Nonequilibrium Statistical Mechanics: Mathematical Understanding and Numerical Simulation

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1 Overview of the Field

1.1 Aims of statistical mechanics

Statistical mechanics is a theory allowing to infer the macroscopic behavior of physical systems from the knowledge of their microscopic description (namely the interaction laws between the elementary constituents of matter, such as atoms in a classical framework). The foundations of this theory date back to the nineteenth century. Major contributors include Maxwell, Boltzmann, Gibbs, Kelvin and Einstein.

The orders of magnitude used in the microscopic description of matter are very different from those of the macroscopic quantities we are used to. For instance, the number of particles under consideration in a macroscopic sample of material is of the order of the Avogadro number $\mathcal{N}_A \sim 10^{23}$, while typical distances are expressed in Å (10^{-10} m), energies are of the order of $k_{\rm B}T \simeq 4 \times 10^{-21}$ J at room temperature, and the typical times are of the order of 10^{-15} s when the proton mass is the reference mass. For practical numerical computations of matter at the microscopic level, following the dynamics of every atom would require simulating $\mathcal{N}_A$ atoms and performing $\mathrm{O}(10^{15})$ time integration steps, which is of course impossible!

Despite its intrinsic limitations on spatial and time-scales, molecular simulations have been used and developed over the past 50 years, and its number of users keeps increasing. It nowadays has two major aims. First, it can be used as a *numerical microscope* to perform "computer" experiments. This was the initial motivation for simulations at the microscopic level: physical theories were tested on computers. This use of molecular simulation is particularly clear in its historic development, which was triggered and sustained by the physics of simple liquids. It is still very helpful to observe numerical trajectories to guide intuition about what is happening in the system. Another major aim of molecular simulation, maybe even more important than the previous one, is to compute macroscopic quantities or thermodynamic properties, typically through averages of some functionals of the system. In this case, molecular simulation is a way to obtain *quantitative* information on a system, instead of resorting to approximate theories, constructed for simplified models, and giving only qualitative answers.

1.2 Nonequilibrium statistical mechanics

Equilibrium statistical mechanics is nowadays a fairly well-understood scientific field, both from theoretical and numerical viewpoints. The situation is dramatically different for nonequilibrium systems, which are subjected flows of energy, momentum, particles, etc. It is often the case that a stationary state is attained

thanks to thermal baths at the boundaries of the system, which model a coupling with an infinite equilibrium system. In this case, the thermodynamic state of the system is described by some probability measure, whose analytical expression is usually unknown.

From a theoretical viewpoint, nonequilibrium systems pose many challenges. First of all, showing the very existence and uniqueness of a stationary measure for the stochastic or deterministic dynamics under consideration turns out to be non-trivial in many cases, *e.g.* [14] and references therein. Once the existence and uniqueness of the invariant measure is obtained, it still remains to connect results with those obtained from linear response theory in order to obtain formulas such as the Green-Kubo formula, which relate time-correlations of some observables to a given transport coefficient such as thermal conductivity, viscosity, etc. From a technical viewpoint, this task is easier when the generator of the dynamics has a spectral gap. The dynamics of many interesting systems, especially infinite systems obtained as the thermodynamic limit of finite size systems, however turn out not to have a spectral gap even when some stochastic perturbation is added to the deterministic Hamiltonian dynamics.

One difficulty for the analysis of nonequilibrium systems is that the stationary measure a priori depends on particular features of the evolution under consideration. In contrast, for equilibrium systems, there are (infinitely) many different dynamics which can be used to sample this measure. For instance, the equilibrium canonical ensemble can be sampled using a Langevin dynamics (with various values of the friction parameter) or Metropolis-Hastings algorithms.

Another difficulty of nonequilibrium systems is the non-locality of the stationary measure. A local perturbation in the force-field of the dynamics will in general globally affect the invariant measure, even far away from the perturbation.

1.3 Simulating nonequilibrium systems

The efficient simulation of nonequilibrium systems is an important issue from a numerical viewpoint.

