}} \left|q_{\varsigma_{-su}-\varsigma}\right|\, d\omega\, du \\ &\leq \|D\|\int_0^1 \|\varsigma_{-su} - \varsigma\|_1 du,\end{aligned}$$

and since the map $s \mapsto \varsigma_s$ is continuous in $\mathcal{T}$, the dominated convergence theorem yields

$$\lim_{s\to 0}\int_0^1 \|\varsigma_{-su} - \varsigma\|_1 du = 0.$$

Part (4) Relation (8) implies that

$$\omega_t(\sigma) = \omega(\sigma_t) = \int_{\mathfrak{X}} q_{\varsigma_t}\, d\omega - \operatorname{tr}(D\varsigma),$$

and formula (34) yields

$$\omega_t(\sigma) = \mathrm{tr}(D(\varsigma_t - \varsigma)) = \mathrm{tr}(\varsigma(D_t - D)).$$

Part (5) Starting from definition (2) and using the cocycle relation (42), we obtain

$$\mathrm{Ent}(\omega_t|\omega) = -\int_{\mathfrak{X}} \ell_{\omega_t|\omega}\, d\omega_t = \int_{\mathfrak{X}} \ell_{\omega_{-t}|\omega}\, d\omega.$$

Eq. (41) and Fubini's theorem further yield

$$\mathrm{Ent}(\omega_t|\omega) = \int_{\mathfrak{X}} \int_0^{-t} \sigma_{-s}\, ds d\omega = -\int_{\mathfrak{X}} \int_0^{t} \sigma_s\, ds d\omega = -\int_0^t \omega_s(\sigma)\, ds.$$

4.3. Proof of Proposition 2.2

Part (1) We have to show that ω_+, the Gaussian measure of covariance D_+, is the weak limit of the net $\{\omega_t\}_{t>0}$. Since the cylinders form a convergence determining class for Borel measures on $\mathfrak{X}$ (see Example 2.4 in [5]), it suffices to show that $\lim_{t\to\infty} \omega_t(C_I(B)) = \omega_+(C_I(B))$ holds for any finite subset $I \subset \Gamma$ and any Borel set $B \subset \mathbb{R}^I$. By Hypotheses (G2)–(G3), one has $\lim_{t\to\infty} D_{t,I} = D_{+,I}$ and

$$e^{-\frac{1}{2}(x, D_{t,I}^{-1} x)} \le e^{-\frac{\|x\|^2}{2M}},$$

for all $x \in \mathbb{R}^I$. It follows that $\lim_{t\to\infty} D_{t,I}^{-1} = D_{+,I}^{-1}$ as well as $\lim_{t\to\infty} \det(2\pi D_{t,I}) = \det(2\pi D_{+,I})$ so that

$$\lim_{t\to\infty} \frac{1}{\sqrt{\det(2\pi D_{t,I})}} \int_B e^{-\frac{1}{2}(x, D_{t,I}^{-1} x)}\, dx = \frac{1}{\sqrt{\det(2\pi D_{+,I})}} \int_B e^{-\frac{1}{2}(x, D_{+,I}^{-1} x)}\, dx,$$

holds by the dominated convergence theorem. The same argument applies to ω_-.
Part (2) Follows directly from Lemma 4.1 (1) and Proposition 2.1 (4).

4.4. Proof of Proposition 2.3

Part (1) Let us note that $\alpha \in J_t$ if and only if

$$D^{-1} + \alpha(e^{-t\mathcal{L}^*} D^{-1} e^{-t\mathcal{L}} - D^{-1}) > 0. \tag{43}$$

It follows that J_t is open. For $\theta \in [0, 1]$, we can write

$$D^{-1} + \theta\alpha(e^{-t\mathcal{L}^*} D^{-1} e^{-t\mathcal{L}} - D^{-1}) = \theta\left(D^{-1} + \alpha(e^{-t\mathcal{L}^*} D^{-1} e^{-t\mathcal{L}} - D^{-1})\right) + (1-\theta)D^{-1},$$

whence $\alpha \in J_t \Rightarrow \theta\alpha \in J_t$ and we can conclude that J_t is an interval. Multiplying (43) by ϑ from the left and the right and using the relations $\vartheta = \vartheta^* = \vartheta^{-1}$, we obtain

$$D^{-1} + \alpha(e^{t\mathcal{L}^*} D^{-1} e^{t\mathcal{L}} - D^{-1}) > 0, \tag{44}$$

whence we see that $\alpha \in J_{-t}$. By symmetry, we conclude that $J_{-t} = J_t$. Furthermore, multiplying (44) by $e^{-t\mathcal{L}^*}$ and $e^{-t\mathcal{L}}$ from the left and the right, respectively, we obtain

$$\alpha D^{-1} + (1-\alpha) e^{-t\mathcal{L}^*} D^{-1} e^{-t\mathcal{L}} > 0.$$

It follows that $1-\alpha \in J_t$, and by symmetry, we conclude that $\alpha \in J_t$ if and only if $1-\alpha \in J_t$. Thus, J_t is an open interval symmetric around $\alpha = \frac{1}{2}$.

Part (2) For any bounded operator $C > 0$ on $\ell^2_{\mathbb{R}}(\Gamma)$ and for any $\alpha, t \in \mathbb{R}$ such that $C^{-1} + \alpha T_t > 0$, formulae (5) and (37) allow us to write

$$e^{\alpha \ell_{\omega_t|\omega}}\, d\omega_C = \sqrt{\frac{\big(\det(I+DT_t)\big)^{\alpha}}{\det(I+\alpha C T_t)}}\, d\omega_{(C^{-1}+\alpha T_t)^{-1}}. \tag{45}$$

By definition $D^{-1} + \alpha T_t > 0$ for $\alpha \in (-\delta_t, 1+\delta_t)$. Taking $C = D$ in (45) and integrating over $\mathfrak{X}$, one easily checks that

$$e_t(\alpha) = \frac{\alpha}{2} \log\det(I+DT_t) - \frac{1}{2}\log\det(I+\alpha DT_t) \tag{46}$$

for all $t \in \mathbb{R}$ and $\alpha \in (-\delta_t, 1+\delta_t)$. The first term on the right-hand side of this identity is linear in α and hence entire analytic.[4] The determinant in the second term is also an entire function of α, and its logarithm is analytic on the set where the operator $I+\alpha DT_t$ is invertible; see Section IV.1 in [17]. Writing $I+\alpha DT_t = D(D^{-1}+\alpha T_t)$, we see that $I+\alpha DT_t$ is invertible for $\alpha \in J_t$. Furthermore, since

$$I + \alpha DT_t = \alpha D^{1/2}(\alpha^{-1} I + D^{1/2} T_t D^{1/2}) D^{-1/2},$$

and the operator $D^{1/2}T_tD^{1/2}$ is self-adjoint, we conclude that $I+\alpha DT_t$ is invertible for $\alpha \in \mathbb{C}\setminus\mathbb{R}$. Hence, the function $e_t(\alpha)$ is analytic in the cut plane $\mathbb{C}_+ \cup \mathbb{C}_- \cup J_t$. Its convexity is a well-known property of Rényi's relative entropy and follows from Hölder's inequality applied to Eq. (13), and relations (14) are easy to check by a direct computation.

It remains to prove that $e_t(\alpha) = +\infty$ for $\alpha \notin J_t$. To this end, we first note that the spectrum of D^{-1} is contained in the interval $[M^{-1}, m^{-1}]$ and that the operator αT_t is compact. By the Weyl theorem on essential spectrum, it follows that the intersection of the spectrum of the self-adjoint operator $D^{-1}+\alpha T_t$ with the complement of $[M^{-1}, m^{-1}]$ consists of isolated eigenvalues. Thus, if $\alpha \notin J_t$, then there are finitely many orthonormal vectors $\{\varphi_j\}$, numbers $\lambda_j \geq 0$, and an operator $B \geq cI$ with $c > 0$ such that

$$D^{-1} + \alpha T_t = -\sum_{j=1}^{n} \lambda_j (\varphi_j, \cdot)\varphi_j + B.$$

It follows that

$$\omega(e^{\alpha \ell_{\omega_t|\omega}}) = \big(\det(I+DT_t)\big)^{\alpha/2} \int_{\mathfrak{X}} \exp\left\{\frac{1}{2}\sum_{j=1}^{n} \lambda_j |(\varphi_j, x)|^2\right\} e^{-(x,Bx)/2}\omega(dx). \tag{47}$$

Since $B - D^{-1} \in \mathcal{T}$ and $D^{-1} + B > 0$, we conclude from (5) that $e^{-(x,Bx)/2}\omega(dx)$ coincides, up to a numerical factor $C > 0$, with a centered Gaussian measure whose

[4] We shall see in the proof of Theorem 2.1 that it is in fact identically equal to zero.

covariance operator is equal to $D' := (D^{-1} + B)^{-1}$. Hence, we can rewrite (47) in the form

$$\omega(e^{\alpha \ell_{\omega_t|\omega}}) = C \int_{\mathfrak{X}} \exp\left\{\frac{1}{2}\sum_{j=1}^{n} \lambda_j |(\varphi_j, x)|^2\right\} \omega_{D'}(dx).$$

Since the support of $\omega_{D'}$ coincides with the entire space, this integral is infinite.

Part (3) Using the cocycle relation (42), we can write[5]

$$\begin{aligned} e_t(1-\alpha) &= \log \omega(e^{\ell_{\omega_t|\omega}} e^{-\alpha \ell_{\omega_t|\omega}}) = \log \omega_t(e^{-\alpha \ell_{\omega_t|\omega}}) \\ &= \log \omega(e^{-\alpha \ell_{\omega_t|\omega} \circ \phi^t}) = \log \omega(e^{\alpha \ell_{\omega_{-t}|\omega}}) = e_{-t}(\alpha). \end{aligned}$$

Now note that, by (G4), the measure ω is invariant under ϑ, whence we conclude that $\omega_{-t} = \omega_t \circ \vartheta$ and $\ell_{\omega_t|\omega} \circ \vartheta = \ell_{\omega_{-t}|\omega}$. It follows that $e_{-t}(\alpha) = e_t(\alpha)$. Combining this with the above relation, we obtain the Evans–Searles symmetry.

4.5. Proof of Theorem 2.1

Part (1) We first prove the existence of limit (15). Let us set

$$D_t(\alpha) = ((1-\alpha)D^{-1} + \alpha D_t^{-1})^{-1} \tag{48}$$

and recall that $e_t(\alpha)$ can be written in the form (46). Using the relations (35), (39), Lemma 4.1 (3) and the chain rule we obtain

$$\begin{aligned} \frac{d}{dt}\log\det(I + \alpha D T_t) &= \operatorname{tr}\big((I + \alpha D T_t)^{-1} \alpha D \dot{T}_t\big) = -2\alpha \operatorname{tr}\big(D_t(\alpha)\varsigma_{-t}\big) \\ &= -2\alpha \operatorname{tr}\big(D_{-t}(1-\alpha)\varsigma\big). \end{aligned} \tag{49}$$

In particular, for $\alpha = 1$ the derivative is equal to zero for any $t \in \mathbb{R}$, whence we conclude that the first term in (46) is identically equal to zero. Let us now fix $\alpha \in \underline{J}$ and choose $t_0 > 0$ so large that $\alpha \in J_t$ for $t \geq t_0$. It follows from (46) and (49) that

$$\frac{1}{t} e_t(\alpha) = \frac{1}{t} e_{t_0}(\alpha) - \frac{2\alpha}{t} \int_{t_0}^{t} \operatorname{tr}\big(D_{-s}(1-\alpha)\varsigma\big) ds. \tag{50}$$

By Assumption (G3)

$$\operatorname*{s\text{-}lim}_{s\to\infty} D_{-s}(1-\alpha) = D_-(1-\alpha) := \big(\alpha D^{-1} + (1-\alpha)D_-^{-1}\big)^{-1},$$

and since ς is trace class, it follows that

$$\lim_{s\to\infty} \operatorname{tr}\big(D_s(1-\alpha)\varsigma\big) = \operatorname{tr}\big(D_-(1-\alpha)\varsigma\big).$$

Combining this with (50), we conclude that for $\alpha \in \underline{J}$,

$$\lim_{t\to+\infty} \frac{1}{t} e_t(\alpha) = -2\alpha \operatorname{tr}\big(D_-(1-\alpha)\varsigma\big). \tag{51}$$

[5]Note that this computation does not use (G4).

Once the existence of limit is known, we can easily obtain the required properties of $e(\alpha)$. The convexity of $e(\alpha)$ and the first and last relations in (16) follow immediately from the corresponding properties of $e_t(\alpha)$. Furthermore, it follows from (40) and the invariance of ω under ϑ that

$$e_t'(0) = \int_{\mathfrak{X}} \ell_{\omega_t|\omega}(x)\,\omega(dx) = \int_{\mathfrak{X}} \int_0^t \sigma_{-s}(x)\,ds\,\omega(dx) = -\int_{\mathfrak{X}} \int_0^t \sigma_s(x)\,ds\,\omega(dx).$$

In view of Part (2), the limit $e(\alpha)$ is analytic on its domain of definition. By Theorem 25.7 in [26],

$$\lim_{t\to\infty} \frac{1}{t} e_t'(\alpha) = e'(\alpha),$$

for $\alpha \in \underline{J}$. Using Fubini's theorem and Part (2) of Proposition 2.2, we derive

$$e'(0) = \lim_{t\to\infty} \frac{1}{t} e_t'(0) = -\lim_{t\to\infty} \frac{1}{t} \int_0^t \omega(\sigma_s)\,ds = -\omega_+(\sigma) = -\mathrm{tr}(\varsigma D_+).$$

The third relation in (16) now follows from the fourth one.

Part (2) The analyticity of $e(\alpha)$ follows from relation (51). We now prove (17).

Let μ be the spectral measure of Q for the linear functional induced by the trace class operator $D_-^{1/2}\varsigma D_-^{1/2}$. In other words, μ is the signed Borel measure such that

$$\int f(q)\mu(dq) = \mathrm{tr}(f(Q)D_-^{1/2}\varsigma D_-^{1/2}), \tag{52}$$

for any bounded continuous function $f : \mathbb{R} \to \mathbb{C}$. By Eq. (21), the measure μ has its support in the interval $[-\overline{\delta}^{-1}, (1+\overline{\delta})^{-1}]$. One easily checks that

$$f \mapsto \int f(q^{-1})q^{-1}\,\mu(dq),$$

defines a continuous linear functional on the Fréchet space $C_0(\mathbb{R})$ of compactly supported continuous functions $f : \mathbb{R} \to \mathbb{C}$. By the Riesz representation theorem (see Chapter 2 in [28]), it follows that there exists a signed Borel measure ν, with support on $(-\infty, -\overline{\delta}] \cup [1+\overline{\delta}, \infty)$, such that

$$\int f(r)\,\nu(dr) = \int f(q^{-1})q^{-1}\,\mu(dq). \tag{53}$$

A standard argument based on the monotone class technique shows that (53) remains valid for any bounded measurable function f. Decomposing the measures μ and ν into their positive and negative parts, we easily deduce from (53) that

$$\int f(r)|\nu|(dr) = \int f(q^{-1})|q|^{-1}|\mu|(dq),$$

for all bounded continuous f. In particular, taking $f(r) = \frac{1}{r}$ outside a small neighbourhood of zero and using (52), we derive

$$\int \frac{|\nu|(dr)}{|r|} = \int |\mu|(dq) \le \|D_-^{1/2}\varsigma D_-^{1/2}\|_1 < \infty.$$

Recalling relation (23) (which will be established below) and using (53) with $f(r) = -\log(1-\alpha r^{-1})$ on the support of ν, we obtain

$$e(\alpha) = -\alpha \operatorname{tr}\bigl(g(\alpha Q) D_-^{1/2} \varsigma D_-^{1/2}\bigr) = -\int \alpha g(\alpha q)\mu(dq)$$
$$= -\int q^{-1}\log(1-\alpha q)\mu(dq) = -\int \log(1-\alpha r^{-1})\nu(dr).$$

This relation coincides with (17).

To prove the uniqueness, let ν_1, ν_2 be two signed Borel measures with support in $\mathbb{R}\setminus \underline{J}$, satisfying $\int |r|^{-1}|\nu_k|(dr) < \infty$, $k = 1, 2$, and such that

$$\int \log(1-\alpha r^{-1})\nu_1(dr) = \int \log(1-\alpha r^{-1})\nu_2(dr)$$

for $\alpha \in \underline{J}$. Differentiating, we derive that

$$\int \frac{d\nu_1(r)}{r-\alpha} = \int \frac{d\nu_2(r)}{r-\alpha} \tag{54}$$

for $\alpha \in \underline{J}$. By analytic continuation (54) holds for all $\alpha \in \mathbb{C}_+ \cup \mathbb{C}_-$. Since the linear span of the set of functions $\{(r-\alpha)^{-1} \mid \alpha \in \mathbb{C}_+ \cup \mathbb{C}_-\}$ is dense in $C_0(\mathbb{R})$, (54) yields that for any $f \in C_0(\mathbb{R})$, $\int f d\nu_1 = \int f d\nu_2$. Hence $\nu_1 = \nu_2$.

Part (3) The fact that I is a convex function taking values in $[0, +\infty]$ follows immediately from the definition. The relation $e'(0) = \omega_-(\sigma) = -\omega_+(\sigma)$ and the regularity of e imply that I vanishes only at $s = \omega_+(\sigma)$. The validity of (18) is a straightforward consequence of the last relation in (16). Let us prove (19).

Consider the following family of random variables $\{\Sigma_t\}_{t\in[0,\infty)}$ defined on the probability space $(\mathfrak{X}, \mathcal{F}, \omega)$,

$$\Sigma_t = \frac{1}{t}\int_0^t \sigma_s\, ds.$$

By Proposition 2.1 (2) and the symmetry relations $\omega = \omega\circ\vartheta$ and $\sigma\circ\vartheta = -\sigma$, we have

$$e_t(\alpha) = \log\omega\bigl(e^{\alpha \ell_{\omega_t|\omega}}\bigr) = \log\omega\bigl(e^{\alpha\int_0^t \sigma_{-s}\,ds}\bigr) = \log\omega\bigl(e^{-\alpha\int_0^t \sigma_s\,ds}\bigr) = \log\omega\bigl(e^{-\alpha t\Sigma_t}\bigr),$$

so that $e_t(-\alpha)$ is the cumulant generating function of the family $\{\Sigma_t\}_{t\in[0,\infty)}$. Applying a local version of the Gärtner–Ellis theorem (see Theorem 4.65 in [22]), we conclude that (19) holds with

$$\varepsilon = \min\bigl(-\omega_+(\sigma) - \partial^+ e(-\underline{\delta}), -\omega_+(\sigma) + \partial^- e(1+\underline{\delta})\bigr)$$
$$= \min\bigl(e'(0) - \partial^+ e(-\underline{\delta}), \partial^- e(1+\underline{\delta}) - e'(1)\bigr),$$

where $\partial^\pm e(\alpha)$ denotes the right/left derivative of $e(\alpha)$. The fact that $\varepsilon > 0$ follows from the convexity and analyticity of $e(\alpha)$.

Part (4) As was shown above, $e_t(-\alpha)$ is the cumulant generating function of $\{\Sigma_t\}$. Therefore, by Bryc's lemma (see [7] or Section 4.8.4 in [22]), the CLT will be

established if we prove that $e_t(\alpha)$ extends analytically to a disc $\mathcal{D}_\varepsilon = \{\alpha \in \mathbb{C} \,|\, |\alpha| < \varepsilon\}$ and satisfies the estimate

$$\sup_{t \geq t_0, \alpha \in \mathcal{D}_\varepsilon} \frac{1}{t} |e_t(\alpha)| < \infty, \tag{55}$$

for some $t_0 > 0$. The analyticity was established in Part (2) of Proposition 2.3. Using the representation (50), one easily sees that in order to prove (55) it suffices to show that

$$\sup_{t \in \mathbb{R}, |1-\alpha| < \varepsilon} \|D_t(\alpha)\| < \infty. \tag{56}$$

An elementary analysis shows that Assumption (G2) implies the lower bound

$$(1-\alpha) D_s^{-1} + \alpha D_t^{-1} \geq \frac{2}{M} \frac{M-m}{M+m} \left(\delta + \tfrac{1}{2} - |\alpha - \tfrac{1}{2}|\right), \tag{57}$$

for $t, s \in \mathbb{R}$ and $\alpha \in [-\delta, 1+\delta]$. Since for $z \in \mathbb{C}$,

$$\operatorname{Re}\left((1-z) D_s^{-1} + z D_t^{-1}\right) = (1 - \operatorname{Re} z) D_s^{-1} + \operatorname{Re} z D_t^{-1},$$

we have the upper bound

$$\| \left((1-z) D_s^{-1} + z D_t^{-1}\right)^{-1} \| \leq \frac{M}{2} \frac{M+m}{M-m} \left(\delta + \tfrac{1}{2} - |\operatorname{Re} z - \tfrac{1}{2}|\right)^{-1} \tag{58}$$

for $s, t \in \mathbb{R}$ and z in the strip $\{z \in \mathbb{C} \,|\, \operatorname{Re} z \in (-\delta, 1+\delta)\}$. Thus, the required estimate (56) holds provided $\epsilon < \delta$.

