

<b>Project acronym</b>	NONSTOPS
<b>Project coordinator</b>	PILLET Claude-Alain
<b>Project Title</b>	Nonequilibrium Stochastic and Open Systems
<b>Titre du projet</b>	Systèmes stochastiques et ouverts hors équilibre
<b>ANR instrument</b>	PRC
<b>ANR challenge</b>	Défi “Des Autres Savoirs”
<b>Multidisciplinary project</b>	No
<b>Research category</b>	Basic research
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## 1 ABSTRACT

From the very beginning of its development statistical mechanics, as a rational approach to the generic behavior of complex systems, has been one of the most fruitful cross-fertilization areas between physics and mathematics. Nowadays its use has pervaded a large spectrum of scientific activities, far beyond its original scope in physics. It provides invaluable tools for the analysis of a variety of phenomena, from the microscopic to the cosmological scale, and from the social sciences to nanotechnology. Besides its many achievements in such applications, statistical mechanics is still under active development. During the last decades researchers have faced new challenges, looking towards a mathematically rigorous approach to non-equilibrium phenomena and to the emerging thermodynamics of irreversible processes. From their works, new fundamental concepts have emerged: current carrying non-equilibrium steady states, entropy production, fluctuation relations, large deviations in the time domain and their relation to linear and non-linear response theory, dynamical phase transitions, thermodynamics at small scales . . . There is no doubt that these and future advances in our understanding of statistical properties of non-equilibrium processes will have considerable impact on various scien-

tific domains outside of physics and foster the development of new research directions in mathematics. The modern framework of dynamical systems and some tightly related domains of probability theory have been major actors in recent developments. Indeed, the Markovian approach to the dynamics of open systems which was for a long time the traditional route to non-equilibrium statistical physics is now linked to the stochastic properties of the microscopic dynamics. In this context, the *chaotic hypothesis* of Gallavotti-Ruelle plays the same role as Boltzmann's ergodic hypothesis of equilibrium statistical physics. In the quantum regime, the framework of  $C^*$  and  $W^*$  dynamical systems and the powerful techniques provided by the modular theory of von Neumann algebras have also played a central role.

This project focuses on some challenging mathematical problems raised by the recent advances in non-equilibrium statistical mechanics mentioned above. From the technical point of view, these problems are mainly concerned with the large time asymptotics and ergodic properties of classical and quantum dynamical systems, with special emphasis on the large deviations of some functionals of these systems related to transport phenomena. From a more conceptual perspective, one of our main main purpose is to confirm the universal nature of the entropic fluctuation relations which are at the forefront of these new developments by extending them to a larger class of dynamical systems. To this aim, we shall follow a strategy based on the canonical construction of well behaved entropic functionals. The mechanism at work in this construction being completely general, it applies to abstract dynamical systems, classical as well as quantum. This generic approach to entropic fluctuations should allow us to deal with a large class of concrete and physically relevant systems. We will consider in particular two directions of research which appear very promising given the present state of the art: classical systems with an infinite number of degrees of freedom described by stochastic PDEs and open quantum systems driven by thermodynamic forces and/or repeated interactions with ancillary systems which may also be the object of repeated measurements. Even though, at first sight, these classical and quantum dynamical systems appear to be only remotely connected, it appears that they share some common features which fit within the framework of a generalized thermodynamic formalism.

To conclude, let us mention that our general strategy is largely based on the use of information theoretic concepts and techniques. Taking advantage of the strong synergy between statistical mechanics and information theory, we also expect to gather some interesting results regarding quantum information theory on our way, such side-effects have already occurred with some of our previous works<sup>JP6, JOPS, ?</sup>.

## 2 STAFF

Partner <sup>1</sup>	Name, first name	Position <sup>2</sup> University	Research area	Person × month	Contribution to the proposal Role
CPT	<i>Boritchev, Alexandre</i>	MC Lyon	Nonlinear PDEs and turbulence	16	Random particle systems
AGM	<i>Bruneau, Laurent</i>	MC Cergy	Mathematical physics	48	Nonequilibrium quantum statistical mechanics, quantum transport
CRM	<i>Chen, Linan</i>	MC McGill	Probability in connection with analysis and geometry	24	Stochastic PDEs, Gaussian measures and information geometry
CRM	<i>Jakšić, Vojkan</i>	PR McGill	Mathematical physics	48	Nonequilibrium statistical mechanics, quantum information <a href="#">Local coordinator</a>
CPT	<i>Joye, Alain</i>	PR Grenoble	Mathematical physics	48	Random quantum walks, spectral analysis, modeling
AGM	<i>Kuksin, Sergei</i>	DR Paris VII	Nonlinear PDEs and turbulence	12	Weak turbulence
AGM	<i>Nersesyan, Vahagn</i>	MC Versailles	Nonlinear PDEs and control theory	24	Large deviation properties of nonlinear stochastic PDEs
CPT	<i>Panati, Annalisa</i>	MC Toulon	Mathematical physics	48	Quantum field theory and statistical mechanics
AGM	<i>Pautrat, Yan</i>	MC Orsay	Quantum probability	16	Nonequilibrium statistical mechanics, quantum information
CPT	<i>Pillet, Claude-Alain</i>	PR Toulon	Mathematical physics	48	Nonequilibrium statistical mechanics, quantum information <a href="#">Project coordinator</a>
AGM	<i>Shirikyan, Armen</i>	PR Cergy	Nonlinear PDEs and control theory	36	Large deviation properties of nonlinear stochastic PDEs <a href="#">Local coordinator</a>

<sup>1</sup> AGM=Laboratoire Analyse , Géométrie et Modélisation (UMR 8088), CNRS, Université de Cergy-Pontoise  
 CPT=Centre de Physique Théorique (UMR 7332), CNRS, Université de Toulon et Aix-Marseille Université  
 CRM=Centre de Recherches Mathématiques (UMI 3457), CNRS, Université de Montréal

<sup>2</sup> PR=Professeur; MC=Maître de Conférence; DR=Directeur de Recherche

### Staff involvement in running research contracts

Name	Person × month	Funding agency, program grant	Project acronym	Coordinator	Start date End date
A. Boritchev	15	ANR PRC €361.300	ISDEEC	R. Joly	January 2017 December 2020
V. Jakšić, V. Nersesyan, C.-A. Pillet, A. Shirikyan	N/A	CNRS PICS €15.000	RESSPDE	V. Nersesyan	January 2017 December 2019
Y. Pautrat	32	ANR PRC €386.000	StoQ	S. Attal	October 2014 September 2019

## 3 CONTEXT AND RESEARCH OBJECTIVES

### 3.1 Context of the proposal

Equilibrium statistical mechanics – as a foundation for equilibrium thermodynamics – is by now a fairly well established subject with solid structural basis, both from the physical and mathematical perspectives. Unfortunately a slight departure from equilibrium carries us into what remains, to a large extent, a *terra incognita*. However, there is light at the end of the tunnel, citing David Ruelle<sup>Ru3</sup>:

*What do we mean by equilibrium? Take a bar of metal in equilibrium at room temperature and watch it closely. Nothing happens. Now impose an electric potential difference at the ends of the*

bar: electric current flows, the bar emits some heat, and it is no longer in equilibrium. If we try to describe the physics of our metallic bar at the microscopic level (the level of atoms and electrons) we find that our fundamental understanding of equilibrium is very good, but our understanding of non-equilibrium states is pretty poor. In one case we can make precise and useful calculations; in the other, hardly any. This situation is unfortunate because the phenomena of life occur far from equilibrium. After 100 years of limited progress in extending the theory of equilibrium to non-equilibrium systems, there are signs that we are finally getting somewhere [...] Our fundamental understanding of non-equilibrium states is moving forwards, but the fact that we cannot yet prove Fourier's law (that heat conduction is inversely proportional to the length of the conductor) from first principles shows how far we still have to go.

Indeed, the last decades have been rich in encouraging advances in our understanding of the microscopic basis of non-equilibrium phenomena, and more specifically of non-equilibrium steady states (NESSs). In the vast phenomenology encountered out of thermodynamic equilibrium, NESSs look in many respects closest to equilibrium in terms of complexity. They are thus a good testing ground for new ideas<sup>?</sup>. Despite the fact that they carry mass/charge/heat currents and hence describe transport phenomena typically absent in equilibrium, they do share with equilibrium states well defined and time-independent properties – mass/charge/energy densities. However, unlike equilibrium states, they are not *characterized* by these properties: there is no microcanonical or canonical ensemble which would provide a universal way to *compute* the NESS of a system under specific constraints. From the thermodynamic point of view, there is no potential which they minimize under these constraints: the fundamental Clausius construction of an entropy function fails out of equilibrium<sup>Ru4</sup>. Appealing alternative variational approaches, like the minimal entropy production principle<sup>Ja</sup>, have also been doomed to failure<sup>La</sup>. Instead, NESS are dynamically selected<sup>?</sup>: while dynamics plays little, if any role in equilibrium statistical mechanics, it becomes the main actor out of equilibrium. In particular, large time asymptotics and statistical properties of dynamical systems, which are the main object of *ergodic theory*, play a central role in the recent developments of non-equilibrium statistical mechanics.