Transport properties can be understood for systems close to equilibrium, using results from linear response theory. There are several general numerical approaches to estimate transport coefficients (shear viscosity, thermal conductivity, autodiffusion constant, etc), based either on (i) equilibrium simulations, where the transport coefficient is obtained by the Green-Kubo formula (integrated equilibrium correlation function) or Einstein formula; (ii) nonequilibrium simulations in a steady-state, with either boundary-driven systems or field-driven dynamics where the response of the system to some mechanical or thermal forcing is measured as a function of the forcing strength; and (iii) the study of transient states, where a system initially at a equilibrium is perturbed, and the relaxation of the perturbation is monitored as a function of time.

2 Recent Developments and Open Problems

2.1 Understanding general properties of nonequilibrium systems

Even when the invariant measure of nonequilibrium systems is unknown it is relevant to attempt to unravel steady-state properties such as the existence of long-range space or time correlations, or appearance of metastable states when a forcing is introduced into the system. Even at a qualitative level a clear picture has not emerged yet, even for the simplest systems on one-dimensional lattices. One of the first theoretical studies of long-range correlations in exclusion processes is [6].

2.2 Thermal transport in general systems

Thermal transport properties can be studied in systems subjected to a temperature gradient (fixed for instance by setting the temperatures at the boundaries) by considering the energy current flowing from the hot to the cold interface. When Fourier's law is applicable, linear temperature profiles are obtained when the temperature difference is small, and the current is proportional to the temperature gradient.

Despite many efforts in the past, our understanding of the microscopic ingredients necessary for the validity of Fourier's law is still scarce (see for instance the review article [4], which is still of contemporary interest). A first distinction to be made is whether the system under consideration is on a lattice or not, and whether its dynamics is deterministic or involves some stochastic perturbation. Of course, studying

systems on a lattice is much easier from a theoretical viewpoint than considering fluid systems without any internal structure. Adding stochastic perturbations helps as well. On the other hand, it may be depressing (or stimulating, depending on one's inclination) to realize that our understanding of thermal transport processes in very simple fluids described by a deterministic mechanical model of hard spheres is almost still as incomplete as it was in 1978 when Joel Lebowitz reviewed the problem in [11]. Even for three dimensional lattices systems, there is no proof at the moment that the conductivity is finite in systems with generic (nonlinear) interaction potentials.

2.3 Thermal transport in one-dimensional systems

The topic of thermal transport in one-dimensional systems has been a very active field of research in the last fifteen years – motivated in part by the carbon nanotube technology, and also by the desire to understand the origin of Fourier's law (or its failure!) in one of the simplest atomic systems. There are many research groups working on this topic around the world, both from theoretical and numerical viewpoints (see for instance the review articles [12, 7]).

Despite the simplicity of the model, it is still not completely clear at the moment which ingredients of the interaction potentials between the particles on the lattice, of externally applied pinning potentials or forces, and of added stochastic perturbations are necessary or sufficient to obtain normal thermal transport. It is however believed that the conservation of invariants in the system, such as the energy, the volume and the momentum, plays an important role.

From a technical viewpoint, the rigorous mathematical results known to this date are mostly upper bounds on the divergence of the thermal conductivity (through upper bounds on the decay of the autocorrelation function of the currents). Obtaining lower bounds is a current important theoretical challenge in this domain.

2.4 Derivation of macroscopic evolution equations for microscopic systems

The thermodynamic limit of transport processes at the microscopic scales can be understood by some limiting process, using appropriate space-time scalings. The system should first be understood in the hyperbolic time-scale, where the system is studied over long times Nt with space renormalized by a factor N^{-1}. Locally, the state of the system is expected to be close to some equilibrium Gibbs measure consistent with the local invariants of the system, such as the energy, the momentum and the volume for Hamiltonian dynamics. In the hyperbolic scaling, a reduced description of the evolution of the microscopic system is given by coupled partial differential equations involving the invariants of the dynamics, known as the hydrodynamic limit (see [10]). The limiting set of equations is often not difficult to obtain formally. To rigorously prove the convergence, the method of choice is the relative entropy method of Yau [16]. Some appropriate ergodicity properties are however required to apply it. It is currently a major open problem to rigorously derive hydrodynamic limits for deterministic systems [4]. The situation is more favorable when the Hamiltonian dynamics is perturbed by appropriate stochastic processes.

