JETC 2025

The 18th Joint European Thermodynamics Conference
Belgrade, Serbia
May 26–30, 2025

Book of Abstracts

Edited by Velimir Ilić

Mathematical Institute of the Serbian Academy of Sciences and Arts

International conference

The 18th Joint European Thermodynamics Conference
Belgrade, Serbia May 26–30, 2025

Book of Abstracts

Velimir Ilić, Editor

Mathematical Institute of the Serbian Academy of Sciences and Arts,
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CONFERENCE PROGRAM

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08:30-9:00	ARRIVALS	REGISTRATION DESK							
09:00-09:20		OPENING		PLENARY TALK Michael Cates	Thermodynamics of small systems	Heat conduction I	Stochastic and information thermodynamics	Thermodynamics of fluids	Closing discussion
09:20-09:40		PLENARY TALK Juan M. R. Parrondo			G. P. Beretta J. Korbel A. Aydın R. Chamberlin	V. A. Cimmelli P. Rogolino D. La Pegna M. Pavelka M. Western M. Costa Reis	E. Roldan S. Liang K. Olsen R. Chakraborty P. Jizba	D. Alt X. Zhang D. Giordano C. Pezzotti M. Pszota S. Buyukdagli	
09:40-10:00				Quantum thermodynamics and quantum information theory Č. Brukner, M. Huber, G. Manzano, P. Jizba					
10:00-10:40		Prigogine Prize							
10:20-11:00		COFFEE BREAK							
11:00-11:10				COFFEE BREAK					END OF CONFERENCE
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11:30-13:10		Foundations and philosophy of thermodynamics P. Ván, G. P. Beretta, F. Barbaresco, R. V. Chamberlin, K. H. Hoffmann, P. M. Mariano, J. Yngvason, M. te Vrügt		Thermodynamics of long-range interacting systems A. Trombettoni, A. Campa, S. Iubini, E. King, V. Pagni	Physics of life M. R. Ejtehadi A. Kolchinsky D. Fessas V. A. F. Costa	Heat conduction II A. Sellitto C. F. Munafo P. M. Mariano K. Seki S. Iubini	Thermodynamics of learning A. Decelle, D. Abranches, C. Furtlehner, C. Maes, P. Rotondo		EXCURSION TO SREMSKI KARLOVCI (OPTIONAL)
13:10-13:30		LUNCH BREAK							
13:30-15:00	REGISTRATION DESK								
15:00-17:00		Nonequilibrium thermodynamics P. Ván C. Maes J. Yngvason F. Barbaresco	Quantum thermodynamics M. Milovanović J. A. Almanza-Marrer B. Aslanbas G. Di Bello	Stochastic thermodynamics in physics and beyond J. Korbel, É. Roldán, D. Das, R. Garcia Millan, A. Kolchinsky, S. Loos, K. Sekimoto	PLENARY TALK Johann Rafelski Thermodynamics in high energy physics T. Bhattacharyya, Airton Deppman, M. Rybczyński, L. Tinti, S. Tripathy		New horizons in continuum mechanics A. Sellitto, V. A. Cimmelli, A. Berezovski, F. Oliveri, V. Romano, M. Sciacca, F. Zullo		
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18:00-19:00	WELCOME TO BELGRADE/ GUIDED TOUR TO KALEMEGDAN								
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20:00-23:30					CONFERENCE DINNER (OPTIONAL)				

PLENARY TALK (PANORAMA)	PRIGOGINE PRIZE (PANORAMA)	TOPICAL SESSION (KLUB)	MINI-SYMPOSIUM (PANORAMA)	SPECIAL SESSION (PANORAMA)
40’ talk (including Q&A)	30’ talk (including Q&A)	20’ (including Q&A) for each regular talk	4’ for each organizer (underlined) 12’ for each panelist ~40’ discussion with audience	40’ (including Q&A) for each invited talk (underlined) 20’ for each regular talk

FOREWORD

Dear Colleagues,

It is my great pleasure to present the Book of Abstracts of the 18th Joint European Thermodynamics Conference (JETC 2025), held from 26 to 30 May 2025 in Belgrade, Serbia, and hosted by the Mathematical Institute of the Serbian Academy of Sciences and Arts.

The Joint European Thermodynamics Conferences were established in 1989 and have since been organised biennially in Europe, with the aim of fostering interaction and integration among the diverse theoretical foundations and application domains of thermodynamics. After 35 years of distinguished scientific tradition, JETC was held for the first time on the Balkan Peninsula, a region located at the historical crossroads of Eastern and Western Europe.

JETC 2025 was attended by 80 participants from abroad, representing more than 20 countries and four continents, and consisted of the following modules, which promoted active exchange throughout the conference: plenary lectures, mini-symposia with focused thematic discussions, special and topical sessions, and a poster session.

During the conference, three awards were presented: the Prigogine Prize for the best doctoral thesis completed within the preceding two years, the Award for the Best Student Poster, and the Award for the Best Mini-Symposium Speaker. I extend my sincere congratulations to all award recipients.

The successful realisation of JETC 2025 would not have been possible without the support of the Steering and Scientific Committees, the dedicated efforts of the mini-symposium organisers, and the invaluable contributions of the plenary lecturers, invited speakers, invited panellists, session participants, and all attendees. I express my sincere gratitude to all those who contributed to making JETC 2025 a success. I would also like to express my special appreciation to the members of the Local Organising Committee for their passionate and seamless efforts in ensuring the smooth and successful organisation of the conference.