### 3.2 State of the art and positioning of the proposal

**NESSs and Fluctuation Theorems.** NESSs, as basic objects of transport theory, have since a long time been subjects of interest in various areas of the physical sciences, from hydrodynamics to solid state physics. More recently, besides the burst of activity related to electronic properties of nanostructures (quantum dots, molecular wires, ...) <sup>MSSL,PC</sup>, NESSs have also become structuring elements in the study of the dynamics and nonequilibrium thermodynamics of small molecular systems<sup>Ri</sup> and biophysical networks<sup>FKD,GQQ</sup>. The emerging theoretical and experimental tools have already found interesting applications in several branches of life sciences: neurodynamics, genome regulation, enzyme kinetics and metabolic processes... However, the vast majority of these works concern computational aspects of steady states and ignore the mathematical status and resulting structural properties of NESSs. The pioneering works of Evans, Cohen, Morriss and Searles on the violation of the second law<sup>ECM,ES</sup>, soon followed by the groundbreaking formulation of the *Fluctuation Theorem* by Gallavotti and Cohen<sup>GC1,GC2</sup> opened a new era in the study of NESSs. The first fluctuation relation in statistical mechanics goes back to 1905 and the celebrated work of Einstein on Brownian motion. The subsequent historical developments are reviewed in<sup>RM</sup>. Virtually all these early works deal with systems subject to weak mechanical and/or thermodynamical forces, and we mention here only the classical results of Onsager, Green and Kubo which are usually referred to as *fluctuation-dissipation relations*. One of the key features of modern Fluctuation Theorems (FTs) is that they hold for systems arbitrarily far from equilibrium and reduce to Green-Kubo formulas and Onsager relations in the linear regime near equilibrium<sup>Ga,LS,AGMT</sup>. The vast body of theoretical, numerical and experimental works that followed the seminal papers<sup>ECM,ES,GC1,GC2</sup> is reviewed in<sup>RM</sup>. Besides a large impact on experimental and theoretical physics, the FT has also triggered the interest of the mathematical physics community. See<sup>?</sup> and references therein for an exposition of the early mathematical developments that took place in the following years. Most notably, a mathematically precise notion of NESS for classical and quantum<sup>Ru2</sup> systems, patterned on the SRB-states of smooth dynamical systems, emerged from these works. Among the decisive steps in the elaboration of the subject, we must mention the

discovery by Jarzynski<sup>Jar1</sup> of a universal relation between the work performed on a system undergoing an arbitrary isothermal transition between two equilibrium states and the free energy difference between these two states. The works of Kurchan<sup>Ku1</sup> and Lebowitz-Spohn<sup>LS</sup> extending the FT to stochastic dynamics and more generally Markov processes opened the way to Crooks<sup>Cr1</sup>, who unveiled the deep relation linking Jarzynski's identity with the FT. We should also mention the work of Maes<sup>Ma</sup> who realized the relation between the FT and the Gibbsian structure of NESSs. Nowadays, after two decades of intense developments, FTs come in several flavors: local/global, transient/stationary, integral/detailed, extended, generalized, . . .<sup>RM,Se</sup>. FT and the corresponding Jarzynski identity for quantum dynamics were first proposed by Kurchan<sup>Ku2</sup> and H. Tasaki<sup>Ta</sup>. More mathematically oriented formulations of quantum FTs appeared in<sup>dR,DdRM,JPW</sup>. On the applicative side, fluctuation relations provide a new way to measure free-energy (differences) through non-reversible processes, e.g. between conformal states of large molecules<sup>Jar2,AMJR,PR</sup>, an important source of valuable data for the life sciences.

**Open systems.** This project is primarily concerned with *open systems* which are the paradigmatic systems of interest in non-equilibrium statistical mechanics and thermodynamics. They consist of a *confined* part  $\mathcal{S}$  coupled to some *extended* environment  $\mathcal{R}$  which may itself consist in several reservoirs with distinct thermodynamic properties. In the classical regime the dynamics of the joint system  $\mathcal{S} + \mathcal{R}$  is Hamiltonian, it is unitary in the quantum regime. Both, classical and quantum dynamics are reversible. Dissipation and fluctuations arise in such systems through the ability of the environment to convey mass/charge/energy to spatial infinity and, conversely, to ensure an inexhaustible feeding of the system  $\mathcal{S}$  with such quantities.

Within the realm of classical physics, Langevin dynamics and stochastic calculus provide an efficient framework for the study of a large variety of non-equilibrium processes. The reduction of Hamiltonian to stochastic dynamics often yields a very good Markovian approximation, in some cases we can even prove that the stochastic description is exact<sup>EPR1</sup>. However, despite this simplification, non-linear effects in boundary driven Hamiltonian networks are still not completely understood to the point that the mere existence of a NESS remains a largely open problem, see<sup>CE</sup> and references therein for recent advances in this question. Another promising direction of research within the domain of classical physics concerns open systems whose confined part  $\mathcal{S}$  have infinitely many degrees of freedom. The non-equilibrium statistical mechanics of stochastic PDEs underwent an important development in the last twenty years. The problem goes back to the pioneering article of Hopf (1952) who initiated the statistical study of 3D Navier–Stokes equations. Mathematical foundation of the theory were laid down by Foias (1972–73) and Vishik–Fursikov–Komech (1975–80). They proved, in particular, the existence of a statistical solution with given initial data and constructed a solution whose law is invariant with respect to translations in space and time. Starting from the mid-nineties, various aspects of qualitative behavior of trajectories for finite- and infinite-dimensional stochastic systems were investigated by a number of research groups. The problem is by now rather well understood if it is considered in a finite volume. Namely, if the stochastic forcing is sufficiently non-degenerate, then the stationary distribution is unique, and it attracts exponentially fast all other trajectories in the sense of convergence in law; see the book<sup>KS</sup> and the references therein. The problem now is to describe the concept of entropy production and to investigate its fluctuations and universal symmetries.

While the above mentioned problems regarding the classical statistical mechanics of open systems are mainly of a technical nature, the corresponding quantum theory is also plagued by conceptual difficulties. The nature of quantum mechanics, the peculiar status of measurements which are intimately connected with the control of quantum mechanical systems, and the interplay of measurement processes and dynamics make the mathematical modeling, analysis and interpretation of dissipation and fluctuations in quantum systems much more problematic than in their classical analogues. These problems also make the quantum theory of open systems richer and more challenging. Repeated or continuous monitoring of quantum systems by direct measurement on  $\mathcal{S}$  or indirect measurements on some parts of its environment  $\mathcal{R}$ , possibly including a feedback control of its dynamics give rise to new classes of dynamical systems of interest<sup>KM,BBB</sup>. Regarding the Markovian approach to the dynamics of open quantum systems, one may think of Einstein's treatment of matter–radiation thermal equilibrium (1917) as a first encounter. Pauli's master equation (1928) extends Einstein's approach to more general systems and paves the way to Markovian quantum dynamics. The mathematical analysis of the



latter goes back to the early 70' (Davies, Lindblad, Gorini-Kossakowski-Sudarshan). More recently, deeper relations between the Markovian approximation of the dynamics of open systems and their "true" unitary quantum evolution have been obtained<sup>JP2,JP3,dR,dRK</sup>. We note however that the status of Markovian approximations of quantum dynamics is less favorable than in the classical regime: non-Markovian effects may become important, particularly for systems  $\mathcal{S}$  of microscopic size which are currently the objects of an intense interest due to the rapid development of nanotechnologies in various areas of physics, chemistry, biology and information science. For this reason, the study of the large time asymptotics and ergodic properties of the unitary dynamics of open quantum systems remains of prime importance.

Among the recent advances in the mathematical theory of open systems, we should mention the existence and uniqueness of the NESS for specific models of classical<sup>EPR1,EPR2,EH,LY1,LY2,CE,JNPS1,JNPS2,JNPS3</sup>, and quantum<sup>JP3,AP,FMU,MMS,JOP1,BD,BP,BJM1,BJM2</sup> systems<sup>1</sup>. A substantial part of these results, as well as basic structural properties of these NESSs<sup>JOP1,JOP2,BDBP,CMP,JaP,JPP1</sup>, have been obtained by members of the consortium, some of them in the framework of the ANR project *HamMark* (2009–2013). The latter, was centered around Markovian vs. Hamiltonian approaches to the dynamics of open quantum systems. Its main objective was the merging of probabilistic, spectral and scattering theoretic and algebraic tools. It has produced a corpus of techniques which form a solid basis for the NONSTOPS project. The members of the present consortium have published around 30 articles mentioning the support of the *HamMark* project in refereed journals. Another ANR project closely related to the topics of this proposal is *STOSYMAP* (2012–2015). The main subject of that project was the problem of turbulence in various media. Three members of Cergy's team were involved in *STOSYMAP*, and the techniques developed by them are relevant for studying the questions discussed here.