Part (5) We first note that the differentiability of $e(\alpha)$ at zero and a local version of Theorems II.6.3 in [11] (which holds with identical proof) implies that, for any $\varepsilon > 0$ and any integer $n \geq 1$,

$$\omega\left(\{x \in \mathfrak{X} \,|\, |\Sigma_n - \omega_+(\sigma)| \geq \varepsilon\}\right) \leq e^{-a(\varepsilon) n},$$

where $a(\varepsilon) > 0$ does not depend on n. By Theorems II.6.4 in [11], it follows that

$$\lim_{n \to \infty} \frac{1}{n} \int_0^n \sigma_s(x)\, ds = \omega_+(\sigma) \tag{59}$$

for ω-a.e. $x \in \mathfrak{X}$. Suppose now we have shown the following inequality for some $r < 1$,

$$\sup_{0 \leq t \leq 1} \left| \int_n^{n+t} \sigma_s(x)\, ds \right| \leq (n+1)^r \qquad \text{for } n \geq n_0(x), \tag{60}$$

where $n_0(x) \geq 0$ is an integer that is finite for ω-a.e. $x \in \mathfrak{X}$. In this case, we can write

$$\left| \frac{1}{t} \int_0^t \sigma_s(x)\, ds - \frac{1}{n} \int_0^n \sigma_s(x)\, ds \right| \leq \frac{1}{n} \left| \int_n^{n+\hat{t}} \sigma_s(x)\, ds \right| + \frac{1}{n^2} \left| \int_0^n \sigma_s(x)\, ds \right|,$$

where n is the integer part of t and $\hat{t} = t - n$. It follows from (60) that the first term on the right-hand side goes to zero for a.e. $x \in \mathfrak{X}$, and the second goes to

zero in view of (59). Combining this with (59), we obtain (20). Thus, it remains to establish (60).

Let us fix an arbitrary $r \in (0,1)$ and denote by $\xi_n(x)$ the expression on the left-hand side of (60). In view of the first relation in (12), we have

$$\xi_n(x) = \sup_{0\le t\le 1}\left|\int_n^{n+t}(e^{s\mathcal{L}}x, \varsigma e^{s\mathcal{L}}x)ds\right| = \sup_{0\le t\le 1}\big|(x, \varsigma_{n,t}\, x)\big|, \qquad \varsigma_{n,t} := \int_n^{n+t}\varsigma_s\, ds.$$

Suppose we have constructed a sequence $\{B_n\}$ of self-adjoint elements of $\mathcal{T}$ such that, for any $n \ge 0$,

$$\sup_{0\le t\le 1}\big|(x, \varsigma_{n,t}\, x)\big| \le (x, B_n x), \qquad \|B_n\|_1 \le C, \tag{61}$$

where $C > 0$ does not depend on n. In this case, introducing the events $A_n = \{x \in \mathfrak{X} \,|\, \xi_n(x) \ge (n+1)^r\}$, for sufficiently small $\varepsilon > 0$, we can write

$$\omega(A_n) \le e^{-\varepsilon(n+1)^r}\omega(e^{\varepsilon\xi_n}) \le e^{-\varepsilon(n+1)^r}\big(\det(I - 2\varepsilon D B_n)\big)^{-1/2}, \tag{62}$$

where we used the fact that the Gaussian measures on $\mathfrak{X}$ with covariance operators $D'_\varepsilon = (D^{-1} - 2\varepsilon B_n)^{-1}$ and D are equivalent, with the corresponding density given by (see (5))

$$\Delta_{D'_\varepsilon|D}(x) = \big(\det(I - 2\varepsilon D B_n)\big)^{1/2} e^{\varepsilon(x, B_n x)}.$$

In view of the second inequality in (61), the determinant in (62) is bounded from below by a positive number not depending on $n \ge 0$ for sufficiently small $\varepsilon > 0$. Thus, the series $\sum_n \omega(A_n)$ converges, and by the Borel–Cantelli lemma, inequality (60) holds with an almost surely finite integer $n_0(x)$.

We now prove (61). From Assumption (G2) we derive

$$M \ge D_t = e^{t\mathcal{L}} D e^{t\mathcal{L}^*} \ge m\, e^{t\mathcal{L}} e^{t\mathcal{L}^*},$$

so that the uniform bound

$$\|e^{t\mathcal{L}}\| \le \left(\frac{M}{m}\right)^{1/2} \tag{63}$$

holds. Since $\varsigma \in \mathcal{T}$ is self-adjoint, one has $|(x, \varsigma x)| \le (x, |\varsigma| x)$ for all $x \in \mathcal{K}$. Hence

$$\sup_{0\le t\le 1}|(x, \varsigma_{n,t}x)| \le \int_n^{n+1}|(e^{s\mathcal{L}}x, \varsigma e^{s\mathcal{L}}x)|ds \le \int_n^{n+1}(e^{s\mathcal{L}}x, |\varsigma| e^{s\mathcal{L}}x)ds = (x, B_n x),$$

where

$$B_n = \int_n^{n+1} e^{s\mathcal{L}^*}|\varsigma| e^{s\mathcal{L}} ds$$

is a self-adjoint element of $\mathcal{T}$ such that

$$\|B_n\|_1 \le \frac{M}{m}\,\|\varsigma\|_1.$$

The proof of Theorem 2.1 is complete.

4.6. Proof of Theorem 2.2

Part (1) Let $\{s_n\}$ be an arbitrary sequence converging to $\overline{\delta}$. Recall that $D^{-1}+\alpha T_{s_n} > 0$ for $\alpha \in J_{s_n}$. Multiplying this inequality by $e^{s_n\mathcal{L}/2}$ from the right and by $e^{s_n\mathcal{L}^*/2}$ from the left, we obtain

$$(1-\alpha)D^{-1}_{-s_n/2} + \alpha D^{-1}_{s_n/2} > 0,$$

for any $\alpha \in J_{s_n}$. Invoking Assumptions (G2)–(G3), we can pass to the limit in the last inequality to get

$$(1-\alpha)D_-^{-1} + \alpha D_+^{-1} \geq 0,$$

for any $\alpha \in \overline{J}$. Taking $\alpha = 1+\overline{\delta}$ and $\alpha = -\overline{\delta}$ and performing some simple estimation, we obtain inequality (21). Furthermore, it follows from (21) that $\alpha Q < 1$ for $\alpha \in (-\overline{\delta}, 1+\overline{\delta})$, whence we conclude that the operator function (22) is analytic in the cut plane $\mathbb{C}_+ \cup \mathbb{C}_- \cup (-\overline{\delta}, 1+\overline{\delta})$.

Part (2) We first prove the existence of the limit in (23). To this end, we shall apply Vitali's convergence theorem to the sequence of functions

$$h_n(\alpha) = \frac{1}{t_n} e_{t_n}(\alpha), \qquad n \geq 1, \qquad \alpha \in J_{t_n}.$$

By the very definition of $\hat{\delta}$, for any $\varepsilon > 0$ there is N_ε such that, for all $n \geq N_\varepsilon$, the function h_n is analytic in the cut plane $\mathbb{C}_- \cup \mathbb{C}_+ \cup \hat{J}_\varepsilon$ where

$$\hat{J}_\varepsilon = (-\hat{\delta}+\varepsilon, 1+\hat{\delta}-\varepsilon) \subset J_{t_n}.$$

By the proof of Part (4) of Theorem 2.1 (more precisely Eq. (58)), the functions h_n are uniformly bounded in any disk or radius less than δ around $\alpha = 0$. By the Cauchy estimate, the same is true of their derivatives h_n'.

Let K_0 be the compact subset of $(\mathbb{C}_- \cup \mathbb{C}_+ \cup \hat{J}_\varepsilon) \setminus \{0\}$ described on the left of Figure 1. From definition (48) we infer

$$D_{t_n}(\alpha) = D^{1/2}(1+\alpha Q_n)^{-1}D^{1/2} = zD^{1/2}(z-Q_n)^{-1}D^{1/2}, \qquad z = -\frac{1}{\alpha},$$

where $Q_n = D^{1/2}T_{t_n}D^{1/2}$ is a self-adjoint element of $\mathcal{T}$. By definition, $\alpha \in J_{t_n}$ iff $I + \alpha Q_n > 0$, i.e.

$$\mathrm{sp}(Q_n) \subset (-(1+\delta_{t_n})^{-1}, \delta_{t_n}^{-1}) \subset (-(1+\hat{\delta}-\varepsilon)^{-1}, (\hat{\delta}-\varepsilon)^{-1}) \tag{64}$$

for all $n \geq N_\varepsilon$. Since the function $\alpha \mapsto z = -1/\alpha$ maps K_0 to a set which is uniformly separated from $\mathrm{sp}(Q_n)$ (see Fig. 1), it follows from the spectral theorem that

$$\sup_{\substack{n\geq N_\varepsilon \\ \alpha\in K_0}} \|D_{t_n}(\alpha)\| \leq \|D\| \sup_{\substack{n\geq N_\varepsilon \\ -z^{-1}\in K_0}} \frac{|z|}{\mathrm{dist}(z, \mathrm{sp}(Q_n))} < \infty.$$

Applying Lemma 4.1 (3) to Eq. (46) (recall that the first term on the right-hand

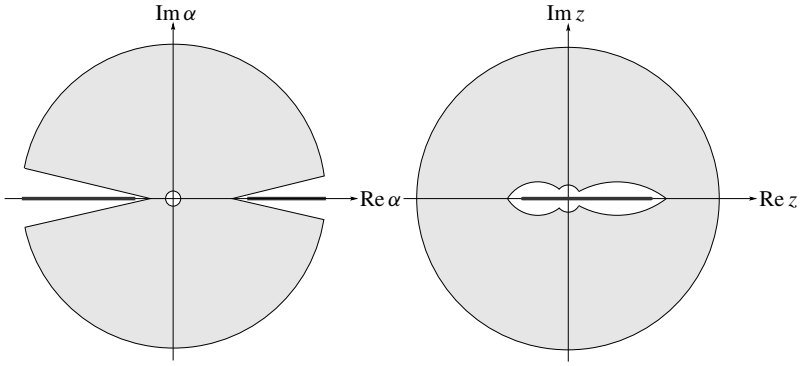

Fig. 1. A compact region $K_0 \subset (\mathbb{C}_- \cup \mathbb{C}_+ \cup \hat{J}_\varepsilon) \setminus \{0\}$ and its image under the map $\alpha \mapsto z = -1/\alpha$. The thick lines in the α-plane are the cuts $\mathbb{R} \setminus \hat{J}_\varepsilon$. By Eq. (64), if $n \geq N_\varepsilon$, then the spectrum of Q_n lies inside the thick line of the z-plane.

side of the latter vanishes) and integrating Eq. (39) to express T_{t_n} we obtain

$$h_n'(\alpha) = -\frac{1}{2t_n}\mathrm{tr}(D_{t_n}(\alpha)T_{t_n}) = \int_0^1 \mathrm{tr}(D_{t_n}(\alpha)\varsigma_{-st_n})ds.$$

The bound (63) further yields

$$|h_n'(\alpha)| \leq \frac{M}{m}\|\varsigma\|_1 \, \|D_{t_n}(\alpha)\|,$$

and the previous estimate allows us to conclude that the sequence $\{h_n'\}_{n\geq N_\varepsilon}$ is uniformly bounded in K_0.

Summing up, we have shown that $\{h_n'\}_{n\geq N_\varepsilon}$ is uniformly bounded on any compact subset of $\mathbb{C}_- \cup \mathbb{C}_+ \cup \hat{J}_\varepsilon$ and since $h_n(0) = 0$, the same is true of the sequence $\{h_n\}_{n\geq N_\varepsilon}$. By Part (1) of Theorem 2.1, the sequence $\{h_n(\alpha)\}$ converges for $\alpha \in \underline{J}$. By Vitali's theorem (see Section I.A.12 in [18]), we conclude that the sequence $\{h_n\}$ converges uniformly on any compact subset of $\mathbb{C}_- \cup \mathbb{C}_+ \cup \hat{J}_\varepsilon$, and the limit is an analytic function on it. Since $\varepsilon > 0$ was arbitrary, we see that the middle term in (23) is well defined for any $\alpha \in \mathbb{C}_- \cup \mathbb{C}_+ \cup \hat{J}$ and is an analytic function on this domain.

To prove the second equality in (23), since both left- and right-hand sides are analytic functions on $\mathbb{C}_- \cup \mathbb{C}_+ \cup \hat{J}$ it suffices to establish it for $\alpha \in \underline{J}$. The lower bound (57) shows that $D_t(\alpha)$ is bounded and strictly positive for all $t \in \mathbb{R}$ and $\alpha \in (-\delta, 1+\delta)$. It follows from Eq. (37) and Lemma 4.1 (1) that $\ell_{\omega_t|\omega} \in L^1(\mathfrak{X}, d\omega_{D_t(\alpha)})$. Moreover, Eq. (45) shows that for $f \in L^1(\mathfrak{X}, d\omega_{D_t(\alpha)})$,

$$\omega_{D_t(\alpha)}(f) = \frac{\omega(e^{\alpha\ell_{\omega_t|\omega}} f)}{\omega(e^{\alpha\ell_{\omega_t|\omega}})}. \tag{65}$$

Using this relation with $f = \ell_{\omega_t|\omega}$, integrating the identity

$$e^{\alpha\ell_{\omega_t|\omega}} = 1 + \int_0^\alpha e^{\gamma\ell_{\omega_t|\omega}}\ell_{\omega_t|\omega}\, d\gamma$$

against ω, and applying Fubini's theorem, we obtain

$$\omega(e^{\alpha \ell_{\omega_t|\omega}}) = 1 + \int_0^\alpha \omega(e^{\gamma \ell_{\omega_t|\omega}}) \omega_{D_t(\gamma)}(\ell_{\omega_t|\omega})\, d\gamma.$$

Resolving this integral equation (which reduces to a linear differential equation) for $\alpha \mapsto \omega(e^{\alpha \ell_{\omega_t|\omega}})$, we derive

$$\omega(e^{\alpha \ell_{\omega_t|\omega}}) = \exp\left(\int_0^\alpha \omega_{D_t(\gamma)}(\ell_{\omega_t|\omega}) d\gamma \right).$$

Taking the logarithm, dividing by t, and using (41), we obtain

$$\begin{aligned} \frac{1}{t} e_t(\alpha) &= \frac{1}{t} \int_0^\alpha \omega_{D_t(\gamma)}(\ell_{\omega_t|\omega})\, d\gamma = \frac{1}{t} \int_0^\alpha \int_0^t \omega_{D_t(\gamma)}(\sigma_{-s})\, ds d\gamma \\ &= \int_0^\alpha \int_0^1 \omega_{D_t(\gamma)}(\sigma_{-ts})\, ds d\gamma. \end{aligned} \tag{66}$$

It follows from (34) and the first relation in (12) that

$$\begin{aligned} \omega_{D_t(\gamma)}(\sigma_{-ts}) = \operatorname{tr}(D_t(\gamma)\, \varsigma_{-ts}) &= \operatorname{tr}\left(e^{-ts\mathcal{L}} D_t(\gamma) e^{-ts\mathcal{L}^*} \varsigma \right) \\ &= \operatorname{tr}\left(\left((1-\gamma) D_{-ts}^{-1} + \gamma D_{t(1-s)}^{-1} \right)^{-1} \varsigma \right). \end{aligned}$$

Combining this with Hypothesis (G3) and a continuity property of the trace, we derive

$$\lim_{t\to\infty} \omega_{D_t(\gamma)}(\sigma_{-ts}) = \operatorname{tr}\left(\overline{D}_\gamma \varsigma \right) = \omega_{\overline{D}_\gamma}(\sigma) \qquad \text{for } \gamma \in (-\delta, 1+\delta),\ s \in (0,1),$$

where we set $\overline{D}_\gamma = ((1-\gamma) D_-^{-1} + \gamma D_+^{-1})^{-1}$. The bound (58) allows us to apply the dominated convergence theorem to Eq. (66), and conclude that

$$\begin{aligned} e(\alpha) = \lim_{t\to\infty} \frac{1}{t} e_t(\alpha) &= \int_0^\alpha \int_0^1 \omega_{\overline{D}_\gamma}(\sigma)\, ds d\gamma \\ &= \int_0^\alpha \operatorname{tr}\left(\overline{D}_\gamma \varsigma \right) d\gamma, \qquad \alpha \in (-\delta, 1+\delta). \end{aligned} \tag{67}$$

Writing $\overline{D}_\gamma = D_-^{1/2} (I - \gamma Q)^{-1} D_-^{1/2}$, we further get

$$e(\alpha) = \int_0^\alpha \operatorname{tr}\left(D_-^{1/2} (I - \gamma Q)^{-1} D_-^{1/2} \varsigma \right) d\gamma,$$

and performing the integral yields Eq. (23) for $\alpha \in (-\delta, 1+\delta)$.

Finally, to prove (24), it suffices to note that if α does not belong to the closure of $\hat{J}$ then, for infinitely many $n \geq 1$, $\alpha \notin J_{t_n}$ and by Proposition 2.3 (2), $e_{t_n}(\alpha) = +\infty$.

Part (3) The required properties of the rate function $\hat{I}$ follow from (16) and elementary properties of the Legendre transform. Thus, we shall only prove (26).

In doing so, we shall assume that the interval $\hat{J}$ is finite; in the opposite case, the result follows immediately from the Gärtner–Ellis theorem; see Section 4.5.3 in [10]. Moreover, we shall consider only the nondegenerate situation in which $\omega_+(\sigma) > 0$. The analysis of the case $\omega_+(\sigma) = 0$ is similar and easier.

Let us extend $\hat{e}(\alpha)$ to the endpoints of the interval $\hat{J}$ by the relation

$$\hat{e}(\alpha) = \limsup_{t\to+\infty} \frac{1}{t} e_t(\alpha), \qquad \alpha \in \{-\hat{\delta}, 1+\hat{\delta}\}.$$

Since the extended function $\hat{e}$ is convex and, hence, continuous at any point where it is finite, the Legendre transform of $e(-\alpha)$ coincides with $\hat{I}$ defined by (25). In view of a well-known result on the large deviation upper bound (e.g. see Theorem 4.5.3 in [10]), the following inequality holds for any closed subset $F \subset \mathbb{R}$,

$$\limsup_{n\to\infty} \frac{1}{t_n} \log \omega\left(\left\{x \in \mathfrak{X} \;\middle|\; \frac{1}{t_n}\int_0^{t_n} \sigma_s(x)\, ds \in F\right\}\right) \le -\inf_{s\in F} \hat{I}(s).$$

Since $\hat{I}$ is also continuous, this upper bound easily implies that (24) will be established if we prove the inequality

$$\liminf_{n\to\infty} \frac{1}{t_n} \log \omega\left(\left\{x \in \mathfrak{X} \;\middle|\; \frac{1}{t_n}\int_0^{t_n} \sigma_s(x)\, ds \in O\right\}\right) \ge -\inf_{s\in O} \hat{I}(s), \tag{68}$$

where $O \subset \mathbb{R}$ is an arbitrary open set. A standard argument shows that it suffices to prove (68) for any open interval $\mathcal{J} \subset \mathbb{R}$. Let us set

$$s^- = -\lim_{\alpha\uparrow 1+\hat{\delta}} \hat{e}'(\alpha), \qquad s^+ = -\lim_{\alpha\downarrow -\hat{\delta}} \hat{e}'(\alpha).$$

In view of the local version of the Gärtner–Ellis theorem (see Theorem 4.65 in[6] [22]), relation (26) is true for any interval $\mathcal{J} \subset (s^-, s^+)$. Thus, it suffices to consider the case when $\mathcal{J} = \mathcal{J}_{s,\varepsilon} = (s-\varepsilon, s+\varepsilon)$, where $\pm(s - s_\pm) \ge 0$. The proof of (68) is divided into several steps.