I look forward to meeting the JETC 2025 participants again at the next Joint European Thermodynamics Conference.

With kind regards,
Velimir Ilić
Mathematical Institute of the
Serbian Academy of Sciences and Arts
Belgrade, Serbia

JETC 2025 Conference Chair

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TWO NOTES ON THE FOUNDATIONS OF THERMODYNAMICS: OBJECTIVITY OF ENTROPY AND THE ORIGIN OF GIANT FLUCTUATIONS

Juan M. R. Parrondo

Dept. Estructura de la Materia, Física Térmica y Electrónica and GISC,
Universidad Complutense de Madrid, Madrid, Spain

ABSTRACT

The standard formulations of statistical mechanics and the explanations of irreversibility rely on the way we describe physical systems. They use concepts such as coarse-graining, macroscopic states, and probabilistic states that depend on the observables we measure, the precision with which we measure them, or the information we have about the microstate of a system. Some of these elements of arbitrariness can be removed from the formulation of statistical mechanics using an observable-dependent entropy that was already used by Einstein in his studies of fluctuations [1]. The observable-dependent entropy, together with the ergodic hypothesis, characterizes the irreversible behavior of specific observables, both micro- or macroscopic [2]. On the other hand, equilibrium and the entropy of a system cannot be defined without choosing the observables used to describe its state, and this choice seems to involve an unavoidable arbitrariness. Finally, we present a new mechanism for the origin of states with low entropy based on symmetry-breaking transitions [2,3]. This mechanism replaces the controversial "past hypothesis" [4], namely, the assumption that the universe started in a low-entropy state, with the simpler scenario of an environment with decreasing temperature.

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MULTIPLE INTERFACIAL TENSIONS IN ACTIVE FIELD THEORIES OF PHASE SEPARATION

Michael Cates[1,2]

[1]University of Cambridge, Cambridge, UK
[2]University of Edinburgh, Edinburgh, UK

ABSTRACT

In thermal equilibrium, the interfacial tension between coexisting phases is a free energy derivative with respect to the interfacial area. Consistent with thermodynamics, many different measurements or definitions of the tension (via, say, the capillary wave spectrum or the Laplace pressure at a curved interface) all give the same answer. There is no such consistency for interfaces in active systems. Indeed a minimal scalar field theory of active phase separation (Active Model B+) gives at least three distinct tensions, some of which can be negative without the interface losing stability. The various tensions have interesting consequences for the phase diagram and also for nucleation, where the quasipotential is calculable at the level of classical nucleation theory. I will describe the various tensions and their roles, and finally argue that their differences are enough to establish that the stationary measure of the field theory is nonlocal.

THERMAL NONEQUILIBRIUM AND QUARK-GLUON PLASMA

Johann Rafelski, Cheng Tao Yang
Department of Physics, The University of Arizona, Tucson, Arizona, USA

ABSTRACT

The Universe folloqing on electroweak transformation at a temperature $T \simeq 125\,\mathrm{GeV}$ was dominated during the folloqing $25\mu s$ by strongly interacting particles [1] quarks and gluons forming a new state of matter, the color deconfined Quark-Gluon Plasma (QGP) for $T > 150\,\mathrm{MeV}$. In the laboratory environment QGP is formed in highly relativistic collisions of heaviest nuclei reaching $T \simeq 0.5\,\mathrm{GeV}$; therefore thermalization of collision energy into thermal motion of a large number of newly created strongly interacting quarks and gluons is required for QGP state formation, a challenging frontier of ongoing research [2].

For the strong QCD force the thermal reaction rates in QGP have been studied in depth [1] as the lifespan of laboratory QGP $O(\infty\prime^{-\in\in}\,\mathrm{s})$ is of comparable magnitude. The expansion of the Universe is described by the Hubble parameter H which is many (*e.g.* 15-18) orders of magnitude slower [3] compared to microscopic reaction rates. Even so, we find that nonequilibrium of physical significance arises both, in the laboratory formed QGP environment, especially during transformation into normal matter gas phase, and in the primordial Universe.

The importance of any nonstationary condition in expanding QGP Universe is that this is the dynamic requirement for baryogenesis: We are searching for the origin of matter. To form matter we need ireversibilitiy among microscopic processes allowing emergence of newly formed baryons. In the study of nonstationary condition we distinguish between two possible nonequilibrium features inherent to QGP: i) The abundance (chemical) nonequilibrium and; ii) the momentum distribution (kinetic) nonequilibrium. The important difference between nonequilibrium and nonstationary condition is that latter requires time dependence, that is expansion of the Universe. I will describe both bottom quark flavor nonstationary condition which arises near to Universe hadronization [3], and Higgs particle dynamics in QGP across a large temperature range [4]. For the Higgs the two salient feature are that it practically does not scatter on low mass QGP particles and its decay channels into virtual gauge mesons are not reversible. The abundance of heavy particles in the Universe is shown in Fig. 1 as a function of Temperature T assuming equilibrium.

The laboratory environment is different [5] due to the rapid expansion-dilution of the high density QGP matter created in in laboratory ultra-relativistic nuclear collisions. Therefore, the laboratory situation allows to use the quark-flavor nonequilibrium to characterize the QGP properties [6], leading to the recognition of QGP as the new state of deconfined matter. To isolate the physical processes a detailed comparison of experimental results with theoretical models allowing for chemical non-equilibrium is required to achieve appropriate level of understanding of all physical mechanisms [7].

