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ACTIVITY REPORT

Project-Team
PARADYSE

PARticles And DYnamical SystEms

IN COLLABORATION WITH: Laboratoire Paul Painlevé (LPP)

DOMAIN

**Applied Mathematics, Computation and
Simulation**

THEME

Numerical schemes and simulations

Inria

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Project-Team PARADYSE

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Computer sciences and digital sciences

- A6.1.1. – Continuous Modeling (PDE, ODE)
- A6.1.2. – Stochastic Modeling
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- A6.2.3. – Probabilistic methods
- A6.5. – Mathematical modeling for physical sciences

Other research topics and application domains

- B3.6. – Ecology
- B3.6.1. – Biodiversity
- B5.3. – Nanotechnology
- B5.5. – Materials
- B5.11. – Quantum systems
- B6.2.4. – Optic technology

1 Team members, visitors, external collaborators

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2 Overall objectives

The PARADYSE team gathers mathematicians from different communities with the same motivation: to provide a better understanding of dynamical phenomena involving particles. These phenomena are described by fundamental models arising from several fields of physics. We shall focus on model derivation, study of stationary states and asymptotic behaviors, as well as links between different levels of description (from microscopic to macroscopic) and numerical methods to simulate such models. Applications include non-linear optics, thermodynamics and ferromagnetism. Research in this direction has a long history, that we shall only partially describe in the sequel. We are confident that the fact that we come from different mathematical communities (PDE theory, mathematical physics, probability theory and numerical analysis), as well as the fact that we have strong and effective collaborations with physicists, will bring new and efficient scientific approaches to the problems we plan to tackle and will make our team strong and unique in the scientific landscape. Our goal is to obtain original and important results on a restricted yet ambitious set of problems that we develop in this document.

3 Research program

3.1 Time asymptotics: Stationary states, solitons, and stability issues

The team investigates the existence of *solitons* and their link with the global dynamical behavior for non-local problems such as the Gross–Pitaevskii (GP) equation which arises in models of dipolar gases. These models, in general, also introduce non-zero boundary conditions which constitute an additional theoretical and numerical challenge. Numerous results are proved for local problems, and numerical simulations allow to verify and illustrate them, as well as making a link with physics. However, most fundamental questions are still open at the moment for non-local problems.

The non-linear Schrödinger (NLS) equation finds applications in numerous fields of physics. We concentrate, in a continued collaboration with our colleagues from the physics department (PhLAM) at Université de Lille (U-Lille) in the framework of the Laboratoire d'Excellence CEMPI, on its applications in non-linear optics and cold atom physics. Issues of orbital stability and modulational instability are central here (see Section 4.1 below).

Another typical example of problem that the team wishes to address concerns the Landau–Lifshitz (LL) equation, which describes the dynamics of the spin in ferromagnetic materials. This equation is a fundamental model in the magnetic recording industry [40] and solitons in magnetic media are of particular interest as a mechanism for data storage or information transfer [41]. It is a quasilinear PDE involving a function that takes values on the unit sphere \mathbb{S}^2 of \mathbb{R}^3 . Using the stereographic projection, it can be seen as a quasilinear Schrödinger equation and the questions about the solitons, their dynamics and potential blow-up of solutions evoked above are also relevant in this context. This equation is less understood than the NLS equation: even the Cauchy theory is not completely understood [30, 39]. In particular, the geometry of the target sphere imposes that the solution has a norm equal to one everywhere, so in particular the boundary conditions cannot be zero, and, even in dimension one, there are kink-type solitons having different limits at $\pm\infty$.

3.2 Derivation of macroscopic laws from microscopic dynamics

The team investigates, from a microscopic viewpoint, the dynamical mechanism at play in the phenomenon of relaxation towards thermal equilibrium for large systems of interacting particles. For instance, a first step consists in giving a rigorous proof of the fact that a particle repeatedly scattered by random obstacles through a Hamiltonian scattering process will eventually reach thermal equilibrium, thereby completing previous works in this direction by the team. As a second step, models similar to the ones considered classically will be defined and analyzed in the quantum mechanical setting, and more particularly in the setting of quantum optics.

Another challenging problem is to understand the interaction of large systems with the boundaries, which is responsible for most energy exchanges (forcing and dissipation), even though it is concentrated in very thin layers. The presence of boundary conditions to evolution equations sometimes lacks understanding from a physical and mathematical point of view. In order to legitimate the choice done at the

macroscopic level of the mathematical definition of the boundary conditions, we investigate systems of particles with different local interactions. We apply various techniques to understand how diffusive and driven systems interact with the boundaries.

Finally, we aim at obtaining results on the macroscopic behavior of large scale interacting particle systems subject to kinetic constraints. In particular, we study the behavior in one and two dimensions of the Facilitated Exclusion Process (FEP), on which several results have already been obtained. The latter is a very interesting prototype for kinetically constrained models because of its unique mathematical features (explicit stationary states, absence of mobile cluster to locally shuffle the configuration). There are very few mathematical results on the FEP, which was put forward by the physics community as a toy model for phase separation.

Our goal is to develop collaboration at the interface between probability and PDE theory, and use the rich PDE background of the team to provide tools to be used on statistical physics problems put forward by the probability side of the team.

3.3 Numerical methods: analysis and simulations

The team addresses both questions of precision and numerical cost of the schemes for the numerical integration of non-linear evolution PDEs, such as the NLS equation. In particular, we aim at developing, studying and implementing numerical schemes with high order that are more efficient for these problems. We also want to contribute to the design and analysis of schemes with appropriate qualitative properties. These properties may as well be “asymptotic-preserving” properties, energy-preserving properties, or convergence to an equilibrium properties. Other numerical goals of the team include the numerical simulation of standing waves of non-linear non-local GP equations. We also keep on developing numerical methods to efficiently simulate and illustrate theoretical results on instability, in particular in the context of the modulational instability in optical fibers, where we study the influence of randomness in the physical parameters of the fibers.