Once the behavior of the system is understood in the hyperbolic space-time scaling, it is possible to study the diffusion of the energy on a longer time-scale – which amounts to understanding the energy fluctuations. If the process has a diffusive behavior consistent with Fourier's law, then the relevant time scale is indeed the diffusive one. However, the energy often "superdiffuses" in one dimensional chains, so that the correct time scaling for time should rather be $N^\alpha t$ for $1 < \alpha < 2$ instead of $N^2 t$ (see for instance [13] for a review of the cases when such statements can be made mathematically rigorous). The macroscopic evolution of the fluctuation fields obtained with this process typically are a coupled system of nonlinear stochastic partial differential equations. Needless to say, giving a mathematical meaning to these limiting objects is already quite a challenge, not to mention rigorously proving the convergence in itself.

2.5 Numerical analysis of simulation methods

In contrast to equilibrium sampling, where many strategies exist to enhance the convergence of longtime averages of appropriate dynamics, only few if any works have considered some kind of importance sampling method for nonequilibrium systems: Numerical studies are often performed by a straightforward longtime integration of the dynamics. In many situations however, these averages are not converging very fast because

of the large variance of the estimator compared to the average value to be computed (see for instance the discussion in [9]). Moreover, in some situations such as thermal transport computations in very long atom chains, long transient regimes have to be removed from the computation of the average.

Variance reduction techniques are used on a daily basis in equilibrium simulations. The use of such techniques is often based on the explicit expression of the invariant measure, and its modification under appropriate perturbations. There are three main strategies: importance sampling, stratification, and the control variate method. None of them can be used as such for nonequilibrium systems. Indeed, the control variate method is an interesting technique for very specific, low dimensional dynamics for which there is a strong coupling (see for instance [8]); while the non trivial modifications of the invariant measure of nonequilibrium systems under perturbations somehow prevent the use of importance sampling and stratification by constrained dynamics.

Let us also mention that the numerical analysis of nonequilibrium sampling methods is rather scarce: we are not aware of a study of the time-step error arising in the numerical discretization of the Green-Kubo formula or in the definition of the transport coefficients as given by linear response results.

3 Presentation Highlights

The speakers were given 40 minutes to deliver their lectures, including 5 minutes question. It was most often the case that questions were asked (and answered!) as they arose during the talk – a very familial and informal way of proceeding, and a nice feature of smaller scale workshops with participants hosted on site and living together for a week.

3.1 Thermal transport

A substantial fraction of the talks were devoted to the study of thermal transport, both from theoretical and numerical angles.

3.1.1 More theoretically oriented studies

Cédric Bernardin (Ecole Normale Supérieure de Lyon) discussed the anomalous diffusion in Hamiltonian systems perturbed by a conservative noise. He actually considered one of the simplest Hamiltonian models, with only two conserved quantities (instead of three in standard Hamiltonian systems). He treated in particular the case of exponential interaction potentials à la Toda, for which refined results can be stated.

Jani Lukkarinen (University of Helsinki) reviewed results for two models satisfying Fourier's law in chains of harmonic oscillators: systems subjected to self-consistent bulk thermostatting mechanisms, and systems perturbed by a non-momentum conserving bulk stochastic noise. In both cases, some new results were given about the hydrodynamical equations for typical macroscopic energy and displacement profiles, as well as their fluctuations and large deviations.

Carlangelo Liverani (Universita Roma Tor Vergata) discussed the statistical properties of a very simple (if not the simplest possible) fast-slow deterministic system of dimension 2. One variable, which should be thought of as the energy, evolves on a much slower time scale than the other, while the other variable evolves according to a mixing dynamics. The motivation for considering this system is to understand how microscopically deterministic system may be described by mesoscopic stochastic evolutions. This would be an important step in rigorously deriving hydrodynamic equations from a weakly interacting microscopic Hamiltonian system.

François Huveneers (Université Paris-Dauphine) presented results on the asymptotic localization of energy in some Hamiltonian chains. Energy transfer in close to integrable Hamiltonian systems can sometimes be much slowed down or even suppressed. Anderson localization, breathers, KAM tori or Nekhoroshev estimates can in some cases be invoked to justify this claim. However, given a chain at positive temperature in the infinite volume limit, it is generally hard to infer any clear picture on heat transfer out of such mathematical results. This can however be studied for nearly integrable Hamiltonian chains in a weak coupling regime, and allows to write rigorous asymptotic estimates suggesting a very rapid fall-off of the thermal conductivity with the coupling strength. Both disorder and strong anharmonicity play a similar role in the considered regime.

