Abstract Book

Solvay Workshop on "Nonequilibrium and nonlinear phenomena in statistical mechanics"

11 - 13 July 2016

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Invited Speakers Abstracts

Adaptive Molecular Sensing

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The binding and unbinding of complex molecules with each other is the basis of all life. One well-studied class of such processes has a lock-and-key character, where particular molecules guiding particular behaviors are sensed and processed by highly specific receptors or circuits. Here, I consider sensing in open environments where the molecular environment is very diverse and dynamically evolving. I discuss two limits of this problem, one which leads to random sensing and another which leads to dynamically adapting sensor repertoires. I argue that these two limits give rise respectively to predictive theories of the organization of the olfactory system and the immune system.

Thermodynamics of boundary driven open quantum systems.

Felipe Barra.

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We consider open quantum systems evolving with a so-called boundary-driven Lindblad equation. These systems have been used as toy models for quantum non-equilibrium systems [1]. We will discuss in simple examples some of the properties that make them attractive models of non-equilibrium systems and also consider them in the context of quantum thermodynamics. We will show that a thermodynamically consistent description of boundary driven Lindblad models can be obtained by simultaneously deriving the Lindblad equation and the appropriate thermodynamic expressions from a unitary description of the system plus the environment [2]. As an example, we show that an XX chain coupled to a left and a right heat baths behaves as a quantum engine, a heater or refrigerator depending on the parameters, with efficiencies bounded by Carnot efficiencies. In the context of the unitary description we discuss the entropy production and work fluctuation theorems [3] and explain why an XX chain coupled in this way to a single heat bath relaxes to thermodynamic-equilibrium while and XY chain does not.

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Current fluctuations in non equilibrium diffusive systems

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This talk will review some results obtained over the last ten years on the fluctuations and the large deviations of the current in diffusive systems. In steady state situations, (open systems in contact with two reservoirs, ring geometry) the distribution of these fluctuations can be fully computed by the macroscopic fluctuation theory. For diffusive systems in non stationnary situations, or mechanical systems the problem is much harder. A simple model where the transport is due to random walkers with Levy distributed fly times seems to reproduce some of the results in these cases.

Hamiltonian chains with dissipation

Jean-Pierre Eckmann

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I plan to speak about a new result, with Noé Cuneo and Gene Wayne:

The idea is to see how the dissipation at one end of a deterministic chain (of coupled rotators) manifests itself at the other end, once one has transformed the system to canonical form. This work (which is not yet quite finished), will illustrate how the role of almost-breathers comes out beautifully, because the system has more and more difficulties in dissipating the energy of a rotator when it is at very high energy. I will also address open problems, when time permits.

Dynamics and Thermodynamics of Open Chemical Reaction Networks

Massimiliano Esposito, Matteo Polettini, Riccardo Rao

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We consider open chemical reaction networks of elementary reactions driven by time-dependent chemostats. Their dynamics is described by deterministic rate equations with mass action kinetics.

We establish an energy and entropy balance and introduce a nonequilibrium Gibbs free energy. The difference between this latter and its equilibrium form represents the minimal work done by the chemostats to bring the network to its nonequilibrium state.

It is minimized in nondriven detailed-balanced networks (i.e. networks which relax to equilibrium states) and has an interesting information-theoretic interpretation.

We further show that the entropy production of complex balanced networks (i.e. networks which relax to special kinds of nonequilibrium steady states) splits in two non-negative contributions: one characterizing the dissipation of the nonequilibrium steady state and the other the transients due to relaxation and driving.

In nonequilibrium steady states, we find that the entropy production strongly depends on the topology of the network and illustrate our findings on a model of monomer-exchange dynamics for glucans. Our theory lays the path to study time-dependent energy and information transduction in biochemical networks.

References:

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2. M. Polettini and M. Esposito, "Irreversible thermodynamics of open chemical networks I: Emergent cycles and broken conservation laws", J. Chem. Phys. 141, 024117 (2014).
3. R. Rao, D. Lacoste and M. Esposito, "Glucans monomer-exchange dynamics as an open chemical network", J. Chem. Phys. 143, 244903 (2015).

SRB: Interpretation, Simulations

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The SRb distribution, as an extension of The Boltzmann-Gibbs distribution for equilibria can be interpreted in terms of the ideas that were at te origin of Statistical Mechanics in the light of Boltzmann's derivation starting from the ergodic hypothesis in its original formulation. Application to stationary fluctuations.

Caustics in Random Media: Universal Properties on Many Scales

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Wave flows propagating through weakly scattering random media exhibit random focusing and branching of the flow as universal phenomena. Examples are found on many scales from ballistic electron flow in semiconductor nanostructures [1-4] to tsunamis traveling through the oceans. Even for very weak disorder in the medium, this effect can lead to extremely strong fluctuations in the wave intensity and to heavy-tailed distributions [4]. Besides statistically characterizing random caustics and extreme events by deriving scaling laws and relevant distribution functions we have recently studied the role of random focusing in the propagation of tsunami waves [5]. We model the system by linearized shallow water wave equations with random bathymetries to account for complex height fluctuations of the ocean floor and determine the typical propagation distance at which the strongest wave fluctuations occur as a function of the statistical properties of the bathymetry. Our results have important implications for the feasibility of accurate tsunami forecasts.