**Quantum walks.** Given the prominent role played by classical random walks in the development of non-equilibrium statistical mechanics, as basic models for diffusion processes, we shall also consider their quantum counterparts. Quantum walks (QW) are at the crossroads of quantum physics, statistical mechanics, theoretical computer science and non-commutative probability<sup>VA</sup>. A QW is a unitary operator on a Hilbert space with basis elements associated to the vertices of an infinite graph, whose matrix elements couple nearest neighbors of the graph only. When the unitary operator is random, one speaks of random quantum walk (RQW). The versatility of QWs makes them efficient models in various circumstances. QWs provide experimentally reliable approximations of the dynamics of physical systems in appropriate regimes: A RQW yields the one time step evolution operator of a quantum particle with spin in a random environment, with corresponding transport and spectral properties related to the original physical model. As an example, RQWs defined on trees display a localization-delocalization transition as the random Anderson model does<sup>HJ1</sup>. In the quantum computing community, the algorithmic simplicity of QWs provides them with a distinguished role: QWs appear as building blocks in the elaboration of quantum algorithms, and they are used as a central tool assessing the probabilistic efficiency of quantum search algorithms<sup>Mo</sup>. The probabilistic interpretation of quantum mechanics promotes QWs to the status of non-commutative analogs of classical random walk whose rich transport properties have attracted the attention of the probability community, see e.g.<sup>Ko,GVWW</sup>. We shall exploit the demonstrated modeling capacities of QW to investigate transport in non-equilibrium quantum statistical mechanics by means of simplified, yet relevant, models closely associated with classical random walks, building up on our recent analysis of thermalization properties of ensembles of fermionic quantum walkers<sup>HJ2</sup>.

**Many body localization.** One of the most important phenomenon in quantum transport theory is Anderson or strong localization which concern the effect of impurities in a regular crystal on its electronic conductance. Neglecting the interactions between electrons, this problem reduces to the spectral analysis of a one-body Schrödinger operator with a random potential. More precisely on the existence/absence of an absolutely continuous part in the spectrum of this operator. Anderson localization for non-interacting electrons has been extensively studied over the last 35 years and at the moment an essentially complete mathematical theory is available in dimension one, and in the large disorder regime in higher dimensions<sup>Ki,AM,FS,GK</sup>. The transport properties of interacting electrons in disordered crystals are by far less understood. There are some theoretical evidences for the existence of a metal-insulator transition at finite temperature<sup>BAA</sup>, but very little, if anything,

<sup>1</sup>These references are not meant to be exhaustive.

is known on the mathematical side about this issue<sup>AW,CS</sup>. The traditional, spectral theoretic approach to Anderson localization is unsuitable in this case and a completely new scheme is needed. Our previous works on the non-interacting case<sup>BJLP1,BJLP2</sup> strongly suggest to characterize the metallic/insulating regimes by the the large size asymptotics of the conductance of finite samples in the framework of open systems.

*Information geometry.* The basic issue of information theory is to quantify and compare the information content of typical samples of given probability distributions. For that purpose, and starting with the foundational contributions of Shannon, various concepts of entropies, relative entropies, and other divergences have been introduced. The study of these concepts, their properties and their interrelations nowadays form the core of information theory, including its quantum counterpart. From a structural point of view, a major problem with these concepts stems from the fact that they do not provide a natural metric structure to the space of probability distributions under consideration. Even though the benefits of a geometrization of the latter for basic problems in statistics were recognized quite early<sup>Ra</sup>, substantial progresses in this task only started much later with the works of Efron<sup>Ef</sup>, Amari<sup>AN</sup> and others. Almost simultaneously and independently, similar considerations concerning the geometry of the set of thermodynamic states have appeared in the physics literature<sup>We,Cr2</sup>. The differential geometry of manifolds of probability distributions is by now a well developed branch of statistics that goes under the name *information geometry*. Primarily aimed at finite-dimensional parametric estimation, it has been extended to infinite-dimensional non-parametric models<sup>PS</sup>.

### 3.3 Objectives, originality and novelty of the proposal

The principal objectives of the project are centered around transport properties of classical and quantum open systems and stochastic models thereof. This includes existence, uniqueness and various structural properties of NESSs. We shall particularly (but not exclusively) focus our interest on FTs, i.e., statistical properties of the fluctuations of entropy production and the associated mass/charge/energy transfers between the system and its environment. From a very general perspective, these problems revolve around major theoretical advances and offer new challenges to mathematical physicists, and a chance to diversify their activities. The main originality of our project, as compared to the vast majority of the literature on the subject, is that we shall investigate these problems for **concrete systems**, aiming at **rigorous mathematical results**, based on **realistic assumptions** on the ergodic/chaotic properties of these systems and with the concern of identifying **canonical constructions** to assess the universality of the aforementioned structural properties despite the obvious discrepancy in the mathematical structure of classical and quantum dynamical systems. This means in particular that: (a) we shall consider physically motivated models; (b) we shall not rely on numerical simulations, except perhaps for the purpose of illustrating analytical results; (c) we shall try, as much as possible, to follow a unified strategy to deal with classical and quantum systems in order to clearly exhibits the structural basis of FTs; (d) we shall also try to disentangle the canonical constructions which are at the origin of the universality of FTs from the technical contingencies which limit their validity. More specifically, we aim at:

*Establishing FTs for classical and quantum open systems.* We adopt the widely accepted point of view that the physically relevant and mathematically non-trivial aspects of FTs consist in: (1) formulating and proving ergodic properties – Strong Law of Large Numbers (SLLN), Central Limit Theorem (CLT), Large Deviation Principle (LDP) – for the fluctuations of *entropy production* and various other individual (mass, charge, heat, ...) currents circulating between a system and its environment; (2) displaying the symmetry relations satisfied by the rate functions of these LDP. Accordingly, we plan to study these two problems for physically relevant models, with the aim at clarifying the mathematical structure at work behind the scene. In our opinion, the thermostated (iso-energetic, iso-kinetic, ...) models frequently used in the literature, while convenient for the purpose of numerical calculations, are not well suited to analytic approaches. They are also not easily transposed to quantum systems. For these reasons, because we aim at a unified treatment of deterministic and stochastic, classical and quantum dynamical systems, and also in view of the consortium expertise, we plan to restrict our studies to: (a) classical open systems described by stochastic PDEs; (b) classical Hamiltonian open systems with a large or infinite number of degrees of freedom; (c) quantum open systems consisting of

a confined part  $S$  coupled to extended fermionic or bosonic free fields at non-vanishing density and subject to various measurement protocols (full statistics of charge/energy transfers, repeated and continuous monitoring of the environment, ...). We are confident that a statistical approach to various direct and indirect measurement protocols in open quantum systems is the key to a better understanding of their non-equilibrium dynamics. Indeed, we have recently done some preliminary works on the large time asymptotics of a general model of repeated quantum measurement<sup>BJPP</sup>. Our results show strong evidences supporting that this limit can be described by a generalized (i.e., non-Gibbsian) thermodynamic formalism. The originality of our approach lies in a consistent use of dynamical system theory which departs from the more traditional probabilistic approach based on martingale convergence theorems.

A conceptual and two major technical difficulties arise in this program. On the conceptual side, the identification of entropy production is a largely open question since entropy itself is ill-defined out of equilibrium. In the seminal works<sup>ECM,ES</sup> and<sup>GC1,GC2</sup>, the role of entropy production was played by the phase space contraction rate. A zoo of path space functionals and FTs has emerged from subsequent studies to a point which, in our opinion, has obscured rather than clarified the whole subject, at least from the perspective of an underlying mathematical structure. We shall follow a novel and radically different approach to this conceptual problem. Based on our previous works<sup>JPR,JOPP</sup> and information theoretic considerations, we have identified a canonical entropic functional which, by construction, satisfies what could be called a *maximal FT*. Our preliminary investigations<sup>JPS1,JPS2</sup> have shown that for a class of simple deterministic and stochastic classical dynamical systems, it is possible to relate this functional to physically interesting quantities like the work performed on the system by non-conservative forces or the heat dissipated in the environment. Moreover, we were able to exploit this relation in order to derive LDPs for their fluctuations. We plan to generalize this original approach to a wider class of open systems including (a)-(c) and to relate our canonical entropic functional to a large part (and we hope all) of the above mentioned zoology. Our ambition is thus to unveil the *mother of FT*, a result which would indeed provide a strongly structuring basis for the recent advances in non-equilibrium statistical mechanics and bring some order into the vast and somewhat hectic literature on this subject.

To complete this program, we will tackle with the two above mentioned technical problems. The first one is generic in ergodic theory and concerns the control of the large time properties of the underlying dynamical systems. The consortium has a very strong expertise in this domain, with some of the world experts in the ergodic theory of stochastic PDEs and classical and quantum open systems. The second technical problem is of purely probabilistic nature and relates to large deviations. In the above mentioned preliminary works, we were able to extend some classical results linking the large time asymptotics of cumulant generating functions to large deviation properties (the Gärtner-Ellis theorem). This was done by exploiting the Gaussian nature of the underlying processes and of their NESSs. We expect that acquiring a suitable control on the NESS should enable us to further extend these results to non-Gaussian cases.