3.1.2 More numerically oriented presentations

Abhishek Dhar (International Centre for theoretical sciences, Bangalore) suggested a Levy walk description of anomalous heat transport. His talk was based on some recent work suggesting that a good description of heat transport in low dimensional systems is obtained by modeling heat carriers as Levy walkers rather than simple random walkers.

Alessandra Iacobucci (Université Paris-Dauphine) presented numerical results obtained for chains of rotors subjected to both thermal and mechanical forcings, in a nonequilibrium steady-state. Unusual nonlinear profiles of temperature and velocities are observed in the system. In particular, the temperature is maximal in the center, which is an indication of the nonlocal behavior of the system. Despite this uncommon behavior, local equilibrium holds for long enough chains. The numerical results also show that, when the mechanical forcing is strong enough, the energy current can be increased by an inverse temperature gradient. This counterintuitive result again reveals the complexity of nonequilibrium states.

Gary Morris (University of New South Wales) was the only speaker this week to consider heat conduction problems in fluid systems, namely quasi-one-dimensional hard disks confined in some narrow channel, using periodic boundary conditions in the orthogonal direction. In his numerical studies, he considered both low and large density systems.

3.2 Non-thermally driven driven systems

Federico Bonetto (Georgia Institute of Technology) presented some results for a simple model of electric conduction in a non equilibrium steady state. The models consists of N particles moving in a periodic array of scatterers under the influence of an electric field and of a Gaussian thermostat keeping the energy fixed. Analytic result for the behavior of the steady state of the system at small electric field can be obtained. In this regime, the velocity distribution becomes independent of the geometry of the scatterers. For a large number of particles, the system can be described by a linear Boltzmann type equation.

Christian Maes (University of Leuven) discussed the extension of Clausius heat theorem to driven systems. Clausius theorem asserts that the heat divided by the temperature is an exact differential for reversible processes. Christian Maes suggested an extension of this thermodynamic fact to simple systems of nonequilibrium statistical mechanics using dynamical large deviations and the excess heat produced when switching from one nonequilibrium state to another.

David Mukamel (Weizmann Institute) presented theoretical and numerical results on long-range correlations in some driven lattice systems, such as the existence of long range-order, spontaneous symmetry breaking and non-local response to local perturbations. He focuses on two cases: particle diffusion processes with localized perturbations of the transitions rates (the aim being then to understand the long-range perturbations of the density), and interface dynamics for spins systems with a line defect.

Martin Evans (University of Edinburgh) reported on the peculiar condensation in one-dimensional particle systems where the hopping between sites of a one dimensional lattice occurs with a rate increasing with the number of particles. Some clusters of particles spontaneously form in the system, and then move at increasing speed as they gain particles. Ultimately, they produce a moving condensate which comprises a finite fraction of the mass in the system. Surprisingly, the relaxation time to steady state decreases with system size.

A focus on discrete nonlinear Schrödinger systems

Stefano Lepri (Istituto dei Sistemi Complessi) introduced a nonequilibrium forcing in the discrete nonlinear one-dimensional Schrödinger equation. This system can be regarded as a minimal model for stationary transport of bosonic particles like photons in layered media or cold atoms in deep optical traps. Due to the presence of two conserved quantities, energy and norm (or number of particles), the model displays coupled transport in the sense of linear irreversible thermodynamics. Numerical studies show that the Onsager coefficients are finite in the thermodynamic limit, *i.e.* transport is normal. Depending on the position in the parameter space, the "Seebeck coefficient" may be either positive or negative. For large differences between the thermostat parameters, density and temperature profiles may display an unusual nonmonotonic shape. This is due to the strong dependence of the Onsager coefficients on the state variables.

Roberto Livi (Universita di Firenze) reported results complementary to the ones presented by Stefano Lepri. More precisely, he focused on another parameter regime leading to the formation and persistence of

breathers (stable nonlinear excitations), which may explain anomalous transport properties. These excitations are also responsible for the appearance of metastable states living over exceedingly long time scales, thus inhibiting any appreciable signal of relaxation to equilibrium, while yielding the formation of ”negative” temperature conditions.