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Fluctuations in stochastic systems with memory

Rosemary J. Harris and Massimo Cavallaro

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I will give a gentle introduction to the effects of long-range temporal correlations in stochastic particle systems, focusing particularly on fluctuations about the typical behaviour. Specifically, in the first part of the talk, I will discuss how long-range memory dependence can modify the large deviation principle describing the probability of rare currents and lead, for example, to superdiffusive behaviour. In the second part of the talk, I will describe a more interdisciplinary project incorporating the psychological "peak-end" heuristic for human memory into a simple discrete choice model from economics. Along the way, I will attempt to indicate connections between different approaches, as well as mentioning recent work on the implementation of the "cloning" procedure for evaluation of large deviations in non-Markovian processes.

References:

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3. Cavallaro M. and Harris, R. J., *Framework for the direct evaluation of large deviations in non-Markovian processes,* preprint http://arxiv.org/abs/1603.05634.

Non-quilibrium fluctuation-induced forces

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Non-equilibrium fluctuations of the quantum electrodynamic (QED) field in the proximity of heated or moving surfaces lead to interesting phenomena. Employing a theoretical formalism that combines scattering theory and "fluctuational QED," we discuss a number of such phenomena:

* The force between two spheres (or a sphere and plate) at different temperatures can be attractive or repulsive.
* Even in vacuum at zero temperature, a rotating sphere loses its kinetic energy to radiation if composed of a lossy material.
* Non-lossy plates in uniform motion can also experience a frictional forces if moving rapidly through an analog of Cherenkov radiation.
* The fluctuating QED forces on a small dielectric are non-Gaussian and may lead to non-diffusive motion.

Quantifying Stability in Complex Networks: From Linear to Basin Stability

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The human brain, power grids, arrays of coupled lasers and the Amazon rainforest are all characterized by multistability. The likelihood that these systems will remain in the most desirable of their many stable states depends on their stability against significant perturbations, particularly in a state space populated by undesirable states. Here we claim that the traditional linearization-based approach to stability is in several cases too local to adequately assess how stable a state is. Instead, we quantify it in terms of basin stability, a new measure related to the volume of the basin of attraction. Basin stability is non-local, nonlinear and easily applicable, even to high-dimensional systems. It provides a long-sought-after explanation for the surprisingly regular topologies of neural networks and power grids, which have eluded theoretical description based solely on linear stability.

Specifically, we employ a component-wise version of basin stability, a nonlinear inspection scheme, to investigate how a grid's degree of stability is influenced by certain patterns in the wiring topology. Various statistics from our ensemble simulations all support one main finding: The widespread and cheapest of all connection schemes, namely dead ends and dead trees, strongly diminish stability. For the Northern European power system we demonstrate that the inverse is also true: `Healing' dead ends by addition of transmission lines substantially enhances stability. This indicates a crucial smart-design principle for tomorrow's sustainable power grids: add just a few more lines to avoid dead ends. Further, we analyse the particular function of certain network motifs to promote the stability of the system. Here we uncover the impact of so-called detour motifs on the appearance of nodes with a poor stability score and discuss the implications for power grid design.

Moreover, it will be shown that basin stability enables uncovering the mechanism for explosive synchronization and understanding of evolving networks.

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Menck, P., Heitzig, J., Kurths, J. and Schellnhuber, H. , Nature Communication 5 (2014), 3969
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Thermodynamic constraints on the equilibrium fluctuations of an order parameter

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Isometric fluctuation relations are deduced for the fluctuations of the order parameter in equilibrium systems of condensed-matter physics with broken discrete or continuous symmetries [1,2]. These relations are similar to their analogues obtained for non-equilibrium systems where the broken symmetry is time reversal. These relations are applied to classic models of statistical physics such as the Curie-Weiss, Heisenberg, and XY models of magnetism, where the continuous rotational symmetry is broken, as well as to the q-state Potts model and the p-state clock models where discrete symmetries are broken. Further applications to mean-field models of nematic liquid crystals will be also mentioned.

Finally, we will also present extensions of this framework to analyze fluctuations of a coarse-grained order parameter, which is obtained from the original one by decimating part of the initial system.

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Response and Fluctuations in Climate Science

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The climate is a complex, chaotic, non-equilibrium system featuring a limited horizon of predictability, variability on a vast range of temporal and spatial scales, instabilities resulting into energy transformations, and mixing and dissipative processes resulting into entropy production. Despite great progresses, we still do not have a complete theory of climate dynamics able to encompass instabilities, equilibration processes, and response to changing parameters of the system[1]. We will outline some applications of the response theory developed by Ruelle for non-equilibrium statistical mechanical systems, showing how it allows for setting in a coherent framework concepts like climate sensitivity and climate response. We show how to predict climate change – both the global averages and the spatial patterns of climatic fields - using suitably defined Green functions constructed for comprehensive global climate models[2]. By using the transfer operator formalism in a reduced space, we also present evidence of the fact that the breakdown of the Ruelle response is associated to being in the vicinity of climatic critical transitions[3]. Finally, we also find evidence in a simple forced and dissipative atmospheric model of a clear violation of the fluctuation-dissipation theorem and clarify theoretical reasons and practical relevance of this result[4].