*Studying the entropic fluctuations of some stochastic PDEs of physical relevance.* To describe the corresponding set of problems, let us consider a Hamiltonian PDE damped by a linear term and perturbed by a stochastic forcing. This type of models arise in many physical problems and include some well-known PDEs, such as the Navier–Stokes system, the complex Ginzburg–Landau equation, and the damped–driven Korteweg–de Vries equation. Under some mild conditions on the stochastic forcing, the large-time behavior of trajectories is now well understood<sup>KS</sup>. Namely, one can prove the existence and uniqueness of a NESS, which is stable in the sense that all the trajectories converge to it in distribution. Moreover, the SLLN, the CLT, and the LDP hold for practically all relevant observables. The problem now is to understand entropy production and its fluctuations in the system and to investigate the behavior of the NESS in the vanishing viscosity/forcing limit. Let us stress again that the very definition of the concept of entropy production is still unclear in the general case and its description reflecting the relevant physical phenomenon is a part of the problem.

Another direction of research in this topic concerns the 2D/3D Vlasov–Poisson–Fokker–Planck equation. This is a (stochastic) kinetic equation that is conceptually different from the previously studied nonlinear models such as the Navier–Stokes, Schrödinger, Korteweg–de Vries, Ginzburg–Landau or Burgers equations. At this point, the problem is treated only in the linear case. Namely, using hypocoercivity estimates<sup>Vi</sup> and under an assumption of smallness for the noise, De Moor, Rodrigues and Vovelle<sup>dMRV</sup> proved the existence and



uniqueness of an invariant measure and established the existence of a spectral gap. On the other hand, the nonlinear case remains completely open.

*Studying the relaxation in Hamiltonian open systems.* This problem is closely related to the previous one. We shall consider the Hamiltonian model of open system consisting of a confined finite-dimensional subsystem  $\mathcal{S}$  coupled to  $M \geq 1$  extended wave fields  $\mathcal{R}_1, \dots, \mathcal{R}_M$ , initially in thermal equilibrium at different temperatures. Under some rather restrictive conditions on the coupling between these subsystems, the relaxation of the joint system  $\mathcal{S} + \mathcal{R}_1 + \dots + \mathcal{R}_M$  towards a (non)-equilibrium steady state is well understood in two special cases: (a) when  $M = 1$ <sup>JP1</sup>; (b) when  $M = 2$  and the system  $\mathcal{S}$  is a weakly pinned chain of anharmonic oscillators<sup>EPR1, EH</sup>. Since the publication of these results more than 15 years ago, and until very recently<sup>CEP, CE</sup>, little progress has been achieved in this direction. Our goal is to investigate this problem under more realistic hypotheses on the coupling in case (a) and for more general system  $\mathcal{S}$  in case (b). In particular, we plan to study the return to equilibrium/relaxation to NESS for these systems, the validity of ergodic theorems (SLLN, CLT, LDP), as well as FTs.

*Studying the kinetic limit in weak turbulence.* Weak turbulence (also called *wave turbulence* in some contexts) is by now a classical subject in physics going back to pioneering articles of V. Zakharov and his collaborators<sup>ZLF</sup>. In mathematical terms, the problem consists in studying the behavior of trajectories of a linear dispersive equation perturbed by a small nonlinear Hamiltonian term and a stochastic forcing and damped by a viscous term of the same order. The problem contains three parameters—the time  $t$ , the viscosity  $\nu$  describing the perturbation, and the size of the physical domain  $L$ , and the aim is to investigate the asymptotic regime  $t \rightarrow \infty, \nu \rightarrow 0, L \rightarrow \infty$ . The order of taking these limits is a part of the problem, and there is no unanimity in the community of physicists dealing with weak turbulence.

*Modeling aspects of quantum transport and non-equilibrium statistical mechanics by means of QWs.* A key feature of QWs is their encoding of the relevant dynamical information within a sparse unitary operator with a band structure. This allows for a relatively simple proof of localization-delocalization transition for RQWs on trees, and thus makes us hopeful to find signatures of this transition on the cubic lattice in large dimension. The mathematical analysis of the venerable (de)localization problem by means of unitary random models is quite recent and we feel RQWs represent a credible alternative to the Anderson model to probe these questions.

Concerning non-equilibrium statistical mechanics, we want to take advantage of the simplicity of QWs to study their effective dynamics, when they interact with a given reactive environment. The goal is to describe quantum friction without resorting to artificial procedures suppressing correlations, and to investigate its links with repeated interaction type models and the recently introduced open quantum walks<sup>APSS</sup>. With a different perspective, we intend to study ensembles of (non-)interacting QWs in contact with several reservoirs in different thermodynamical states, and analyze the induced NESS, in keeping with<sup>HJ2</sup> which deals with QWs in contact with one reservoir. In particular, we want to define this way a quantum version of the celebrated classical exclusion processes describing such NESSs, see<sup>DLS</sup>, making use of the analogy between random walks and QWs. We plan on describing the FT of the particle currents and of the entropy production. The relative algorithmic simplicity of the dynamics of QWs should allow for a detailed analysis on these fundamental questions in quantum statistical mechanics.

While QWs have been the object of many investigations by now, there are no mathematical works devoted to their behavior under the influence of an environment. The consortium having a strong expertise in the definition and analysis of discrete (random) dynamical systems given as QWs, repeated interaction systems, or unitary band matrices, see e.g.<sup>BHJ, HJS, BJM1, BJM2, ABJ, HJPR, J2</sup>, and on the basis of present investigations on ensembles of QWs interacting with reservoirs<sup>HJ2</sup>, we expect to progress significantly on this new set of questions regarding the dynamics of QWs and, in return to cast new light on the physics of non-equilibrium statistical mechanics by means of these models.

*Further developing scattering theoretic techniques for  $C^*$ -dynamical systems.* The use of such techniques in the analysis of locally interacting fermionic systems was initiated in<sup>FMU, JOP1, JPP</sup>. We plan to extend these approaches in order to investigate the large size asymptotics of the conductivity of finite samples. Defining localization/conducting regimes of interacting electrons in a one-dimensional disordered crystal by ways of our characterization of these regimes in the non-interacting case<sup>BJLP1, BJLP2</sup> will allow us to investigate the possible existence of a localized regime in weakly interacting systems at zero temperature. This would be a first step in the mathematical analysis of many-body localization. This is a very challenging problem given its physical relevance, the absence of mathematical results and the well known difficulties in dealing with interacting systems in the thermodynamic limit. The proposed approach is original and may lead to a breakthrough in the timely subject of many-body localization.

*Exploring the information geometry of NESSs.* Unlike equilibrium states which form a finite dimensional manifold parametrized by a small number of well defined thermodynamic parameters, the geometric nature of NESSs is a largely unexplored domain. Among the various geometries which can be assigned to the set of NESSs, the entropic connection introduced by Ruelle<sup>Ru4</sup> is particularly appealing since its curvature vanishes at equilibrium (a geometric formulation of Clausius construction of the entropy function), providing a clear criterion distinguishing equilibrium from non-equilibrium. We plan to investigate this entropic geometry, starting with some simple tractable models, with the aim at establishing the first links between information geometry and non-equilibrium statistical mechanics. Using geometry to study families of probability distributions is a novel approach which has not yet received much attention in statistical mechanics and thus has a high potential for innovation.

## 4 SCIENTIFIC PROGRAM AND PROJECT ORGANIZATION

### 4.1 Project structure

The structure of the project follows the standards for a cooperative work in mathematics. The broad objectives described in Section 3.3 have been transcribed into more precise and essentially independent tasks delineated in Section 4.3. A subset of the consortium, chosen for its particular expertise, is initially assigned to each of these tasks. Members working on a given task exchange information on the status of their contribution. They invite or visit experts outside of the consortium to keep updated on the current scientific developments on the subject and eventually start new collaborations. Given the high activity in the field, these contacts are essential for the success of the project and a substantial part of the budget is devoted to support it. Whenever required, members of the consortium meet to discuss more delicate technical, conceptual or strategic issues. Regular annual meetings of the consortium are also scheduled in order to assess the global advancement of the project, to share the technical and conceptual difficulties encountered and foster new collaborations between the partners, to discuss potential strategic issues, including possible reassignment or reorientation of a task. Whenever possible, these meetings will be coupled to, or included in other scientific events in order to optimize their added value (see Section 5). Each task will produce, as end result, one or several publications which will be submitted to international refereed journals and posted on internet archives. These results will also be communicated in international workshops and conferences. A web site will be dedicated to the project. It will feature a short description of our objectives, the list of the members of the consortium with links to their homepages, a list of the meetings organized and/or supported by ANR through our project and the updated list of publications. A final 2 weeks meeting featuring an international workshop and a summer school will be organized in July 2021 in order to promote the achievements of the consortium and propose a survey of the current state of the art, with particular emphasis towards young researchers.

### 4.2 A brief portrait of the consortium

We refer to the separate Appendix to this document for short CVs of the coordinators of the 3 partners of this project. The purpose here is to clearly establish the ability of the consortium to work together for the

success of the project and to emphasize the coherence of this consortium with its objectives. In preamble, let us mention that prior to submit this project to ANR, we have performed some preliminary works in the framework of the 3 years CNRS PICS grant **RESSPDE** (2014-2016, renewed for the period 2016-2018). The main objective was to foster collaboration between the Canadian partner and members of the former ANR projects HamMark and STOSYMAP, and to perform exploratory investigations in preparation of the present project.