3.3 Hydrodynamic limits and kinetic models

3.3.1 Derivation of hydrodynamic limits

In connection with the lectures by Jani Lukkarinen and Cédric Bernardin, Marielle Simon (Ecole Normale Supérieure de Lyon) derived hydrodynamic equations of diffusion type for atom chains subjected to velocity-flipping processes. The proof of convergence uses the relative entropy of the law of the process with respect to the local equilibrium Gibbs state appropriately modified by a second order correction term. A crucial technical step to use the relative entropy method is to control the energy moments. This can fortunately be done thanks to the very specific structure of the invariant measure of the system.

On a related topic, Milton Jara (IMPA) presented results beyond the hydrodynamic limit, on the fluctuations of one-dimensional chains of oscillators perturbed by a noise that conserves the energy and momentum. When the strength of the noise is tuned properly (the so-called weakly asymmetric scaling), the scaling limit of the fluctuations of the conserved quantities is given by a system of stochastic Burgers equations, which corresponds to a generalization of the celebrated KPZ equation.

Makiko Sasada (Keio University) reviewed stochastic energy exchange systems of locally confined particles in interaction. These systems have been extensively studied recently since they can be seen as accessible models for the rigorous study of the derivation of Fourier’s law from microscopic dynamics of mechanical origin. As a generalization of these dynamics, Grigo et al. introduced a class of pure jump Markov processes of energies and studied the spectral gap of their generator under the assumption that the rate function of the energy exchange is uniformly positive. The results presented by Makiko Sasada are an extension to the case where the rate function does not have a uniform lower bound. Obtaining a spectral gap is a first mandatory step in the rigorous derivation the hydrodynamic behavior.

Johannes Zimmer (University of Bath) proposed a formulation of hydrodynamic limits in a more analytical framework. He first recalled that the diffusion equation, obtained as an appropriate scaling limit of Brownian motion, can be reformulated as gradient flow of the entropy in the Wasserstein metric. The latter formulation is physically very appealing, since it reveals in a mathematically rigorous way that the entropy can be seen as a driving force out of equilibrium. The connection with the original particle system is however quite cumbersome. Johannes Zimmer proposed to combine a Large Deviation principle with Gamma-convergence techniques to make the connection more straightforward.

3.3.2 Boltzmann-type approaches

Herbert Spohn (Technische Universität München) introduced the Hubbard Hamiltonian, which describes electrons on a lattice with on-site interactions. He showed that for small interactions the dynamics is well approximated by a kinetic equation, the matrix-valued Hubbard-Boltzmann equation. He discussed general features of this equation and, for one dimensional chains with nearest neighbor hopping, presented simulation results of the spatially homogeneous equation and its approach to the steady state.

Chanwoo Kim (Cambridge University) reported his results on thermally forced systems described by a Boltzmann equation. The first issue is to construct steady-state solutions in a general bounded domain with diffuse reflection boundary conditions corresponding to a non-isothermal temperature of the wall. This is done in a perturbative regime. Further investigation shows that Fourier’s law does not hold in the kinetic regime corresponding to rarefied gases.

3.4 Numerical methods

3.4.1 Efficient simulation

Tony Lelièvre (Ecole des Ponts) presented the mathematical analysis of two numerical methods to accelerate the sampling of metastable dynamics where the system remains for very longtime in a region of the con-

figuration space before hopping to another one. The first method consists in adding a non-gradient force to an equilibrium overdamped Langevin dynamics, so that the invariant measure is unchanged, and to optimize the non-gradient field to maximize the spectral gap. The analysis can be rigorously performed for harmonic systems. The second method is the parallel replica algorithm proposed by A. Voter, whose properties can be studied using properties of quasi-stationary distributions.

Carsten Hartmann (Freie Universität Berlin) reviewed some ideas of risk-sensitive optimal control theory, and showed how to apply them to efficiently bias a system. A typical application is the computation of exit times out of metastable states. Using appropriate biasing forces (which amount in simple one dimensional cases to a tilting of double well potentials), the transitions from one metastable to the other are dramatically enhanced. It turns out that the non-gradient forces applied to the system to bias it are in fact gradient forces at optimum.

David Sanders (National University of Mexico) reported on the development of efficient algorithms for simulating deterministic dynamics in a quenched (fixed) random environment of obstacles on a lattice, such as a Lorentz lattice gas or mirror model. The focus is on the low densities of obstacles for which a straightforward simulation of the dynamics becomes computationally prohibitive.