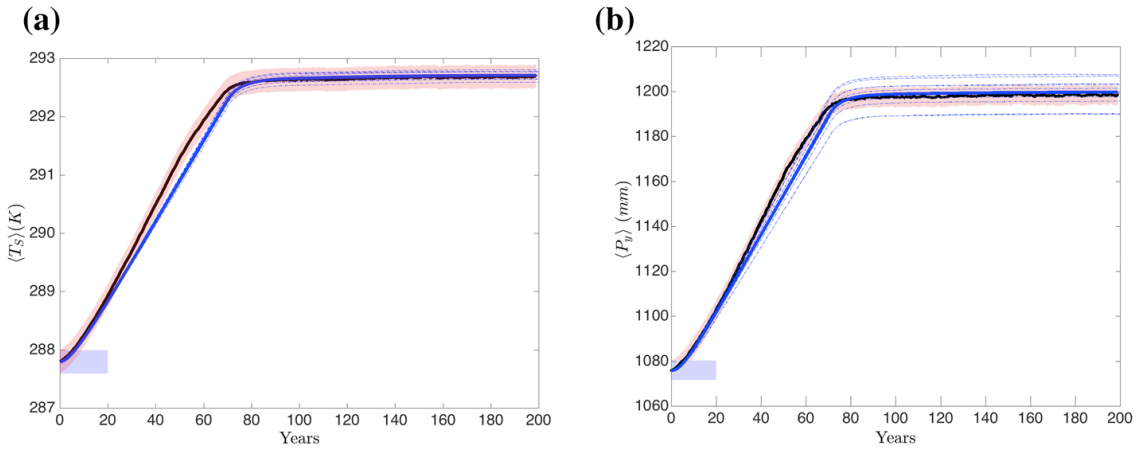

Figure 1: Climate change projections for a) the globally averaged mean annual surface temperature ‹T_S›, and b) the globally averaged annual total precipitation ‹P_Y›. The black line shows the ensemble-average of an experiment of climate change performed using a general circulation model. The thick blue line is the projection obtained using the Ruelle response theory. The dashed lines correspond to projections performed using limited information. The shading refers to the fluctuations. From Ref. 2.

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Irreversibility and the arrow of time in a quenched quantum systems

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Irreversibility is one of the most intriguing concepts in physics. While microscopic physical laws are perfectly reversible, macroscopic average behavior has a preferred direction in time. According to the second law of thermodynamics, this arrow of time is associated with a positive mean entropy production. We discuss the nonequilibrium entropy produced in an isolated spin-1/2 system following fast quenches of an external magnetic field measured using a nuclear magnetic resonance setup. We demonstrate that it is equal to the entropic distance, expressed by the Kullback-Leibler divergence, between a microscopic process and its time reversal.

References:

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Emergent Long-Range Couplings in Arrays of Fluid Cells

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Recent experimental work by Gasparini and coworkers [1,2] examined small cubical boxes of about 1 nm edge inscribed in a regular pattern on a silicon wafer and filled with liquid ^{4}He. The boxes are then coupled by addition of more ^{4}He to form a thin supernatant film or via channels. Something most remarkable happens: even though the boxes have a mesoscopic spacing, calorimetric measurements show clear evidence of coupling between different boxes. The authors did not offer any theoretical analysis, but they made the intriguing suggestion that action at a distance effects of this type might be a common feature of critical systems, both quantum (like ^{4}He) and classical. In our work, we have constructed a theoretical model of boxes containing a fluid phase below its critical temperature but at coexistence. The boxes are coupled together by rods (of arbitrary length) also containing the fluid; in this way, we can assemble lattices of coupled boxes like those of Gasparini et al. We have analysed this model using mesoscopic description and by Monte-Carlo simulation, which confirms our phenomenological results [3]. We have shown that, by appropriate tuning of parameters, the lattice of boxes develops long ranged order, even though the rods are very long compared to their lateral dimensions; the simulations produce associated thermodynamic signatures. If we consider two boxes coupled by a single rod, then we have a model system that may have relevance as a potential mechanism for biological control. Our ideas may also be useful for networks in social science. Finally, we suspect that our ideas extend to quantum spin models and maybe even to systems of coupled quantum dots.

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Transport phenomena in one-dimensional systems

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Non-equilibrium stationary processes are discussed in chains of nonlinear oscillators. Heat conduction in one-dimensional systems is first reviewed, introducing various universality classes, and recalling the conditions for the occurrence of anomalous (diverging) transport coefficients. The open problems are also briefly recalled.

Then I discuss physical setups where two quantities are simultaneously transported and mutually interact. In this second part, I mostly refer to two models: coupled rotors (XY chain), where energy and angular momentum play a major role and the discrete nonlinear Schrödinger equation, where angular momentum is replaced by the norm (or mass). In this latter case a specific discussion on the definition of appropriate thermostats is also provided.

Finally, I analyze the emergence of non-extensive non-equilibrium states in the presence of a torque when the external heat baths are set to zero temperature. An analogy with synchronization transition is also presented.

References:

Lepri S (ed) 2016 *Thermal transport in low dimensions: from statistical physics to nanoscale heat transfer*, Lect. Notes Phys **921** (Springer-Verlag, Berlin Heidelberg)

Mechanical Yield to Plastic Flow in Amorphous Materials

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Materials that exhibit a "yield" phenomenon response elastically to small strainsor stresses, but at some critical value of the stress they yield mechanically and exhibit a complex plastic flow. The search of criteria to distinguish the properties of the material before and after the yield was long and futile; none of the standard signatures like correlation functions, Voronoi tesselations or any other "structural" measure succeeded to clarify the difference between pre-yield and post-yield configurations. I will explain in this talk how to construct a new order parameter that allows us to show that the yield phenomenon is a bona-fide first order thermodynamic phase transition, shedding an entirely new light on the phenomenon.