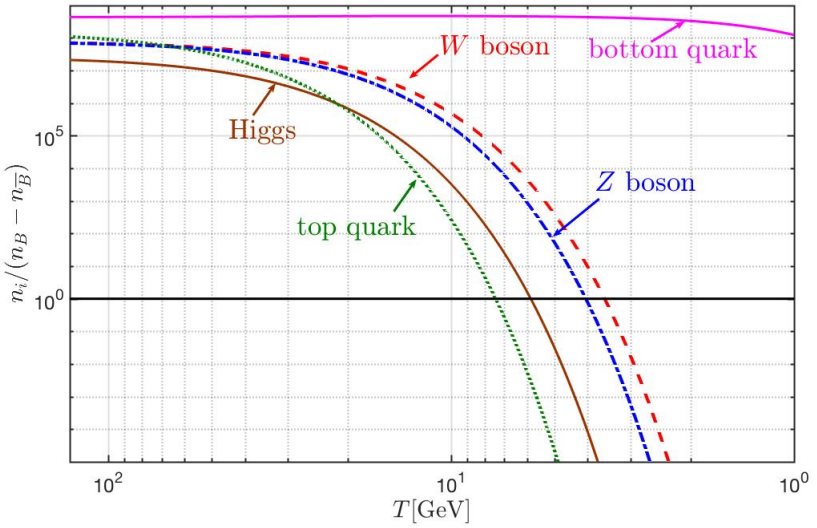

Figure 1: Thermal primordial QGP heavy particle abundances normalized by the net baryon abundance $n_B - \bar{n}_B$ as a function of Universe temperature T.

Keywords: quark deconfinement, quark-gluon plasma, Higgs particle, baryogenesis

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STOCHASTIC THERMODYNAMIC TREATMENT OF THERMAL ANISOTROPY

Olga Movilla Miangolarra
University of La Laguna, Spain

ABSTRACT

Anisotropy in temperature fields, chemical potentials, and ion concentration gradients provide the fuel that feeds dynamical processes that sustain life. At the same time, anisotropy is a root cause of incurred losses manifested as entropy production. In this talk, we shed light on the delicate balance between energy extraction and entropic losses by considering an overdamped stochastic thermodynamic system in an anisotropic temperature heat bath. Specifically, we show that path lengths traversed in the manifold of thermodynamic states, measured in a suitable Riemannian metric (the Wasserstein-2 metric), represent dissipative energy losses, while area integrals of a work-density quantify work being extracted. Thus, the maximal amount of work that can be extracted relates to an isoperimetric problem in the Wasserstein space, trading off area against the length of an encircling path. Furthermore, we provide a geometric decomposition of entropy production, where dissipation is distinguished from seepage of energy between ambient anisotropic heat sources by way of the system dynamics. We show that, in the presence of anisotropy, minimization of entropy production can be expressed via a modified Optimal Mass Transport (OMT) problem. However, in contrast to the isotropic situation that leads to a classical OMT problem and Wasserstein length, entropy production may not be identically zero when the thermodynamic state remains unchanged, unless one has control over non-conservative forces.

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MINI-SYMPOSIUM

Foundations and Philosophy of Thermodynamics

Organisers:
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Karl Heinz Hoffmann (Germany)
Paolo Maria Mariano (Italy)
Jakob Yngvason (Austria)
Michael te Vrügt (Germany)

JETC 2025

TRANSVERSE SYMPLECTIC FOLIATION STRUCTURE FOR DISSIPATIVE THERMODYNAMICS BASED ON SOURIAU MODEL OF STATISTICAL MECHANICS

Frédéric Barbaresco

THALES Land & Air Systems, Vélizy-Villacoublay, France

ABSTRACT

Jean-Marie Souriau's model, known as "Lie groups Thermodynamics," is a symplectic model of statistical mechanics. This framework integrates geometric methods into statistical mechanics, where Gibbs states of a system are represented as points in a symplectic manifold, and Lie groups describe the symmetries of the system. We give an original interpretation of "Lie groups Thermodynamics" with a symplectic foliation generated by coadjoint orbit of the Lie group acting on the system, where the Entropy is characterized as an invariant Casimir Function. Transverse to this symplectic foliation, considered as level sets of Entropy, we can associate a Riemannian foliation as level set of Energy. These transverse foliations define a webs structure. We explain dynamics along both transverse leaves by a metriplectic flow mixing Poisson bracket on symplectic leaves (level sets of Entropy), describing non-dissipative phenomenon by preserving Entropy, and metric bracket on Riemannian leaves (level sets of Energy), characterizing non-dissipative phenomenon by Entropy production. In the framework of Information Geometry for statistical manifolds, we can associate to the symplectic foliation the Fisher metric, and to the Riemannian foliation the dual of the Fisher metric (hessian of Entropy).