The team also designs simulation methods to estimate the accuracy of the physical description via microscopic systems, by computing precisely the rate of convergence as the system size goes to infinity. One method under investigation is related to cloning algorithms, which were introduced very recently and turn out to be essential in molecular simulation.

4 Application domains

4.1 Optical fibers

In the propagation of light in optical fibers, the combined effect of non-linearity and group velocity dispersion (GVD) may lead to the destabilization of the stationary states (plane or continuous waves). This phenomenon, known under the name of modulational instability (MI), consists in the exponential growth of small harmonic perturbations of a continuous wave. MI has been pioneered in the 60s in the context of fluid mechanics, electromagnetic waves as well as in plasmas, and it has been observed in non-linear fiber optics in the 80s. In uniform fibers, MI arises for anomalous (negative) GVD, but it may also appear for normal GVD if polarization, higher order modes or higher order dispersion are considered. A different kind of MI related to a parametric resonance mechanism emerges when the dispersion or the non-linearity of the fiber are periodically modulated.

As a follow-up of our work on MI in periodically modulated optical fibers, we investigate the effect of random modulations in the diameter of the fiber on its dynamics. It is expected on theoretical grounds that such random fluctuations can lead to MI and this has already been illustrated for some models of the randomness. We investigate precisely the conditions under which this phenomenon can be strong enough to be experimentally verified. For this purpose, we investigate different kinds of random processes describing the modulations, taking into account the manner in which such modulations can be created experimentally by our partners of the fiber facility of the PhLAM. This necessitates a careful modeling of the fiber and a precise numerical simulation of its behavior as well as a theoretical analysis of the statistics of the fiber dynamics.

This application domain involves in particular S. De Bièvre and G. Dujardin.

4.2 Ferromagnetism

The Landau–Lifshitz (LL) equation describes the dynamics of the spin in ferromagnetic materials. Depending on the properties of the material, the LL equation can include a dissipation term (the so-called Gilbert damping) and different types of anisotropic terms. The LL equation belongs to a larger class of non-linear PDEs which are often referred to as geometric PDEs, and some related models are the Schrödinger map equation and the harmonic heat flow. We focus on the following aspects of the LL equation.

Solitons In the absence of Gilbert damping, the LL equation is Hamiltonian. Moreover, it is integrable in the one-dimensional case and explicit formulas for solitons can be given. In the easy-plane case, the orbital and asymptotic stability of these solitons have been established. However, the stability in other cases, such as in biaxial ferromagnets, remains an open problem. In higher dimensional cases, the existence of solitons is more involved. In a previous work, a branch of semitopological solitons with different speeds has been obtained numerically in planar ferromagnets. A rigorous proof of the existence of such solitons is established using perturbation arguments, provided that the speed is small enough. However, the proof does not give information about their stability. We would like to propose a variational approach to study the existence of this branch of solitons, that would lead to the existence and stability of the whole branch of ground-state solitons as predicted. We also investigate numerically the existence of other types of localized solutions for the LL equation, such as excited states or vortices in rotation.

On the other hand, with the inclusion of the Gilbert damping, the Landau-Lifshitz-Gilbert (LLG) equation becomes (partially) dissipative. Interestingly, in the one-dimensional case, the same solitons, referred to as *domain walls*, emerge as significant structures. Not only do they demonstrate asymptotic stability, even in the presence of a small magnetic field ([36]), but they also serve as crucial building blocks for various stable configurations, such as 2-domain wall structures ([35]). Numerical simulations further suggest that any general solution should decompose over time into a superposition of domain walls, though this still presents an open problem at the theoretical level. Exploring the scenario of a notched nanowire ([34]) reveals yet another context where generalized domain walls manifest. They exhibit an even better asymptotic stability compared to their non-notched counterparts, which may lead to applications in information storage.

Approximate models An important physical conjecture is that the LL model is to a certain extent universal, so that the non-linear Schrödinger and Sine-Gordon equations can be obtained as its various limit cases. In a previous work, A. de Laire has proved a result in this direction and established an error estimate in Sobolev norms, in any dimension. A next step is to produce numerical simulations that will enlighten the situation and drive further developments in this direction.

Self-similar behavior Self-similar solutions have attracted a lot of attention in the study of non-linear PDEs because they can provide some important information about the dynamics of the equation. While self-similar expanders are related to non-uniqueness and long time description of solutions, self-similar shrinkers are related to a possible singularity formation. However, there is not much known about the self-similar solutions for the LL equation. A. de Laire and S. Gutierrez (University of Birmingham) have studied expander solutions and proved their existence and stability in the presence of Gilbert damping. We will investigate further results about these solutions, as well as the existence and properties of self-similar shrinkers.

This application domain involves in particular A. de Laire, G. Dujardin and G. Ferriere.

4.3 Bose-Einstein condensates and nonlinear optics

In quantum physics and nonlinear optics, the Gross-Pitaevskii equation with non-zero boundary conditions is employed to describe the behavior of quantum fluids and Bose-Einstein condensates. The primary challenges are to comprehend new realistic physical effects, such as nonlocal interactions, quasilinear effects and variations in the width of the domain.

In order to establish a rigorous understanding of the dynamics of these models, the study of particular solutions such as dark solitons, which play a key role in the large-time behavior, is a crucial first step.