Arnold diffusion in a driven optical lattice

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The effect of time-periodic forces on matter has been a topic of growing interest since the advent of lasers because, with laser radiation, it is possible to control and cool matter. On the other hand, it has been known since Arnold's classic work [1] that dynamical systems with 2.5 or more degrees of freedom (DoF) are intrinsically unstable. As a consequence, time-periodic driven systems can experience large excursions in energy. In order to clarify some of these issues for optical lattices, we have analyzed the classical and quantum dynamics of atoms confined to a time-periodic optical lattice with 2.5 DoF. When the laser polarizations are orthogonal, the system consists of two uncoupled 1.5 DoF optical lattices, which already have been studied both experimentally [2] and theoretically [3]. These 1.5 DoF systems remain stable. However, when laser polarizations are turned away from orthogonal, an Arnold web forms and the dynamics undergoes a fundamental change. For parallel laser polarizations, we find large random excursions in the atomic energies and significant entanglement of energies in the quantum dynamics [4].

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Typical fast thermalization processes in closed many-body systems

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Lack of knowledge about the detailed many-particle motion on the microscopic scale is a key issue in any theoretical description of a macroscopic experiment. For systems at or close to thermal equilibrium, statistical mechanics provides a very successful general framework to cope with this problem. Far from equilibrium, only very few quantitative and comparably universal results are known. Here, a new quantum mechanical prediction of this type is derived and verified against various experimental and numerical data from the literature. It quantitatively describes the entire temporal relaxation towards thermal equilibrium for a large class (in a mathematically precisely defined sense) of closed many-body systems, whose initial state may be arbitrarily far from equilibrium.

Far-from-equilibrium activated processes

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We analyze the kinetics of activated processes under far-from-equilibrium conditions, when the system is subjected to external driving forces or gradients or at high values of the affinities. When a force is applied, the reaction rate depends on the force. In the case of a chemical reaction at high affinity values, the reaction rate is no longer constant but depends on the affinity, which implies that the law of mass action is no longer valid. This result is in good agreement with the kinetic theory of reacting gases, which uses a Chapman-Enskog expansion for the probability distribution. We analyze the case of ion transport through a protein channel induced by entropic forces.

References:

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Transitions in Network co-evolution dynamics

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In coevolving networks, the dynamics of the states of the nodes of a network is coupled to the dynamics of the network topology (network plasticity). Coevolution leads generically to network fragmentation transitions. The coevolving voter model is a prototype model for consensus dynamics that exhibits such transitions at some critical value of the parameter measuring network plasticity [1]. Two new questions will be addressed: the robustness of this transition under stochastic perturbations [2], and the role of a multilayer network where each layer evolves according to its own temporal scale [3]. In both situations a new type of anomalous transition, named shattered fragmentation, is found.

As a second example of transitions in coevolving networks we study infection propagation in two interconnected networks with adaptive rewiring between them. We characterize a transition from endemic to healthy phases for a critical value of the rewiring rate [4].

References:

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3- M. Diakonova et al *Absorbing and Shattered Fragmentation Transitions in Multilayer Coevolution* , Physical Review E **89**, 06218 (2014)
4-F. Vázquez et al. *Rescue of endemic states in interconnected networks with adaptive coupling*, arXiv 1511.05606

Pacman has a new exponent

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In the 1980s arcade game Pacman, the player moves a particle (pacman) through a maze which is filled with food. The game is won when all food is consumed. We study the dynamics of this system assuming that pacman is an active particle such as a bacterium, i.e. not controlled by an external player, that swims through a two-dimensional percolating cluster and preferably moves towards food. We present the average squared distance traveled and the amount of food eaten as a function of pacman's propensity to move towards food. We observe that pacman's mean squared displacement follows a power law with an exponent that differs both from that of a self avoiding random walk as well as a random walk on a percolating cluster.

Stochastic Models of Self-propelled Particles

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I will review models of self-propelled particles from a viewpoint of statistical physics. Special attention is payed to the influence of noise on the dynamics of single particles and on the exhibition of spatial structures in groups of interacting moving particles. In detail, the determination of velocity distribution function and of the diffusion coefficients for special kinds of noise will be discussed. I sketch the connection between the stochastic micro-dynamics of the self-moving entities and the balance equation for macroscopic characterization as density, mean velocity and effective temperature, I will show that properties of swarming depend crucially on the kind of applied noise.

Nonequilibrium self-assembly of polymeric nanoparticles in flow

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Polymeric nanoparticles are of increasing interest in nanotechnology and nanomedicine. One promising approach to preparing nanoparticles in a controlled manner is to use microfluidic devices. Nanoparticles then form as the result of a self-assembly process under conditions far from equilibrium, and parameters like mixing speed and shear rate can be used to control the size and shape of the particles.