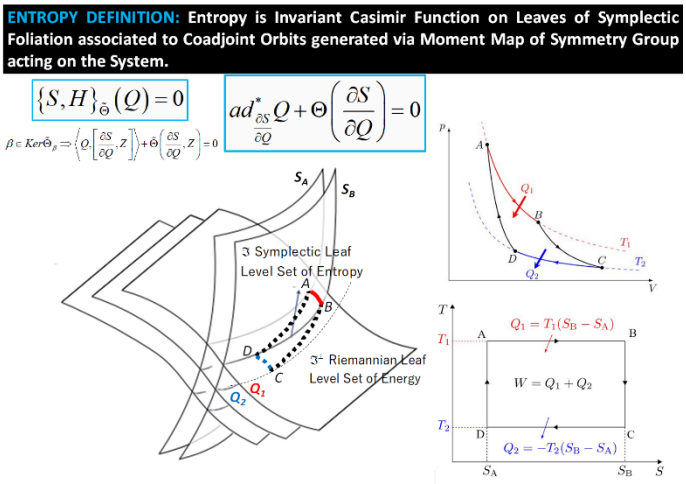

Figure 1: Entropy as Casimir function on Symplectic leaves (level set of entropy) generated by coadjoint orbits and transverse Riemannian leaves (level sets of Energy). Sadi Carnot Cycle on transverse foliations.

We develop this foliation model of thermodynamics, making the link with the notion of metriplectic flow, compatible with Onsager relations, describing the dynamics along each of the leaves. We show that to the symplectic foliation of Souriau, we can associate a transverse Riemannian foliation by the energy level sets, which describe the dissipative phenomena and the generation of Entropy of the 2nd principle of Sadi Carnot. We recall that the physicist Baptiste Coquinot has established the compatibilities of metriplectic flow with the Onsager relations that describe dissipa-tive phenomena. We also recall that Günther Vojta had studied first Onsager rela-tions within the framework of symplectic geometry. We conclude with physicist Herbert B. Callen's insight into thermodynamics as the Science of symmetry. We recall avenues of study opened by Callen to explore more deeply the role of symmetry in thermodynamics.

Keywords: thermodynamics, 2nd principle, symplectic foliation, Riemannian foliation, Lie groups, Lie algebra cohomology, entropy, Casimir function, Pfaff forms

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STABLE NANOTHERMODYNAMICS: BEYOND BOLTZMANN'S FACTOR FOR THERMAL EQUILIBRIUM AND NANOSCALE FLUCTUATIONS

Ralph V. Chamberlin

Department of Physics, Arizona State University, Tempe, AZ, USA

ABSTRACT

In his lectures on statistical mechanics [1] Feynman calls Boltzmann's factor a "fundamental law," but then he lists several assumptions needed for a system to obey this "law." Two key assumptions are 1) the system must be coupled to an ideal heat bath yielding temperature (T) and 2) this coupling must be very weak, yet faster than any fluctuations in local energy. Now it is known that many measurements and computer simulations show clear deviations from these assumptions [2]. Most deviations are due to localized energy fluctuations that are too fast to fully couple to the heat bath, so that conservation of local energy dominates over the very weak coupling needed for Boltzmann's factor. In such cases, we have found that it may be necessary to return to the fundamental laws of thermodynamics to understand the thermal behavior. For example, local energy fluctuations are often best analyzed in a microcanonical ensemble (Fig. 1A, upper left), because conservation of local energy is a more-basic law than Boltzmann's factor.

Hill's theory of small system thermodynamics [3] has been called "the most extensive addition to equilibrium thermodynamics since Gibbs." Indeed, Hill and Gibbs made mathematically similar (and comparably important!) contributions to the laws of thermodynamics. Specifically, conservation of energy during reversible processes (equation in inset of Fig. 1B) requires the term introduced by Gibbs (μdN_t) if the total number of particles changes ($dN_t \neq 0$), plus the term introduced by Hill ($\varepsilon d\eta$) if the number of independent clusters of interacting particles ("subsystems") changes ($d\eta \neq 0$). Gibbs' chemical potential is set to zero ($\mu = 0$) for the stable equilibrium of quantized waves, e.g. photons or phonons. Similarly, Hill's subdivision potential is set to zero ($\varepsilon = 0$) to minimize the free energy (Fig. 1B) for the stable equilibrium of independent subsystems in the nanocanonical ensemble. Hill discussed this stability condition at length in section 10-3 of his 1964 book. To my knowledge, since 1964 only our group has applied $\varepsilon = 0$ to any system, allowing us to solve, resolve, or at least clarify several "unsolved" problems in physics [2]. Here I will focus on the stable solution (Fig. 1C) of Ising's original (1925) model for finite chains of interacting binary degrees of freedom ("spins"), which goes beyond Boltzmann's factor by utilizing $\varepsilon = 0$. Ising could not have found this solution 40 years before Hill's work.