NONSTOPS has grown around the long term research program started in the 90' by **Vojkan Jakšić** and **Claude-Alain Pillet** on mathematical problems of non-equilibrium statistical mechanics. Several breakthroughs have been achieved by this program: the first proofs of return to equilibrium<sup>JP2</sup> and of relaxation towards a NESS<sup>JP3</sup> for a small quantum system coupled to extended reservoirs in thermal equilibrium, a general definition of entropy production in quantum open systems<sup>JP4</sup>, the proof of the Landauer-Büttiker formula<sup>AJPP</sup>, ... More generally, V. Jakšić and C.-A. Pillet have developed algebraic techniques, exploiting the modular theory of von Neumann algebras, to deal with various ergodic problems in quantum statistical mechanics<sup>JP5, JOPP</sup>. These 2 researchers bring their broad expertise of the subject and their deep knowledge of the various analytic and algebraic techniques which are needed to cope with the difficult problems related to the large time asymptotics of classical and quantum open systems. They will be leading Tasks **Q1, Q3, Q4, Q5, Q6**.

**Sergei Kuksin** and **Armen Shirikyan** are preeminent experts in dynamical systems defined by non-linear PDEs and Hamiltonians with infinitely many degrees of freedom. Their important contributions to the ergodic theory of dissipative non-linear stochastic PDEs have been decisive in the field and are widely recognized by the international community. S. Kuksin is also one of the founders of the research direction *KAM for PDEs*, which is closely related to the topics of this proposal; see<sup>Kuk1</sup>. A. Shirikyan has contributed to the control theory for PDEs and used successfully<sup>Shi</sup> various ideas from it to investigate stochastic problems. They are the authors of the monograph<sup>KS</sup>, devoted to the investigation of turbulence in two-dimensional Navier–Stokes system. These researchers will be leading Tasks **C1** and **C2**. Their competence will also be crucial for Tasks **C3, C4** and **C5**.

**Alain Joye** is a leading expert in spectral analysis and quantum dynamics. He became interested in open quantum systems after the development, in the framework of algebraic quantum mechanics, of the spectral approach to the ergodic theory of open quantum systems. He has been actively involved in the applications of these techniques to repeated interaction systems and is now internationally recognized as an expert in this class of quantum open systems. The latter being closely related to repeated quantum measurements, his expertise is crucial for the success of Task **Q6**. His wide knowledge of disordered quantum systems will also be relevant to Tasks **Q3** and **Q4** while his competences regarding adiabatic quantum evolution will also be exploited in Task **Q1**. More recently A. Joye has been involved in the burst of activities around quantum walks, a subject which fits perfectly with the other objectives of this proposal. He will be leading Task **Q2**.

Under the guidance of S. de Bièvre, **Laurent Bruneau** wrote his Ph.D. thesis in Lille on some Hamiltonian models of classical and quantum open systems. After a first postdoc in Warsaw with J. Dereziński, where he worked on some mathematical problems of quantum field theory, L. Bruneau spent a year in Grenoble and started what became a regular collaboration with A. Joye on repeated interaction systems. More recently, L. Bruneau got involved in a fruitful collaboration with V. Jakšić, Y. Last and C.-A. Pillet on the characterization of the absolutely continuous spectrum of semi-infinite 1D Jacobi matrices through the transport properties of finite samples. He will be strongly involved in Tasks **Q3** and **Q4** which are deep refinements of these works. His expertise in the spectral theory of disordered systems will also be exploited for Task **Q2**.

**Yan Pautrat** is a non-commutative probabilist who wrote his Ph.D. thesis on quantum stochastic calculus under the supervision of S. Attal in Grenoble. A part of this thesis is devoted to the continuum limit of repeated interaction systems and the emergence of quantum Langevin dynamics. After his thesis, he spent a year as a CRM-postdoc of V. Jakšić at McGill. During this period he started to work on some probabilistic aspects of the NESS of interacting fermionic systems. Since then he has been a regular collaborator of V. Jakšić and C.-A. Pillet on several projects. In parallel, he has been working on open quantum walks, a different type of QW recently introduced by S. Attal, F. Petruccione and C. Sabot. The expertise of Y. Pautrat in quantum probability will be essential for Tasks **Q1, Q2** and **Q6**.

**Annalisa Panati** did her Ph.D. in Orsay under the direction of C. Gérard on mathematical problems of rel-

ativistic quantum field theory on a curved background. She continued working on inhomogeneous quantum field theory in the spectral analysis group of CPT, after her hiring as Maître de Conférence in Toulon in 2009. In 2011, she got a 1 year CNRS delegation to CRM where she started a reorientation towards non-equilibrium statistical mechanics under the guidance of V. Jakšić. Taking a leave of absence from her home university, she stayed in Montreal until 2016 and has been actively working on various problems in quantum transport. Her combined competences in interacting quantum field theory and algebraic quantum mechanics will be exploited in Tasks Q1 and Q3.

**Vahagn Nersesyan** was a Ph.D. student of A. Shirikyan. He wrote his thesis on control and ergodic theory of stochastic Ginzburg–Landau and Schrödinger equations. More recently, he presented a HDR thesis on mixing properties and large deviations of stochastic nonlinear dissipative PDEs and global control of nonlinear Schrödinger equation and 3D Navier–Stokes equation. V. Nersesyan was a very active and efficient member of the first PICS RESSPDE (2014-16) and took over the responsibility of its renewal (2017-19). He has now acquired a solid expertise in ergodic theory and large deviations for stochastic PDEs which will be essential for the success of Tasks C1, C5.

Before being hired as a Maître de Conférence in Lyon in 2014, **Alexandre Boritchev** obtained his Ph.D. in 2012, with a thesis on randomly forced generalised Burgers equation with small viscosity directed by S. Kuksin. As a postdoc, he spent 1 year with F. Merle in Cergy and 1 year with J.-P. Eckmann in Geneva. After his thesis, A. Boritchev has been working on mathematical problems related to turbulence, more specifically properties of the stochastic Burgers equations. He will be working on Task C3.

**Linan Chen** did her Ph.D. thesis at MIT under the supervision of D.W. Stroock. After a 2 year postdoc at McGill, she was hired there as an Assistant Professor in 2014. She is a probabilist interested in connections with analysis and geometry, including partial differential equations, functional analysis, Gaussian measures and applications in random geometry. Very recently, L. Chen started investigation of the behavior of trajectories of particles in the 2D stochastic Navier–Stokes flow. Her competences will be important in Task Q5 and also in some developments of Task C1.

Collaborations among members of the consortium have a long and fruitful history. Joint publications being too numerous to be cited individually, we give some representative numbers: The first joint paper dates back to 1995, since then a total of 63 papers have been cosigned by at least 2 members of the consortium. All members, apart from the two youngest ones, have at least 2 joint publications and five members have more than 10. We count 44 joint publications between the French and Canadian partners. We also mention a book: S. KUKSIN, A. SHIRIKYAN, *Mathematics of Two-Dimensional Turbulence*, Cambridge University Press, Cambridge, 2012; and a series of lecture notes edited by S. ATTAL, A. JOYE, C.-A. PILLET, *Open Quantum Systems I, II and III*, Lecture Notes in Mathematics 1880, 1881 and 1882, Springer, Berlin, 2006.

We also have recently started to develop students exchanges. Two master students of V. Jakšić spent a month with A. Joye in Grenoble in 2015 and came back to France for six more weeks in 2016, one in Grenoble and the other in Orsay with Y. Pautrat. This exchange directly lead to the paper<sup>HJPR</sup>. Moreover, one student will start a PhD in the Fall of 2017 co-supervised by V. Jakšić and A. Joye, while the other has just started a PhD in Cambridge, informally co-supervised by Y. Pautrat. This practice will be continued in the future.

The consortium also has good records in scientific animation. The summer schools “*Open Quantum Systems*” (Grenoble 2003) and “*Advances in Open Quantum Systems*” (Autrans 2013) were organised by S. Attal, A. Joye and C.-A. Pillet and attended by several Canadian master students. A joint semester “*Frontiers in Mathematical Physics*” was organized in May–July 2011 in Cergy and Montreal by L. Bruneau, V. Jakšić, R. Livi, C.-A. Pillet and R. Seiringer (the proceedings appeared in the special issue of *J. Math. Phys.* 55 (2014)). L. Bruneau and V. Jakšić were also organizers of the workshops “*Entropy in Quantum Mechanics: Recent Advances*” held in Cergy, June 25–26, 2013. A semester “*Current Topics in Mathematical Physics*” was organized in May–July 2014 in Montreal by V. Jakšić, A. Panati, R. Seiringer and A. Shirikyan. Finally, we mention that V. Jakšić is the convenor of the next *International Congress of Mathematical Physics, Montreal 2018*. This largest meeting of our community will be followed, in the Fall 2018, by a Thematic Semester at CRM entitled “*Analysis in Mathematical Physics*” and featuring 5 workshops (2 of them directly related to this project), and two Winter schools. During the semester, V. Jakšić will teach a lecture on *entropy* and C.-A. Pillet, who will apply for a CNRS delegation to UMI 3457, will run a weekly research seminar.