For instance, proving the stability of dark solitons, based on various physical considerations, implies that these structures are good candidates to be controlled experimentally and to be considered in new applications.

Although the properties of dark solitons are well-known in classical models described by the Gross-Pitaevskii equation, the situation becomes more intricate when adding terms to model new realistic physical effects. Each characteristic introduces a range of new theoretical and numerical difficulties. This complexity emphasizes the need for a careful and detailed examination to enhance our understanding of these intricate systems.

This application domain involves in particular A. de Laire, G. Dujardin and G. Ferriere.

4.4 Cold atoms

The cold atoms team of the PhLAM Laboratory is reputed for having realized experimentally the so-called Quantum Kicked Rotor, which provides a model for the phenomenon of Anderson localization. The latter was predicted by Anderson in 1958, who received in 1977 a Nobel Prize for this work. Anderson localization is the absence of diffusion of quantum mechanical wave functions (and of waves in general) due to the presence of randomness in the medium in which they propagate. Its transposition to the Quantum Kicked Rotor goes as follows: a freely moving quantum particle periodically subjected to a “kick” will see its energy saturate at long times. In this sense, it “localizes” in momentum space since its momenta do not grow indefinitely, as one would expect on classical grounds. In its original form, Anderson localization applies to non-interacting quantum particles and the same is true for the saturation effect observed in the Quantum Kicked Rotor.

The challenge is now to understand the effects of interactions between the atoms on the localization phenomenon. Transposing this problem to the Quantum Kicked Rotor, this means describing the interactions between the particles with a Gross-Pitaevskii equation, which is a NLS equation with a local (typically cubic) non-linearity. So the particle's wave function evolves between kicks following the Gross-Pitaevskii equation and not the linear Schrödinger equation, as is the case in the Quantum Kicked Rotor. Preliminary studies for the Anderson model have concluded that in that case the localization phenomenon gives way to a slow subdiffusive growth of the particle's kinetic energy. A similar phenomenon is expected in the non-linear Quantum Kicked Rotor, but a precise understanding of the dynamical mechanisms at work, of the time scale at which the subdiffusive growth will occur and of the subdiffusive growth exponent is lacking. It is crucial to design and calibrate the experimental setup intended to observe the phenomenon. The analysis of these questions poses considerable theoretical and numerical challenges due to the difficulties involved in understanding and simulating the long term dynamics of the non-linear system. A collaboration of the team members with the PhLAM cold atoms group is currently under way.

This application domain involves in particular S. De Bièvre and G. Dujardin.

4.5 Modelling shallow water dynamics

The understanding of the propagation of waves in shallow water is of importance for the modelling of tsunamis and other rogue waves. This requires a better understanding of dispersive shallow water systems as ABCD systems, that are related to the classical Boussines systems, and classifying particular travelling waves solutions for these systems. To deal with systems is at forefront of research. Analogous questions for single equations as KdV equations are well-documented.

A. de Laire and O. Goubet are involved in these topics, together with researchers in Chile : Claudio Muñoz (Universidad de Chile), María Eugenia Martínez (University of Chile) and Felipe Poblete (Austral University of Chile). The applications for tsunamis is of interest for people in Chile.

4.6 Qualitative and quantitative properties of numerical methods

Numerical simulation of multimode fibers The use of multimode fibers is a possible way to overcome the bandwidth crisis to come in our worldwide communication network consisting in singlemode fibers. Moreover, multimode fibers have applications in several other domains, such as high power fiber lasers and femtosecond-pulse fiber lasers which are useful for clinical applications of non-linear optical

microscopy and precision materials processing. From the modeling point of view, the envelope equations are a system of non-linear non-local coupled Schrödinger equations. For a better understanding of several physical phenomena in multimode fibers (e.g. continuum generation, condensation) as well as for the design of physical experiments, numerical simulations are a suitable tool. However, the huge number of equations, the coupled non-linearities and the non-local effects are very difficult to handle numerically. Some attempts have been made to develop and make available efficient numerical codes for such simulations. However, there is room for improvement: one may want to go beyond MATLAB prototypes, and to develop an alternative parallelization to the existing ones, which could use the linearly implicit methods that we plan to develop and analyze. In link with the application domain 4.1, we develop in particular a code for the numerical simulation of the propagation of light in multimode fibers, using high-order efficient methods, that is to be used by the physics community.

This application domain involves in particular G. Dujardin and A. Roget.

Qualitative and long-time behavior of numerical methods We contribute to the design and analysis of schemes with good qualitative properties. These properties may as well be “asymptotic-preserving” properties, energy-preserving properties, decay properties, or convergence to an equilibrium properties. In particular, we contribute to the design and analysis of numerically hypocoercive methods for Fokker–Planck equations [38], as well as energy-preserving methods for hamiltonian problems [32].

This application domain involves in particular G. Dujardin.

High-order methods We contribute to the design of efficient numerical methods for the simulation of non-linear evolution problems. In particular, we focus on a class of linearly implicit high-order methods, that have been introduced for ODEs and generalized to PDEs [25]. We wish both to extend their analysis to PDE contexts, and to analyze their qualitative properties in such contexts.

This application domain involves in particular G. Dujardin.

4.7 Modeling of the liquid-solid transition and interface propagation

Analogously to the so-called Kinetically Constrained Models (KCM) that have served as toy models for glassy transitions, stochastic particle systems on a lattice can be used as toy models for a variety of physical phenomena. Among them, the kinetically constrained lattice gases (KCLG) are models in which particles jump randomly on a lattice, but are only allowed to jump if a local constraint is satisfied by the system.