Step 1: Reduction. We first show that the required inequality will be established if we prove that, for any $\hat{s} \in \mathbb{R}$ satisfying the inequality $\pm(\hat{s} - s_\pm) \ge 0$ and any $\varepsilon > 0$,

$$\liminf_{n\to\infty} \frac{1}{t_n} \log \omega\big(B_n(\hat{s}, \varepsilon)\big) \ge -\hat{I}(\hat{s} \pm \varepsilon), \tag{69}$$

where $B_n(\hat{s}, \varepsilon) = \{x \in \mathfrak{X} \,|\, |t_n^{-1}\ell_{\omega_{t_n}|\omega} + \hat{s}| < \varepsilon\}$. Indeed, we have

$$\hat{I}(s) = \begin{cases} -(1+\hat{\delta})s - e^- & \text{for } s \le s^-, \\ \hat{\delta}s - e^+ & \text{for } s \ge s^+, \end{cases} \tag{70}$$

[6]In the formulation of Theorem 4.65 in [22], it is required that the limit of $t_n^{-1}e_{t_n}(\alpha)$ as $n \to \infty$ should exist for any α in the closure of $\hat{J}$. However, the same proof works also in the case when the limits exist only for $\alpha \in \hat{J}$.

where e^- (respectively, e^+) is the limit of $\hat{e}(\alpha)$ as $\alpha \uparrow 1+\hat{\delta}$ (respectively, $\alpha \downarrow -\hat{\delta}$). In particular, the rate function $\hat{I}$ is everywhere finite and continuous. It follows from (69) and inequality (68) with $\mathcal{J} \subset (s^-, s^+)$ that

$$\lim_{\varepsilon\to 0^+} \liminf_{n\to\infty} \frac{1}{t_n} \log \omega\left(\left\{x \in \mathfrak{X} \;\middle|\; \frac{1}{t_n}\int_0^{t_n} \sigma_s(x)\,ds \in \mathcal{J}_{\hat{s},\varepsilon}\right\}\right)$$
$$= \lim_{\varepsilon\to 0^+} \liminf_{n\to\infty} \frac{1}{t_n} \log \omega\big(B_n(\hat{s},\varepsilon)\big) \geq -\hat{I}(\hat{s}),$$

where $\hat{s} \in \mathbb{R}$ is any point. A well-known (and simple) argument implies the required lower bound (68) for any interval $\mathcal{J} \subset \mathbb{R}$. Thus, we need to establish (69). To simplify the notation, we shall consider only the case when $\hat{s} \geq s_+$ (assuming that $s_+ < \infty$).

Step 2: Shifted measures. Let us fix $\hat{s} \geq s^+$ and denote $\tilde{e}_t(\alpha) = e_t(-\alpha)$ and $\tilde{e}(\alpha) = \hat{e}(-\alpha)$. Since $\tilde{e}'_{t_n}$ is a monotone increasing function mapping the interval $-J_{t_n} = (-1-\delta_{t_n}, \delta_{t_n})$ onto $(-\infty, \infty)$ (see (46)), for any $n \geq 1$ there is a unique number $\alpha_n \in -J_{t_n}$ such that $\tilde{e}'_{t_n}(\alpha_n) = t_n\hat{s}$. Following a well-known idea in the theory of large deviations, let us define a sequence of measures ν_n on $\mathfrak{X}$ by their densities

$$\Delta_{\nu_n|\omega} = \exp\big(-\alpha_n \ell_{\omega_{t_n}|\omega} - \tilde{e}_{t_n}(\alpha_n)\big).$$

Suppose we have proved that

$$\liminf_{n\to\infty} \nu_n\big(B_n(\hat{s},\varepsilon)\big) > 0. \tag{71}$$

In this case, assuming that $\alpha_n > 0$, we can write

$$\omega\big(B_n(\hat{s},\varepsilon)\big) = \int_{B_n(\hat{s},\varepsilon)} \exp\big(\alpha_n \ell_{\omega_{t_n}|\omega} + \tilde{e}_{t_n}(\alpha_n)\big) d\nu_n$$
$$\geq \exp\big(t_n\alpha_n(-\hat{s}-\varepsilon) + \tilde{e}_{t_n}(\alpha_n)\big)\nu_n\big(B_n(\hat{s},\varepsilon)\big),$$

whence it follows that

$$\liminf_{n\to\infty} \frac{1}{t_n} \log \omega\big(B_n(\hat{s},\varepsilon)\big) \geq \liminf_{n\to\infty}\Big(\alpha_n(-\hat{s}-\varepsilon) + \frac{1}{t_n}\tilde{e}_{t_n}(\alpha_n)\Big). \tag{72}$$

If we know that

$$\lim_{n\to\infty} \alpha_n = \hat{\delta}, \qquad \liminf_{n\to\infty} \frac{1}{t_n}\tilde{e}_{t_n}(\alpha_n) \geq e^+, \tag{73}$$

then $\alpha_n > 0$ for n large enough and inequality (72) and relation (70) immediately imply the required result (69). Thus, we need to prove (71) and (73).

Step 3: Proof of (73). Since $\alpha_n \in -J_{t_n}$ and $\delta_{t_n} \to \hat{\delta}$, the first relation in (73) will be established if we show that

$$\liminf_{n\to\infty} \alpha_n = \hat{\delta}. \tag{74}$$

Suppose this is not the case. Then there is $\varepsilon > 0$ and a sequence $n_k \to +\infty$ such that $-1 \leq \alpha_{n_k} \leq \hat{\delta} - \varepsilon$, where the first inequality follows from the fact that

$\tilde{e}'_{t_n}(\alpha_n) \geq 0$ and $\tilde{e}'_{t_n}(-1) \leq 0$. To simplify notation, we assume that the entire sequence $\{\alpha_n\}$ satisfies this inequality. It follows that

$$s^+ \leq \hat{s} = \frac{1}{t_n}\tilde{e}'_{t_n}(\alpha_n) \leq \frac{1}{t_n}\tilde{e}'_{t_n}(\hat{\delta} - \varepsilon) \qquad \text{for any } n \geq 1. \tag{75}$$

Since $\frac{1}{t_n}e_{t_n}(\alpha)$ are convex functions converging to the smooth function $\tilde{e}(\alpha)$ for $\alpha \in -\hat{J}$, by Theorem 25.7 in [26], we have

$$\lim_{n\to\infty} \frac{1}{t_n}\tilde{e}'_{t_n}(\alpha) = \tilde{e}'(\alpha) \qquad \text{for any } \alpha \in -\hat{J},$$

and the limit is uniform on any compact subset of $-\hat{J}$. Comparing this with (75), we see that $s^+ \leq \tilde{e}'(\hat{\delta} - \varepsilon)$. It follows that $\tilde{e}'$ is constant on the interval $[\hat{\delta} - \varepsilon, \hat{\delta}]$ and, hence, by analyticity and the first relation in (16), the function $e(\alpha)$ vanishes. This contradicts the assumption that $\omega_+(\sigma) > 0$ and proves (74).

We now establish the second relation in (73). For any $\gamma \in (0, \hat{\delta})$, we have

$$\tilde{e}_{t_n}(\alpha_n) = \tilde{e}_{t_n}(\gamma) + \int_\gamma^{\alpha_n} \tilde{e}'_{t_n}(\alpha)\, d\alpha \geq \tilde{e}_{t_n}(\gamma) + (\alpha_n - \gamma)\tilde{e}'_{t_n}(0),$$

where we used the facts that $\tilde{e}'$ is nondecreasing and that $\alpha_n > \gamma$ for sufficiently large $n \geq 1$, in view of the first relation in (73). It follows that

$$\liminf_{n\to\infty} \frac{1}{t_n}\tilde{e}_{t_n}(\alpha_n) \geq \tilde{e}(\gamma) + (\hat{\delta} - \gamma)\tilde{e}'(0).$$

Passing to the limit as $\gamma \to \hat{\delta}$, we obtain the required inequality.

Step 4: Proof of (71). Let us introduce trace class operators

$$Q_n = D^{1/2}T_{t_n}D^{1/2}, \qquad M_n = t_n^{-1}(I - \alpha_n Q_n)^{-1}Q_n, \qquad n \geq 1.$$

Since $\alpha_n \in -J_{t_n}$, the operator $I - \alpha_n Q_n$ is strictly positive and M_n is well defined. Suppose we have shown that

$$\nu_n\big(f(X_n)\big) = \mu\big(f(Y_n)\big), \qquad X_n = -t_n^{-1}\ell_{\omega_{t_n}|\omega}, \qquad Y_n = \frac{1}{2}(x, M_n x), \qquad n \geq 1, \tag{76}$$

where $f : \mathbb{R} \to \mathbb{R}$ is an arbitrary bounded measurable function and μ is the centered Gaussian measure on $\mathfrak{X}$ with the covariance operator I. In this case, taking f to be the indicator function of the interval $\mathcal{J}_{\hat{s},\varepsilon}$, we can write

$$\nu_n\big(B_n(\hat{s}, \varepsilon)\big) = \mu\big(\{x \in \mathfrak{X} \,|\, |Y_n(x) - \hat{s}| < \varepsilon\}\big) =: p_n(\varepsilon) \qquad \text{for any } n \geq 1.$$

Thus, the required assertion will be established if we prove that

$$\inf_{n\geq 1} p_n(\varepsilon) > 0 \qquad \text{for any } \varepsilon > 0. \tag{77}$$

To this end, let us assume that we have proved that

$$\mathfrak{M} := \sup_{n\geq 1} \|M_n\|_1 < \infty, \qquad \mathrm{tr}(M_n) = 2\hat{s}. \tag{78}$$

We now use the following lemma, whose proof is given in the end of this subsection (cf. Lemma 2 in [8, Section 3].)

LEMMA 4.2. *Let μ be the centered Gaussian measure on $\mathfrak{X}$ with the covariance operator I. Then for any positive numbers κ and ε there is $p(\kappa,\varepsilon) > 0$ such that*

$$\mu\big(\{x \in \mathfrak{X} \,|\, |(x, Mx) - \mathrm{tr}(M)| < \varepsilon\}\big) \geq p(\kappa,\varepsilon) \tag{79}$$

for any self-adjoint operator $M \in \mathcal{T}$ satisfying the inequality $\|M\|_1 \leq \kappa$.

In view of (78), we have

$$Y_n(x) - \hat{s} = \big(x, \tfrac{1}{2}M_n x\big) - \mathrm{tr}\big(\tfrac{1}{2}M_n\big).$$

Applying Lemma 4.2 with $\kappa = 2\mathfrak{M}$, we see that (77) holds. Thus, to complete the proof of the theorem, it remains to establish (76) and (78).

Step 5: Proof of the auxiliary assertions. Simple approximation and analyticity arguments show that, to prove (76), is suffices to consider the case in which $f(x) = e^{\gamma x}$, where $\gamma \in \mathbb{R}$ is sufficiently small. Thus, we need to check that

$$\nu_n\big(\exp(-\gamma t_n^{-1}\ell_{\omega_{t_n}|\omega})\big) = \mu\big(e^{\gamma Y_n}\big). \tag{80}$$

Recalling the construction of α_n and using the relation $\tilde{e}_t(\alpha) = -\frac{1}{2}\log\det(I - \alpha Q_t)$ (see (46)), we write

$$\begin{aligned}\nu_n\big(\exp(-\gamma t_n^{-1}\ell_{\omega_{t_n}|\omega})\big) &= \int_{\mathfrak{X}} \exp\big(-(\gamma t_n^{-1} + \alpha_n)\ell_{\omega_{t_n}|\omega} - \tilde{e}_{t_n}(\alpha_n)\big)\omega(dx)\\ &= \exp\big(\tilde{e}_{t_n}(\gamma t_n^{-1} + \alpha_n) - \tilde{e}_{t_n}(\alpha_n)\big) = \det\big(I - \gamma M_n\big)^{-1/2}.\end{aligned}$$

This expression coincides with the right-hand side of (80).

Finally, to prove (78), we first note that the equality follows immediately from the choice of α_n and the relation $\tilde{e}_t'(\alpha) = \frac{1}{2}\mathrm{tr}\big((I - \alpha Q_t)^{-1}Q_t\big)$. To establish the inequality, we start by using (39) and (63) to get the bound

$$\|Q_n\|_1 \leq \int_0^{t_n} \|D^{1/2}\varsigma_{-s}D^{1/2}\|_1 ds \leq \frac{M^2}{m} t_n \|\varsigma\|_1. \tag{81}$$

Writing the spectral decomposition of the compact self-adjoint operator M_n, we easily show that

$$M_n^- = t_n^{-1}(I + \alpha_n Q_n^-)^{-1}Q_n^-,$$

where A^+ and A^- stand the positive and negative parts of a self-adjoint operator A, and we used that fact that $\alpha_n > 0$ for sufficiently large n (see (74)). Combining this relation with (81), we derive

$$\mathrm{tr}(M_n^-) = t_n^{-1}\mathrm{tr}\big((I + \alpha_n Q_n^-)^{-1}Q_n^-\big) \leq \frac{M^2}{m}\|\varsigma\|_1.$$

Recalling the second relation in (78), we conclude that

$$\|M_n\|_1 = \operatorname{tr}(|M_n|) = \operatorname{tr}(M_n + 2M_n^-) \le 2\left(\hat{s} + \frac{M^2}{m}\|\varsigma\|_1\right).$$

The proof of Theorem 2.2 is complete. □

Proof of Lemma 4.2. We set $Y(x) = (x, Mx)$ and note that $\mu(Y) = \operatorname{tr}(M)$. Let us denote by $\{P_I, I \subset \mathbb{R}\}$ the family of spectral projections for M and, given a number $\theta > 0$, write $M = M^{\le\theta} + M^{>\theta}$, where $M^{\le\theta} = MP_{[-\theta,\theta]}$. Accordingly, we represent Y in the form

$$Y(x) = Y^{\le\theta}(x) + Y^{>\theta}(x), \qquad Y^{\le\theta}(x) = \big(x, M^{\le\theta}x\big) - \operatorname{tr}\big(M^{\le\theta}\big).$$

Now note that the random variables $Y^{\le\theta}$ and $Y^{>\theta}$ are independent under the law μ. It follows that the probability $P(M,\varepsilon)$ given by the left-hand side of (79) satisfies the inequality

$$\begin{aligned} P(M,\varepsilon) &\ge \mu\big(\{|Y^{>\theta}| < \varepsilon/2, |Y^{\le\theta}| < \varepsilon/2\}\big) \\ &= \mu\big(\{|Y^{>\theta}| < \varepsilon/2\}\big)\mu\big(\{|Y^{\le\theta}| < \varepsilon/2\}\big). \end{aligned} \tag{82}$$

We claim that both factors on the right-hand side of this inequality are separated from zero. Indeed, to estimate the first factor, we note that

$$\kappa \ge \|M\|_1 \ge \theta \operatorname{rank}\big(M^{>\theta}\big), \tag{83}$$

where $\operatorname{rank}(M^{>\theta}) =: N_\theta$ stands for the rank of $M^{>\theta}$. Denoting by λ_j the eigenvalues of M indexed in the nonincreasing order of their absolute values, we see that

$$|Y^{>\theta}(x))| = \left|\sum_{j=1}^{N_\theta} \lambda_j (x_j^2 - 1)\right| \le \kappa \sum_{j=1}^{N_\theta} |x_j^2 - 1|,$$

where $\{x_j\}$ are the coordinates of x in the orthonormal basis formed of the eigenvectors of M. Combining this with (83), we derive

$$\begin{aligned} \mu\big\{|Y^{>\theta}(x))| < \varepsilon/2\big\} &\ge \mu\left\{\sum_{j=1}^{N_\theta} |x_j^2 - 1| < \frac{\varepsilon}{2\kappa}\right\} \\ &\ge \prod_{j=1}^{N_\theta} \mu\big\{|x_j^2 - 1| < (2\kappa N_\theta)^{-1}\varepsilon\big\} \ge p\big(\delta\big)^{\kappa/\theta}, \end{aligned}$$

where $\delta = \varepsilon\theta/(2\kappa^2)$, and $p(\delta) > 0$ is the probability of the event $|x^2 - 1| < \delta$ under the one-dimensional standard normal law. To estimate the second factor in (82), we use the Chebyshev inequality

$$\begin{aligned} \mu\big\{|Y^{\le\theta}(x)| < \varepsilon/2\big\} &= 1 - \mu\big\{Y^{\le\theta}(x) \ge \varepsilon/2\big\} - \mu\big\{-Y^{\le\theta}(x) \ge \varepsilon/2\big\} \\ &\ge 1 - \mu\big(\exp(\gamma Y^{\le\theta} - \gamma\varepsilon/2)\big) + \mu\big(\exp(-\gamma Y^{\le\theta} - \gamma\varepsilon/2)\big), \end{aligned} \tag{84}$$

where $\gamma > 0$ is sufficiently small and will be chosen later. We have

$$\begin{aligned}\mu\big(\exp(\gamma Y^{\preceq\theta})\big) &= \exp\big\{-\gamma\operatorname{tr}\big(M^{\preceq\theta}\big) - \tfrac{1}{2}\log\det\big(I - \gamma M^{\preceq\theta}\big)\big\}\\ &= \exp\big\{-\tfrac{1}{2}\operatorname{tr}\big(2\gamma M^{\preceq\theta} + \log(I - 2\gamma M^{\preceq\theta})\big)\big\}. \end{aligned} \tag{85}$$

Now note that if $4|\gamma|\theta \le 1$, then

$$2\gamma M^{\preceq\theta} + \log(I - 2\gamma M^{\preceq\theta}) = \sum_{n=2}^{\infty} \frac{\big(-2\gamma M^{\preceq\theta}\big)^n}{n}.$$

Recalling that $\|M^{\preceq\theta}\| \le \theta$ and $\|M^{\preceq\theta}\|_1 \le \kappa$ and using the inequality $|\operatorname{tr}(AB)| \le \|A\|_1\|B\|$, it follows that

$$\big|\operatorname{tr}\big(2\gamma M^{\preceq\theta} + \log(I - 2\gamma M^{\preceq\theta})\big)\big| \le \sum_{n=2}^{\infty} |2\gamma\theta|^{n-1} 2|\gamma|\kappa \le 8\kappa\gamma^2\theta.$$

Substituting this into (85), we see that, if $|\gamma| \le (4\theta)^{-1}$, then $\mu\big(\exp(\gamma Y^{\preceq\theta})\big) \le \exp\big(4\kappa\gamma^2\theta\big)$. A similar estimate holds for $\mu\big(\exp(-\gamma Y^{\preceq\theta})\big)$. Combining these inequalities with (84) and choosing $\gamma = \frac{\varepsilon}{16\kappa\theta}$, we derive

$$\mu\big\{|Y^{\preceq\theta}(x)| < \varepsilon/2\big\} \ge 1 - 2\exp\big(4\kappa\gamma^2\theta - \gamma\varepsilon/2\big) = 1 - 2\exp\left(-\frac{\varepsilon^2}{64\kappa\theta}\right).$$

The right-hand side of this inequality can be made greater than zero by choosing a sufficiently small $\theta > 0$ which will depend only on κ and ε. □

4.7. Proof of Theorem 2.3

The proof of this result is very similar to that of Theorems 2.1 and 2.2, and we shall only outline the proof.

Part (1) Follows from Hölder's inequality as in the proof of Proposition 2.3 (2).

Part (2) Since $0 \in J_t^+$, the fact that J_t^+ is an interval follows immediately from the following property: if $\alpha \in J_t^+$, then $\theta\alpha \in J_t^+$ for $\theta \in (0, 1)$. To prove the analyticity, note that, by Eq. (45), one has

$$e^{-\alpha\ell_{\omega_t|\omega}} d\omega_+ = \sqrt{\frac{\big(\det(I + DT_t)\big)^{-\alpha}}{\det(I - \alpha D_+ T_t)}}\, d\omega_{(D_+^{-1} - \alpha T_t)^{-1}}.$$

This relation implies that the function

$$\begin{aligned} e_{t+}(\alpha) &= -\frac{\alpha}{2}\log\det(I + D_+T_t) - \frac{1}{2}\log\det(I - \alpha D_+T_t)\\ &= -\frac{\alpha}{2}\log\det(I + D^{1/2}T_tD^{1/2}) - \frac{1}{2}\log\det(I - \alpha D_+^{1/2}T_tD_+^{1/2}) \end{aligned} \tag{86}$$

is real analytic in α on the open interval defined by the condition $I - \alpha D_+^{1/2}T_tD_+^{1/2} > 0$ and takes the value $+\infty$ on its complement (where the intersection of the spectrum

of $I - \alpha D_+^{1/2} T_t D_+^{1/2}$ with the negative half-line is nonempty). The above inequality coincides with the one defining J_t^+.