### 4.3 Description by task

#### 4.3.1 Classical systems

##### [C1] Stochastic PDEs arising in mathematical physics.

Let us describe this problem in mathematical terms. Consider a Markovian random dynamical system  $\{\varphi_t\}$  in a Polish space  $X$ . This means that the mappings  $\varphi_t : X \rightarrow X$  depend on a random parameter belonging to a probability space  $(\Omega, \mathcal{F}, \mathbb{P})$ , and the trajectories of  $\varphi_t$  parametrized by initial points form a Markov process in  $X$ . We assume in addition that the random flow  $\varphi_t$  is *mixing* in the following sense: there is a unique probability measure  $\mu$  on  $X$  such that, for any bounded continuous function  $f : X \rightarrow \mathbb{R}$ , we have

$$\mathbb{E} f(\varphi_t(u)) \rightarrow (f, \mu) \quad \text{as } t \rightarrow \infty, \quad (1)$$

where  $u \in X$  is an arbitrary initial point and  $(f, \mu)$  stands for the mean value of  $f$  with respect to  $\mu$ . In this case,  $\mu$  is called a *stationary measure* for  $\{\varphi_t\}$ . If convergence (1) is sufficiently fast, then the SLLN is also true:

$$\langle f \rangle_t := \frac{1}{t} \int_0^t f(\varphi_s(u)) \, ds \rightarrow (f, \mu) \quad \text{as } t \rightarrow \infty. \quad (2)$$

Suppose now that the system in question possesses a natural *entropy production* functional  $\sigma : X \rightarrow \mathbb{R}$ . If there is a good control of  $\sigma$  at infinity, then the SLLN (2) holds with  $f = \sigma$ . The *Gallavotti–Cohen fluctuation theorem* (see<sup>GC1,GC2,LS</sup>) describes the variations of the time average  $\langle \sigma \rangle_t$  around the spatial average  $(\sigma, \mu)$ . More precisely, it claims a universal symmetry that can be written in the form

$$\frac{\mathbb{P}\{\langle \sigma \rangle_t = -r\}}{\mathbb{P}\{\langle \sigma \rangle_t = +r\}} \sim e^{-rt} \quad \text{as } t \rightarrow \infty, \quad (3)$$

where  $r \in \mathbb{R}$  is any number. In other words, the probability of observing a negative fluctuation of the entropy is exponentially small with respect to the probability of symmetric positive fluctuation. This type of results, as well as their local versions, are well known for various deterministic and stochastic systems with good mixing properties. Very recently, these results were extended to infinite-dimensional Markov processes associated with randomly forced PDEs with strong dissipation; see<sup>JNPS2</sup>. Our goal is to establish the Gallavotti–Cohen fluctuation theorem for stochastic PDEs of mathematical physics, such as the complex Ginzburg–Landau equation and the 2D Navier–Stokes equation with random perturbation white in time and smooth in space variables.

**Staff involved:** L. Chen, V. Jakšić, V. Nersisyan, C.-A. Pillet, A. Shirikyan.

##### [C2] Weak turbulence.

Consider the following nonlinear PDE on the torus  $\mathbb{T}_L^d = \mathbb{R}^d / (L\mathbb{Z}^d)$ ,  $L \geq 1$ :

$$\dot{u} + i\Delta u + \varepsilon \rho i |u|^2 u = -\nu(-\Delta u + 1)^p u + \sqrt{\nu} \langle \text{random force} \rangle. \quad (4)$$

Here  $u = u(t, x)$  ( $t \geq 0$ ,  $x \in \mathbb{T}_L^d$ ) is an unknown complex function, the parameters  $\varepsilon, \nu, \rho$  satisfy the inequalities  $0 < \varepsilon \leq 1$ ,  $0 \leq \nu \leq 1$ ,  $\rho \geq 1$ , and  $p$  is an integer, “not too small in terms of  $d$ .” The random force is smooth in  $x$  and is a white noise as a function of  $t$ . The wave turbulence (WT) studies solutions of this equation for large  $t$  when  $\varepsilon, \nu \ll 1$  and  $L \gg 1$ . Classically  $\nu = 0$ , and in this case (4) becomes the defocusing NLS equation; see<sup>ZLF</sup>. The stochastic model (4) <sub>$\nu > 0$</sub>  was suggested by Zakharov–L’vov<sup>ZLF</sup>. Natural relation between  $\varepsilon$  and  $\nu$  is  $\nu = \varepsilon^2$ , if  $\nu > 0$ . In the stochastic equation (4), let us pass to the slow time  $\tau = \nu t = \varepsilon^2 t$  and denote  $\lambda_k = (|k|^2 + 1)^p$ . Then the equation, written in terms of the Fourier coefficients  $v_k$ , reads

$$\frac{d}{d\tau} v_k(\tau) + i|k|^2 \nu^{-1} v_k = -i\rho \sum_{k_1+k_2=k_3+k} v_{k_1} v_{k_2} \bar{v}_{k_3} - \lambda_k v_k + b_k \frac{d}{d\tau} \beta_k(\tau). \quad (5)$$

Here  $\{\beta_k, k \in \mathbb{Z}_L^d\}$  are independent standard complex Wiener processes and the real numbers  $b_k$  are non-zero and fast converge to zero when  $|k| \rightarrow \infty$ . This equation is well posed and mixing.



Denote  $n_k^L(\tau) = \frac{1}{2} \mathbb{E}|a_k^L(\tau)|^2$ ,  $k \in \mathbb{Z}_L^d$ . One of the main conjectures of the WT is to prove that when  $\nu \ll 1, L \gg 1$ ,  $\rho$  is properly scaled in terms of  $\nu$  and  $L$  and the time is large, the function  $n_k^L(\tau)$  converges to a solution of a certain kinetic equation for  $n_k^L(\tau)$  with  $k \in \mathbb{R}^d$ . The papers<sup>Kuk1, KM</sup> suggested a program how to prove this conjecture in the stochastic setting, and a number of publications, quoted in<sup>Kuk1, KM</sup>, proved “one/half” of it. The main goal of the planned research is to complete the proof along the lines, indicated in<sup>KM</sup>.

**Staff involved:** *S. Kuksin, A. Shirikyan.*

[C3] *Non-entropic conservation laws, random particle systems and the KPZ limit.*

The KPZ equation describes a random dynamics representing the scaling limit of several stochastic models, such as growth models, polymers, interacting particles, which are said to fall in the KPZ universality class. Early convergence results to KPZ were established<sup>BG</sup>, more recently analytical aspects were investigated in<sup>Ha</sup>. The long time behavior of random dynamics in the KPZ universality class is expected to be described by the so called KPZ fixed point process. Several properties of such a process have been investigated in the last decades, see<sup>CQR</sup> for a review, however a full description is still missing.

Several quantities in the KPZ universality class (e.g. correlation functions) feature a non trivial long time behavior. These limits can informally be regarded as the corresponding quantities of a limit process, the so-called KPZ fixed point. Its existence as a random field is not proved yet<sup>CQR</sup>. While the KPZ equation is formally equivalent to the stochastic Burgers’s equation, it is possible, at least at a formal level, to consider the KPZ fixed point as a random, distribution-valued solution to the (deterministic) Burgers equation  $u_t + uu_x = 0$ . Many features (e.g. correlation functions, scaling properties, invariant measures, marginal distributions) of the KPZ fixed point have been investigated exploiting explicit formulas in the long time limit for processes that are thought to fall within the KPZ universality class<sup>CQR</sup>. Following this direction, our main target consists in exploiting a one-to-one correspondence between piecewise constant solutions to Burgers’ equation, and a rather rich dynamics of a new family of stochastic particles systems. Particles can be either repulsive or attractive, are grouped in stacks. Stacks of particles perform a non-local deterministic dynamics, but they can randomly split, merge and be created. We aim to investigate long-time behavior and a suitable scaling limit of such particle systems, aiming to a better comprehension of the KPZ fixed point. As a first step in this direction, we plan to prove existence of (and convergence to) an invariant measure for the above particle systems.