3.4.2 Nonequilibrium techniques for computing equilibrium properties

Rémi Joubaud (Imperial College London) showed how to use Langevin dynamics to compute the shear viscosity of a system. Such computations are often performed with deterministic dynamics using Nosé-Hoover or Gaussian thermostats. The interest of the Langevin dynamics is that its generator has a spectral gap, which allows to rigorously prove linear response results. In particular, following the seminal work of Irving and Kirkwood, it is possible to prove a conservation equation relating the variations of the stress tensor and of the average velocity. An important issue is the dependence of the transport coefficient on the parameters of the dynamics. Rémi Joubaud exposed some new results on the asymptotic behavior of the shear viscosity coefficient for large frictions, based on asymptotic analysis of an appropriate Poisson equation. These theoretical results were illustrated by numerical simulations of a bi-dimensional Lennard-Jones system.

The Langevin dynamics used by Rémi Joubaud can actually be seen as the limit of some mechanical model, as suggested by Frédéric Legoll (Ecole des Ponts). In fact, the proof is done for a single large particle, placed in an ideal gas heat bath composed of point particles that are distributed consistently with the background flow field and interact with the large particle through elastic collisions. In the limit of small bath atom masses, the large particle dynamics converges to a Langevin-type stochastic dynamics, which is parametrized by the background flow field. This derivation follows the ideas of D. Dürr, S. Goldstein and J. Lebowitz.

Mathias Rousset (INRIA Rocquencourt) showed how to use constrained, time-inhomogeneous Langevin dynamics to compute equilibrium free energy differences from nonequilibrium switching processes where the system is driven from one state to another. The method first requires a proper definition of the work function, and then a fluctuation identity (known as the Jarzynski-Crooks relation) relating the statistics of forward and backward switchings. Consistent numerical schemes allowing to evaluate the work without time-step error were also presented.

3.4.3 Using theoretical concepts of nonequilibrium statistical mechanics for numerical analysis

In his talk, Yannis Pantazis (University of Massachussetts) presented recent results allowing to quantify the degree of non-reversibility induced by the discretization of reversible Markov processes. Despite an extensive literature on the numerical analysis for SDE's, their stability properties, strong and/or weak error estimates, large deviations and infinite-time estimates, no quantitative results were known on the lack of reversibility of the discrete-time approximation process. Such quantitative estimates can be provided by the relative entropy production rate of the process, where forward and time-reversed trajectories are compared. Crucially, from a numerical point of view, the entropy production rate is an *a posteriori* quantity, hence it can be computed in the course of a simulation as the ergodic average of a certain functional of the process (the so-called Gallavotti-Cohen action functional). The method was illustrated for various numerical schemes for the overdamped and underdamped Langevin dynamics.

4 Scientific Progress Made

4.1 General knowledge dissemination to younger and more isolated researchers

Let us first mention that the workshop was an outstanding opportunity for many researchers to meet and work together: the community of researchers interested in fundamental issues of nonequilibrium systems is indeed a rather small one, and every occasion to efficiently interact with fellow colleagues is welcome. One of the participants (who has a position in Mexico) for instance mentioned that this was the first conference in two years where he really felt his topics fit in. Needless to say, he benefited from many inspiring discussions.

As organizers we also took care of inviting younger researchers, so that several PhD students and post-docs were present. We believe that they gained awareness on the issues and interesting open problems in the field, and that this meeting helped them to obtain a broader view on how their work fits in the general scientific stage.

4.2 Specific progress arising from discussions held at the workshop

Most of the lectures gave rise to passionate discussions during the coffee breaks or lunches and dinners. On top of these informal discussions whose long term impact is difficult to estimate, let us mention some illustrative examples of situations in which the diversity of the backgrounds of the researchers in the audience was beneficial.

4.2.1 Space-time scalings for thermal transport

During the presentation, or rather, the discussion session led by Lebowitz on thermal transport, an important issue was raised by Stefano Olla about the importance of space-time scalings in thermal transport studies. Indeed, many studies (especially numerical ones) focus on the study of properties in the nonequilibrium steady-state where the time scales have disappeared. A notable exception are the recent results by Ahbishek Dhar, who presented numerical simulations backing up an interpretation of the anomalous space-time scalings of energy transport using a simplified model based on Levy walks of energy carriers. The relevance of the study of space-time scalings arose several times during the conference, and is an important concern of more theoretically oriented researchers who have the feeling that the numerical validation of the prediction based on hydrodynamic limits is not as extensive as it should be.