Here we use field-based simulations to investigate some of the main physical mechanisms underlying this control. First, we examine the size control in the so-called co-solvency method, where a collapse of polymeric nanoparticles from solution is induced by mixing bad solvent into apolymer dispersion. Experimentally, it is found that the particle size can be controlled by varying the mixing speed. We show that this control essentially happens in the initial stage of polymer-solvent demixing and derive scaling laws which are in agreement with experiments. Then, we study the effect of high shear rates on self-assembly. Shear mainly affects the later stages of self-assembly. It can reduce potential barriers for particle fusion, and thus assist the production of larger particles. Furthermore, it can induce irreversible shape changes in the particles and be exploited to make particles with unconventional shapes.

Universal features of NESS-fluctuations of single molecules and small networks

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I will review our recent work dealing with universal aspects of fluctuations in non-equilibrium steady states using concepts from stochastic thermodynamics. Slow hidden degrees of freedom lead to a modification of the fluctuation theorem [1,2]. The precision of any bio-molecular process is universally constrained by its thermodynamic cost [3]. Current fluctuations in any Markovian network are universally bounded by entropy production and, even more stronger, by topology and affinity dependent bounds [4]. Finally, measurements of the response and correlations of a driven single DNA-molecule and their theoretical analysis have revealed the range of validity for the concept of an effective temperature [5].

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Universal distributions for growing interfaces in one dimension

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Growing interfaces, as modelled by the Kardar-Parisi-Zhang equation, are paradigmatic systems for non-equilibrium processes. Since the turn of the century, in a variety of simplify models, asymptotic universal probability densify functions have been computed. I will provide an introduction and add a very recent surprising item, also of relevance for experimental realizations. For stationary initial conditions and long times, the height at the origin has a random amplitude of size t^(1/3) distributed according to Baik-Rains. We will explain what happens for almost stationary initial conditions, in the sense that they still have a wandering exponent ½ but the 'wrong' variance.

Proteins as learning amorphous matter: dimension and spectrum of the genotype-to-phenotype map

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Genes are transcribed and translated into three-dimensional configurations of amino acids that make functional proteins. This sequence-to-function map is hard to decrypt since it involves intricate genetic and physical interactions. Furthermore, evolution has to find the tiny fraction of functional sequences in an enormous, high dimensional universe, which implies that protein is a non-generic, information-rich matter, outside the scope of standard statistical methods. Therefore, although structure and forces within a protein have been extensively studied, the fundamental question is still open: How does a functional protein originate from a linear DNA sequence?

To address this question, we will discuss a simple mechanistic model of proteins as amorphous learning matter, which reveals the basic geometry of the genotype-to-phenotype map. The model describes how the gene adapts the amino acid interaction network to generate long-range modes in the protein, which are known to be central to its function, especially in allosteric proteins. We will show how this evolutionary learning process projects the high-dimensional sequence space onto a low-dimensional space of mechanical modes, thereby explaining the observed dimensional reduction between genotype and phenotype spaces of proteins.

The model provides an explicit map between sequence, configuration, and function of proteins whose computational simplicity allows for a massive survey of the sequence universe. In particular, we will discuss the strong correspondence found between patterns in the sequence space and the mechanical modes of the protein. Spectral analysis further explains how the biophysical constraint of obtaining a specific protein function is mirrored in sequence space as correlation ripples. These findings propose a testable basic principle of the protein as a biophysical object whose dynamics encode the evolutionary learning process.

Macroscopic effects in heterogeneous stochastic systems

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We consider stochastic particle systems made up of heterogeneous units. Heterogeneity can arise, amongst other factors, as as result of each unit being represented by a different set of parameters in the model (quenched noise) or by a different connectivity pattern (complex networks). We introduce a general framework suitable to analytically study this kind of systems and apply it to particular models of interest in economy and epidemiology [1]. As a further illustration, we study the noisy voter model, a modification of the original voter model including random changes of state [2]. The proposed method is able to unfold the dependence of the model not only on the mean degree (the mean-field prediction) but also on more complex averages over the degree distribution. We find that particle heterogeneity can enhance or decrease the size of the collective fluctuations depending on the system, and that it is possible to infer some properties of the heterogeneity distribution in the system by measuring only macroscopic, global, variables and their fluctuations. Our work shows that, in some cases, heterogeneity among the units composing a system can be fully taken into account without losing analytical tractability.

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Main quantum fluctuation theorems and work–energy relationshipswith due regard for convergence, dissipation and irreversibility

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In this paper, firstly the fluctuation theorem (FT) for *expended work* in a driven nonequilibrium system, isolated or thermostatted, as formulated originally by Crooks and Tasaki [1, 2], together with the ensuing Jarzynski work–energy (W–E) relationship [3], with clarifications by various authors among whom Kawai, Parrondo and Van den Broeck [4] – will be discussed and reobtained. Secondly, the fluctuation theorems for *entropy flow* due to Evans, Cohen and Morris [5] with extensions by many researchers, a.o. Galavotti and Cohen [6], (Kurchan [7, 8], Lebowitz and Spohn [9], Evans and Searles [10] and Harris and Schütz [11]). Our treatment will be fully quantum-statistical, being an extension of our previous research reported in Phys. Rev. E, 2012 [12].