**Staff involved:** *A. Boritchev, V. Nersesyan, A. Shirikyan.*

[C4] *Relaxation of open Hamiltonian systems.*

Consider a finite-dimensional Hamiltonian system (the small system) coupled to the wave equation in  $\mathbb{R}^d$  (the large system). We thus deal with the phase space  $\mathcal{H} = \mathbb{R}^{2d} \oplus (H^1 \times L^2)$  (where Lebesgue and Sobolev spaces are considered over  $\mathbb{R}^d$ ) and the Hamiltonian

$$H(p, q, \varphi, \pi) = \frac{|p|^2}{2} + V(q) + \frac{1}{2} \int_{\mathbb{R}^d} (|\nabla \varphi|^2 + |\pi|^2) dx + q \cdot \int_{\mathbb{R}^d} \rho(x) \nabla \varphi(x) dx, \quad (6)$$

where the canonical variables  $(p, q) \in \mathbb{R}^{2d}$  and  $(\varphi, \pi) \in H^1 \times L^2$  correspond to the small and large systems, respectively, and  $\rho(x)$  stands for the charge density. The last term in Hamiltonian (6) describes the interaction between the two systems in the dipolar approximation. Assuming that the initial state of the wave field is distributed according to the Gaussian measure describing its thermal equilibrium at a given positive temperature, and under some hypotheses on the function  $\rho$  expressed in terms of the representation of its Fourier transform as a Blaschke product, one can introduce some new variables  $r_k$  and reduce (at least, formally) the Hamiltonian system defined by (6) to an infinite-dimensional stochastic system of the form<sup>EPR1</sup>

$$\dot{q} = p, \quad \dot{p} = -\nabla_q G(p, q, r), \quad \dot{r}_k = -\gamma_k \nabla_{r_k} G(p, q, r) + \lambda_k \dot{w}_k, \quad (7)$$

where  $r = (r_k, k \geq 1)$ ,  $G$  is a Hamiltonian,  $\gamma_k > 0$  and  $\lambda_k$  are real numbers, and  $w_k$  denote independent standard Brownian motions. We plan to begin with the justification of the above-mentioned reduction and the investigation of the well-posedness of the Cauchy problem for (7). Once these results are established, we shall

study the mixing properties of the corresponding random flow. We shall then also consider entropy production and FTs for finite dimensional Hamiltonian systems coupled to several wave fields at different temperatures.

**Staff involved:** V. Jakšić, V. Nersesyan, C.-A. Pillet, A. Shirikyan, Postdoc.

#### [C5] NESS of strongly pinned chains of oscillators.

Boundary driven chains of anharmonic oscillators are special cases of the Hamiltonian systems considered in Task C4. These models have been more extensively studied for their relevance in the modeling of heat conduction. The case of weakly pinned chains is quite well understood<sup>EPR2,EH</sup>: they relax exponentially fast to a NESS<sup>RT1</sup> satisfying the FT<sup>RT2</sup>. Chains of strongly pinned oscillators or rotors are known to exhibit a much slower relaxation<sup>HM</sup>. A proof of the existence of a NESS for a chain of 3 and 4 rotors (which can be thought as infinitely pinned oscillators) has been obtained last year<sup>CEP,CE</sup> as part of the Ph.D. thesis of N. Cuneo. Motivated by these advances, we shall investigate the existence and unicity of the NESS of chains of  $N$  rotors and strongly pinned oscillators. Given the complexity of the argument needed to treat the cases of  $N = 3$  and  $N = 4$ , the extension of the results of<sup>CEP,CE</sup> to arbitrary  $N$  is a very challenging problem with a non-negligible risk of failure. However, a success or a counterexample would definitively have a large impact on the subject, and we believe that the risk is worth to be taken.

**Staff involved:** A. Shirikyan, Postdoc.

### 4.3.2 Quantum systems

#### [Q1] Quantum transfer operators and entropic fluctuations.

The Ruelle-Perron-Frobenius transfer operators play a central role in the thermodynamic formalism of classical chaotic dynamical systems. Their spectral properties are linked to the ergodic properties of natural (or physical) steady states (i.e., SRB-measures) of these systems. The object of this task is to show that *quantum transfer operators* appear as natural objects of modular theory in the framework of  $C^*$  or  $W^*$  dynamical systems. Like their classical cousins, they provide an access to the ergodic properties of these dynamical systems and encode information on their NESSs and hence on the transport properties of the underlying physical systems. We have developed the conceptual foundations of this approach in<sup>JOPP</sup>.

Since the seminal works of Levitov and Lesovik, counting statistics of charge transport has been the subject of a large amount of publications in the theoretical and experimental physics literature. However the mathematical status of this theory and in particular its relation to the algebraic framework of quantum statistical mechanics is still unclear. We shall relate the counting statistics of entropy transport to quantum transfer operators and study their large time asymptotics for simple but physically relevant models of the spin-fermion/boson type. This is, in our opinion, the most appealing approach to FTs for quantum systems. As a *proof of concept*, we have performed in<sup>JPPP</sup> a study of the statistics of energy transfers in equilibration processes. The extension of these results to non-equilibrium situations is of course more challenging, but we are confident that the techniques developed in the HamMark project should allow us to fulfill this task. In particular, energy/entropy FTs will be investigated for the adiabatic repeated interaction quantum systems recently introduced in<sup>HJPR</sup>.

**Staff involved:** V. Jakšić, A. Panati, Y. Pautrat, C.-A. Pillet.

#### [Q2] Random quantum walks.

Notwithstanding applications for quantum computing, the main focus on QWs will concern their ability to model quantum transport, their link with probability theory, and their thermodynamical properties.

(i) *Deeper analysis of the fine spectral properties of RQW*, in the spirit of ongoing research on Anderson type models. Thanks to the heuristic link between the Anderson model and RQW described in<sup>J2</sup> and to the relative simplicity of the RQW, an ambitious long term goal would be to exhibit evidence of a localization-delocalization transition on the cubic lattice in large dimension. A first step in that direction consists in analyzing the behavior of the exponential localization length of certain RQW as a function of the dimension of the underlying lattice, by resorting to a classical random walk expansion of the evolution operator, exploiting the relative algorithmic simplicity of RQW.

(ii) *QWs evolving in a reactive environment.* This study aims at describing the overall effects of an environment as quantum friction in the light of simplified quantum models. The prototypical environment consists in a field of spins attached to the vertices of the underlying graph with which the quantum particle interacts in a unitary fashion. The exchanges between the environment and the quantum walker will influence the transport properties of the latter, whose effective dynamics is obtained by tracing out the degrees of freedom of the environment. We want to compare the effective dynamics with repeated interaction models introduced to study the effective dynamics of a particle in a thermal environment<sup>BDBP, BJM1</sup>, and with the open quantum walks introduced by<sup>APSS</sup>. Further tracing out the spin degrees of freedom of the quantum walker, we get a time dependent family of discrete probability distributions giving the probability to find the particle at a vertex of the underlying graph. We shall analyze the transport properties of the particle, in particular the transitions between ballistic and diffusive or localized and diffusive regimes, depending on the initial state of the spin field.

(iii) *Ensemble of QWs in contact with several reservoirs.* This item is part of the non equilibrium statistical mechanics concerned with the description of particle flows between different thermodynamical reservoirs, through a quantum sample. The goal is to introduce a quantum version of "simple exclusion processes" providing classical stochastic models of interacting particles with nontrivial thermodynamic properties in some regimes<sup>DLS</sup>. Following<sup>HJ2</sup> which deals with one reservoir only, we will consider an ensemble of non interacting fermionic quantum walkers on a finite dimensional sample coupled to reservoirs of infinitely many particles in states characterized by their particle density. The Fermi statistics is chosen to introduce an exclusion mechanism and the coupling conserves the total number operator. We will consider in particular the reduced one body density matrix of quantum walkers, the density profile of those particles and the flux observables between the reservoirs. The setup considered being in keeping with the approach developed in paragraph Q3, we shall also address the localization/delocalization of QWs along those lines.

**Staff involved:** L. Bruneau, A. Joye, Y. Pautrat.

### [Q3] Transport in interacting fermionic systems.

We plan to study localization/delocalization in interacting electronic systems using the ideas and techniques that have recently emerged in the mathematically rigorous literature on non-equilibrium quantum statistical mechanics. The main idea is to link the localization property of interacting fermions in a disordered sample to the transport properties of the NESS which builds up when thermal reservoirs initially at different thermodynamic parameters are attached to the sample. For fermionic systems on a one-dimensional lattice the proposed approach can be summarized as follows:

1. Consider the sequence of locally interacting fermionic system, indexed by  $L$ , in which two electronic reservoirs, at zero temperature and chemical potential  $\mu_l, \mu_r$ , are attached at the end points of the finite sample obtained by restricting the Hamiltonian of the system to the sublattice  $\{1, \dots, L\}$ . The voltage differential  $\mu_r - \mu_l$  then generates an electronic current through the sample with the steady state value  $\langle \mathcal{J}_L \rangle_+$ .
2. Define the localization regime through the large  $L$  behavior of  $\langle \mathcal{J}_L \rangle_+$ :  $(\mu_l, \mu_r)$  is in the localization regime if  $\limsup_{L \rightarrow +\infty} \langle \mathcal{J}_L \rangle_+ = 0$ , it is in the conducting regime if  $\liminf_{L \rightarrow +\infty} \langle \mathcal{J}_L \rangle_+ > 0$ .

This characterization of Anderson localization is physically natural and it has recently been shown<sup>BJLP1</sup> that the above proposed definition reduces to the standard (spectral) one in the case of non-interacting fermions and for arbitrary (deterministic) potential: localization/conducting regime coincide with the absence/presence of absolutely continuous spectrum. We plan in particular to use this approach to investigate the question of localization for interacting one-dimensional random systems.

On the mathematical side, the Landauer–Büttiker approach allowing to deduce transport properties of non-interacting fermions from scattering theory, this idea calls for the development of a new algebraic scattering theory for singularly time-correlated perturbations needed to tackle interacting systems. We are hopeful that this new approach would lead to a novel research direction in mathematical physics.