Part (3) The fact that $\underline{J}^+$ is an interval follows immediately from its definition. To prove that $J_t^+ \supset (-\delta, \delta)$, note that, in view of Hypothesis (G2), for any $t, \alpha \in \mathbb{R}$ we have

$$I - \alpha D_+^{1/2} T_t D_+^{1/2} = D_+^{1/2}(D_+^{-1} - \alpha(D_t^{-1} - D^{-1}))D_+^{1/2} \geq \frac{\delta - |\alpha|}{\delta + 1}.$$

This expression is positive for $|\alpha| < \delta$.

To prove the existence of limit (28) and its analyticity on $\underline{J}^+$, we repeat the argument used in the proof of Theorem 2.2 (2). Namely, let us introduce the family of operators $D_t^+(\alpha) = (D_+^{-1} - \alpha T_t)^{-1}$, which are well defined for $\alpha \in (-\delta, \delta)$. Then the following analogue of relation (65) is valid,

$$\omega_{D_t^+(\alpha)}(f) = \frac{\omega(e^{-\alpha \ell_{\omega_t|\omega}} f)}{\omega(e^{-\alpha \ell_{\omega_t|\omega}})} \qquad \text{for } f \in L^1(\mathfrak{X}, d\omega_{D_t^+(\alpha)}).$$

The argument used in the derivation of (66) gives that

$$\frac{1}{t} e_{t+}(\alpha) = -\int_0^\alpha \int_0^1 \omega_{D_t^+(\gamma)}(\sigma_{-ts})\, ds d\gamma,$$

while Hypothesis (G2) and the relation $e^{r\mathcal{L}} D_+ e^{r\mathcal{L}^*} = D_+$ valid for $r \in \mathbb{R}$ imply that

$$e^{-ts\mathcal{L}} D_t^+(\gamma) e^{-ts\mathcal{L}^*} = \left(D_+^{-1} - \gamma(D_{t(1-s)}^{-1} - D_{-ts}^{-1})\right)^{-1} \leq M\left(1 - \frac{|\gamma|}{\delta}\right)^{-1}.$$

Following again the argument in the proof of Theorem 2.2 (2), for $\alpha \in (-\delta, \delta)$ we derive

$$e_+(\alpha) = \lim_{t\to\infty} \frac{1}{t} e_{t+}(\alpha) = -\int_0^\alpha \omega_{\overline{D}_{1-\gamma}}(\sigma)\, d\gamma. \tag{87}$$

Now note that $\overline{D}_{1-\gamma} = \vartheta \overline{D}_\gamma \vartheta$, whence it follows $\omega_{\overline{D}_{1-\gamma}}(\sigma) = \omega_{\overline{D}_\gamma}(\sigma \circ \vartheta) = -\omega_{\overline{D}_\gamma}(\sigma)$. Substituting this into (87) and recalling (67), we see that

$$e_+(\alpha) = \int_0^\alpha \omega_{\overline{D}_\gamma}(\sigma)\, d\gamma = e(\alpha) \qquad \text{for } \alpha \in (-\delta, \delta). \tag{88}$$

We have thus established the existence of limit (28) on the interval $(-\delta, \delta) \subset \underline{J}^+$. The fact that it exists for any $\alpha \in \underline{J}^+$ and defines a real-analytic function can be proved with the help of Vitali's theorem (cf. proof of Part (2) of Theorem 2.2). Finally, relation (29) is established by the same argument as (24).

Parts (4–6) The proofs of the large deviation principle, central limit theorem, and strong law of large numbers for the time average of the entropy production functional under the limiting law ω_+ are exactly the same as for ω (see Parts (3–5) of Theorem 2.1), and therefore we will omit them.

Part (7) The fact that the functions $e_+(\alpha)$ and $e(\alpha)$ coincide on the intersection $\underline{J}^+ \cap \underline{J}$ follows from (88) and their analyticity. The equality of the corresponding

rate functions on a small interval around $\omega_+(\sigma)$ is a straightforward consequence of (88) and the definition of the Legendre transform. □

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LINEAR AND NONLINEAR DISSIPATIVE DYNAMICS

B. ZEGARLIŃSKI

Imperial College London, 180 Queens Gate, London SW7 2AZ, UK
(e-mail: b.zegarlinski@imperial.ac.uk

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In this paper we introduce and study new dissipative dynamics for large interacting systems.

Keywords: Dunkl type generators, infinite dimensions, noncommutative and nonlinear dynamics, ergodicity.

1. Introduction

The theory of large dissipative systems has a long and growing mathematical history. Some of the classical literature one could find e.g. in [24] and [37]; see also references therein. In this paper we focus on dissipative dynamics with noncompact configuration space and their counterparts in noncommutative algebras.

A construction of Markov semigroups on the space of continuous functions with an infinite-dimensional underlying space well suited to study strong ergodicity problems can be found in [51] in case of fully elliptic generators. More recently it was extended to subelliptic situation in [16, 31] and Lévy type generators [35]. An interesting approach via stochastic differential equations one can find in [15] and some recent extension to subelliptic generators in [50] (see also [3, 4] and references therein). Another approach via Dirichlet forms theory which is well adapted to L_2 theory, can be found e.g. in [1, 45] and reference therein.

For symmetric semigroups, after a recent progress in proving the log-Sobolev inequality for infinite-dimensional Hörmander type generators $\mathcal{L}$ symmetric in $L_2(\mu)$ defined with a suitable nonproduct measure μ ([25–28, 32, 43]), one can expect an extension of the established strategy [51] for proving strong pointwise ergodicity for the corresponding Markov semigroups $P_t \equiv e^{t\mathcal{L}}$ (respectively in the uniform norm in case of the compact spaces as in [24] and references therein). One could obtain more results in this direction, including configuration spaces given by infinite products of general noncompact nilpotent Lie groups other than Heisenberg type groups, by conquering a (finite-dimensional) problem of sub-Laplacian bounds (of the corresponding control distance) which for a moment remains still very hard.

The ergodicity theory in case when an invariant measure is not given in advance, in noncompact subelliptic setup is an interesting and challenging problem which was initially studied in [16] and was extended in new directions in [31] developing further

strategy based on generalised gradient bounds. We remark that in fully elliptic case a strategy based on classical Bakry–Emery arguments involving restricted class of interactions can be achieved. In case of the stochastic strategy of [15], the convexity assumption enters via dissipativity condition in a suitable Hilbert space and does not improve the former one as far as ergodicity is concerned; (on the other hand it allows to study a number of stochastically natural models). In subelliptic setup involving subgradient this strategy faces serious obstacles, see e.g. comments in [6].

In noncommutative setup the development of mathematical description of infinite dissipative systems is much less developed. Some description of infinite-dimensional dissipative dynamics of jump type which are not symmetric with respect to a given Gibbs state as well as some results on theirs ergodicity can be found in [54]; see also references therein and [14, 23, 38] on constructions associated to classical Gibbs states (where interaction potential is classical). In [40] a construction and ergodicity results were provided for an interesting class where generator of jumps part corresponds to a classical potential, but additionally the generator contains a conservative part corresponding to a different possibly nonclassical potential. In general, for an infinite-dimensional system still no construction of jump type dynamics exists which would be symmetric for a Gibbs state associated to a generic nonclassical potential. Some interesting general constructions, based on application of Dirichlet form theory [13], are provided in [14, 44] (see also references therein).

A study of diffusion type dynamics providing a construction and ergodicity results were given in [34], including generators associated to a family of noncommuting fields, but not a priori symmetric with respect to an $\mathbb{L}_2$ scalar product associated to a given state.

Another recent examples of dissipative dynamics for infinite boson systems can be found in [7, 41].

One of the important techniques developed to study ergodicity of dissipative dynamics of infinite classical interacting systems is based on use of hypercontractivity property or its infinitesimal form encoded in log–Sobolev inequality ([24] and references therein). A noncommutative basis for such theory was introduced in [42]. Since then, in noncommutative setup some progress was achieved in studying certain directions ([2, 9, 11, 12]) with interesting new results emerging in connection to quantum information theory ([29, 30]). Still many important technical aspects necessary to effective implementation of the theory remain elusive in noncommutative world. (This includes e.g. the product and perturbation properties of log–Sobolev inequality.)

In Sections 2 and 3, we study finite- and infinite-dimensional systems for which we construct dissipative dynamics described by Dunkl type generators and provide certain basic ergodicity results. In Section 4 we give an example of such dissipative dynamics in noncommutative setup. In Section 5 we discuss some nonlinear classical dissipative dynamics and theirs noncommutative counterparts. In Appendix we provide some discussion of monotone convergence in noncommutative $\mathbb{L}_p$ spaces.

2. Dunkl type Markov generators and semigroups

In this section we discuss linear dissipative dynamics associated to Markov generators of the following form

$$\mathcal{L} \equiv \sum_{i\in\mathcal{R}} \mathcal{L}_i$$

defined on a dense domain of the space of bounded continuous functions $\mathcal{C}(\Omega)$ on a product space $\Omega \equiv \times_{i\in\mathcal{R}}\Omega_i$ with $\Omega_i \sim \Omega_0$ is a smooth manifold of finite dimension n, where the indices i form a countable, possibly infinite, set $\mathcal{R}$, and

$$\mathcal{L}_i \equiv \mathbb{T}_i^2 - \beta_i \cdot \mathbb{T}_i$$

with $\mathbb{T}_i \equiv \nabla_i + A_i$, where ∇_i denotes the gradient operator and

$$(A_i f)_l \equiv \frac{\kappa}{x_{i,l}}(f - f\circ\sigma_{i,l})$$

with $\sigma_{i,l}\circ\sigma_{i,l} = \mathrm{id}$, $\sigma_{i,l}(x_{i,l}) = -x_{i,l}$, $l = 1,\ldots,n$, are both acting on i-th coordinate, while β_i's are dependent possibly on many coordinates and are continuously differentiable. First of all we notice that we have

$$\Gamma_{\mathcal{L}_i}(f) \equiv \frac{1}{2}(\mathcal{L}_i f^2 - 2f\mathcal{L}_i f) = |\nabla_i f|^2 + \frac{1}{2\kappa}(A_i f)^2 - \beta_i \cdot \frac{1}{2}(A_i f^2 - 2f A_i f).$$

We note that, unlike as in the diffusion case, the first-order term gives a nontrivial contribution. Since for A type component we have

$$\begin{aligned} A_{i,l} f^2 - 2f A_{i,l} f &= \frac{\kappa}{x_{i,l}}((f^2 - f^2\circ\sigma_{i,l}) - 2f(f - f\circ\sigma_{i,l})) \\ &= -\frac{\kappa}{x_{i,l}}(f - f\circ\sigma_{i,l})^2 = -\frac{x_{i,l}}{\kappa}(A_{i,l} f)^2, \end{aligned}$$

so we get

$$\Gamma_{\mathcal{L}}(f) \equiv \sum_i \left(|\nabla_i f|^2 + \sum_l \frac{1}{2\kappa_l}(1 + \beta_{i,l}\cdot x_{i,l})(A_{i,l} f)^2 \right)$$

which is nonnegative if for all i, l we have

$$1 + \beta_{i,l}\cdot x_{i,l} \geq 0.$$

Next we note that at a minimum point $\tilde{\omega}$ for which components are outside reflection set, we have

$$-\beta_{i,l}\cdot A_{i,l} f = +\beta_{i,l}\cdot x_{i,l}\kappa_l \left(\frac{f\circ\sigma_{i,l}(\tilde{\omega}) - f(\tilde{\omega})}{x_{i,l}^2} \right).$$

Thus, assuming $\nabla_{i,l} x_{i,l} = 1$, we have

$$(\mathbb{T}_{i,l}^2 - \beta_{i,l}\mathbb{T}_{i,l}) f = (\tilde{\omega}),$$

$$\nabla_{i,l}^2 f(\tilde{\omega}) + \frac{2\kappa_l}{x_{i,l}}\nabla_{i,l} f(\tilde{\omega}) + \frac{\kappa_l}{x_{i,l}^2}(f\circ\sigma_{i,l}(\tilde{\omega}) - f(\tilde{\omega})) - \beta_{i,l}\cdot\nabla_{i,l} f(\tilde{\omega})$$

$$+\beta_{i,l}\cdot x_{i,l}\frac{\kappa_l}{x_{i,l}^2}(f\circ\sigma_{i,l}(\tilde{\omega}) - f(\tilde{\omega})) = \nabla_{i,l}^2 f(\tilde{\omega}) + \frac{\kappa_l}{x_{i,l}^2}(1+\beta_{i,l}\cdot x_{i,l})(f\circ\sigma_{i,l}(\tilde{\omega}) - f(\tilde{\omega})) \geq 0$$

under the same condition for the coefficients as before. Using suitable limiting procedure, one obtains similar result if any component of the minimum point belongs to the reflection invariant set.
Hence we get the following condition for $\mathcal{L}$ being a Markov generator.

THEOREM 1. *Suppose for all i, l we have*

$$1 + \beta_{i,l} x_{i,l} \geq 0.$$

Then

$$\Gamma_{\mathcal{L}}(f) \geq 0$$

and $\mathcal{L}$ satisfies the minimum principle, i.e. at a minimum point $\tilde{\omega} \in \Omega$,

$$(\mathcal{L}f)(\tilde{\omega}) \geq 0.$$

REMARK 1. Note that positivity of canonical quadratic form implies minimum principle for functions f for which $(f - \min f)^{1/2}$ is in the domain of the generator.

EXAMPLE 1. Suppose $\Omega \equiv \mathbb{R}^{\mathcal{R}}$ and

$$A_i f = \frac{\kappa}{\omega_i}(f - f \circ \sigma_i)$$

with $\kappa > 0$ and $\sigma_i(\omega)_j = (-1)^{\delta_{ij}} \omega_j$. Suppose

$$\beta_i = a_{2n+1}\omega_i^{2n+1} + \sum_{m=2,..,2n} a_m \omega_i^m + \tilde{M}\omega_i + \sum_{O: O \ni i} b_O \prod_{k \in O} \varsigma(\omega_k),$$

where $a_{2n+1} > 0$, $a_m \in \mathbb{R}$, $n \geq 1$, and $b_O \in \mathbb{R}^+$, with finite sets O, and $\sup_j \sum_{O: O \ni j} |b_O| < \infty$, where $\varsigma(x) = x\chi_{x \in [-1,+1]} + \chi_{x \in [+1,\infty]} - \chi_{x \in (-\infty,-1]}$ and with $\tilde{M} > 0$. Then conditions of the above theorem are satisfied provided the coefficients $a_m, m = 2, .., 2n$, are sufficiently small in absolute value. (It should be clear that one can add to such βs a sufficiently small continuous bounded functions without harming the conditions of the theorem.)

Since $\mathcal{L}$ is densely defined and vanishes on constants, it is a Markov (pre-) generator. Thus one can expect that the corresponding semigroup $P_t \equiv e^{t\mathcal{L}}$ can be well-defined C_0-Markov semigroup on the space of bounded (uniformly-)continuous functions. If the dimension of the space is finite this is fine; in infinite dimensions this requires more arguments which will be discussed later.

3. Generalised gradient bounds

Given a Markov semigroup introduced in the previous section and assuming that it provides some mild smoothing properties, it would be interesting to consider a problem when the following generalised gradient type bounds can be satisfied

$$\tilde{\Gamma}(P_t f)^q \leq C e^{-mt} P_t \tilde{\Gamma}(f)^q,$$

where $\tilde{\Gamma}$ is a quadratic form involving first-order operators, $C \in \mathbb{R}^+, m \in \mathbb{R}$ and $q \in [\frac{1}{2}, 1]$ are constants independent of f and $t \in \mathbb{R}^+$. In particular, one could

ask this question for the canonical Γ form associated to the Markov generator or a form $|\mathbb{T}f|^2 \equiv \sum_i |\mathbb{T}_i f|^2$. Similar bounds involving differential operators may have a variety of applications including ergodicity theory (cf. [16]) or certain smoothing properties of the semigroup (see e.g. [5, 6, 17, 27, 36] and references therein). Even in the case of diffusion operators in finite dimensions it is a hard problem for which a relatively satisfactory solution currently only exists in case of (products of) Heisenberg type groups; for $q = \frac{1}{2}$ the other groups constitute a formidable challenge. Therefore one can expect that our case is even more challenging. Thus, to gain at least some intuition, we discuss here a simplified situations starting from a case of single field and one reflection.

With a function η such that $\eta \circ \sigma = -\eta$ and $X\eta = \varepsilon$, for some constant $\varepsilon \in (0, \infty)$, we set

$$A_\sigma(f) \equiv A(f) \equiv \frac{f - f \circ \sigma}{\eta}, \qquad T \equiv X + A$$

and

$$\mathcal{L} \equiv T^2 - \beta\eta T, \qquad \beta > 0.$$

Then one has

$$(Tf) \circ \sigma = -T(f \circ \sigma), \qquad (\mathcal{L}f) \circ \sigma = \mathcal{L}(f \circ \sigma).$$

Now for $f_s \equiv P_s f$, we have

$$\begin{aligned}\partial_s P_{t-s}|Tf_s|^2 &= P_{t-s}(-\mathcal{L}|Tf_s|^2 + 2Tf_s \cdot T\mathcal{L}f_s)\\ &= P_{t-s}(-2\Gamma(Tf_s) + 2Tf_s \cdot [T, \mathcal{L}]f_s) \le P_{t-s}(2Tf_s \cdot [T, \mathcal{L}]f_s)\end{aligned}$$

with use of

$$-2\Gamma(Tf_s) \equiv -\mathcal{L}|Tf_s|^2 + 2Tf_s \cdot \mathcal{L}Tf_s \le 0.$$

Next note that

$$[T, \mathcal{L}]g = [T, T^2 - \beta\eta T]g = -\beta[T, \eta]Tg = -\beta(\varepsilon Tg + 2(Tg) \circ \sigma).$$

Thus

$$\partial_s P_{t-s}|Tf_s|^2 \le -2\beta P_{t-s}(Tf_s \cdot (\varepsilon Tf_s + 2(Tf_s) \circ \sigma)). \tag{1}$$

Repeating our computation for $f_s \circ \sigma \equiv (P_s f) \circ \sigma$,

$$\begin{aligned}\partial_s P_{t-s}(|(Tf_s)|^2 \circ \sigma) &= P_{t-s}(-\mathcal{L}(|Tf_s|^2 \circ \sigma) + 2(Tf_s) \circ \sigma (T\mathcal{L}f_s) \circ \sigma)\\ &= P_{t-s}(-2\Gamma((Tf_s) \circ \sigma) + 2(Tf_s) \circ \sigma ((T\mathcal{L}f_s) \circ \sigma - \mathcal{L}(Tf_s \circ \sigma)))\\ &= P_{t-s}(-2\Gamma((Tf_s) \circ \sigma) + 2(Tf_s) \circ \sigma (([T, \mathcal{L}]f_s) \circ \sigma))\\ &\le -2\beta P_{t-s}((Tf_s) \circ \sigma \cdot (2(Tf_s) + \varepsilon(Tf_s) \circ \sigma))).\end{aligned} \tag{2}$$

Adding (1) and (2), we obtain

$$\partial_s P_{t-s}(|(Tf_s)|^2 + |(Tf_s)|^2 \circ \sigma) \le -2(2 + \varepsilon)\beta P_{t-s}(|(Tf_s)|^2 + |(Tf_s)|^2 \circ \sigma).$$

Integrating this differential inequality, yields

$$(|(Tf_s)|^2 + |(Tf_s)|^2 \circ \sigma) \le e^{-2(2+\varepsilon)\beta t} P_t(|Tf|^2 + |Tf|^2 \circ \sigma).$$

Next, (although there is no doubt that what follows below can be done for general case of classical (finite) Coxeter groups of Dunkl theory), to focus our attention we consider the case of products of real lines each with a single natural reflection. That is we consider

$$T_i f \equiv (\nabla_i + A_i) f$$

with ∇_i denoting partial derivative with respect to i-th coordinate and

$$A_i f \equiv \kappa \frac{f - f \circ \sigma_i}{\omega_i}$$

with a reflection defined by

$$(\sigma_i \omega)_j \equiv (-1)^{\delta_{ij}} \omega_j.$$

In this setup we note the following relation, in which we set $f_s \equiv P_s f$,

$$\begin{aligned} \partial_s P_{t-s} |T_i f_s|^2 &= P_{t-s}(-\mathcal{L}|T_i f_s|^2 + 2T_i f_s \cdot T_i \mathcal{L} f_s) \\ &= P_{t-s}(-2\Gamma(T_i f_s) + 2T_i f_s \cdot [T_i, \mathcal{L}] f_s) \\ &\leq P_{t-s}(2T_i f_s \cdot [T_i, \mathcal{L}] f_s) \end{aligned}$$

where in the last step we have used the fact that

$$-2\Gamma(T_i f_s) \equiv -\mathcal{L}|T_i f_s|^2 + 2T_i f_s \cdot \mathcal{L} T_i f_s \leq 0.$$