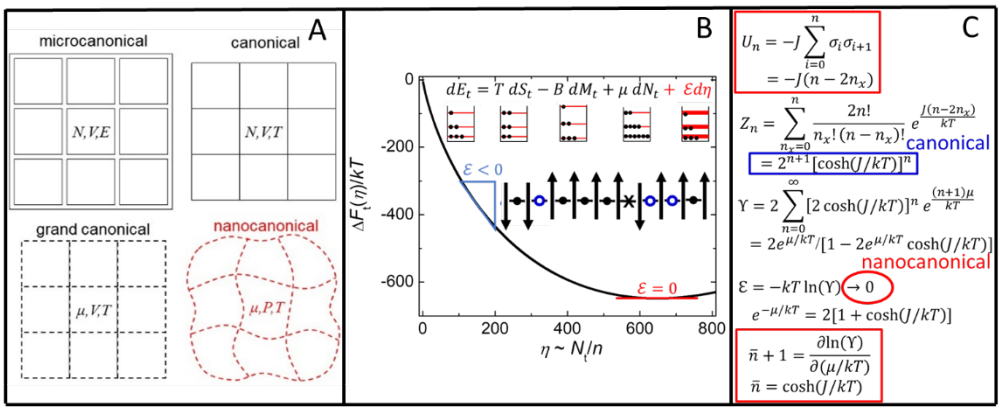

Figure 1: A) Sketch of various ensembles, from subdividing a larger system into $\eta = 9$ subsystems, with their environmental variables for a simple gas. B) Main figure shows the total free energy versus number of subdivisions for a system of $N_t = 1000$ Ising spins at $kT/J = 1$. The system subdivides until it reaches its stable equilibrium at $\varepsilon = 0$, yielding subsystems of average size $\bar{n}+1 \approx 1000/642+1 \approx 2.54$ spins. Upper inset gives the fundamental equation of thermodynamics, including Hill's pair of conjugate variables (in red), with a simple (three-energy-level) diagram showing how energy might change from each term in the equation. Other inset shows $N_t = 10$ Ising spins with low-energy (•) and high-energy (**X**) interactions, plus no-energy "breaks" (o) that subdivide the system into $\eta = 4$ subsystems. C) The Ising model requires $\varepsilon = 0$ for stability in the nanocanonical ensemble.

Keywords: nanothermodynamics, nanocanonical ensemble, nanoscale fluctuations, stable equilibrium, Ising model

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ENDOREVERSIBLE THERMODYNAMICS

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Technische Universität Chemnitz, Chemnitz, Germany

ABSTRACT

Usually, thermodynamic processes are performed within a finite time interval or with non-vanishing rates. For such processes the classical equilibrium results like the Carnot efficiency as the maximum achievable efficiency no longer apply. Instead a new approach adapted to the non-equilibrium exchanges is required. From an application point of view such an adapted approach is needed to optimize technically relevant thermodynamic processes (which all operate with finite rates). The optimization needs two ingredients: an optimization goal and a description which allows one to quantify the dissipation occurring in the process. While the optimization objective is a matter of choice and might be for instance "maximum power", an appropriate modelling of the processes occurring in detail is mandatory for a quantitative treatment. Only when the dissipation (or entropy production) can be quantitatively determined, does a quantitative optimization become possible.

Endoreversible Thermodynamics provides a framework, which allows to do that by viewing a system as a network of internally reversible (endoreversible) subsystems exchanging energy in an irreversible fashion. All irreversibilities are confined to the interaction between the subsystems. The concept of 'endoreversibility' has proven to be a powerful tool for the construction of models with the desired qualities. A proper modelling of the transport equations between the subsystems allows to quantify the dissipation associated with the energy exchange. The assumption of endoreversibility simplifies the expenditure for the analysis essentially. This concept of 'endoreversibility' has been successfully applied to a wide variety of thermodynamic systems and led to remarkable results [1, 2].

An important problem in the analysis of endoreversible systems is how to deal with the time dependence of process variables and parameters, i.e. how the dynamics of a system evolves during a process. This problem has first been investigated in relatively simple models, which lacked the richness in technological detail of sophisticated engine models. However, while it was this approach which made insights into thermodynamic path optimization feasible, endoreversible thermodynamics as a general theory provides a framework to deal with thermodynamical systems at all levels of detail and is thus a universal approach also ranging to very elaborate and complex models [3].

Here we will present this modelling approach and show, how the quantitative determination of the entropy production is performed. This approach is adapted to systems consisting of discrete units like reservoirs, engines or reactors, which exchange thermodynamic extensities like volume, mole number or charge in the form of fluxes. This approach can also handle momentum or angular momentum fluxes and can thus seamlessly incorporate mechanical exchange processes. The potential of Endoreversible Thermodynamics becomes apparent in real world thermodynamic optimization problems [4,5].

Keywords: endoreversible thermodynamics, finite-time thermodynamics, quantification of entropy production

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FLUCTUATING BOUNDARIES BETWEEN MECHANICS AND THERMODYNAMICS

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ABSTRACT

Is there any fixed boundary from what we call mechanics and what we describe in terms of heat along general processes? To try to formulate at least an attempt at an answer, consider a molecular cluster and a related discrete-to-continuum approach to its dynamics. We can first associate with averages the structures that we attribute to mechanics (say those described by the balance equations of forces and couples), so that heat is described by fluctuations [1]. However, in a multi-scale view of the discrete-to-continuum transition, we can also decompose in some way the fluctuations, considering a portion of them (one defined in appropriate way) as contributing to mechanics while the remaining part of fluctuations as associated with heat [2], [3]. We discuss both circumstances and the related notions of temperature that may be defined.

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ENTROPY AND ADIABATIC ACCESSIBILITY

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ABSTRACT

In 1856 Rudolf Clausius coined the word entropy as a suitable name for what he had been calling the 'transformational content of a body'. The new word made it possible to state the second law of thermodynamics in the brief but alarming form: The entropy of the universe tends toward a maximum. Thus, entropy is originally related to possible changes, not to chaos and probability as in subsequent work by Boltzmann and Gibbs. In my contribution to the mini-symposium a modern version of this view on entropy, developed in joint work with Elliott Lieb already 25 years ago, will be sketched. The key concept is the relation of adiabatic accessibility between pairs of states of macroscopic bodies. It turns out that an essentially unique entropy for equilibrium states emerges from a few basic properties of this relation. The situation is different for non-equilibrium states, however, where as a rule more than one entropy function is required to delimit adiabatic accessibility. A recent exposé of this work can be found in [1].

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IS THERMODYNAMICS FUNDAMENTAL?