4.2.2 Normal conductivity of one-dimensional atom chains?

On tuesday evening, several physicists and mathematicians gathered to discuss the recent numerical results obtained by Zhao et al. [17], which tend to show that the thermal conductivity of some one dimensional atom chains are finite provided the interaction potential is of FPU type, with a sufficient level of anharmonicity (parameter α sufficiently large). The discussion first focused on technical details of the simulations in order to critically assess the reliability of the result. The computations are currently being checked both by the italian group featuring Roberto Livi and Stefano Lepri, and by Ahbishek Dhar in India. Preliminary results however seem to confirm the surprising results of [17].

The second part of the discussion attempted to provide more convincing physical explanations than the one proposed in [17]. Unfortunately, no satisfactory understanding emerged in spite of the stimulating interactions among the participants – this problem nonetheless remains as a stimulating counter-example to some of the currently well-accepted theories accounting for the divergent thermal conductivity of one dimensional chains. The discussion was a perfect advertisement tribune for many people who were not aware of the results [17] before the workshop. There is no doubt that future work in this direction will be strongly influenced by the findings in this article.

4.2.3 Are some previous simulation data in contradiction with new theoretical results?

The presentation by Cédric Bernardin led to a discussion on the relationship between the new theoretical results [2], which seem to indicate that the divergence of the thermal conductivity in one dimensional systems perturbed by a stochastic exchange process preserving energy and momentum should not depend on the

intensity of the exchange process; whereas previous related numerical studies [1, 9, 3] documented such a dependence.

One important point is that the theoretical study [2] is performed for an infinite system at equilibrium, at variance with numerical simulations performed on finite systems, either at equilibrium [1] or in a nonequilibrium setting [9, 3]. It is common folklore that there should be a simple relationship between the slow long-time tail decay of the autocorrelation of the current in the Green-Kubo formula (described by some power law decay) and the divergence of the thermal conductivity of open systems in their steady states. The argument is that the autocorrelation should be integrated over times of order N. There is however no clear mathematical result backing up this belief. Even worse, it even not clear from a physical viewpoint whether the scaling for the cut-off time in the Green-Kubo formula indeed is N in the presence of a strong noise (which tends to reduce the mean free path of non-interacting phonons) rather than a more general dependence N^α, with α depending on the noise strength.

During this discussion, a question arose: can it even be shown that the current vanishes in the thermodynamic limit in one-dimensional chains, as we expect? (except for the trivial case of harmonic chains with mass disorder for which it is known that the conductivity decreases exponentially with the system size) It seems that, although the steps in the proof of this statement are quite clear, there are still subtle mathematical obstructions to answering this quite natural and simple question. Needless to say, even less is known at the theoretical level about a possible scaling the thermal conductivity with the system size.

5 Outcome of the Meeting

5.1 Interactions among subgroups of participants

The feedback we received from workshop participants is overwhelmingly positive. The workshop aimed at gathering a mixed audience, composed of mathematicians, physicists and computer scientists, studying nonequilibrium systems from a theoretical viewpoint or through numerical simulations. Many researchers appreciated the diversity of the viewpoints of the audience. Answering questions about the numerical counterpart of your theoretical results is always refreshing for those more interested in theoretical aspects, while the researchers focusing on applications benefited both from the feedback from mathematicians developing a fundamental understanding of the various phenomena arising in nonequilibrium systems, and from applied mathematicians caring about the numerical accuracy and efficiency of the simulation techniques.

It is indeed our belief that there is a strong interplay between theoretical considerations, which may trigger numerical validations or extensions, and numerical simulations. It is often the case that some ad-hoc dynamics invented for a given application turns out to be of much broader interest; also, numerical experiments may motivate new theoretical results or investigations. We believe that gathering practitioners (physicists and mathematicians) from different fields and theoreticians (again, physicists and mathematicians) fostered new insights and cross-fertilization.