We remark that in the current setup where all directions in the tangent space are represented in the generator, we can afford to disregard otherwise vital nonpositive term $-2\Gamma(T_i f_s)$. Next we note that, by our current assumption

$$\begin{aligned} [T_i, \mathcal{L}_j] g &= [T_i, T_j^2 - \beta_j T_j] g = -[T_i, \beta_j] T_j g \\ &= -(\nabla_i \beta_j) T_j g - A_i(\beta_j)(T_j g) \circ \sigma_i. \end{aligned}$$

Combining this with our previous bounds, we obtain the relation

$$\begin{aligned} \partial_s P_{t-s} |T_i f_s|^2 \leq & -2P_{t-s}((\nabla_i \beta_i)|T_i f_s|^2) - 2P_{t-s}\left(A_i(\beta_i) T_i f_s \cdot (T_i f_s) \circ \sigma_i\right) \\ & - 2\sum_{j \neq i} P_{t-s}\left((\nabla_i \beta_j) T_i f_s \cdot T_j f_s\right) \\ & - 2\sum_{j \neq i} P_{t-s}\left(A_i(\beta_j) T_i f_s \cdot (T_j f_s) \circ \sigma_i\right). \end{aligned}$$

As compared to a conventional situation, where reflections are not in the game, we have now got a trouble in the form of terms containing reflected factors. In case when $\beta_j = \sum_k G_{jk} \omega_k + \eta_j$ with $G_{ii} > 0$ and G_{jk} sufficiently small, and η_j are sufficiently small cylinder functions, at this point we could use quadratic inequality to separate terms containing $|T_i f_s|^2$ and get the following bound,

$$\begin{aligned} \partial_s P_{t-s} |T_i f_s|^2 \leq & -2\alpha P_{t-s} |T_i f_s|^2 + P_{t-s}\left(A_i(\beta_i)|T_i f_s \circ \sigma_i|^2\right) \\ & + \sum_{j \neq i} P_{t-s}\left(|\nabla_i \beta_j| |T_j f_s|^2\right) + \sum_{j \neq i} P_{t-s}\left(|A_i(\beta_j)| |(T_j f_s) \circ \sigma_i|^2\right) \end{aligned}$$

with a constant

$$\alpha \le \inf_i \Big(\nabla_i \beta_i - \frac{1}{2} \sum_{j \neq i} |\nabla_i \beta_j| - \frac{1}{2} \sum_j |A_i(\beta_j)| \Big).$$

Solving this inequality with respect to $P_{t-s}|T_i f_s|^2$, after integration with respect to $s \in [0,t]$ and using supremum bounds for the coefficients, we arrive at

$$|T_i f_t|^2 \le e^{-\alpha t} P_t |T_i f|^2 + \|A_i(\beta_i)\|_\infty \int_0^t ds e^{-\alpha(t-s)} P_{t-s} |T_i f_s \circ \sigma_i|^2$$
$$+ \sum_{j \neq i} \|A_i(\beta_j)\|_\infty \int_0^t ds e^{-\alpha(t-s)} P_{t-s} |(T_j f_s) \circ \sigma_i|^2.$$

At this stage, if P_t is a Markov semigroup, one can pass to the following supremum bounds,

$$\|T_i f_t\|_\infty^2 \le e^{-\alpha t} \|T_i f\|_\infty^2 + \|A_i(\beta_i)\|_\infty \int_0^t ds e^{-\alpha(t-s)} \|T_i f_s\|_\infty^2$$
$$+ \sum_{j \neq i} \|A_i(\beta_j)\|_\infty \int_0^t ds e^{-\alpha(t-s)} \|T_j f_s\|_\infty^2.$$

This relation allows us to show existence of a semigroup in infinite dimensions as well as uniform ergodicity in sup norm if additionally $\alpha > 0$ ([16, 52]).

Unbounded drifts

In what follows we would like to improve on that above by allowing nonlinear unbounded drifts β_i's as well as getting suitable pointwise bounds. To this end we will keep on an assumption that symmetric parts $(\beta_j + \beta_j \circ \sigma_i)$ are zero or sufficiently small. Now we propose to consider simultaneously reflected terms, as follows,

$$\partial_s P_{t-s} |T_i f_s \circ \sigma_i|^2 = P_{t-s}(-\mathcal{L}|T_i f_s \circ \sigma_i|^2 + 2(T_i f_s) \circ \sigma_i \cdot (T_i \mathcal{L} f_s) \circ \sigma_i)$$
$$= P_{t-s}(-2\Gamma(T_i f_s \circ \sigma_i) + 2(T_i f_s) \circ \sigma_i \cdot ([T_i, \mathcal{L}] f_s) \circ \sigma_i$$
$$+ 2(T_i f_s) \circ \sigma_i \cdot ((\mathcal{L} T_i f_s) \circ \sigma_i - \mathcal{L}(T_i f_s \circ \sigma_i)))$$
$$= P_{t-s}(-2\Gamma(T_i f_s \circ \sigma_i) + 2(T_i f_s) \circ \sigma_i \cdot \{(-(\nabla_i \beta_i) T_i f_s - A_i(\beta_i)(T_i f_s) \circ \sigma_i) \circ \sigma_i\})$$
$$+ \sum_{j \neq i} 2 P_{t-s}((T_i f_s) \circ \sigma_i \cdot \{(-(\nabla_i \beta_j) T_j f_s - A_i(\beta_j)(T_j f_s) \circ \sigma_i) \circ \sigma_i\})$$
$$+ P_{t-s} 2 \Big((T_i f_s) \circ \sigma_i \cdot \Big((\beta_i + \beta_i \circ \sigma_i) T_i((T_i f_s) \circ \sigma_i) + \sum_{j \neq i} (\beta_j + \beta_j \circ \sigma_i) T_j((T_i f_s) \circ \sigma_i) \Big) \Big).$$

Since, with some constant $C \in (0, \infty)$, one has

$$|T_i g|^2 \le C \Gamma_i(g),$$

as long as $\gamma \equiv \sup_i \sum_j ||\beta_j + \beta_j \circ \sigma_i||^2_\infty < \infty$, with the use of quadratic inequality we see that

$$
\begin{aligned}
&-2\Gamma(T_i f_s \circ \sigma_i) \\
&+2\Big((T_i f_s)\circ\sigma_i \cdot \Big((\beta_i + \beta_i\circ\sigma_i)T_i((T_i f_s)\circ\sigma_i) + \sum_{j\neq i}(\beta_j + \beta_j\circ\sigma_i)T_j((T_i f_s)\circ\sigma_i)\Big)\Big) \\
&\qquad\qquad \leq \frac{C}{2}\gamma |T_i f_s \circ \sigma_i|^2.
\end{aligned}
$$

This allows us to get

$$
\begin{aligned}
\partial_s P_{t-s}|T_i f_s \circ \sigma_i|^2 \leq\ & -2P_{t-s}\left(\left((\nabla_i\beta_i)\circ\sigma_i - \frac{C}{4}\gamma\right)|T_i f_s\circ\sigma_i|^2\right) \\
& -2P_{t-s}((A_i(\beta_i)\circ\sigma_i)(T_i f_s)\circ\sigma_i\cdot(T_i f_s)) \\
& -2\sum_{j\neq i} P_{t-s}\left((T_i f_s)\circ\sigma_i\cdot\left\{\left(((\nabla_i\beta_j)\circ\sigma_i)(T_j f_s)\circ\sigma_i + A_i(\beta_j)\circ\sigma_i(T_j f_s)\right)\right\}\right).
\end{aligned}
$$

This together with similar bound for $\partial_s P_{t-s}(T_i f_s)$ obtained before, yields

$$
\begin{aligned}
&\partial_s P_{t-s}(|T_i f_s|^2 + |T_i f_s\circ\sigma_i|^2) \\
&\quad\leq -2P_{t-s}((\nabla_i\beta_i)|T_i f_s|^2) - 2P_{t-s}\left(\left((\nabla_i\beta_i)\circ\sigma_i - \frac{C}{4}\gamma\right)|T_i f_s\circ\sigma_i|^2\right) \\
&\qquad -2P_{t-s}\left((A_i(\beta_i) + A_i(\beta_i)\circ\sigma_i)T_i f_s\cdot(T_i f_s)\circ\sigma_i\right) \\
&\qquad -2\sum_{j\neq i} P_{t-s}\left((\nabla_i\beta_j)T_i f_s\cdot T_j f_s\right) - 2\sum_{j\neq i} P_{t-s}\left(A_i(\beta_j)T_i f_s\cdot(T_j f_s)\circ\sigma_i\right) \\
&\qquad -2\sum_{j\neq i} P_{t-s}\left(((\nabla_i\beta_j)\circ\sigma_i)(T_i f_s)\circ\sigma_i\cdot(T_j f_s)\circ\sigma_i\right) \\
&\qquad -2\sum_{j\neq i} P_{t-s}\left(A_i(\beta_j)\circ\sigma_i(T_i f_s)\circ\sigma_i\cdot(T_j f_s)\right).
\end{aligned}
$$

We can simplify that by using the quadratic inequality to have

$$
\begin{aligned}
\partial_s P_{t-s}(|T_i f_s|^2 + |T_i f_s\circ\sigma_i|^2) \leq\ & -2M P_{t-s}(|T_i f_s|^2 + |T_i f_s\circ\sigma_i|^2) \\
& + \sum_{j\neq i}\gamma_{ij} P_{t-s}(|T_j f_s|^2 + |(T_j f_s)\circ\sigma_i|^2)
\end{aligned}
$$

provided that

$$
(\nabla_i\beta_i) + (\nabla_i\beta_i)\circ\sigma_i - \frac{1}{2}|A_i(\beta_i) + A_i(\beta_i)\circ\sigma_i| - \frac{1}{2}\sum_{j\neq i}\gamma_{ij} - \frac{C}{4}\gamma \geq M
$$

and where we set

$$
\gamma_{ij} \equiv \|\nabla_i\beta_j\|_\infty + \|A_i(\beta_j)\|_\infty.
$$

Now we are in much better shape than before. This is because the first condition allows for β_i other than linear, for example including

$$\beta_i = a_{2n+1}\omega_i^{2n+1} + \sum_{l=2,..,2n} a_l\omega_i^l + \tilde{M}\omega_i + \sum_{k\neq i} G_{ik}\omega_k + \sum_{O:O\ni i} b_O \prod_{k\in O} \varsigma(\omega_k),$$

where $a_{2n+1} > 0$, $n \geq 1$, and $a_l, b_O \in \mathbb{R}$, with finite sets O, and $\sup_j \sum_{O:O\ni j} |b_O| < \infty$, where $\varsigma(x) = x\chi_{x\in[-1,+1]} + \chi_{x\in[+1,\infty]} - \chi_{x\in(-\infty,-1]}$ and finally with $\tilde{M} > 0$. Thus, for such drift coefficients β_i, integration with respect to s of our differential inequality yields the following,

$$|T_i f_t|^2 + |T_i f_t \circ \sigma_i|^2 \leq e^{-2Mt} P_t(|T_i f|^2 + |T_i f \circ \sigma_i|^2) + \sum_{j\neq i} \gamma_{ij} \int_0^t ds e^{-2M(t-s)} P_{t-s}(|T_j f_s|^2 + |(T_j f_s) \circ \sigma_i|^2).$$

From this we get the the following bound as a simple implication.

LEMMA 1.

$$\|T_i f_t\|_\infty^2 \leq 2e^{-2Mt}\|T_i f\|_\infty^2 + \sum_{j\neq i} 2\gamma_{ij} \int_0^t ds e^{-2M(t-s)} \|T_j f_s\|_\infty^2.$$

With this inequality, via standard arguments, see e.g. [16, 49, 51] and references therein, one obtains finite speed of propagation of information which allows to show the existence of the semigroup in infinite dimensions and, under additional assumptions, existence of invariant measure and strong ergodicity. That is one has the following result.

THEOREM 2. *Suppose* $M, \gamma_{ij} \in \mathbb{R}$ *with* $\gamma_{ij} > 0$ *and* $\sup_i \sum_j \gamma_{ij} < \infty$. *Then the Markov semigroup* P_t *is well defined in infinite dimensions. Moreover, if* $M > 0$ *and* $\sup_i \sum_j \gamma_{ij} > 0$ *is sufficiently small, then there exists* $m \in (0, \infty)$ *such that*

$$\|\mathbb{T} f_t\|_\infty^2 \leq 2e^{-2mt}\|\mathbb{T} f\|_\infty^2$$

with

$$\|\mathbb{T} g\|_\infty^2 \equiv \sum_i \|T_i g\|_\infty^2.$$

In this case there exists a unique measure μ *with finite moments such that*

$$\|f_t - \int f d\mu\|_\infty^2 \leq e^{-2mt} C(\|\mathbb{T} f\|_\infty)$$

for any cylinder function f *with bounded* $\|T_i f\|_\infty^2$ *with some constant* $C(\|\mathbb{T} f\|_\infty) \in (0, \infty)$ *independent of* $t \in (0, \infty)$.

Now we get back to our symmetrised with respect to σ_i inequality in our claim and notice that, at least when our Coxeter group generated by reflections is

finite, one could consider full symmetrisation to get after resummation the following Gronwal type inequality

$$\|\mathbb{T} f_t\|^2_{\mathrm{Cox}} \leq e^{-2\hat{M}t} P_t \|\mathbb{T} f\|^2_{\mathrm{Cox}} + \sum_{j\neq i} \hat{\gamma}_{ij} \int_0^t ds e^{-2\hat{M}(t-s)} P_{t-s} \|\mathbb{T} f_s\|^2_{\mathrm{Cox}}$$

with

$$\|\mathbb{T} g\|^2_{\mathrm{Cox}} \equiv \sum_i \sum_{c\in \mathrm{Cox}} |T_i g \circ c|^2$$

A simple application of this yields the following bound.

CLAIM. *With some* $\hat{m} \in \mathbb{R}$,

$$\|\mathbb{T} f_t\|^2_{\mathrm{Cox}} \leq e^{-2\hat{m}t} P_t \|\mathbb{T} f\|^2_{\mathrm{Cox}}.$$

One may expect that similar bound could be possible for square of a seminorm in which we sum over i and composition with c is replaced by projections (on subspaces obtained via symmetrisation subordinated to Cox). One may hope that the last could possibly survive also in the case when the Coxeter group is infinite (at least on some smaller class of functions which are sufficiently quickly decreasing to zero with the size of $c \in \mathrm{Cox}$). This is for a moment an interesting, challenging and widely open problem.

REMARK 2. A theory of dissipative semigroups generated by Dunkl type operators associated to noncommutative groups was recently developed in [52] and [53].

4. Quantum Dunkl type generators

In this section we provide a description of linear dissipative semigroup with Dunkl type generators in a noncommutative algebra $\mathcal{A}$. While the principal objective here is to provide a new noncommutative model, one could also potentially hope for a possible application of such models to quantum information theory.

Let $\sigma_j \in \mathcal{A}$, $j \in \mathcal{I}$, be such that $\sigma_j^* = \sigma_j$, $\sigma_j^2 = 1$ and $\{\sigma_j, \sigma_k\} = 0$. Define maps

$$\mathcal{A} \ni f \to \mathfrak{S}_{jk}(f) \equiv \sigma_j f \sigma_k \in \mathcal{A}.$$

Then we have

$$\mathfrak{S}^2_{jk} = I \qquad \text{and} \qquad \mathfrak{S}_{jk}(fg) = \mathfrak{S}_{jk}(f)\mathfrak{S}_{kk}(g) = \mathfrak{S}_{jj}(f)\mathfrak{S}_{jk}(g).$$

Define

$$A^L_{jk}(f) \equiv \kappa_{jk}(f - \mathfrak{S}_{jk}(f)) \qquad \text{and} \qquad A^R_{jk}(f) \equiv (f - \mathfrak{S}_{jk}(f))\tilde{\kappa}_{jk}$$

with $\mathfrak{S}_{jj}(\kappa_{jk}) = -\kappa_{jk}$ and $\mathfrak{S}_{kk}(\tilde{\kappa}_{jk}) = -\tilde{\kappa}_{jk}$. Then we have

$$\begin{aligned} A^L_{jk}(A^L_{jk}(f)) &= A^L_{jk}(\kappa_{jk}(f - \mathfrak{S}_{jk}(f))) \\ &= \kappa_{jk}(\kappa_{jk}(f - \mathfrak{S}_{jk}(f)) - \mathfrak{S}_{jk}(\kappa_{jk}(f - \mathfrak{S}_{jk}(f)))). \end{aligned}$$

Since

$$\begin{aligned}\mathfrak{S}_{jk}(\kappa_{jk}(f-\mathfrak{S}_{jk}(f))) &= -\kappa_{jk}(\mathfrak{S}_{jk}(f)-\mathfrak{S}_{jk}^2(f)) = -\kappa_{jk}(\mathfrak{S}_{jk}(f)-f)\\ &= \kappa_{jk}(f-\mathfrak{S}_{jk}(f))\end{aligned}$$

we obtain

$$A_{jk}^L(A_{jk}^L(f)) = 0.$$

Similarly we have

$$A_{jk}^R(A_{jk}^R(f)) = 0.$$

We also note that

$$\begin{aligned}A_{jk}^R(A_{jk}^L(f)) &= A_{jk}^R(\kappa_{jk}(f-\mathfrak{S}_{jk}(f)))\\ &= (\kappa_{jk}(f-\mathfrak{S}_{jk}(f)) - \mathfrak{S}_{jk}(\kappa_{jk}(f-\mathfrak{S}_{jk}(f))))\tilde{\kappa}_{jk}\\ &= (\kappa_{jk}(f-\mathfrak{S}_{jk}(f)) - (\kappa_{jk}(f-\mathfrak{S}_{jk}(f))))\tilde{\kappa}_{jk} = 0\end{aligned}$$

and similarly

$$A_{jk}^L(A_{jk}^R(f)) = 0.$$

Next consider a derivation $\delta_l(f) \equiv [\sigma_l, f]$, which satisfies

$$\delta_l(\sigma_j) = 2\sigma_l\sigma_j(1-\delta_{lj}).$$

Then, for $l \neq j, k$, we have

$$\begin{aligned}\delta_l(\mathfrak{S}_{jk}(f)) &= \delta_l(\sigma_j f \sigma_k) = \delta_l(\sigma_j) f\sigma_k + \sigma_j\delta_l(f)\sigma_k + \sigma_j f\delta_l(\sigma_k)\\ &= -2\sigma_j\sigma_l f\sigma_k + \sigma_j\delta_l(f)\sigma_k + \sigma_j f 2\sigma_l\sigma_k = -\sigma_j\delta_l(f)\sigma_k\\ &= -\mathfrak{S}_{jk}(\delta_l(f)).\end{aligned}$$

That is $\mathfrak{S}_{jk}$ is a reflection in the sense of [52, 53] (in the direction of "tangent vector" δ_l). Using this we can introduce the following generalised derivations,

$$\mathbb{T}f \equiv \nabla f + \mathbb{A}(f)$$

with components $\mathbb{T}_l \equiv \nabla_l + \mathbb{A}_l$, $l \in \mathcal{I}$, defined by $\nabla_l = \delta_l$ and

$$\mathbb{A}_l \equiv A_{jk}^L + A_{jk}^R.$$

We define an operator

$$\mathcal{L}_l f \equiv \mathbb{T}_l^2 f = (\delta_l^2 + \delta_l\mathbb{A}_l + \mathbb{A}_l\delta_l)f \equiv \mathcal{L}_0 f + \{\nabla_l, \mathbb{A}_l\}f$$

and its associated quadratic form

$$\Gamma_{\mathcal{L}_l}(f) \equiv \frac{1}{2}(\mathcal{L}_l(f^*f) - \mathcal{L}_l(f^*)f - f^*\mathcal{L}_l(f)).$$