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University of Mainz, Mainz, Germany

ABSTRACT

The answer to this question depends very strongly on what one takes ‘thermodynamics’ and ‘fundamental’ to mean. A typical interpretation of ‘fundamental’ would be ‘not being reducible to something else’, and based on this interpretation it is often held that thermodynamics is not fundamental because it can be reduced to the behavior of individual particles in the framework of statistical mechanics. These reductions, however, do at a closer look often rely on assumptions or concepts that come from thermodynamics, implying that thermodynamics - while not being in conflict with the microscopic laws of physics - also can tell us something over and above what we learn from these microscopic laws. A good illustration of this is the problem of explaining the irreversible approach to thermodynamic equilibrium from the reversible Hamiltonian equations. It turns out that these explanations rely on assumptions that Hamilton’s equations themselves cannot justify. Moreover, also here one faces terminological issues: The way one can explain the approach to equilibrium depends strongly on what one takes ‘equilibrium’ to mean.

MINI-SYMPOSIUM

Quantum Thermodynamics and Quantum Information Theory

Organiser:
Časlav Brukner (Austria)

Invited panelists:
Maximilian Lock (Austria)
Gonzalo Manzano (Spain)
Petr Jizba (Czech Republic)

THE EMERGENCE OF IRREVERSIBILITY IN QUANTUM THEORY: ENTROPY AND MEASUREMENT

Maximilian P. E. Lock
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ABSTRACT

Irreversible entropy growth implied by the second law of thermodynamics appears to conflict with the unitary, entropy-preserving evolution of isolated quantum systems. Effective irreversibility emerges in large isolated systems due to the mismatch between the effective dimension of the microscopic unitary dynamics and the resolving power of the observables in question. A quantum version of the second law can be recovered, with equilibrium fluctuations that are found to shrink as system size increases. The apparent irreversibility of quantum measurement can then argued to be a thermodynamic effect, leading to criteria for when a physical system functions as an observer.

QUANTUM STOCHASTIC THERMODYNAMICS

Gonzalo Manzano
Institute for Cross Disciplinary Physics and Complex Systems (IFISC) UIB-CSIC, Spain

ABSTRACT

In the last decades, the formalism of stochastic thermodynamics have been successfully applied to describe small nonequilibrium systems where fluctuations become important, giving important insights about the nature of irreversibility and the second law. In this talk I will discuss the extension of stochastic thermodynamics to open quantum systems that are continuously monitored using the formalisms of quantum trajectories [1]. This framework allows the derivation of universal fluctuation relations, from the famous "fluctuation theorems" for entropy production to more advanced relations based on Martingle theory [2, 3]. These allow us to split entropy production into classical and quantum contributions and can be used in applications with first passage times such as in quantum clocks [4].

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NEW CLASSES OF ENTROPIC UNCERTAINTY RELATIONS

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[2]Sussex Centre for Quantum Technologies, University of Sussex, Falmer, UK

ABSTRACT

Historically, the most widely used quantifier of quantum uncertainty has been the variance. While variance effectively captures uncertainty in terms of fluctuations (or spread) around the mean — and is well-suited for many types of state distributions — it fails to provide a meaningful measure in certain important cases, such as multimodal or heavy-tailed distributions.

Among the various alternative (non-variance-based) measures of uncertainty employed in quantum mechanics, information entropies play a particularly prominent role. In this talk, I will explore the use of entropy power, specifically the Rényi and Tsallis entropy powers, to derive one-parameter families of information-theoretic uncertainty relations for pairs of conjugate observables in infinite-dimensional Hilbert spaces.

These families form an infinite hierarchy of uncertainty relations based on higher-order statistics, which — in principle — enable the reconstruction of the underlying information distribution by measuring the associated entropy powers. I will demonstrate improvements over traditional uncertainty relations based on variance and Shannon entropy and briefly discuss their implications and applications in quantum mechanics.

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MINI-SYMPOSIUM

Thermodynamics of Long-Range Interacting Systems

Organisers:

Andrea Trombettoni (Italy)
Alessandro Campa (Italy)

Invited panelists:

Stefano Iubini (Italy)
Emma C. King (Germany)
Valerio Pagni (Switzerland)

HEAT TRANSPORT IN LONG-RANGE INTERACTING NONLINEAR LATTICES

Stefano Iubini[1*], Stefano Lepri[1], Stefano Ruffo[1,2]

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[2]SISSA – International School for Advanced Studies, Trieste, Italy

ABSTRACT

Nonlinear low-dimensional assemblies of classical coupled oscillators have been extensively studied as paradigmatic models of heat transport since many years. While for short-range forces there is currently a detailed understanding of the dynamical mechanisms leading to the establishment of the Fourier law or to its breakdown, the case of long-range interacting systems has received less attention. I will analyze the basic mechanisms underlying heat transport processes in such systems. After a general overview, I will focus on the case of a ϕ^4 chain with long-range interactions decaying as a power α of the intersite distance. Depending on α, both diffusive and superdiffusive transport regimes are identified by means of a dynamical scaling analysis of energy structure factors and excess energy correlations. An effective simplified model of transport based on Lévy flights describes successfully the numerical results. Final considerations will be drawn about possible hydrodynamic universality classes.