Whereas a true explosion of papers took place after the initial articles around the turn of the century referred to above ([1-11]), virtually all of these suffered from one or more of the following deficiencies: (i). The arguments are fully based on classical trajectories in phase space; this is true for Christopher Jarzynski's original work [3], as well as for Crooks' cited paper [1]; better fares Tasaki's quantum treatment in the arXiv [2]. (ii). A large number of quantum treatments for the work FT and the W–E relationships involve the 'pure' von Neumann equation or 'non-reduced' Heisenberg operators; this is regrettable, particularly for an otherwise beautiful derivation based on symmetry and extension in the complex plane by Talkner and Hänggi [13]. The basic point here is that correlation functions for non-reduced Heisenberg operators do not converge. As the author has pointed out in many papers and in her recent book [14]: Kubo Linear Response Theory (LRT) is a *hollow shell* until proper randomization (Kubo: 'stochasticization') [15] is introduced and carried out. Thus, we must explicitly consider the interactions λV with the reservoir or internal scatterers. Taking the trace over these, the resulting semigroup has complete positivity, shows non-unitarity for the time evolution, exhibits dissipation and irreversibility, with the general result being the Lindblad quantum master equation (QME) [16]. In the physical literature a more explicit result is obtained after application of the 'weak coupling–long time' limit, developed long ago by Leon Van Hove [17, 18]. (iii). While a few dozen papers do use a stochastic approach with some Master Equation as guiding *leitmotiv*, this author found most treatments wanting and not in accord with the general tenets spelled out by Lindblad and others (see e.g. Breuer and Petruccione [19]). Note that a QME must also be employed for a correct and fully quantum mechanical version of the entropy FT; a stochastic treatment with 'jump-induced' random trajectories – see [11] – is begging the question.

We now come to the contents of *this* paper. Our presentation will have three parts. *A*. In the introduction we shall briefly dwell on the reasons for re-formulation as argued above. *B*. We shall present our way of obtaining the *quantum work FT and W–E relationships* based on the non-stationary ME derived in [12] with convergent correlation functions for Heisenberg operators; this largely follows our previous study, offering some new refinements. *C*. From our ME, as also found in a paper by Gaspard [20], we shall establish various *quantum entropy FT's* for thermostatted systems. A number of useful relationships of Harris and Schütz [11]) will still gainfully be employed; however, the Markov conditional probability $P(\sigma', t|$

σ, t_0) shall only denote the two state-points, with no reference whatsoever to 'stochastic trajectories', these being meaningless in a quantum description. Also, contrary to our treatment in [12], the 'quantum Hamiltonian' approach of their studies is fully dropped and a straightforward reasoning gives the desired results.

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Extending Landauer's Bound from Bit Erasure to Arbitrary Computation

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Recent advances in nonequilibrium statistical physics have led to great strides in the thermodynamics of computation, allowing the calculation of the minimal thermodynamic work required to implement a computation $\boldsymbol{\pi}$ when two conditions hold:

i) The output of $\boldsymbol{\pi}$ is independent of its input (e.g., as in bit erasure);
ii) We use a physical computer C to implement $\boldsymbol{\pi}$ that is tailored to the precise distribution over $\boldsymbol{\pi}$'s inputs, P_0.

First I extend these analyses to calculate the minimal work required even if the output of $\boldsymbol{\pi}$ depends on its input. I then show that stochastic uncertainty about P_0 increases the minimal work required to run the computer.

Next I show that if C will be re-used, then the minimal work to run it depends only on the logical map $\boldsymbol{\pi}$, independent of the physical details of C. This establishes a formal identity between the thermodynamics of (re-usable) computers and theoretical computer science. I use this identity to prove that the minimal work required to compute a bit string $\boldsymbol{\sigma}$ on a universal Turing machine U is

$$\begin{aligned}&\text{Kolmogorov complexity}_U(\boldsymbol{\sigma})\\ &\qquad +\\ &\log(\text{Bernoulli measure of the set of input strings that compute } \boldsymbol{\sigma})\\ &\qquad +\\ &\log(\text{halting probability of } U)\end{aligned}$$

This can be viewed as a thermodynamic "correction" to Kolmogorov complexity.

I end by using these results to relate the free energy flux incident on an organism / robot / biosphere to the maximal amount of computation that the organism / robot / biosphere can do per unit time.

Dense Granular Flow of Frictional Particles

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A jamming scenario of frictional particles is discussed and interpreted in terms of a nonequilibrium first order phase transition (1). Results of numerical simulations will be presented and analyzed in the framework of a simple model which can account for both, the continuous frictionless case and the discontinuous frictional case. The most important features of the frictional phase diagram are reentrant behavior and a critical jamming point at finite stress. In the simulations, we observe that small systems settle into a stationary state, whereas large systems do not relax to a stationary state on the timescale of observation, but rather display chaotic time dependence (2). We propose a hydrodynamic model which couples stress relaxation to a scalar variable accounting for the microstructure of the packing. Linear stability analysis reveals an extended phase diagram which in addition to regions of stationary flow and jammed states displays chaos. We also develop a microscopic picture of reentrant flow and shear thickening, which emphasizes the role of friction.

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Poster Presentations Abstracts

Fluctuation out of Equilibrium

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A generalization of the fluctuation-dissipation formula for systems with slowly varying parameters is given using the Langevin approach [1] and momentum method [2]. It is shown that spectral function of the fluctuations in these systems is determined not only by the dissipation but also by the derivations of the dispersion. The non Joule dispersion contribution is characterized by a new nonlocal effect originating from an additional phase shift between the force and response of the system. That phase shift results from the parametric control to the system. The general formalism is illustrated for an oscillating electrical circuit. It is shown that in that systems the dispersive contributions strongly affect the quality factor.