Note that

$$\Gamma_{\mathcal{L}_l}(f) \equiv -(\delta_l(f))^*\delta_l(f) + \Gamma_{\{\delta_l, \mathbb{A}_l\}}(f)$$

where

$$\Gamma_{\{\delta_l,\mathbb{A}_l\}}(f) \equiv \frac{1}{2}(\{\delta_l,\mathbb{A}_l\}(f^*f) - \{\delta_l,\mathbb{A}_l\}(f^*)f - f^*\{\delta_l,\mathbb{A}_l\}(f)) = \Gamma_{\{\delta_l,\mathbb{A}_l^L\}}(f) + \Gamma_{\{\delta_l,\mathbb{A}_l^R\}}(f).$$

Since, using reflection property $\delta_l(\mathfrak{S}_{jk}(f)) = -\mathfrak{S}_{jk}(\delta_l(f))$, we have

$$\{\delta_l,\mathbb{A}_l^L\}(f) = 2\kappa_{jk}\delta_l(f) + \delta_l(\kappa_{jk})(f - \mathfrak{S}_{jk}(f))$$

so

$$\frac{1}{2}(\{\delta_l,\mathbb{A}_l^L\}(f^*f) - \{\delta_l,\mathbb{A}_l^L\}(f^*)f - f^*\{\delta_l,\mathbb{A}_l^L\}(f)) = 2[\kappa_{jk,}f^*]\delta_l(f)$$
$$+\frac{1}{2}\left(\delta_l(\kappa_{jk})(f^*f - \mathfrak{S}_{jk}(f^*f)) - \delta_l(\kappa_{jk})\left(f^* - \mathfrak{S}_{jk}(f^*)\right)f - f^*\delta_l(\kappa_{jk})(f - \mathfrak{S}_{jk}(f))\right).$$

The second part on the right-hand side can be represented as

$$\frac{1}{2}\left(\delta_l(\kappa_{jk})(f^*f - \mathfrak{S}_{jk}(f^*f)) - \delta_l(\kappa_{jk})\left(f^* - \mathfrak{S}_{jk}(f^*)\right)f - f^*\delta_l(\kappa_{jk})(f - \mathfrak{S}_{jk}(f))\right)$$
$$= -\frac{1}{2}\delta_l(\kappa_{jk})(f^* - \mathfrak{S}_{jk}(f^*)) \cdot (f - \mathfrak{S}_{jk}(f))$$
$$+\frac{1}{4}\delta_l(\kappa_{jk})(\mathfrak{S}_{jk}(f^*)(\mathfrak{S}_{jk}(f) - \mathfrak{S}_{kk}(f)) + (\mathfrak{S}_{jk}(f^*) - \mathfrak{S}_{jj}(f^*))\mathfrak{S}_{jk}(f))$$
$$+\frac{1}{2}([\delta_l(\kappa_{jk}), f^*](f - \mathfrak{S}_{jk}(f))).$$

In particular, we see that for a special case $j = k$, we obtain

$$\frac{1}{2}\left(\delta_l(\kappa_{jk})(f^*f - \mathfrak{S}_{jk}(f^*f)) - \delta_l(\kappa_{jk})\left(f^* - \mathfrak{S}_{jk}(f^*)\right)f - f^*\delta_l(\kappa_{jk})(f - \mathfrak{S}_{jk}(f))\right)$$
$$= -\frac{1}{2}\delta_l(\kappa_{jj})(f - \mathfrak{S}_{jj}(f))^* \cdot (f - \mathfrak{S}_{jj}(f)) + \frac{1}{2}([\delta_l(\kappa_{jj}), f^*](f - \mathfrak{S}_{jj}(f))),$$

and hence we have

$$\Gamma_{\{\delta_l,\mathbb{A}_l^L\}}(f) = -2([\kappa_{jj,}f])^*\delta_l(f) - \frac{1}{2}\delta_l(\kappa_{jj})(f - \mathfrak{S}_{jj}(f))^* \cdot (f - \mathfrak{S}_{jj}(f))$$
$$+\frac{1}{2}([\delta_l(\kappa_{jj}), f^*](f - \mathfrak{S}_{jj}(f))).$$

Similarly, we have

$$\Gamma_{\{\delta_l,\mathbb{A}_l^R\}}(f) = 2\delta_l(f^*)[\tilde{\kappa}_{jk}, f]$$
$$+\frac{1}{2}\left((f^*f - \mathfrak{S}_{jk}(f^*f))\delta_l(\tilde{\kappa}_{jk}) - \left(f^* - \mathfrak{S}_{jk}\left(f^*\right)\right)\delta_l(\tilde{\kappa}_{jk})f - f^*(f - \mathfrak{S}_{jk}(f))\delta_l(\tilde{\kappa}_{jk})\right)$$

and

$$\frac{1}{2}\left((f^*f - \mathfrak{S}_{jk}(f^*f))\delta_l(\tilde{\kappa}_{jk}) - \left(f^* - \mathfrak{S}_{jk}\left(f^*\right)\right)\delta_l(\tilde{\kappa}_{jk})f - f^*(f - \mathfrak{S}_{jk}(f))\delta_l(\tilde{\kappa}_{jk})\right)$$
$$= -\frac{1}{2}((f^* - \mathfrak{S}_{jk}(f^*))(f - \mathfrak{S}_{jk}(f)))\delta_l(\tilde{\kappa}_{jk})$$
$$+ \frac{1}{4}\left(\left(\mathfrak{S}_{jk}(f^*)(\mathfrak{S}_{jk}(f) - \mathfrak{S}_{kk}(f)) + \left(\mathfrak{S}_{jk}(f^*) - \mathfrak{S}_{jj}(f^*)\right)\mathfrak{S}_{jk}(f)\right)\delta_l(\tilde{\kappa}_{jk})\right)$$
$$+ \frac{1}{2}(f^* - \mathfrak{S}_{jk}(f^*))[\delta_l(\tilde{\kappa}_{jk}), f].$$

Again, for $j = k \neq l$, we can simplify this expression as

$$\frac{1}{2}\left((f^*f - \mathfrak{S}_{jk}(f^*f))\delta_l(\tilde{\kappa}_{jk}) - \left(f^* - \mathfrak{S}_{jk}\left(f^*\right)\right)\delta_l(\tilde{\kappa}_{jk})f - f^*(f - \mathfrak{S}_{jk}(f))\delta_l(\tilde{\kappa}_{jk})\right)$$
$$= -\frac{1}{2}((f^* - \mathfrak{S}_{jj}(f^*))(f - \mathfrak{S}_{jj}(f)))\delta_l(\tilde{\kappa}_{jj}) + \frac{1}{2}(f^* - \mathfrak{S}_{jj}(f^*))[\delta_l(\tilde{\kappa}_{jj}), f].$$

Hence we get

$$\Gamma_{\{\delta_l, \mathbb{A}_l^R\}}(f) = -2(\delta_l(f))^*[\tilde{\kappa}_{jj}, f] - \frac{1}{2}(f - \mathfrak{S}_{jj}(f))^* \cdot (f - \mathfrak{S}_{jj}(f))\delta_l(\tilde{\kappa}_{jj})$$
$$+ \frac{1}{2}(f^* - \mathfrak{S}_{jj}(f^*))[\delta_l(\tilde{\kappa}_{jj}), f].$$

Assuming

$$\kappa_{jj} = \kappa\sigma_l \quad \text{and} \quad \tilde{\kappa}_{jj} = \tilde{\kappa}\sigma_l,$$

combining our calculations we arrive at

$$\Gamma_{\mathcal{L}_l}(f) = -(1 - 2\kappa - 2\tilde{\kappa})(\delta_l(f)^*)\delta_l(f)$$

which is nonpositive provided $2\kappa + 2\tilde{\kappa} \leq 1$. Thus an operator

$$\mathcal{L}f \equiv \mathbb{T}^2 f \equiv \sum_l \mathbb{T}_l^2 f$$

is Markovian. We remark that in general the operators $\mathbb{T}_l$ may not commute (and thus we are in general setup of [53]).

5. On nonlinear dissipative dynamics

To begin we mention first that in [48] an interesting nonlinear dissipative dynamics of jump type was introduced and studied for infinite interacting systems of classical spins on a lattice. The generator of this dynamics is formally given by

$$\mathcal{L}f \equiv \sum_{l \in \mathbb{Z}^d} (\mathbb{E}_l - \mathbb{I})(f)$$

where

$$\mathbb{E}_l f \equiv \frac{1}{\beta} \log E_{X+l} e^{\beta f}$$

with E_{X+l} denotes a conditional expectation given a configuration of the system in $\mathbb{Z}^d \setminus \{X + l\}$ associated to a Gibbs measure and $\beta \in \mathbb{R} \setminus \{0\}$. (The elementary operator in the sum can be understood as a Glauber type generator corrected by the relative entropy part.) One can show that the corresponding semigroup $\mathcal{P}_t \equiv e^{t\mathcal{L}}$ preserves unit and positivity and it was demonstrated there that, under suitable mixing condition, the corresponding dynamics is exponentially ergodic [48]. Without getting into more detail, a more extensive description can be found in [55], such kind of dynamics could prove to be interesting in relation to certain optimization problems, see also a work [39] for some other application of nonlinear averages to economy.

A desire to construct and understand nonlinear noncommutative dissipative dynamics led to the paper [33] where in particular the following result was proved. For $E_i, i = 1, ..., n$, being linear, positive and unital operators on a C^* algebra $\mathcal{A}$, we define $\mathcal{L} : D(F) \to \mathcal{A}$,

$$\mathcal{L}(x) = \sum_{i=1}^{n} \alpha_i \log E_i(e^x) - x,$$

with

$$D(F) = \mathcal{A}_{\text{sa}} \cap K(x, r) \equiv \{y \in \mathcal{A} : \|x - y\| < r\}, \qquad r > 0,$$

and $\alpha_i \geq 0, \sum_{i=1}^{n} \alpha_i = 1$. Note that $\mathcal{L} - (e^r - 1)I$ is strictly dissipative because

$$\| \log E_i(e^{x_2}) - \log E_i(e^{x_1}) \| \leq e^r \|x_2 - x_1\|,$$

and so,

$$\forall \varphi \in J(x_2 - x_1) \equiv (\text{tangent} \quad \text{functionals} \quad \text{at} \quad x_2 - x_1),$$

$$\begin{aligned} \Re\langle \varphi, F(x_2) - F(x_1) \rangle &= \sum_{i=1}^{n} \alpha_i \Re\langle \varphi, \log E_i(e^{x_2}) - \log E_i(e^{x_1}) \rangle - \|x_2 - x_1\| \\ &\leq \sum_{i=1}^{n} \alpha_i \| \log E_i(e^{x_2}) - \log E_i(e^{x_1}) \| - \|x_2 - x_1\| \\ &\leq (e^r - 1)\|x_2 - x_1\|. \end{aligned}$$

Moreover, one-point dissipativity also holds

$\forall x \in D(F) \setminus \{0\} \forall \varphi \in J(x)$,

$$\Re\langle \varphi, F(x) \rangle = \sum_{i=1}^{n} \alpha_i \Re\langle \varphi, \log E_i(e^x) \rangle - \|x\| \leq \sum_{i=1}^{n} \alpha_i \| \log E_i(e^x) \| - \|x\| \leq 0.$$

Hence we have the following result (see [33] for details).

THEOREM 3. *The operator*

$$\mathcal{L}(x) = \sum_{i=1}^{n} \alpha_i \log E_i(e^x) - x,$$

generates a Lipschitz semigroup $S_t : D(F) \to D(F)$ *which is contractive and preserves unit and positivity, i.e.* $(S_t)_{t\geq 0}$ *is a conservative Markov semigroup.*

It is a challenging problem to obtain an infinite-dimensional extension of this result and ergodicity theory for the corresponding semigroup.

REMARK 3. It is also an interesting open question, if it could be possible to extend a classical nonlinear annealing algorithm of [55] to study a challenging problem of determining ground states for large interacting quantum systems.

A theory of nonlinear dissipation for infinite-dimensional interacting systems has been developed over time in [18, 21] and recently in [19]. In particular in the last work we have used log-Sobolev inequality to provide a solution of reaction-diffusion (R-D) type problem when, first of all the underlying space is infinite-dimensional and secondly, when one can have different type of mixing. That is we have studied a system

$$\partial_t u_i = L_i u_i + (\beta_i - \alpha_i)\left(k \prod_{j=1}^{q} u_j^{\alpha_j} - l \prod_{j=1}^{q} u_j^{\beta_j}\right),$$

where $i = 1, \ldots, q$; $\alpha_i, \beta_i \in \mathbb{R}^+$, $\beta_i \neq \alpha_i$; and L_i an operator which models how the i-th substance diffuses, with a key assumption being that these generators satisfy the log-Sobolev inequality

$$\mu\left(f^2 \log \frac{f^2}{\mu f^2}\right) \leq c_i \mu(f(-L_i f))$$

with a given probability measure μ and a constant $c_i \in (0, \infty)$ independent of a function f.

This inequality played in the past an essential role in the development of ergodicity theory for infinite spin systems on a lattice, see e.g. [24, 47], and it is expected that it will be similar in the discussed case of R-D systems [20].

As we mentioned in Introduction, a general theory for the log-Sobolev inequality and associated hypercontractivity property for corresponding linear dissipative semigroups in noncommutative algebras was introduced and initially studied in [42]. In general there is still a number of elements well known for classical case, but hard to get in the noncommutative case. One of them, the equivalence of the log-Sobolev inequality to Sobolev–Orlicz type inequalites (as introduced in [8]), was recently obtained in [2], but still there are many other (including perturbation and product property) awaiting to be understood. One of the possibly promising direction of the progress should be the one including the systems with classical potentials for which jump type dynamics can be well defined for the infinite system.

In this case one can expect that for any local observable f we have the following limit

$$\lim_{n\to\infty} E_{i_n} \dots E_{i_1} f = \omega(f),$$

where E_j denotes a completely positive map given by a generalised conditional expectation which is symmetric in $\mathbb{L}_{2,1/2}(\omega)$ space, with suitable sequence $(i_k)_{k\in\mathbb{N}}$ "going infinitely many times through each site of a lattice" in the sense of [51]. (In Appendix we discuss briefly some matters related to this and other type of limits involving generalised conditional expectation given by completely positive map.)

Appendix. Towards the martingale convergence theorem in noncommutative $\mathbb{L}_p$ spaces

At this point it is interesting to notice the joint monotonicity inequalities for $\mathbb{L}_{p,1/2}(\omega)$ norms obtained in [2], with $\omega \equiv \mathrm{Tr}(\rho\cdot) \equiv \mathrm{Tr}(P^{-1}\cdot)$ where $P = P^* > 0$ with $\mathrm{Tr}\, P^{-1} = 1$.

THEOREM 4. $\forall \alpha \in [0,1],\ \forall r = 2n,\ n \in \mathbb{N}$,

$$\mathrm{Tr}\,|\varphi(P)^{-(1-\alpha)/r}\varphi(f)\varphi(P)^{-\alpha/r}|^r \le \mathrm{Tr}\,|P^{-(1-\alpha)/r} f P^{-\alpha/r}|^r \equiv \|f\|_{P^{-1},\alpha,r}$$

where φ is a completely positive mapping.

Let

$$\langle f, g\rangle_{P,\alpha} \equiv \mathrm{Tr}(P^{-(1-\alpha)} f^* P^{-\alpha} g) = \mathrm{Tr}((P^{-\alpha/2} f P^{-(1-\alpha)/2})^*(P^{-\alpha/2} g P^{-(1-\alpha)/2}))$$

and

$$E_{X,\alpha}(f) \equiv \mathrm{Tr}_X(\gamma^*_{X,\alpha,L} f \gamma_{X,\alpha,R})$$

with

$$\gamma_{X,\alpha,R} \equiv P^{-(1-\alpha)}(\mathrm{Tr}_X\, P^{-1})^{-(1-\alpha)} \equiv \gamma^*_{X,1-\alpha,L}.$$

Then we have

$$\langle E_{X,\alpha}(f), E_{X,\alpha}(g)\rangle_{E_{X,\alpha}(P),\alpha} = \mathrm{Tr}(E_{X,\alpha}(P)^{-(1-\alpha)} E_{X,\alpha}(f)^* E_{X,\alpha}(P)^{-\alpha} E_{X,\alpha}(g))$$

with

$$\begin{aligned} E_{X,\alpha}(P) &= \mathrm{Tr}_X(((\mathrm{Tr}_X\, P^{-1})^{-\alpha})\, P^{-\alpha} P P^{-(1-\alpha)} (\mathrm{Tr}_X\, P^{-1})^{-(1-\alpha)}) \\ &= \mathrm{Tr}_X((\mathrm{Tr}_X\, P^{-1})^{-1}) = (\mathrm{Tr}_X\, P^{-1})^{-1}. \end{aligned}$$

In particular, for $\alpha = \frac{1}{2}$, we have $E_{X,\alpha}(\cdot)$ is a completely positive map.

The product case

We consider first a product state given by

$$P \equiv \otimes_{k=1}^n P_k,$$

where $P_k \equiv P_{X_k} \in \mathcal{A}_{X_k}$, $k = 1, \dots, n$, are commuting positive matrices s.t. $\mathrm{Tr}_{X_k} P_k^{-1} = 1$, and for $n > j \in \mathbb{N}$ set $P_{\ge j} \equiv \otimes_{k=1}^j I_k \otimes_{k=j+1}^n P_k$ and $P_{\ge n} \equiv I$.

Then, we have

$$\prod_{k=1}^{j} E_{X_k,\alpha}(P) \equiv E_{\geq j,\alpha}(P) = P_{\geq j}.$$

In the current situation

$$\gamma_{X_k,\alpha,R} \equiv P^{-(1-\alpha)}(\mathrm{Tr}_{X_k} P^{-1})^{-(1-\alpha)} = P_{X_k}^{-(1-\alpha)},$$
$$E_{X_k,\alpha}(f) = \mathrm{Tr}_{X_k}(P_{X_k}^{-\alpha} f P_{X_k}^{-(1-\alpha)}) = \mathrm{Tr}_{X_k}(P_{X_k}^{-1} f).$$

In a special case $\alpha = \frac{1}{2}$, we will omit the index α writing $E_{X_k}(f) \equiv E_{X_k,1/2}(f)$ and $\|f\|_r \equiv \|f\|_{1/2,r}$. The monotonicity result above, yields

$$\|E_{\geq j}(f)\|_{E_{\geq j}(P)^{-1},r} = \|E_{X_j} E_{\geq j-1}(f)\|_{E_{X_j} E_{\geq j-1}(P)^{-1},r}$$
$$\leq \|E_{\geq j-1}(f)\|_{E_{\geq j-1}(P)^{-1},r}.$$

For $j = n$, we have

$$\|E_{\geq n}(f)\|_{E_{\geq n}(P)^{-1},r} = \|E_{\geq n}(f)\|_{I,r}$$

and

$$E_{\geq n}(f) = \mathrm{Tr}(P^{-1} f) \equiv \omega(f).$$

Naturally this can be generalised to infinite product states with the claim that

$$\lim_{j\to\infty} \|E_{\geq j}(f)\|_{E_{\geq j}(P)^{-1},r} = |\omega(f)|$$

for any local observable f.