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OPTIMAL SPATIAL SEARCHES WITH LONG-RANGE TUNNELING

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[2]Institut fuer Theoretische Physik, Universität zu Köln, Köln, Germany

ABSTRACT

A quantum walk on a lattice is a paradigm of a quantum search in a database. The database qubit strings are the lattice sites, qubit rotations are tunneling events, and the target site is tagged by an energy shift [1–3]. For continuous-time quantum walks, the walker diffuses across the lattice and the search ends when it localizes at the target site. The search time T can exhibit Grover's optimal scaling [4,5] with the lattice size N, namely, $T \sim \sqrt{N}$, on an all-connected, complete lattice. For finite-range tunneling between sites, instead, Grover's optimal scaling is warranted when the lattice is a hypercube, as illustrated in Fig. 1(a), of dimension $d > 4$ [3]. In this symposium, we will show that Grover's optimum can be reached in lower dimensions on lattices of long-range interacting particles, when the interaction strength scales algebraically with the distance r as $1/r^{\alpha}$ and $0 < \alpha < 3d/2$, see Fig. 1(b) [6]. For $\alpha < d$ the dynamics mimics the one of a globally connected graph. For $d < \alpha < d+2$, the quantum search on the graph can be mapped to a short-range model on a hypercube with spatial dimension $d_s = 2d/(\alpha - d)$, indicating that the search is optimal for $d_s > 4$. The critical spectral dimension $d_s = 4$ corresponds to exponent $\alpha = \alpha_c = 3d/2$, which is associated with a phase transition in the time complexity of the search problem. The corresponding order parameter χ_α, with its squared value being the fidelity, is shown in Fig. 2. Our work [6] hereby identifies an exact relation between criticality of long-range and short-range systems, it provides a quantitative demonstration of the resources that long-range interactions provide for quantum technologies, and indicates when existing experimental platforms can implement efficient analog quantum search algorithms.

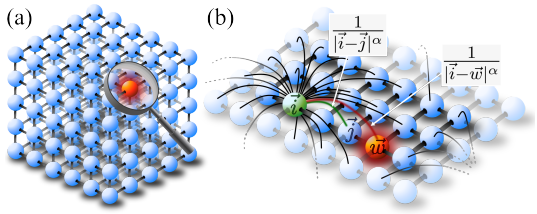

Figure 1: (a) Illustrative graphic of search on a cubic lattice (hypercube with $d = 3$) with nearest-neighbor couplings ($\alpha \to \infty$). Target node for which we search is depicted in red. (b) Schematic of the power-law scaling of the connectivity of a single site $\vec{i}$ in a two-dimensional cubic lattice.

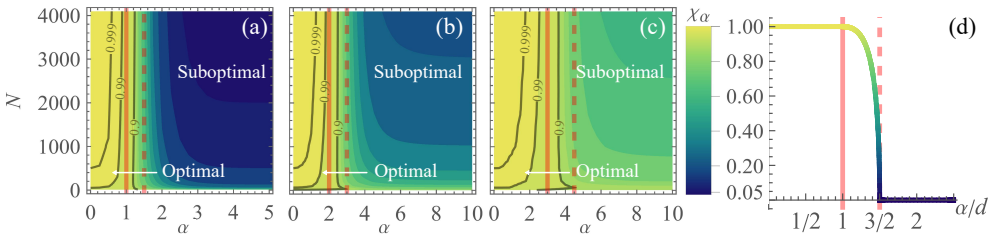

Figure 2: *Upper bound to the search fidelity:* χ_α as a function of the number of lattice sites N and long-range tunneling exponent α for (a) $d = 1$, (b) $d = 2$, and (c) $d = 3$. Vertical lines correspond to $\alpha = d$ (solid) and $\alpha = \alpha_c = 3d/2$ (dashed). (d) Asymptotic behavior of χ_α in the limit $N \to \infty$ as a function of α/d. For $0 < \alpha < d$, $\chi_\alpha = 1$, while for $d < \alpha < 3d/2$ it decreases monotonically to zero as $\chi_\alpha = \sqrt{3 - 2\alpha/d}/(2 - \alpha/d)$.

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CRITICAL AGING AND RELAXATION DYNAMICS IN LONG-RANGE SYSTEMS

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ABSTRACT

We investigate the dynamical scaling properties of a long-range O(N) model subjected to a sudden quench to its critical temperature [1], with a particular emphasis on the resulting aging behavior and the broader implications for non-equilibrium statistical mechanics. In systems with long-range interactions characterized by a power-law decay, the interplay between spatial correlations and temporal evolution presents rich and tunable dynamical regimes [2]. By systematically varying the range of interactions, we demonstrate that the aging exponent of the system can be effectively controlled, revealing a direct mechanism for modifying the dynamical scaling properties. This tunability offers a powerful means to explore a wide spectrum of non-equilibrium behaviors, ranging from those characteristic of short-range interacting systems to novel scaling regimes unique to long-range models.

To unravel these properties in a controlled and systematic manner, we first consider a continuous field-theoretical description of the problem and then we develop a functional renormalization group (fRG) approach specifically inspired by boundary critical phenomena. The fRG formalism provides a natural framework for analyzing systems where time-translation invariance is explicitly broken, making it particularly well suited for studying the aging dynamics of critical systems following a quench. Unlike traditional perturbative approaches, our fRG treatment allows for a non-perturbative picture, capturing crucial scaling behavior even in regimes where standard approximations break down [3]. This approach is further reinforced by benchmarking our findings against the exactly solvable large-N limit of the model, which serves as a valuable reference point for validating the predictions obtained from the renormalization group analysis.