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Extended local equilibrium approach to stochastic thermodynamics

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Over recent years, a new field of statistical physics called stochastic thermodynamics has emerged, which aims at describing small systems subjected to fluctuations [1]. In this description, the temporal evolution of thermodynamic quantities (e.g. work, entropy, ...) follows a fluctuating trajectory. Recently a new approach in the definition of stochastic thermodynamic variables was proposed by De Decker *et al.* [2] based on an extension of the local equilibrium hypothesis. The essence of this method is to make the state variables stochastic by adding a noise term to their deterministic (i.e. macroscopic) evolution equation.
This method allows us to extend quite naturally the macroscopic non-equilibrium thermodynamics to small scale systems. Furthermore we can easily compute the probability distribution of stochastic thermodynamic quantities or relate them to macroscopic parameters. This new formulation seems promising to describe mesoscopic systems.

Using this new framework we investigated in particular the entropy production associated with chemical reactions and heat transfer in steady states. Entropy production is knew to play a central role in the stability criterion and is a measure of efficiency for small systems. We will present how the fluctuations can induce novelties in its behavior. For instance it can be showed that the mean of entropy production (i.e. the experimentally accessible measurement) can slightly differ from the deterministic prediction in the case of non-linear chemical reactions. We can go a step further and also obtain the probability distribution of entropy production in and out equilibrium, which allows us to derive fluctuation theorems[3]. Deviations of the mean behavior can be so completely characterized.

Current efforts are made to complete this formalism and apply it to other quantities (e.g. work) as well as more sophisticated problems (thermodiffusion, complex chemical reactions).

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Emergence of Brownian Motor

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Emergence of motion out of thermal equilibrium will be discussed. Significant effort was dedicated to the research of mechanisms of motion out of thermal equilibrium. Mechanical system, such as Brownian ratchet, generates motion out of thermal fluctuations if spatial symmetry is broken and if the ratchet is coupled to several thermal bathes. Brownian ratchet is a leading physical model for molecular motors. To the best of my knowledge, the question of emergence and thermodynamic stability of Brownian Ratchets remains open.

One can ask a question: if Brownian ratchet can be either in symmetric or asymmetric states whether thermodynamic forces favor transition to asymmetric state and, therefore, favor emergence of motion? Answering this question will help estimating required conditions and universality of directed motion out of thermal equilibrium. These conditions and universality may be an important link between non-equilibrium thermodynamics and Origin of Life as well as a guide to micro-fabrication of the novel nano motors.

Here, I'll present detailed analysis of emergence Brownian Motor using Triangula model[1] of Brownian ratchet. The results are general to any system with multiple degrees of freedom, for instance molecules. Consequently, this work provides a universal extension of Onsager relations to non linear regime.

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Universal trade-off inequality between power and efficiency

Naoto Shiraishi, Keiji Saito, and Hal Tasaki

The thermodynamic efficiency and power (extracted work per a unit time) are two of the main properties of heat engines. Most scientists believe that these two quantities are complementary: There exists a trade-off relation which prohibits engines with high efficiency and large power. However, such a trade-off relation has not been discovered yet. Even worse, maybe surprisingly, whether a heat engine at finite power attains the Carnot efficiency η_{Carnot} has still been an open problem, though its opposite was established by Carnot 200 years ago. Conventional equilibrium thermodynamics provides no restriction on the speed of processes, and even in linear response regime the linear irreversible thermodynamics at the formal level allows devices with the Carnot efficiency at finite power if time-reversal symmetry is broken [1]. By contrast, all studies based on specific dynamical models have arrived at the same result that within these specific models the Carnot efficiency and finite power are incompatible [2-5]. As seen from this, since such a basic problem has still been an open problem, general relation between efficiency and power has completely been missing.

In this presentation, we demonstrate a universal trade-off inequality between efficiency and power, which holds even beyond the linear response regime and even with broken time-reversal symmetry [6]. We first derive a crucial inequality between heat flux from the system to the ν-th bath and total entropy production denoted by J_ν and σ_{tot}, respectively:

$$\sum_{\nu=1}^{\mathrm{n}} |J_\nu| \le \sqrt{\Theta \sigma_{tot}}$$

where Θ is a finite quantity which reflects the property of the system. This inequality means that quick energy exchange between the system and a bath inevitably causes much dissipation. For the case of cyclic processes with two thermal baths with inverse temperature β_{H} and β_{L} ($\beta_{\mathrm{H}} < \beta_L$), this inequality leads to the trade-off inequality between efficiency η and power P:

$$\mathrm{P} \le \overline{\Theta} \beta_L \eta (\eta_{Carnot} - \eta)$$

where $\overline{\Theta}$ is a time average of Θ. This inequality clearly shows that power P goes to zero as efficiency η approaching the Carnot efficiency η_{Carnot}.