Next consider a family of completely positive operator of the form

$$E_X(f) = \mathrm{Tr}_X(\gamma_X^* f \gamma_X), \qquad X \subset\subset \mathfrak{R}$$

which are symmetric in $\mathbb{L}_2(\omega) \equiv \mathbb{L}_{2,\frac{1}{2}}(\omega)$ and unital. Let us assume that there exists a commutative subalgebra $\mathcal{A}_c$ such that $\gamma_X \in \mathcal{A}_c$ and $E_X(\mathcal{A}_c) \subseteq \mathcal{A}_c$. Suppose a family $\{E_X\}_{X\in\mathfrak{R}_0}$, for some countable $\mathfrak{R}_0 \subsetneq \mathfrak{R}$, is ergodic in the sense that

$$\forall f \in \mathcal{A}_c, \qquad \lim_{n\to\infty} E_{X_n} \dots E_{X_1}(f) = \omega(f) \tag{3}$$

and $\forall g \in \mathcal{A}_0$, with a dense subalgebra $\mathcal{A}_0 \subset \mathcal{A}$, $\exists n \in \mathbb{N}$, $E_{X_n} \dots E_{X_1}(g) \in \mathcal{A}_c \cap \mathcal{A}_0$. Then, for $f = E_{X_m} \dots E_{X_1}(g) \in \mathcal{A}_c \cap \mathcal{A}_0$ given by $g \in \mathcal{A}_0$ with some $m \in \mathbb{N}$, we have

$$\lim_{n\to\infty} E_{X_n} \dots E_{X_1}(f) = \omega(f) = \omega(E_{X_m} \dots E_{X_1}(g)) = \langle \mathbb{1}, E_{X_m} \dots E_{X_1}(g)\rangle_{2,\omega}.$$

Since by our assumption E_X are symmetric and unital, by induction we get

$$\langle E_{X_m}(\mathbb{1}), E_{X_{m-1}} \dots E_{X_1}(g)\rangle_{2,\omega} = \langle \mathbb{1}, E_{X_{m-1}} \dots E_{X_1}(g)\rangle_{2,\omega} = \langle \mathbb{1}, g\rangle_{2,\omega} = \omega(g).$$

In particular, this idea can be used for a system with classical interaction, i.e. when

for $f \in \mathcal{A}_0$,

$$\omega(f) \equiv \lim_{\Lambda \to \mathfrak{R}} \mathrm{Tr}(e^{-U_\Lambda} f) / \mathrm{Tr}(e^{-U_\Lambda})$$

with

$$U_\Lambda \equiv \sum_{X \cap \Lambda \neq \emptyset} \Phi_X, \text{ and } \Phi_X \in \mathcal{A}_c \cap \mathcal{A}_0 \text{ with } \sup_{i \in \mathfrak{R}} \sum_{X \subset \mathfrak{R},\ X \ni i} \|\Phi_X\|_{\mathcal{A}} < \infty;$$

and one is given a family

$$\{\mathrm{Tr}_X : X \subset \mathfrak{R}, |X| < \infty | \mathrm{Tr}(\mathrm{Tr}_X(f)) = \mathrm{Tr}(f),\ \mathrm{Tr}_X \mathrm{Tr}_X(f) = \mathrm{Tr}_X(f), \mathrm{Tr}_X(\mathbb{1}) = \mathbb{1}\}.$$

When restricted to $\mathcal{A}_c$, the corresponding structure reduces to the one known in the classical Gibbs measure theory. In particular all E_X act as the classical conditional expectations and one can formulate for them conditions which assure that the ergodicity (3) holds (cf. [24]).

In similar spirit one can also discuss more general sequences $(E_{\Lambda_n} : \Lambda_n \subset \Lambda_{n+1})$. ∘

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NON-MARKOVIAN QUANTUM EVOLUTION: TIME-LOCAL GENERATORS AND MEMORY KERNELS

DARIUSZ CHRUŚCIŃSKI and PAWEŁ NALEŻYTY

Institute of Physics, Faculty of Physics, Astronomy and Informatics,
Nicolaus Copernicus University, Grudziądzka 5, 87-100, Toruń, Poland
(e-mails: darch@fizyka.umk.pl, nalezyty.pavel@gmail.com)

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In this paper we provide a basic introduction to the topic of quantum non-Markovian evolution presenting both time-local and memory kernel approach to the evolution of open quantum systems. We start with the standard notion of a classical Markovian stochastic process and generalize it to classical Markovian stochastic evolution which in turn becomes a starting point of the quantum setting. Our approach is based on the notion of P-divisible, CP-divisible maps and their refinements to k-divisible maps. Basic methods enabling one to detect non-Markovianity of the quantum evolution are also presented. Our analysis is illustrated by several simple examples.

Keywords: open quantum systems, Markovian semigroups, non-Markovian evolution.

1. Introduction

Isolated quantum systems are governed by the celebrated Schrödinger equation. This, however, is rarely encountered in nature, as one is never able to perfectly shield the system of interest from all kinds of interactions with the external world, e.g. thermal photons, cosmic radiation, solar neutrinos or even quantum vacuum [1–5]. Moreover, inclusion of the environment leads to several new phenomena like decoherence, dissipation and the Lamb shift of energy levels, which are of exceptional importance in many fields of science. The usual approach to the dynamics of an open quantum system consists of applying the Born–Markov approximation [1, 2, 6], which leads to a local master equation for the Markovian semigroup [7, 8]. However, recent technological progress and modern laboratory techniques call for a more refined approach which takes into account memory effects completely neglected in the description based on Markovian semigroups. There are several approaches to the so-called *non-Markovian* evolution (see the recent reviews [9, 10], a collection of articles [11], and a recent comparative analysis [12]). In recent years the issue of non-Markovianity in quantum mechanics has observed an increasing attention — there are more than 400 papers published recently on the arXiv having *non-Markovianity* in the title.

In this paper we analyze basic mathematical properties of quantum evolution of open quantum systems. The structure of this paper is the following. In Section 2

we briefly recall the notion of classical Markovian stochastic process and introduce Markovian stochastic evolution represented by the so-called P-divisible classical dynamical map (a family of stochastic matrices). We discuss both time-local description and nonlocal one governed by the corresponding memory kernel. This provides the starting point for the analysis of the quantum setting in Section 3, where the concept of quantum Markovian evolution is represented by the so-called CP-divisible maps. Interestingly, there is possibility to introduce a whole hierarchy of k-divisibilities which characterize how much the quantum evolution departs from the Markovian one. Section 4 provides simple methods which enable one to detect whether the corresponding evolution is non-Markovian. These methods basically use monotonicity property of well-known quantities under Markovian evolution. Hence, any violation of monotonicity witnesses non-Markovianity of the corresponding evolution. Finally, Section 5 discusses nonlocal approach governed by the quantum memory kernel. We provide an analogue of the well-known Bernstein theorem replacing positive functions by completely positive maps. The whole discussion is illustrated by a family of simple and instructive examples.

2. Classical setting

The concept of Markovian evolution was originally introduced on the level of classical stochastic processes. Let us recall that a stochastic process $\{X_t \mid t \in T\}$ is fully determined by the family of joint probability distributions $p(x_n, t_n; x_{n-1}, t_{n-1}; \ldots; x_0, t_0)$ [13–15]. The process $\{X_t \mid t \in T\}$ is called Markovian (or memoryless) if and only if the family of conditional probability distributions $p(x_n, t_n|x_{n-1}, t_{n-1}; \ldots; x_0, t_0)$ satisfy

$$p(x_n, t_n|x_{n-1}, t_{n-1}; \ldots; x_0, t_0) = p(x_n, t_n|x_{n-1}, t_{n-1}) \tag{1}$$

for all $t_0 < t_1 < \ldots < t_n$. Quite remarkably, for Markovian processes one can reconstruct an arbitrary multi-point probability distribution knowing only the initial state of the system and two-point conditional probabilities

$$p(x_n, t_n; \ldots; x_0, t_0) = \prod_{i=1}^{n} p(x_i, t_i|x_{i-1}, t_{i-1})\, p(x_0, t_0). \tag{2}$$

One has the following well-known theorem.

THEOREM 1. *Conditional probabilities of a Markov process satisfy celebrated Chapman–Kolmogorov equation*

$$p(x_3, t_3|x_1, t_1) = \sum_{x_2} p(x_3, t_3|x_2, t_2)\, p(x_2, t_2|x_1, t_1). \tag{3}$$

Consider now the stochastic evolution of a probability vector $\mathbf{p} \in \mathbb{R}^n$,

$$\mathbf{p}(t) = T(t)\mathbf{p}, \tag{4}$$

where $T(t)$ is a family of stochastic matrices satisfying $T(0) = \mathbb{I}_n$ ($n \times n$ identity matrix). Recall, that a matrix T is stochastic if $T_{ij} \geq 0$ and $\sum_i T_{ij} = 1$. If additionally

$\sum_j T_{ij} = 1$ it is called bistochastic or doubly stochastic. One calls a family $T(t)$ a *classical dynamical map*. In what follows we assume that $T(t)$ satisfies linear differential equation

$$\frac{d}{dt}T(t) = L(t)T(t), \qquad T(0) = \mathbb{I}_n, \tag{5}$$

with time-local generator $L(t)$, or linear integro-differential

$$\frac{d}{dt}T(t) = \int_0^t K(t-\tau)T(\tau)d\tau, \qquad T(0) = \mathbb{I}_n, \tag{6}$$

with nonlocal memory kernel $K(t)$.

2.1. Time-local approach

The simplest example of time-local description corresponds to Markovian semigroup $T(t) = e^{Lt}$, where L is time-independent generator.

DEFINITION 1. An $n \times n$ real matrix L satisfies *Kolmogorov conditions* iff $L_{ij} \geq 0$ for $i \neq j$, and $\sum_{i=1}^n L_{ij} = 0$.

It is well known [13] that e^{Lt} defines a legitimate semigroup of stochatic matrices if and only if L satisfies Kolmogorov conditions. Note that if $T(t) = e^{Lt}$, then

$$T(t) = T(t-s)T(s) =: T(t|s)T(s),$$

for any $t \geq s$. a natural generalization of the above property is provided by the definition.

DEFINITION 2. A classical dynamical map $T(t)$ is *P-divisible* if

$$T(t_2) = T(t_2|t_1)T(t_1), \tag{7}$$

and $T(t_2|t_1)$ provides a stochastic matrix for an arbitrary choice of $t_2 > t_1 \geq 0$.

It is clear that for P-divisible evolution a map $T(t_2|t_1)$ is an analog of a conditional probability for a stochastic process and equation (7) is an analogue of Chapman–Kolmogorov equation. Therefore we have the following definition.

DEFINITION 3. A classical stochastic evolution is *Markovian* if and only if the corresponding classical dynamical map $T(t)$ is P-divisible.

It should be stressed that the above definition of Markovianity uses only a 2-point conditional probability $T(t_2|t_1)$ and hence is much weaker than the original definition of the Markovian stochastic process (cf. [18]). Note that if the map $T(t)$ is invertible, then $T(t_2|t_1) = T(t_2)T^{-1}(t_1)$. Moreover, the time-local generator $L(t)$ in (5) reads $L(t) := \dot{T}(t)T^{-1}(t)$. One has the following well-known result.

THEOREM 2. *A map $T(t)$ satisfying classical master equation* (5) *is P-divisible iff the time-local generator $L(t)$ satisfies Kolmogorov conditions for $t \geq 0$.*

Introducing $\pi_{kl}(t) := L_{kl}(t)$ for $i \neq j$ one can rewrite (5) as the following Pauli rate equation

$$\dot{p}_k(t) = \sum_{l=1}^{n} [\pi_{kl}(t) p_l(t) - \pi_{lk}(t) p_k(t)], \tag{8}$$

where $\pi_{kl}(t)$ denotes the rate of transition from l to k.

EXAMPLE 1. Consider

$$L(t) = \frac{1}{2}\gamma(t)\begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}, \tag{9}$$

which satisfies Kolmogorov condition iff $\gamma(t) \geq 0$. One easily finds for the dynamical map

$$T(t) = e^{-\Gamma(t)}\mathbb{I} + (1 - e^{-\Gamma(t)})\mathbb{J}, \tag{10}$$

where $\Gamma(t) = \int_0^t \gamma(u)du$ and $\mathbb{J}_{kl} = \frac{1}{2}$. It is clear that $T(t)$ provides a legitimate dynamical map iff $\Gamma(t) \geq 0$ and it is P-divisible (i.e. Markovian) iff $\gamma(t) \geq 0$. This simple example shows that $\gamma(t)$ needs not be positive for all t and hence cannot be interpreted as a transition rate between two states.

EXAMPLE 2. The above example may be generalized as follows: consider a stochastic $n \times n$ matrix $\mathcal{P}$ such that $\mathcal{P}^2 = \mathcal{P}$ and define

$$L(t) = \gamma(t)[\mathcal{P} - \mathbb{I}_n]. \tag{11}$$

One finds for the corresponding map

$$T(t) = e^{-\Gamma(t)}\mathbb{I}_n + (1 - e^{-\Gamma(t)})\mathcal{P}, \tag{12}$$

which is stochastic if $\Gamma(t) \geq 0$.

For $\mathbf{x} \in \mathbb{R}^n$ one defines the family of ℓ_p norms

$$||\mathbf{x}||_p := \left(\sum_{k=1}^{n} |x_k|^p\right)^{1/p}, \tag{13}$$

for $p \geq 1$. A stochastic matrix satisfies

$$||T\mathbf{x}||_1 \leq ||\mathbf{x}||_1, \tag{14}$$

that is, it is a contraction in ℓ_1 norm. Hence, defining the Kolmogorov distance between two probability vectors $\mathbf{p}_1$ and $\mathbf{p}_2$

$$D[\mathbf{p}_1, \mathbf{p}_2] := \frac{1}{2}||\mathbf{p}_1 - \mathbf{p}_2||_1, \tag{15}$$

one has for any stochastic matrix T

$$D[T\mathbf{p}_1, T\mathbf{p}_2] \leq D[\mathbf{p}_1, \mathbf{p}_2]. \tag{16}$$

Following [19] this property may be used as the following definition of Markovian evolution.

DEFINITION 4 ([19]). *Dynamical map $T(t)$ is Markovian* iff

$$\frac{d}{dt}D[T(t)\mathbf{p}_1, T(t)\mathbf{p}_2] \leq 0 \tag{17}$$

for all pairs of probability vectors $\mathbf{p}_1, \mathbf{p}_2$.

Actually, P-divisibility implies (17) but the converse in general is not true [9]. One proves [9] the following theorem.

THEOREM 3. *An invertible map $T(t)$ is P-divisible if and only if*

$$\frac{d}{dt}||T(t)\mathbf{x}||_1 \leq 0 \tag{18}$$

for all vectors $\mathbf{x} \in \mathbb{R}^n$.

Note that in (18) one has $\mathbf{x} = \mathbf{p}_1 - \mathbf{p}_2$ which implies that $\sum_k x_k = 0$.

EXAMPLE 3. Consider $T(t)$ defined in (10). Taking $\mathbf{x} = (1, -1)^T$ one finds $||T(t)\mathbf{x}||_1 = 2e^{-\Gamma(t)}$ and hence condition (18) is satisfied if and only if $\gamma(t) \geq 0$. For this simple example both definitions of Markovianity coincide.

2.2. Nonlocal master equation

Consider now the master equation for $T(t)$ which is nonlocal in time

$$\frac{d}{dt}T(t) = \int_0^t K(t-\tau)T(\tau)d\tau, \qquad T(0) = \mathbb{I}_n, \tag{19}$$

where the so-called *memory kernel* $K(t)$ encodes all dynamical features of the system. Performing the Laplace transform

$$f(t) \quad \rightarrow \quad \widetilde{f}(s) := \int_0^\infty f(t)e^{-st}dt, \tag{20}$$

one finds

$$\widetilde{T}(s) = \frac{1}{s - \widetilde{K}(s)}. \tag{21}$$

PROBLEM 1. *There is a natural question: what are the properties of $\widetilde{K}(s)$ which guarantee that inverting $\widetilde{T}(s) \rightarrow T(t)$ one obtains a legitimate dynamical map $T(t)$ in the time domain?*

Interestingly, this problem is related to a class of the so-called completely monotone functions [16].

DEFINITION 5. A function $f : \mathbb{R}_+ \rightarrow \mathbb{R}$ is called *completely monotone* (*CM*) iff it satisfies

$$(-1)^n \frac{d^n}{dx^n} f(x) \geq 0, \tag{22}$$

for $n = 0, 1, 2, \ldots$.

THEOREM 4 (Bernstein). *A function* $f:\ \mathbb{R}_+ \to \mathbb{R}$ *is CM iff*

$$f(s) = \int_0^\infty g(t)e^{-st}dt, \tag{23}$$

for $s \geq 0$ *with* $g(t) \geq 0$*, that is, CM function is a Laplace transform of a positive function.*

Now, it is clear that $K(t)$ is a legitimate memory kernel iff its Laplace transform $\widetilde{K}(s)$ gives rise to $\widetilde{T}(s)$ such that

$$(-1)^n \frac{d^n}{ds^n}\widetilde{T}(s) \tag{24}$$

is a stochastic matrix for $s \geq 0$ and $n = 0,\ 1,\ 2, \ldots$. One may call $\widetilde{T}(s)$ satisfying an infinite hierarchy of constrains (24) a *CM-stochastic*. It shows that the nonlocal master equation (6) simplifies in the Laplace transform domain. However, the price one pays for this simplification is an infinite hierarchy of constrains (24) for $\widetilde{T}(s)$ instead of a single condition for $T(t)$.

EXAMPLE 4. Let us consider the stochastic evolution generated by

$$K(t) = k(t)[\mathcal{P} - \mathbb{I}_n], \tag{25}$$

where $\mathcal{P}$ is a stochastic matrix satisfying $\mathcal{P}^2 = \mathcal{P}$ (cf. Example 2). One finds for the solution

$$T(t) = \left(1 - \int_0^t f(\tau)d\tau\right)\mathbb{I}_n + \int_0^t f(\tau)d\tau\mathcal{P}, \tag{26}$$

where the function $f(t)$ is related to the memory function $k(t)$ as follows

$$\widetilde{k}(s) = \frac{s\widetilde{f}(s)}{1 - \widetilde{f}(s)}. \tag{27}$$

This shows that for any function $f(t)$ satisfying $0 \leq \int_0^t f(\tau)d\tau \leq 1$ gives rise to the legitimate memory kernel *via* formula (27). It shows that we have two natural representations of $T(t)$: one coming from time-local $L(t)$ defined and another one coming from the memory kernel $K(t)$. Note that condition $\int_0^t f(\tau)d\tau \geq 0$ implies that $\frac{1}{s}\widetilde{f}(s)$ is CM. Moreover, condition $1 - \int_0^t f(\tau)d\tau \geq 0$ implies that $\frac{1}{s}(1 - \widetilde{f}(s))$is CM as well. Using (27) one arrives at the following condition for the memory function $k(t)$: $k(t)$ is legitimate if

$$\frac{1}{s}\frac{\widetilde{k}(s)}{s + \widetilde{k}(s)}, \quad \frac{1}{s + \widetilde{k}(s)}$$

are CM. This condition is sufficient but not necessary.

EXAMPLE 5. Let us specify the above example for $n = 2$,

$$K(t) = k(t)\begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}, \tag{28}$$

and consider the map

$$T(t) = \frac{1}{2}\begin{pmatrix} 1+\cos t & 1-\cos t \\ 1-\cos t & 1-\cos t \end{pmatrix} \tag{29}$$

corresponding to $f(t) = \sin t$. One easily finds for the memory function

$$k(t) = \cosh(\sqrt{2}t). \tag{30}$$

Note that in this case

$$1 - \int_0^t f(\tau)d\tau = \cos t$$

is not positive, that is, condition $1 - \int_0^t f(\tau)d\tau \geq 0$ is sufficient but not necessary.

An interesting class of $T(t)$ satisfying nonlocal master equation is provided by the so-called semi-Markov evolution [20–24]: it is uniquely determined by a collection of waiting time distributions $q_{ij}(t) \geq 0$ such that $q_{ij}(t)dt$ defines the probability of jump from from a state 'j' to 'i' no later than $t + dt$ (assuming that it arrives at 'j' at time t). It gives rise to a collection of survival probabilities

$$g_j(t) = 1 - \sum_{i=1}^{n} \int_0^t q_{ij}(\tau)d\tau. \tag{31}$$

Now, one constructs the solution

$$T(t) = n(t) + (n * q)(t) + (n * q * q)(t) + \cdots, \tag{32}$$

where $n_{ij}(t) = g_i(t)\delta_{ij}$. Assuming that $\sum_{j=1}^{n} \int_0^t q_{ij}(\tau)d\tau \leq 1$, the above series is convergent for $t \geq 0$. The corresponding nonlocal master equation for the probability vector reads

$$\frac{d}{dt}p_i(t) = \sum_{j=1}^{d} \int_0^t [W_{ij}(t-\tau)p_j(\tau) - W_{ji}(t-\tau)p_i(\tau)]d\tau, \tag{33}$$

where $W_{ij}(t)$ are defined in terms of the Laplace transform as follows

$$\widetilde{W}_{ij}(s) = \frac{\widetilde{q}_{ij}(s)}{\widetilde{g}_j(s)}. \tag{34}$$

EXAMPLE 6. Consider 2-state evolution with $q_{ij}(t) = \frac{1}{2}f(t)$ and $\int_0^\infty f(t)dt \leq 1$. The corresponding semi-Markov evolution is defined by (26) with

$$\mathcal{P} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}.$$

It is therefore clear that semi-Markov evolution defines only a subclass of (26) satisfying $f(t) \geq 0$ and $\int_0^\infty f(t)dt \leq 1$.

More examples of semi-Markov evolution may be found in [17].