Because of the hard constraint, the typical local behavior of KCLGs will differ significantly depending on the value of local conserved fields (e.g. particle density), because the constraint will either be typically satisfied, in which case the system is locally diffusive (liquid phase), or not, in which case the system quickly freezes out (solid phase).

Such a toy model for liquid-solid transition is investigated by C. Erignoux, M. Simon and their co-authors in [3] and [33]. The focus of these articles is the so-called facilitated exclusion process, which is a terminology coined by physicists for a specific KCLG, in which particles can only jump on an empty neighbor if another neighboring site is occupied. They derive the macroscopic behavior of the model, and show that in dimension 1 the hydrodynamic limit displays a phase separated behavior where the liquid phase progressively invades the solid phase.

Both from a physical and mathematical point of view, much remains to be done regarding these challenging models: in particular, they present significant mathematical difficulties because of the way the local physical constraints put on the system distort the equilibrium and steady-states of the model. For this reason, C. Erignoux and A. Roget are currently working with M. Simon (Institut Camille Jordan, Université Lyon 1) and A. Shapira (MAP5, Paris) to generate numerical results on generalizations of the facilitated exclusion process, in order to shine some light on the microscopic and macroscopic behavior of these difficult models.

This application domain involves in particular C. Erignoux and A. Roget.

4.8 Mathematical modeling for ecology

This application domain is at the interface of mathematical modeling and numerics. Its object of study is a set of concrete problems in ecology. The landscape of the south of the Hauts-de-France region is made of agricultural land, encompassing forest patches and ecological corridors such as hedges. The issues are

- the study of the invasive dynamics and the control of a population of beetles which damages the oaks and beeches of our forests;
- the study of native protected species (the purple wireworm and the pike-plum) which find refuge in certain forest species.

Running numerics on models co-constructed with ecologists is also at the heart of the project. In our model, the timescales of animals and plants compare. The life cycle of a tree is one year. For animals we consider mainly insects whose life cycle is also of one year, even for the propagation of insects. Beetle larvae spend a few years in the earth before moving. As a by-product, the mathematical model may tackle other major issues such as the interplay between heterogeneity, diversity and invasibility.

The models use Markov chains at a mesoscopic scale and evolution advection-diffusion equations at a macroscopic scale.

This application domain involves O. Goubet. Interactions with PARADYSE members concerned with particle models and hydrodynamic limits are planned.

5 New software, platforms, open data

5.1 New software

5.1.1 MM_Propagation

Name: MultiMode Propagation

Keywords: Optics, Numerical simulations, Computational electromagnetics

Functional Description: This C++ software, which is interfaced with MatLab, simulates the propagation of light in multimode optical fibers. It takes into account several physical effects such as dispersion, Kerr effect, Raman effect, coupling between the modes. It uses high order numerical methods that allow for precision at reasonable computational cost.

URL: https://github.com/alexandreroget/MM_Propagation

Contact: Alexandre Roget

6 New results

Participants: Quentin Chauleur, Stephan De Bièvre, André de Laire, Guillaume Du-jardin, Clément Erignoux, Olivier Goubet, Christopher Langrenez, Erwan Le Quiniou.

Some of the results presented below overlap several of the main research themes presented in section 3. However, results presented in paragraphs 6.1-6.4 are mainly concerned with research axis 3.1, whereas paragraphs 6.5-6.8 mostly concern axis 3.2. Paragraphs 6.9-6.13 are related to quantum information and computing, and Paragraphs 6.14-6.18 concern numerics-oriented results, so that they are all encompassed in axis 3.3.

6.1 Exotic traveling waves for a quasilinear Schrödinger equation with nonzero background

A. de Laire and E. Le Quiniou have studied a quasilinear Schrödinger equation with nonzero conditions at infinity in dimension one. This quasilinear model corresponds to a weakly nonlocal approximation of the nonlocal Gross–Pitaevskii equation, and can also be derived by considering the effects of surface tension in superfluids. When the quasilinear term is neglected, the resulting equation is the classical Gross–Pitaevskii equation, which possesses a well-known stable branch of subsonic traveling waves solution, given by dark solitons.

In the preprint [28], they investigate how the quasilinear term affects the traveling-waves solutions. They provide a complete classification of finite energy traveling waves of the equation, in terms of the two parameters: the speed and the strength of the quasilinear term. This classification leads to the existence of dark and antidark solitons, as well as more exotic localized solutions like dark cuspons, compactons, and composite waves, even for supersonic speeds. Depending on the parameters, these types of solutions can coexist, showing that finite energy solutions are not unique. Furthermore, they prove that some of these dark solitons can be obtained as minimizers of the energy, at fixed momentum, and that they are orbitally stable.

6.2 Travelling waves for the Gross–Pitaevskii equation on the strip

In one space dimension, the Gross–Pitaevskii equation possesses a family of finite energy travelling waves, called dark solitons. These solitons extend trivially to the strip given by the product space $\mathbb{R} \times \mathbb{T}_L$, where $L > 0$ and \mathbb{T}_L is the torus $\mathbb{T}_L = \mathbb{R}/L\mathbb{Z}$. In this two-dimensional context, the dark solitons are called planar (or line) dark solitons. However, it is well-known in the physics literature that these planar solitons can be unstable due to the tendency to develop distortions in their transverse profile. In addition, experimental observations have shown that the dynamics of planar dark solitons are stable when they are sufficiently confined in the transverse direction L , but unstable otherwise. In the latter case, the creation of vortices can occur.