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Propagating chemical fronts with Marangoni flows

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When the two reactants of an A + B → C reaction are brought into contact, a reaction front is formed and the spatially localized zone where the reaction occurs evolves in time due to the interdiffusion of A and B. The properties of such fronts are well studied in reaction-diffusion systems where no flow can affect the dynamics [1, 2]. Here we consider horizontal aqueous solutions where the three species A, B, and C can affect the surface tension of the solution, thereby driving Marangoni flows (see **Fig. 1**). The resulting dynamics is studied by numerically integrating the incompressible Navier-Stokes equations coupled to reaction-diffusion-convection equations for the three chemical species. We show that the front propagation cannot be predicted anymore on the sole basis of the reaction-diffusion properties as was still possible in the presence of buoyancy-driven flows around such fronts [3]. We relate this observation to the structure of the Marangoni-driven flow. Based on an analytical description, we propose a classification of the convective effects on A + B → C reaction-diffusion fronts as a function of the different Marangoni numbers quantifying the effect of each species on the surface tension (see **Fig. 2**).

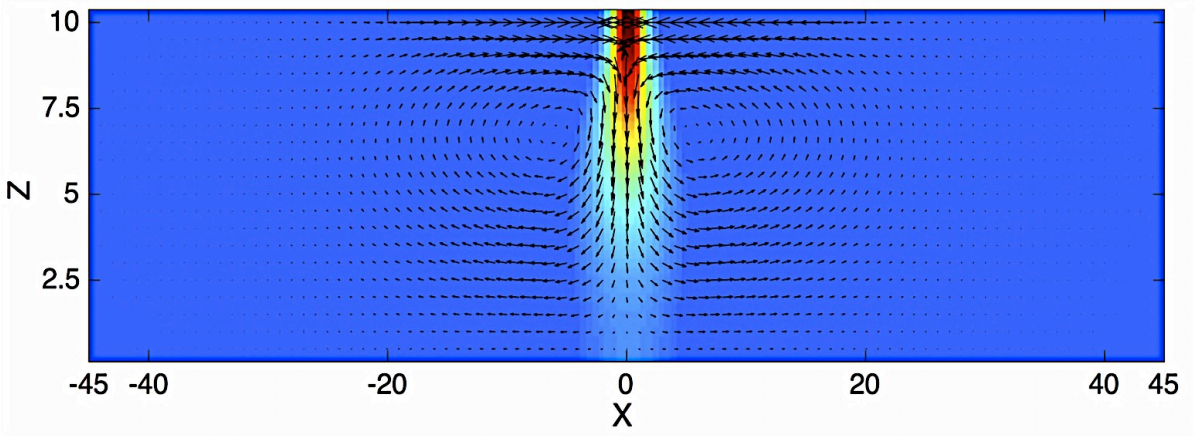

FIG. 1: Focus on the convection rolls centered on the reaction front shown at t = 30. The fluid velocity field is superimposed on a 2D plot of the production rate which ranges between its maximum value (reaction front), ab_{max} shown in red, and its minimum value, ab_{min} = 0, shown in blue. The z-direction has been magnified to see the details of the velocity field. The velocity vectors are here tripled compared to their effective length. The results are shown for M_a = 20, M_b = 40, M_c = 30 and ab_{max} = 0.050, where $M_{a,b,c}$ are the Marangoni numbers of each species A, B, C.

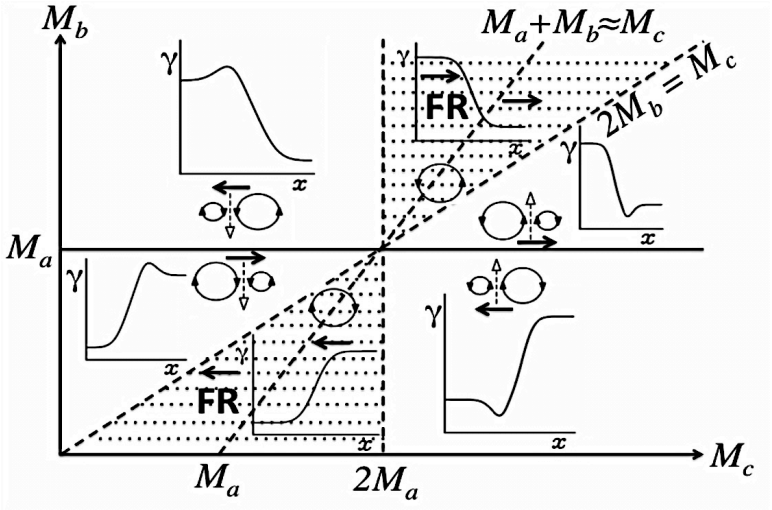

FIG. 2: Classification of the different observed dynamics in the (M_b, M_c) parameter plane at fixed M_a. Typical surface tension profiles as well as a sketch of the observed vortex dynamics are illustrated within the corresponding regions. The dark filled arrow indicates the initial direction of propagation of the front. For $M_c < M_a + M_b$ in the shaded regions, we surprisingly observe the possibility of a front reversal (FR), i.e. the front changes its direction in the course of time.

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Thermodynamics vs. Dynamics: Perspectives from phase transitions

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Thermodynamics successfully describes natural phenomena under equilibrium, but principles of dynamics are invoked for nonequilibrium systems. In this poster we discuss phase transition in a dynamical perspective. Here we show how a single framework based on large-scale modes successfully explains hysteresis at zero temperature, and two-state coexistence (as in phase transition) in the presence of noise induced by temperature. Our model also explains how the width of a hysteresis loop shrinks in the presence of noise, as well as show how initial condition can play a significant role in bistable transitions.