We mentioned in the proposal that one of the aims of this workshop was to motivate more work on the mathematical understanding of simulation techniques, for instance by suggesting some appropriate importance sampling or variance reduction methods for nonequilibrium dynamics. Although this very challenging topic has not been addressed during the presentations in the conference, there were many discussions between applied mathematicians and practitioners about possible work tracks in this direction, especially for the more demanding thermal transport simulations. These discussions seemed to motivate several applied mathematicians to carefully consider the development of more efficient numerical methods for the computation of properties of nonequilibrium systems, in particular transport coefficients. In addition, several PhD students or post-docs, working on theoretical aspects of statistical mechanics, expressed interest in learning techniques of numerical simulation in order to perform computations on their own. This would no doubt be a very efficient way of focusing more mathematical attention on the proper design of efficient numerical techniques rather than seeing simulations as some black-box tool to confirm theoretical results.

5.2 On a more ethical note

Let us finally mention the “concerned scientist” session led by Joel Lebowitz, who took opportunity of the presence of researchers from various backgrounds to spread awareness about human right violations in gen-

eral (using a current brochure from Amnesty international), and situations involving scientists in particular. He presented more precisely two organizations aiming at defending the rights of scientists and supporting their families, namely the Committee of concerned scientists [5] (whom he is a co-chair of) and the Scholars at Risk Network [15].

References

[1] G. Basile, L. Delfini, S. Lepri, R. Livi, S. Olla, and A. Politi, Anomalous transport and relaxation in classical one-dimensional models, *Eur. Phys. J. Special Topics* **151** (2007), 85–93.

[2] C. Bernardin and P. Gonçalves, Anomalous fluctuations for a perturbed Hamiltonian system with exponential interactions, *arXiv preprint* **1205.1879** (2012).

[3] C. Bernardin and G. Stoltz, Anomalous diffusion for a class of systems with two conserved quantities, *Nonlinearity* **25** (2012), 1099- 1133.

[4] F. Bonetto, J. L. Lebowitz, and L. Rey-Bellet, Fourier's law: a challenge for theorists. In *Mathematical Physics 2000* (A. Fokas, A. Grigoryan, T. Kibble, and B. Zegarlinsky, eds.), 128–151, Imperial College Press, 2000.

[5] Committee of Concerned Scientists, http://concernedscientists.org/

[6] B. Derrida, J. L. Lebowitz, and E. R. Speer, Large deviation of the density profile in the steady state of the open symmetric simple exclusion process, *J. Stat. Phys.* **107**(3/4) (2002), 599–634.

[7] A. Dhar, Heat transport in low-dimensional systems, *Adv. Phys.* **57** (2008), 457–537.

[8] J. B. Goodman and K. K. Lin, Coupling control variates for Markov chain Monte Carlo, *J. Comput. Phys.* **228** (2009), 7127–7136.

[9] A. Iacobucci, F. Legoll, S. Olla and G. Stoltz, Thermal conductivity of the Toda lattice with conservative noise, *J. Stat. Phys.* **140**(2) (2010), 336-348.

[10] C. Kipnis and C. Landim, *Scaling limits of interacting particle systems*, Springer, 1999.

[11] J. Lebowitz, Exact results in nonequilibrium statistical mechanics: Where do we stand?, *Suppl. Prog. Theor. Phys* **64** (1978), 35–49.

[12] S. Lepri, R. Livi, and A. Politi, Thermal conduction in classical low-dimensional lattices, *Phys. Rep.* **377** (2003), 1–80.

[13] S. Olla, Energy diffusion and superdiffusion in oscillators lattice networks. In *New Trends in Mathematical Physics* (V. Sidoravicius, ed.), 539–547, Springer, 2009.

[14] L. Rey-Bellet, Open classical systems. In *Open Quantum Systems II* (S. Attal, A. Joye, and C.-A. Pillet, eds.), *Lecture Notes in Mathematics* **1881**, 41–78, Springer, 2006.

[15] Scholars at Risk Network, http://scholarsatrisk.nyu.edu/

[16] H. T. Yau, Relative entropy and hydrodynamics of Ginzburg-Landau models, *Lett. Math. Phys.* **22**(1) (1991), 63–80.

[17] Y. Zhong, Y. Zhang, J. Wang, and H. Zhao, Normal heat conduction in one-dimensional momentum conserving lattices with asymmetric interactions, *Phys. Rev. E* **85**(6) (2012), 060102.