In the articles [20] and [19], A. de Laire, P. Gravejat and D. Smets provide a rigorous framework for studying this kind of phenomenon. Precisely, they prove the existence of nonconstant finite energy travelling wave solutions to the Gross–Pitaevskii equation on the strip $\mathbb{R} \times \mathbb{T}_L$, obtained as minimizers of the energy at fixed momentum. Moreover, by studying the associated variational problem, they deduce that these minimizers are exactly the planar dark solitons when L is less than a critical value, and that they are genuinely two-dimensional solutions otherwise. In particular, planar solitons do not minimize the energy in the presence of a large transverse direction. The proof of the existence of minimizers is based on the compactness of minimizing sequences, relying on a new symmetrization argument that is well-suited to the periodic setting.

6.3 Logarithmic Gross–Pitaevskii equation

The logarithmic nonlinearity in the context of Schrödinger equations has recently regained interest in various domains of physics. For instance, this model may generalize the Gross–Pitaevskii equation, used in the case of two-body interaction, to the case of three-body interaction. R. Carles and G. Ferriere study this equation, named the logarithmic Gross–Pitaevskii equation (or logGP), on the whole space \mathbb{R}^d in [12]. As the first mathematical study of this equation in this framework, they focus on its global wellposedness in the energy space, which turns out to correspond to the energy space for the standard Gross–Pitaevskii equation with a cubic nonlinearity in small dimensions, and on the characterization of solitary and traveling waves in the one-dimensional case. This work opens the door to further studies on this equation, especially on its asymptotic and long-time dynamics : multidimensional solitary and traveling waves and their orbital stability, scattering, multi-solitons, convergence towards other models...

6.4 The logarithmic Schrödinger equation with spatial white noise on the full space

The logarithmic Schrödinger appears as a fundamental model in quantum gravity and nuclear physics, and adding a white noise potential can model strong media disorder. In [22], Q. Chauleur and A. Mouzard

prove the existence and uniqueness of solutions to the stochastic logarithmic Schrödinger. The proof relies on a particular exponential transform which have proved being useful in several contexts, in particular in models arising from quantum field theory.

6.5 Asymmetric attractive zero-range process with particle destruction at the origin

In [14], C. Erignoux, M. Simon and L. Zhao investigate the macroscopic behavior of asymmetric attractive zero-range processes on \mathbb{Z} where particles are destroyed at the origin at a rate of order $N\beta$, where $\beta \in \mathbb{R}$ and $N \in \mathbb{N}$ is the scaling parameter. They prove that the hydrodynamic limit of this particle system is described by the unique entropy solution of a hyperbolic conservation law, supplemented by a boundary condition depending on the range of β . Namely, if $\beta \geq 0$, then the boundary condition prescribes the particle current through the origin, whereas if $\beta < 0$, the destruction of particles at the origin has no macroscopic effect on the system and no boundary condition is imposed at the hydrodynamic limit.

6.6 Large deviations principle for the SSEP with weak boundary interactions

Efficiently characterizing non-equilibrium stationary states (NESS) has been in recent years a central question in statistical physics. The Macroscopic Fluctuations Theory [31] developed by Bertini et al. has laid out a strong mathematical framework to understand NESS, however fully deriving and characterizing large deviations principles for NESS remains a challenging endeavour. In [11], C. Erignoux and his collaborators proved that a static large deviations principle holds for the NESS of the classical Symmetric Simple Exclusion Process (SSEP) in weak interaction with particles reservoirs. This result echoes a previous result by Derrida, Lebowitz and Speer [37], where the SSEP with strong boundary interactions was considered. In [11], it was also shown that the rate function can be characterized both by a variational formula involving the corresponding dynamical large deviations principle, and by the solution to a non-linear differential equation. The obtained differential equation is the same as in [37], with different boundary conditions corresponding to the different scales of boundary interaction.

6.7 Mapping hydrodynamics for the facilitated exclusion and zero-range processes

In [15], C. Erignoux, M. Simon and L. Zhao derive the hydrodynamic limit for two degenerate lattice gases, the facilitated exclusion process (FEP) and the facilitated zero-range process (FZRP), both in the symmetric and the asymmetric case. For both processes, the hydrodynamic limit in the symmetric case takes the form of a diffusive Stefan problem, whereas the asymmetric case is characterized by a hyperbolic Stefan problem. Although the FZRP is attractive, a property that they extensively use to derive its hydrodynamic limits in both cases, the FEP is not. To derive the hydrodynamic limit for the latter, they exploit that of the zero-range process, together with a classical mapping between exclusion and zero-range processes, both at the microscopic and macroscopic level. Because the FEP is degenerate, we had to develop new mapping tools to prove hydrodynamic in the asymmetric case. In the symmetric case, a proof already existed [33] for the hydrodynamic limit, however our mapping arguments further provide an alternative, simpler proof.

6.8 Stationary fluctuations for the facilitated exclusion process

In [27], C. Erignoux and L. Zhao derive the stationary fluctuations for the Facilitated Exclusion Process (FEP) in one dimension in the symmetric, weakly asymmetric and asymmetric cases. The proof relies on the mapping between the FEP and the zero-range process, and extends the same strategy as in previous works, where hydrodynamic limits were derived for the FEP, to its stationary fluctuations. Their results thus exploit works on the zero-range process's fluctuations, but they also provide a direct proof in the symmetric case, for which they derive a sharp estimate on the equivalence of ensembles for the FEP's stationary states.