3. Quantum setting

A treatment of non-Markovian evolution in quantum physics is much more involved than in the classical case. Even the sole definition is problematic. The reason is simple. The very concept of conditional probabilities is not well defined in quantum mechanics [25]. Current approaches towards defining quantum Markovianity are based on generalizations of certain properties of classical dynamical maps, which luckily can be translated to the language of quantum mechanics. Let us consider a quantum system living in $\mathcal{H} = \mathbb{C}^n$. The evolution of the quantum state (a density operator) ρ is represented by a family of completely positive trace-preserving (CPTP) maps $\Lambda_t : \mathfrak{B}(\mathcal{H}) \to \mathfrak{B}(\mathcal{H})$ *via*

$$\rho \quad \to \quad \rho_t = \Lambda_t[\rho], \tag{35}$$

such that $\Lambda_0 = \mathrm{id}$ (identity map in $\mathfrak{B}(\mathcal{H})$ — *quantum dynamical map*). In this paper we analyze only finite-dimensional Hilbert spaces. Let us recall [26] that a linear map $\Phi : \mathfrak{B}(\mathcal{H}) \to \mathfrak{B}(\mathcal{H})$ is positive if $\Phi[X] \geq 0$ for $X \geq 0$. It is k-positive if the map

$$\mathrm{id}_k \otimes \Phi : M_k(\mathbb{C}) \otimes \mathfrak{B}(\mathcal{H}) \to M_k(\mathbb{C}) \otimes \mathfrak{B}(\mathcal{H}), \tag{36}$$

defined by $\mathrm{id}_k \otimes \Phi : M_k(\mathbb{C})[A \otimes B] = a \ \otimes \Phi[B]$ is positive. Finally, it is completely positive (CP) if it is k-positive for $k = 1, 2, \ldots$. It is well known that if $\dim\mathcal{H} = n$, then Φ is CP iff it is n-positive.

EXAMPLE 7. Let us consider a family of trace-preserving maps $\Phi_f : M_n(\mathbb{C}) \to M_n(\mathbb{C})$ defined by

$$\Phi_f[X] := \frac{1}{n - f}(\mathbb{I}_n \mathrm{tr}X - fX). \tag{37}$$

One proves that Φ_f is k-positive but not $(k+1)$-positive iff $\frac{1}{k+1} < f \leq \frac{1}{k}$. In particular for $f = 1$ one reconstructs the so-called reduction map well known in quantum information theory. Reduction map is positive but not 2-positive.

Any CP map Φ possesses Kraus representation

$$\Phi[\rho] = \sum_i K_i \rho K_i^\dagger. \tag{38}$$

This map is trace-preserving if the Kraus operators K_i satisfy $\sum_i K_i^\dagger K_i = \mathbb{I}$. Let Λ_t be a quantum dynamical map. Then we have the following definition.

DEFINITION 6. Λ_t is called *k-divisible* iff for any $t > u$ there exists a k-positive propagator $\Lambda_{t,u}$ such that

$$\Lambda_t = \Lambda_{t,u}\Lambda_u. \tag{39}$$

1-divisible maps is called P-divisible and if $\dim\mathcal{H} = n$, then n-divisible map is called CP-divisible.

In this paper we accept the following definition.

DEFINITION 7 ([9, 27–29]). *A dynamical map* Λ_t *is Markovian* iff it is CP-divisible.

This definition is a direct generalization of Definition 3 for the classical Markovian evolution. Suppose now that the dynamical map Λ_t satisfies time-local master equation

$$\dot{\Lambda}_t = L_t \Lambda_t, \qquad \Lambda_0 = \mathrm{id}, \tag{40}$$

where the time-local generator L_t has the following structure

$$L_t[\rho] = -i[H(t), \rho] + \frac{1}{2}\sum_i \gamma_i(t)\left([V_i(t)\rho, V_i^\dagger(t)] + [V_i(t), \rho V_i^\dagger(t)]\right), \tag{41}$$

with arbitrary noise operators $V_i(t)$, Hermitian effective Hamiltonian $H(t)$, and real $\gamma_i(t)$. This structure guarantees that Λ_t is trace-preserving and hermiticity-preserving. However, it does not guarantee that Λ_t is CP (not even positive). Clearly, if $\gamma_i(t) = 0$, then (40) generates unitary evolution with time-dependent Hamiltonian $H(t)$.

THEOREM 5. *Dynamical map* Λ_t *satisfying* (40) *is CP-divisible (Markovian) if and only if* $\gamma_i(t) \geq 0$ [2, 30].

REMARK 1. If $L_t = L$ is time independent then Theorem 5 reproduces the celebrated result for the structure of the generator of Markovian semigroup [7, 8].

REMARK 2. It should be stressed that condition $\gamma_i(t) \geq 0$ is necessary (and sufficient) for CP-divisibility but it is not necessary to have Λ_t which is CP. Consider

$$L_t[\rho] = \frac{1}{2}\gamma(t)(\sigma_z \rho \sigma_z - \rho). \tag{42}$$

One easily finds

$$\Lambda_t[\rho] = \frac{1}{2}(1 + e^{-\Gamma(t)})\rho + \frac{1}{2}(1 - e^{-\Gamma(t)})\sigma_z \rho \sigma_z, \tag{43}$$

which is CP iff $\Gamma(t) = \int_0^t \gamma(\tau)d\tau \geq 0$. Hence, if $\gamma(t) \ngeq 0$ but $\Gamma(t) \geq 0$, then Λ_t represents quantum non-Markovian evolution.

COROLLARY 1. *If the solution* Λ_t *of the time-local master equation* (40) *defined by the following Dyson series*

$$\Lambda_t = \mathcal{T}\exp\left(\int_0^t L_u du\right) = \mathrm{id} + \int_0^t dt_1 L_{t_1} + \int_0^t dt_1 \int_0^{t_1} dt_2 L_{t_1} L_{t_2} + \ldots, \tag{44}$$

is CP but $\gamma_i(t) \ngeq 0$, *then* Λ_t *is non-Markovian.*

PROBLEM 2. *One of the open problems in the theory of open quantum systems is the characterization of admissible time-local generators* L_t *which leads to CPTP* Λ_t *which is not CP-divisible.*

4. Witnessing non-Markovianity of quantum evolution

The natural question one may pose is *how to check weather given evolution is Markovian*? A similar problem one faces in the theory of quantum entanglement. The basic idea behind witnessing entanglement is to construct a linear operator $W \in \mathfrak{B}(\mathcal{H}_1 \otimes \mathcal{H}_2)$ such that $\langle \psi_1 \otimes \psi_2 | W | \psi_1 \otimes \psi_2 \rangle \geq 0$ but $\mathrm{tr}(W\rho) < 0$ for some entangled state living in $\mathcal{H}_1 \otimes \mathcal{H}_2$ (see [32] for a recent review). Construction of entanglement witnesses utilizes the fact that the set of separable states is convex, so that the Hahn–Banach separation theorem [33] applies and such linear operator W always exists. On the other hand, the set of Markovian evolutions is not convex even in the classical case, as one can easily prove by a direct calculation, therefore non-Markovianity witness cannot be constructed in this simple fashion [29].

Let us introduce the trace norm $\| a \|_{\mathrm{tr}}$ of an operator $A \in \mathfrak{B}(\mathcal{H})$ as follows

$$\| X \|_{\mathrm{tr}} = \mathrm{tr} \sqrt{X^\dagger X}. \tag{45}$$

Note that for a normal operator A with spectrum $\mathrm{spec}\, a = \{\lambda_1, \ldots, \lambda_n\}$ one has

$$\| a \|_{\mathrm{tr}} = \sum_i |\lambda_i|. \tag{46}$$

The importance of the trace norm in the theory of quantum non-Markovian evolution arises from the following fundamental theorem, proved originally in [34].

THEOREM 6. *A trace preserving map $\mathcal{E}$ is positive iff*

$$\| \mathcal{E}[X] \|_{\mathrm{tr}} \leq \| X \|_{\mathrm{tr}} \tag{47}$$

for all Hermitian operators X.

Suppose now that a dynamical map Λ_t is invertible (as a linear map) and let $\Lambda_{t,s} := \Lambda_t \Lambda_s^{-1}$. One has the following result.

THEOREM 7 ([35]). *Λ_t is k-divisible if and only if*

$$\| (\mathrm{id}_k \otimes \Lambda_{t,s})[X] \|_{\mathrm{tr}} \leq \| X \|_{\mathrm{tr}} \tag{48}$$

for any Hermitian $X \in \mathcal{B}(\mathcal{H} \otimes \mathbb{C}^k)$ and arbitrary $t > s$. Equivalently, Λ_t is k-divisible if and only if

$$\frac{d}{dt} \| (\mathrm{id}_k \otimes \Lambda_t)[X] \|_{\mathrm{tr}} \leq 0 \tag{49}$$

for any Hermitian $X \in \mathcal{B}(\mathcal{H})$.

Hence violation of (49) for some observable X witnesses that Λ_t is not k-divisible. A special case corresponding to $X = \rho_1 - \rho_2$ was considered in [19]. For any pair of density operators ρ_1 and ρ_2 one defines the so-called trace distance

$$D[\rho_1, \rho_2] = \frac{1}{2} || \rho_1 - \rho_2 ||_{\mathrm{tr}}. \tag{50}$$

DEFINITION 8 ([19]). *A quantum dynamical map* Λ_t *is Markovian* if

$$\frac{d}{dt} D[\Lambda_t[\rho_1], \Lambda_t[\rho_2]] \leq 0 \tag{51}$$

for all pairs of states ρ_1, ρ_2.

Hence, (51) defines a special case of (49) corresponding to $\mathrm{tr}X = 0$. It is, therefore, clear that BPL condition (51) is in general weaker than P-divisibility condition (49) with $k = 1$. This approach, however, has a clear advantage, as it does not really require the knowledge of the dynamical map – a situation very appealing from an experimentalist point of view e.g. when the state tomography is easier to perform than a full process tomography.

EXAMPLE 8. Consider Λ_t defined in (43),

$$\rho(t) = \Lambda_t[\rho] = \begin{pmatrix} \rho_{11} & e^{-\Gamma(t)}\rho_{12} \\ e^{-\Gamma(t)}\rho_{21} & \rho_{22} \end{pmatrix}. \tag{52}$$

One finds

$$D[\rho_1(t), \rho_2(t)] = \sqrt{\Delta_{11}^2 + |\Delta_{12}|^2 e^{-2\Gamma(t)}}, \tag{53}$$

with $\Delta_{ij} = (\rho_1 - \rho_2)_{ij}$. It is clear that $\frac{d}{dt} D[\rho_1(t), \rho_2(t)] \leq 0$ iff $\gamma(t) \geq 0$. Hence in this simple example both definitions of Markovianity coincide.

EXAMPLE 9 (Pauli channels). Consider a qubit evolution defined by

$$\Lambda_t[\rho] = \sum_{\alpha=0}^{3} p_\alpha(t)\sigma_\alpha \rho \sigma_\alpha, \tag{54}$$

with $p_\alpha(t)$ being probability vector with $p_\alpha(0) = \delta_{\alpha 0}$, and $\{\sigma_0 = \mathbb{I}_2, \sigma_1, \sigma_2, \sigma_3)$ are Pauli matrices. The corresponding time-local generator reads

$$L_t[\rho] = \frac{1}{2} \sum_{k=1}^{3} \gamma_k(t)(\sigma_k \rho \sigma_k - \rho). \tag{55}$$

It is clear that Λ_t is CP-divisible (Markovian) if and only if

$$\gamma_1(t) \geq 0, \quad \gamma_2(t) \geq 0, \quad \gamma_3(t) \geq 0. \tag{56}$$

One may prove [36, 37] that Λ_t is P-divisible if and only if much weaker conditions are satisfied

$$\gamma_1(t) + \gamma_2(t) \geq 0, \quad \gamma_2(t) + \gamma_3(t) \geq 0, \quad \gamma_3(t) + \gamma_1(t) \geq 0. \tag{57}$$

Summarising: for the Pauli channel evolution (54) Markovianity (= CP-divisibility) is controlled by (56), whereas P-divisiblity which is in this case equivalent to BLP-Markovianity is controlled by (57).

EXAMPLE 10. An interesting example of Λ_t which violates (56) but satisfies (57) was recently proposed in [38],

$$\gamma_1(t) = \gamma_2(t) = 1, \qquad \gamma_3(t) = -\tanh t. \tag{58}$$

Note that $\gamma_3(t)$ is always negative and hence $\Gamma_3(t) = \int_0^t \gamma_3(\tau)d\tau < 0$. Nevertheless, the map Λ_t is CP and P-divisible due to (57).

5. Memory kernels—quantum case

As in the classical case let us now consider quantum dynamical map Λ_t satisfying nonlocal equation

$$\dot{\Lambda}_t = \int_0^t K_{t-\tau}\Lambda_\tau d\tau, \qquad \Lambda_0 = \mathrm{id}, \tag{59}$$

where K_t is the corresponding memory kernel encoding dynamical properties of the quantum system. Note that when $K_t = 2\delta(t)L$ and L has the form of a time-independent generator, then (59) reduces to the standard local master equation for the Markovian semi-group. Using the same arguments as in the classical case one finds the following relation in the Laplace transform domain

$$s\widetilde{\Lambda}_s - \mathrm{id} = \widetilde{K}_s\widetilde{\Lambda}_s, \tag{60}$$

and hence

$$\widetilde{\Lambda}_s = \frac{1}{s - \widetilde{K}_s}, \tag{61}$$

which is the analog of (21).

PROBLEM 3. *There is a natural question: what are the properties of $\widetilde{K}_s$ which guarantee that inverting $\widetilde{\Lambda}_s \to \Lambda_t$ one obtains a legitimate dynamical map Λ_t in the time domain?*

The answer is provided by the "quantum analog" of the Bernstein theorem.

THEOREM 8. *a Laplace transform $\widetilde{K}_s$ gives rise to a legitimate dynamical map Λ_t if and only if*

$$(-1)^n \frac{d^n}{ds^n}\frac{1}{s - \widetilde{K}_s} \tag{62}$$

is CP for $n = 1, 2, \ldots$, and $s \geq 0$.

It shows that it is very hard to control whether $\widetilde{K}_s$ provides a legitimate memory kernel — one needs to control the infinite hierarchy of nontrivial conditions (62).

REMARK 3. A function $\widetilde{\Lambda}_s$ such that

$$(-1)^n \frac{d^n}{ds^n}\widetilde{\Lambda}_s \tag{63}$$

defines a completely positive map for $n = 1, 2, \ldots$, and $s \geq 0$ one may call CM-CP map.

COROLLARY 2. *Note that when* $K_t = \delta(t)L$, *then* $\widetilde{K}_s = L$ *and hence* (63) *implies that*

$$(-1)^n \frac{d^n}{ds^n} \frac{1}{s - L} \tag{64}$$

is positive for $n = 0, 1, 2, \ldots$, *and* $s \geq 0$. *In particular one has for* $n = 0$

$$\frac{1}{s - L} = \frac{1}{s}\left(\mathrm{id} + \frac{L}{s} + \frac{L^2}{s^2} + \ldots\right), \tag{65}$$

and for general $n \geq 1$,

$$(-1)^n \frac{d^n}{ds^n} \frac{1}{s - L} = \frac{1}{s^{n+1}}\left(\frac{n!}{0!}\mathrm{id} + \frac{(n+1)!}{1!}\frac{L}{s} + \frac{(n+2)!}{2!}\frac{L^2}{s^2} + \ldots\right). \tag{66}$$

Note that (65) *and* (66) *provide another natural representation of a CP map. It should be stressed that the well-known exponential representation*

$$e^{tL} = \mathrm{id} + tL + \frac{1}{2}t^2L^2 + \frac{1}{3!}t^3L^3 + \cdots, \tag{67}$$

guarantees that the map is CPTP whereas (65) *and* (66) *are not trace-preserving.*

EXAMPLE 11 (Pauli channel—memory kernel). Consider a memory kernels of the following form

$$K_t[\rho] = \frac{1}{2}\sum_{i=1}^{3} k_i(t)(\sigma_i \rho \sigma_i - \rho). \tag{68}$$

Let $\kappa_i(t)$ denote the eigenvalues of K_t

$$K_t[\sigma_i] = \kappa_i(t)\sigma_i, \qquad i = 1, 2, 3. \tag{69}$$

One has the following relations:

$$\begin{aligned} k_1(t) &= \frac{1}{2}(\kappa_1(t) - \kappa_2(t) - \kappa_3(t)), \\ k_2(t) &= \frac{1}{2}(-\kappa_1(t) + \kappa_2(t) - \kappa_3(t)), \\ k_3(t) &= \frac{1}{2}(-\kappa_1(t) - \kappa_2(t) + \kappa_3(t)). \end{aligned} \tag{70}$$

In [39] we proposed the following construction: let $a_1, a_2, a_3 > 0$ such that

$$\begin{aligned} \frac{1}{a_1} + \frac{1}{a_2} &\geq \frac{1}{a_3}, \\ \frac{1}{a_2} + \frac{1}{a_3} &\geq \frac{1}{a_1}, \\ \frac{1}{a_3} + \frac{1}{a_1} &\geq \frac{1}{a_2}. \end{aligned} \tag{71}$$

Let $f(t)$ be a real function satisfying

$$0 \leq \int_0^t f(\tau)d\tau \leq 4\left(\frac{1}{a_1}+\frac{1}{a_2}+\frac{1}{a_3}\right)^{-1}. \tag{72}$$

Then

$$\tilde{\kappa}_k(s) = \frac{-s\tilde{f}(s)}{a_k - \tilde{f}(s)} = \frac{-s\tilde{f}_k(s)}{1-\tilde{f}_k(s)}, \tag{73}$$

with $f_k(t) = f(t)/a_k$, gives rise to the legitimate memory kernel. Interestingly, within this class of memory kernels one may easily control both P- and CP-divisibility. One proves [39] that such kernel gives rise to a P-divisible evolution iff $f(t) \geq 0$ and

$$\int_0^\infty f(t)dt \leq \min\{a_1, a_2, a_3\}. \tag{74}$$

Moreover, it gives rise to a P-divisible evolution iff $f(t) \geq 0$ and

$$\int_0^\infty f(\tau)d\tau \leq a_1 - \sqrt{(a_2-a_1)(a_3-a_1)}, \tag{75}$$

where we assumed $a_1 \leq a_2 \leq a_3$. Note that in the isotropic case $a_1 = a_2 = a_3 =: a$ one has $k_1(t) = k_2(t) = k_3(t)$ and P-divisibility coincides with CP-divisibility, i.e. $\int_0^\infty f(t)dt \leq a$. In particular taking $a_1 = a_2 = 1$, $a_3 = \frac{1}{2}$, and

$$f(t) = e^{-2t}, \tag{76}$$

one finds

$$K_t[\rho] = \frac{1}{2}\left\{\delta(t)(\sigma_1\rho\sigma_1 + \sigma_2\rho\sigma_2 - 2\rho) + e^{-t}(\sigma_3\rho\sigma_3 - \rho)\right\}, \tag{77}$$

which generates the evolution corresponding to (58) in time-local description [39]. Interestingly, this evolution turns out to be a convex combination of two Markovian semi-groups

$$\Lambda_t = \frac{1}{2}(e^{tL_1} + e^{tL_2}), \tag{78}$$

where

$$L_k[\rho] = \frac{1}{2}(\sigma_k\rho\sigma_k - \rho). \tag{79}$$

This example shows that taking a convex combination of Markovian semi-groups one constructs a dynamical map with nontrivial memory kernel.

Qubit evolution within memory kernel approach was also analyzed e.g. in [22, 40, 41] (see also [42, 43]).

6. Conclusions

We provided a basic mathematical introduction to the non-Markovian quantum evolution based on the concept of CP-divisible maps. This concept defines a natural

generalization of P-divisible classical stochastic evolution which is closely related to classical Markovian stochastic process. We analyzed both time-local approach based on local generators and nonlocal approach governed by the corresponding memory kernel known in the literature as the Nakajima–Zwanzig master equation. Non-Markovian evolution is usually linked to realistic description of a variety of complex physical systems where the standard Born–Markov type of approximations are no longer suitable. The problem of non-Markovian evolution is also interesting from the point of view of precise control of quantum systems which is extremely important for modern quantum technologies.

It should be stressed that there are other approaches to quantum non-Markovian evolution (see recent review [10]). The advantage of mathematical approach advocated in this paper is a clear characterization of Markovian evolution in terms of time-local generators. Other approaches like for example the one based on distinguishability of quantum states [10] are more physically oriented as can be experimentally verified. The verification of CP-divisibility is very demanding and requires in general full process tomography. This shows that quantum non-Markovianity is a complex multi-facet phenomenon which still deserves further analysis.

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