**Staff involved:** L. Bruneau, V. Jakšić, A. Panati, C.-A. Pillet.

[Q4] *Conductance and full counting statistics scaling.*

A few years after Anderson's pioneering work on localization, the need for a simple quantity to discriminate between localized or non-localized regimes arose. For an extended system the usual, and certainly most precise, definition of Anderson localization is that the spectrum is pure point (dense) with exponentially localized eigenfunctions. In experiments, systems are however finite. The idea introduced by Edwards and Thouless in 1972 is to consider as a measure of localization of a finite system the ratio  $g_{\text{Th}} = \frac{\delta E}{\Delta E}$ , now known as the *Thouless conductance* and where  $\delta E$  represents the sensitivity to a change a boundary condition (near the Fermi level) and  $\Delta E$  is the level spacing. They argued that in a large system the energy of a localized state should be insensitive to a change of boundary condition, at least if the center of localization is not too close to the boundary, so that the ratio  $g_{\text{Th}}$  should be small. They moreover argued that this quantity could be interpreted as a measure of the conductance of the system.

The derivation of  $g_{\text{Th}}$  and in particular its interpretation as a conductance is, however, extremely heuristic. On one hand it has now been widely accepted both by theoretical and experimental physicists as a signature of localization, and plays an important role in the scaling theory of localization. On the other hand its interpretation as a conductance has been the subject of many debates in the physics literature. When trying to compare the Thouless conductance  $g_{\text{Th}}(L)$ ,  $L$  referring to the size of the system, to the conductance of the system obtained from transport consideration *à la Landauer*, it has been argued mainly based on numerical simulation that, while this interpretation is correct in the diffusive regime, in the localized regime the true conductance should rather scale like  $g_{\text{Th}}(L)^\beta$  in the limit of large  $L$ . No universal value of  $\beta$  seems to be accepted, the value  $\beta = 2$  being the most commonly cited.

On the mathematical side, no mathematically rigorous proof of the Thouless formula were available until recently hampering mathematical development. Its recent derivation from the first principles of quantum mechanics<sup>BJLP1</sup> have opened the way to a systematic study of the above mentioned facts, and the recent results<sup>BJLP2</sup> show that the behavior of  $g_{\text{Th}}$  is indeed a measure of localization. The next step is to compare the respective scaling behaviors of the Thouless conductance and of the conductance obtained from the Landauer-Büttiker formula by coupling the system to fermionic reservoirs at zero temperature and chemical potential  $\mu_l/\mu_r$ , that is the quantity  $g_{\text{LB}}(L) = \frac{\langle \mathcal{J}_L \rangle_+}{\mu_r - \mu_l}$  where  $\langle \mathcal{J}_L \rangle_+$  is the steady state value of the electronic current through the sample. In this direction the analysis of one-dimensional ergodic systems seems very promising. The sample Hamiltonian is  $h_\omega = -\Delta + \lambda v_\omega$  where  $v_\omega(n) = f(T^n \omega)$ ,  $\omega \in \Omega$ , where  $\Omega$  is a probability space,  $f : \Omega \rightarrow \mathbb{R}$  is a bounded measurable map,  $T$  is an ergodic invertible transformation of  $\Omega$ , and  $\lambda$  is a coupling constant. Random and quasi-periodic potentials are examples of such ergodic potentials which both exhibit absence of absolutely continuous spectrum (provided the coupling constant  $\lambda$  is large enough in the quasi-periodic case) and hence give a nice framework to analyze the localized regime. We wish to analyze precisely the large  $L$  behavior of the associated Thouless and Landauer conductances: how they scale in terms of the Lyapunov exponents, what is their respective scaling, is there a universal scaling such as  $g_{\text{LB}}(L) \sim g_{\text{Th}}(L)^2$  in the localized regime?

The behavior of the Landauer conductance in the limit of large samples amounts to that of the steady state expectation value  $\langle \mathcal{J}_L \rangle_+$  of the electronic charge current. A deeper understanding of the transport properties lies at the level of the counting statistics of the charge transport, also called full counting statistics. In connection to Task Q1 we wish to investigate how the localization properties of the system are reflected at the level of the full counting statistics, in particular at zero temperature where no thermal fluctuations are present (the so-called shot noise inherent to the nature of quantum systems).

**Staff involved:** L. Bruneau, V. Jakšić, C.-A. Pillet, Postdoc.

[Q5] *Information geometry and thermodynamics of non-equilibrium steady states.*

This research project concerns the concept of "entropy" for physical systems far from equilibrium. Although in general it is quite likely that such a concept is neither physically nor mathematically well defined, we believe that in various special situations (like open quantum systems) a satisfactory result with possibly far reaching physical and mathematical implications can be obtained by combining the geometric ideas of Ruelle<sup>Ru4</sup> con-

cerning *entropic connection and curvature* with the the recent developments of information geometry<sup>AN</sup>. An interesting related set of ideas has appeared in the physics literature. This subject is riddled with conceptual difficulties and we plan to start with a detailed analysis of exactly solvable models like open XY-chains and simplified models like open quantum systems in the van Hove weak coupling limit. The preliminary results are encouraging and we anticipate that over the next four years this project will evolve in scope, size and depth into a major research direction.

**Staff involved:** *L. Chen, V. Jakšić, C.-A. Pillet.*

[Q6] *Statistical properties of repeated measurement processes.*

The Nobel prize winning experiments of Haroche’s group at ENS have given a new incentive to theoretical investigation of statistical properties of repeated quantum measurements. This research project concerns study of entropic aspects of the processes involving repeated quantum measurements of finite quantum systems. In the first step we will study the entropy production (EP) that quantifies the irreversibility of the measurement process and is linked to the entropy transferred from the system to the environment in the same process. We plan to develop a suitable variant of dynamical systems thermodynamic formalism for the EP and use it to study fine aspects of irreversibility related to the hypothesis testing of the arrow of time. Under a suitable chaoticity assumption, we plan to establish a Large Deviation Principle and a Fluctuation Theorem for the EP. The preliminary results suggest that the thermodynamic formalism variational principle that characterizes the fluctuations of the entropy production may naturally lead to a mathematical definition of "coherent structures associated to rare fluctuations" anticipated in the physics literature, and shed a light on dynamical phase transitions linked to these rare fluctuations. Although these topics have been much studied in the recent theoretical and experimental physics literature, a mathematically rigorous theory is lacking.

As an application of the thermodynamic formalism for the EP we plan to study the notion of quantum detailed balance for completely positive maps. In the literature, one can find many different definitions of the quantum detailed balance that arise by "quantization" of the relations defining its classical counterpart. We plan to adopt a more physical route and link the quantum detailed balance to vanishing of the entropy production of all quantum instruments (that is, measurement processes) that sum up to a given completely positive map. The preliminary results suggest that the vanishing of EP singles out the unique "quantization" of the classical detailed balance condition accompanied by an intuitive and natural KMS structure.

In the final stage of the project we plan to refine the thermodynamic formalism and use the new techniques to study the Rényi entropy, large deviations, and fractal dimensions of repeated quantum measurements.

**Staff involved:** *V. Jakšić, Y. Pautrat, C.-A. Pillet.*

4.4 *Time schedule and work-plan*

The following table gives an approximate schedule when we expect to have some results for the tasks of this projects.

Task	Partners involved	Year 1	Year 2	Year 3	Year 4
C1	Cergy, Montreal, Toulon	★	★	★	★
C2	Cergy	★	★	★	★
C3	Cergy	★	★	★	
C4	Cergy, Montreal, Toulon			★	★
C5	Cergy, Montreal, Toulon		★	★	★
Q1	Cergy, Montreal, Toulon	★	★		
Q2	Cergy, Toulon	★	★	★	★
Q3	Cergy, Montreal, Toulon			★	★
Q4	Cergy, Montreal, Toulon	★	★		
Q5	Cergy, Montreal, Toulon			★	★
Q6	Montreal, Toulon			★	★



## 5 EXPECTED IMPACT, EXPLOITATION AND PROTECTION OF INTELLECTUAL PROPERTY

NONSTOPS is a basic research program in mathematical physics. It will produce definitions and theorems related to timely problems in statistical mechanics. Although no immediate technological, economic or social outcome is expected, there is no doubt that the advances of non-equilibrium statistical mechanics and thermodynamics to which the project will contribute will have a significant impact in physics and in other fields of science and technology, including life sciences and quantum engineering. As already mentioned in Section 4.1, the exploitation of our results will follow the standards of our community: publication in refereed journals and on internet archives, communications in international conferences. A substantial part of the budget is dedicated to the organization of scientific meetings which will provide opportunities to advertise the achievements of the consortium:

Fall 2018	The 1 <sup>st</sup> annual meeting will take place during the Thematic Semester “ <i>Analysis in Mathematical Physics</i> ” at CRM.
Summer 2019	The 2 <sup>nd</sup> annual meeting will be organized in Toulon.
Spring 2020	The 3 <sup>rd</sup> annual meeting will be organized in Cergy.
July 2021	The final, 2 weeks event will take place in south of France and combine an international workshop and a summer school.

Regarding the protection of intellectual property we shall follow the applicable CNRS guidelines:

- The partners keep the co-ownership of the results they have contributed to elaborate.
- The team members keep the right to publish their results.

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