6.9 Kirkwood-Dirac distributions

The Kirkwood-Dirac (KD) quasiprobability distribution can describe any quantum state with respect to the eigenbases of two observables A and B . KD distributions behave similarly to classical joint probability

distributions but can assume negative and nonreal values. In [13] S. De Bièvre provides an in-depth study of the notion of completely incompatible observables that he recently introduced and of its links to the support uncertainty and to the Kirkwood-Dirac nonclassicality of pure quantum states. The latter notion has recently been proven central to a number of issues in quantum information theory and quantum metrology. In this last context, it was shown that a quantum advantage requires the use of Kirkwood-Dirac nonclassical states. S. De Bièvre establishes sharp bounds of very general validity that imply that the support uncertainty is an efficient Kirkwood-Dirac nonclassicality witness for pure states. When adapted to completely incompatible observables that are close to mutually unbiased ones, this bound allows to fully characterize the Kirkwood-Dirac classical pure states as the eigenvectors of the two observables. In [29], De Bièvre, C. Langrenez and D. Arvidsson (Cambridge) provide an analysis of the geometry of the KD-positive and -nonpositive pure and mixed states. They characterize the dependence of the full convex set of states with positive KD distributions on the eigenbases of A and B.

6.10 Photon-added/subtracted states: nonclassicality

Photon addition and subtraction render Gaussian states of the quantized optical field non-Gaussian. In [17], S. De Bièvre and A. Hertz (Toronto-Ottawa) provide a quantitative analysis of the change in the so-called nonclassicality produced by these processes by analyzing the Wigner negativity and quadrature coherence scale (QCS) of the resulting states. The QCS is a recently introduced measure of nonclassicality [PRL 122, 080402 (2019), PRL 124, 090402 (2020)], that we show to undergo a relative increase under photon addition/subtraction that can be as large as 200%.

6.11 Interferometric measurement of the QCS

In [16], S. De Bièvre and his collaborators from the Université Libre de Bruxelles provided an experimental procedure for directly accessing the QCS of the quantum state of an optical field, with the help of only a simple linear interferometer involving two replicas (independent and identical copies) of the state $\hat{\rho}$ supplemented with photon-number-resolving measurements. The proposed protocol has since been implemented with success on the cloud quantum computer of Xanadu, by a team of physicists from the Universities of Toronto and Ottawa.

6.12 Modulational

In [9] S. De Bièvre, G. Dujardin and their collaborators (physicists from the PhLAM laboratory in Lille) study modulational instability in a dispersion-managed system where the sign of the group-velocity dispersion is changed at uniformly distributed random distances around a reference length. An analytical technique is presented to estimate the instability gain from the linearized nonlinear Schrödinger equation, which is also solved numerically. The comparison of numerical and analytical results confirms the validity of their approach. Modulational instability of purely stochastic origin appears.

6.13 Approach to equilibrium in quantum systems

Rigorous derivations of the approach of individual elements of large isolated systems to a state of thermal equilibrium, starting from arbitrary initial states, are exceedingly rare. This is particularly true for quantum mechanical systems. In [23], S. De Bièvre and his collaborators demonstrate how, through a mechanism of repeated scattering, an approach to equilibrium of this type actually occurs in a specific quantum optics system.

6.14 Growth of Sobolev norms and strong convergence for the discrete nonlinear Schrödinger equation

As it is known, the nonlinear Schrödinger stands as a prime model in order to describe the propagation of waves in nonlinear optics or the dynamics of a superfluid in Bose-Einstein condensates. Its discretization in space stands as a first step in order to perform reliable and efficient numerical simulations. Q. Chauleur studies the convergence of the discrete nonlinear Schrödinger equation on a lattice $h\mathbb{Z}^d$ towards the

continuous model as the step size of the lattice h tends to zero in [21]. The proof of the convergence relies on uniform dispersive estimates in order to control the growth of the discrete Sobolev norms of the solution, as well as bilinear estimates of the Shannon interpolation.

6.15 Numerical computation of dark solitons of a nonlocal nonlinear Schrödinger equation

The existence and decay properties of dark solitons for a large class of nonlinear nonlocal Gross-Pitaevskii equations with nonzero boundary conditions in dimension one has been established recently by A. de Laire and S. López-Martínez in [8]. Mathematically, these solitons correspond to minimizers of the energy at fixed momentum and are orbitally stable. In the paper [18], A. de Laire, G. Dujardin and S. López-Martínez provide a numerical method to compute approximations of such solitons for these types of equations, and give actual numerical experiments for several types of physically relevant nonlocal potentials. These simulations allow them to obtain a variety of dark solitons, and to comment on their shapes in terms of the parameters of the nonlocal potential. In particular, they suggest that, given the dispersion relation, the speed of sound and the Landau speed are important values to understand the properties of these dark solitons. They also allow them to test the necessity of some sufficient conditions in the theoretical result proving existence of the dark solitons.

6.16 Linearly implicit high-order numerical methods for evolution problems

G. Dujardin and his collaborator introduced a new class of numerical methods for the time integration of evolution equations set as Cauchy problems of ODEs or PDEs, in the research direction detailed in Section 3.3. The systematic design of these methods mixes the Runge–Kutta collocation formalism with collocation techniques, in such a way that the methods are linearly implicit and have high order. A specific analysis of Runge–Kutta collocation methods for this purpose was carried out by G. Dujardin and his collaborator [24]. The fact that these methods are implicit allows to avoid CFL conditions when the large systems to integrate come from the space discretization of evolution PDEs. Moreover, these methods proved to be efficient since they only require to solve one linear system of equations at each time step, and efficient techniques from the literature can be used to do so [25].

6.17 Exponential integrators for the stochastic Manakov system

The Manakov system is a system of dispersive stochastic PDEs modelling the propagation of light in optical fibers taking into account the polarization mode dispersion effects. In [10], G. Dujardin and his collaborators developed and analyzed an exponential integrator for the numerical solution of this stochastic PDE system. In particular, they proved that this exponential integrator has strong order $1/2$ for a truncated nonlinearity and they inferred that it also has order $1/2$ in probability and order $1/2$ almost surely, for general nonlinearities. Moreover, they provided several numerical experiments illustrating their theoretical results as well as the efficiency of their numerical integrator.

6.18 Uniform estimates for numerical schemes applied to parabolic problems with Neumann boundary conditions

In [26], G. Dujardin and his collaborator tackled the problem of proving uniform-in-time order estimates for a scheme integrating the linear heat equation with homogeneous pure Neumann boundary conditions on a bounded interval. Despite the lack of consistency of the discretization of the boundary condition with the Laplace operator, they proved that the scheme they consider is of order 1 in space and time *uniformly-in-time*. They applied this result to the question of the numerical computation of stationary states to nonhomogeneous heat equations.

7 Partnerships and cooperations

Participants: Quentin Chauleur, Stephan De Bièvre, André de Laire, Guillaume Dujardin, Olivier Goubet.

7.1 International research visitors

7.1.1 Visits of international scientists

Salvador López-Martínez

Status: Researcher

Institution of origin: Universidad Autónoma de Madrid

Country: Spain

Dates: July 17-21

Context of the visit: Research collaboration with A. de Laire and G. Dujardin

Mobility program/type of mobility: Research stay

7.1.2 Visits to international teams

Research stays abroad

Clément Erignoux

Visited institution: Università Roma Tre

Country: Italy

Dates: Feb. 6-8, 2023

Context of the visit: **Closing conference** of Alessandro Giuliani's ERC grant.

André de Laire

Visited institution: Universidad Autónoma de Madrid

Country: Spain

Dates: Feb. 20-27, 2023

Context of the visit: Research collaboration with S. López-Martínez

Clément Erignoux

Visited institution: Weierstrass Institute Berlin

Country: Germany

Dates: May 11-17, 2023

Context of the visit: Scientific collaboration with Robert Patterson and Julian Kern.

Clément Erignoux**Visited institution:** Newton Institute, Cambridge University**Country:** United Kingdom**Dates:** July 3-11, 2023**Context of the visit:** Invited speaker to the workshop *Building a bridge between non-equilibrium statistical physics and biology*, collaboration with Robert Jack, Maria Bruna, and James Mason**Olivier Goubet****Visited institution:** Universidad de Chile**Country:** Chile**Dates:** Sep. 8-15, 2023**Context of the visit:** Research collaboration with C. Muñoz**Stephan De Bièvre****Visited institution:** Cambridge University**Country:** UK**Dates:** Dec. 1-10, 2023**Context of the visit:** Research collaboration with D. Arvidsson**André de Laire****Visited institution:** Universidad de Chile**Country:** Chile**Dates:** Dec. 18-26, 2023**Context of the visit:** Research collaboration with C. Muñoz and participation to the *Annual Meeting of the Chilean Mathematical Society***7.2 National initiatives****7.2.1 LabEx CEMPI**

Through their affiliation to the Laboratoire Paul Painlevé of Université de Lille, PARADYSE team members benefit from the support of the **LabEx CEMPI**. In addition, the LabEx CEMPI is funding the post-doc of Quentin Chauleur in the team, in an interdisciplinary initiative between PhLAM and LPP.

Title: Centre Européen pour les Mathématiques, la Physique et leurs Interactions

Partners: Laboratoire Paul Painlevé (LPP) and Laser Physics department (PhLAM), Université de Lille

ANR reference: 11-LABX-0007

Duration: February 2012 - December 2024 (the project has been renewed in 2019)

Budget: 6 960 395 euros

Coordinator: Emmanuel Fricain (LPP, Université de Lille)

The "Laboratoire d'Excellence" CEMPI (Centre Européen pour les Mathématiques, la Physique et leurs Interactions), a project of the Laboratoire de mathématiques Paul Painlevé (LPP) and the laboratoire de Physique des Lasers, Atomes et Molécules (PhLAM), was created in the context of the "Programme d'Investissements d'Avenir" in February 2012. The association Painlevé-PhLAM creates in Lille a research unit for fundamental and applied research and for training and technological development that covers a wide spectrum of knowledge stretching from pure and applied mathematics to experimental and applied physics. The CEMPI research is at the interface between mathematics and physics. It is concerned with key problems coming from the study of complex behaviors in cold atoms physics and nonlinear optics, in particular fiber optics. It deals with fields of mathematics such as algebraic geometry, modular forms, operator algebras, harmonic analysis, and quantum groups, that have promising interactions with several branches of theoretical physics.

8 Dissemination

Participants: Stephan De Bièvre, André de Laire, Guillaume Dujardin, Clément Erignoux, Olivier Goubet.

8.1 Promoting scientific activities

8.1.1 Scientific events: organisation

- **Nonlinear Analysis and PDE in Lille**, held at the Centre Inria de l'Université de Lille, on February 1-3, 2023. Organizers: A. de Laire and P. Gravejat.
- **Journée des Doctorants en Mathématiques de la région Hauts-de-France**, held at Université de Technologie de Compiègne, on September 15, 2023. Organizers: S. Biard, M. Davila, A. de Laire, A. El Mazouni, R. Ernst, B. Testud.
- **Colloque à la mémoire d'Ezzeddine Zahrouni**, held at the University of Monastir (Tunisia). Organizers: O. Goubet et al.

8.1.2 Journal

Member of the editorial boards

- S. De Bièvre is associate editor of the Journal of Mathematical Physics (since January 2019).
- O. Goubet is the editor-in-chief of the North-Western European Journal of Mathematics.
- O. Goubet is associate editor of ANONA (Advances in Nonlinear Analysis).
- O. Goubet is associate editor of the Journal of Mathematical Study.

Reviewer - reviewing activities All permanent members of the PARADYSE team work as referees for many of the main scientific publications in analysis, partial differential equations, probability and statistical physics, depending on their respective fields of expertise.

8.1.3 Invited talks

All PARADYSE team members take active part in numerous scientific conferences, workshops and seminars, and in particular give frequent talks both in France and abroad.

8.1.4 Research administration

- S. De Bièvre and A. de Laire are both members of the “Conseil de Laboratoire Paul Painlevé” at Université de Lille.
- S. De Bièvre is a member of the executive committee of the LabEx CEMPI.
- A. de Laire is a member of the “Fédération de Recherche Mathématique des Hauts-de-France”.
- A. de Laire is a member of the “Domain Board” of the Graduate School MADIS.
- G. Dujardin is a member of the Executive Committee of the CPER WaveTech.
- O. Goubet is a member of the "Conseil de département de mathématiques" at Université de Lille.
- O. Goubet is a member of the "Bureau du HUB numérique" of the I-Site U-Lille.
- O. Goubet, former President of SMAI, is a member of the "Conseil d'Administration de la SMAI".

8.2 Teaching - Supervision - Juries

8.2.1 Teaching

The PARADYSE team teaches various undergraduate level courses in several partner universities. We only make explicit mention here of the Master courses (level M1-M2) and the doctoral courses.

- Master: A. de Laire, "Analyse numérique pour les EDP", M1 (Université de Lille, 60h).
- Master: A. de Laire, "Modeling", M2 (Université de Lille, 20h).
- Master: A. de Laire, "Prerequisites in Numerical Analysis", M2 (Université de Lille, 20h).
- Master: O. Goubet, "Exemples de problèmes elliptiques et paraboliques", M1 (Université de Lille, 24h).
- Doctoral School: S. De Bièvre, "Quantum information" (Université de Lille, 24h).

8.2.2 Supervision

- During the period April-July 2023, C. Erignoux co-supervised with M. Simon (Lyon 1) the M2 Internship of Hugo Da Cunha (ENS Lyon), titled "Processus d'exclusion facilité en contact avec des réservoirs".
- During the period April-July 2023, C. Erignoux supervised the M2 Internship of Brune Massoulié (École Polytechnique), titled "Temps de transience du processus d'exclusion facilité".
- During the period April-September 2023, O. Goubet supervised the M2 Internship of Céline Wang (ECL and U-Lille), titled "Modélisation mathématique d'une dynamique invasive", and has been supervising her PhD thesis since October 2023, titled "Modèles mathématiques pour la reproduction et la migration d'espèces forestières".
- During the period May-June 2023, O. Goubet (and C. Calgari) supervised the M1 internship of Abdoul Aziz Diallo (U-Lille) on the modelling of the migration of an insect species.
- S. De Bièvre is supervising the PhD thesis of Christopher Langrenez on "KD nonclassicality", during 2022-2025.
- A. de Laire and O. Goubet are supervising the PhD thesis of Erwan Le Quiniou on the "Study of a quasilinear Gross-Pitaevskii equation", during 2022-2025.
- G. Dujardin co-supervised with D. Cohen the PhD thesis of Andre Berg (University of Umeå, 2018-2023), entitled "Numerical analysis and simulation of stochastic partial differential equations with white noise dispersion". The defense took place on September 25, 2023.

8.2.3 Juries

A. de Laire served as reviewer for the PhD thesis of Anatole Guérin (University Paris-Saclay, June 9, 2023), entitled "Dispersive and focussing results for the Schrödinger equation and applications to the binormal flow", supervised by Nicolas Burq and Valeria Banica.

O. Goubet served as reviewer for the PhD thesis of Dieunel Dor (U. Poitiers, December 4, 2023), entitled "Mathematical models for growing cancer tumors", supervised by Alain Miranville.

O. Goubet served as reviewer for the PhD thesis of Cheikou Oumar Diaw, (U. Cergy, November 30, 2023), entitled "viscosity solutions for degenerated fully nonlinear equations", supervised by Françoise Demengel.

O. Goubet served as reviewer for the PhD thesis of Lu Li (U. Poitiers, March 10, 2023), entitled "The PDE type models for the growth of glial cells", supervised by Alain Miranville and Rémy Guillevin

9 Scientific production

9.1 Major publications

- [1] R. Ahmed, C. Bernardin, P. Gonçalves and M. Simon. 'A Microscopic Derivation of Coupled SPDE's with a KPZ Flavor'. In: *Annales de l'Institut Henri Poincaré* 58.2 (2022). DOI: [10.1214/21-AIHP1196](https://doi.org/10.1214/21-AIHP1196). URL: <https://hal.archives-ouvertes.fr/hal-02307963>.
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9.2 Publications of the year

International journals

- [9] A. Armaroli, G. Dujardin, A. Kudlinski, A. Mussot, S. De Bièvre and M. Conforti. 'Modulational instability in randomly dispersion-managed fiber links'. In: *Physical Review A* 108.2 (Aug. 2023), p. 023510. DOI: [10.1103/PhysRevA.108.023510](https://doi.org/10.1103/PhysRevA.108.023510). URL: <https://hal.science/hal-03911304>.

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