Furthermore, we extend the so-called effective dimension [4] framework—originally formulated to establish a mapping between short-range and long-range interacting systems in equilibrium—to the non-equilibrium setting. This generalization provides deeper insight into the universality of dynamical critical phenomena and elucidates the connections between different classes of interacting systems far from equilibrium. By leveraging this framework, we gain a more comprehensive understanding of how long-range interactions modify the fundamental scaling properties that govern relaxation and aging in classical dissipative systems.

Finally, we broaden our analysis to quantum systems by incorporating the Keldysh formalism within the fRG framework. This extension enables us to study the prethermal evolution of quantum long-range systems following a quantum quench to their dynamical critical point, shedding light on the role of quantum fluctuations in shaping non-equilibrium dynamics. By systematically addressing both classical and quantum regimes, our work provides a unified perspective on long-range interacting systems far from equilibrium, offering new theoretical insights with potential implications for experimental realizations in ultracold atomic gases, trapped ions, and other platforms exhibiting tunable long-range interactions [2].

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MINI-SYMPOSIUM

Stochastic Thermodynamics in Physics and Beyond

Organisers:

Jan Korbel (Austria)
Édgar Roldán (Italy)

Invited panelists:

Debraj Das (Italy)
Ken Sekimoto (France)
Rosalba Garcia Millan (UK)
Artemy Kolchinsky (Spain & Japan)
Sarah Loos (UK & Germany)

QUANTUM RUN-AND-TUMBLE MEASUREMENT ENGINE

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[2]SISSA – International School for Advanced Studies, Trieste, Italy

ABSTRACT

We introduce a single-qubit quantum measurement engine powered by backaction energy input. This engine utilizes the fundamental principles of quantum measurement and feedback to harness work from the single-qubit system. To reduce the energetic costs associated with information processing, we introduce a lazy feedback mechanism [1]. The lazy feedback step stochastically utilizes measurement outcomes, prescribed by a designated *laziness* probability. As a result, we show that the cumulative work extracted over successive cycles of the engine exhibits a second-order Markov process, analogous to a classical run-and-tumble process with transient anomalous diffusion. We derive exact analytical expressions for finite-time moments of the extracted work and key statistical measures, including first-passage-time distributions. Furthermore, we obtain the optimal laziness probability that maximizes the mean power extracted per cycle from the quantum engine. All analytical results on the extracted work are readily applicable to the run-and-tumble process, for which obtaining first-passage-time distributions is highly nontrivial. Our work thus highlights hitherto-unexplored links between quantum engine and active matter.

Keywords: quantum measurement engine, run-and-tumble dynamics, nonequilibrium work statistics, quantum thermodynamics, active matter

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INTRINSIC PHYSICAL ASPECTS OF MARTINGALE - MARTINGALE DRIFT AND CLASSICAL CANONICAL SPIN DISTRIBUTION

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ABSTRACT

Martingale property is a concept widespread in mathematics and statistical mechanics. Is there any intrinsic physical aspect hidden in the martingale beyond just a tool? We have shown analytically that, when the evolution of the drift function is a martingale associated with the histories generated by the very Langevin equation, the drift function of the d-dimensional Langevin equation is the Langevin function with a properly chosen scale factor. Moreover, we numerically demonstrated that those generated histories from a common initial data, which become asymptotically ballistic, show their orientations to obey the classical canonical spin statistics under the external field corresponding to the initial data. Finally we showed that the canonical density of a d-dimensional spin evolves as martingale associated with the process generate by the above mentioned Langevin equation. This finding, as a byproduct, leads to an analytical proof of the above numerical finding. These results elucidate a ”physical link” between the martingale and canonical spin statistics.

OPTIMAL CLOSED-LOOP CONTROL OF ACTIVE PARTICLES

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ABSTRACT

Minimising the energetic cost of moving an active particle in a confining trap over a target distance is a fundamental problem of optimal control of active matter. The control is a closed-loop protocol if it involves information about the particle state, such as its initial position or self-propulsion, and it is an open-loop protocol otherwise. In this talk, I will present recent analytical results where we derive the optimal time-dependent protocol that minimises its associated average work [1, 2]. I will show that, while the optimal open-loop protocol is independent of the particle's activity, the optimal closed-loop protocol utilises the initial self-propulsion to lower the overall accumulated work. Depending on parameters, the associated work becomes negative, indicating that the activity of the particle can be harvested to extract work from the system. Moreover, the extractable work reaches a maximum at a finite persistence time.

I will further present a minimal active information engine based on a periodic optimal closed-loop protocol and compare its performance when run by a Run and Tumble Particle or by an Active Ornstein-Uhlenbeck Particle. While the average work is identical in both cases, the work distribution, its fluctuations and the information efficiency of the engine are advantageous when the engine is run by a Run and Tumble Particle.

Keywords: optimal control, active matter, work extraction, information engine

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THERMODYNAMIC INFERENCE: CYCLE AFFINITY, CROSS-CORRELATION ASYMMETRY AND BEYOND

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[1]Pompeu Fabra University, Barcelona, Spain
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ABSTRACT

I will discuss the problem of *thermodynamic inference*, which aims to infer thermodynamic quantities from statistics of fluctuating systems. Most work in the field has focused on the inference of *entropy production*, a measure of thermodynamic dissipation that depends on microscopic kinetics. However, one may also consider a different — and complementary — problem of inferring *cycle affinity*, a measure of nonequilibrium driving strength that does not depend on microscopic parameters.

In this context, I will introduce our recent work [1] which derived a simple inequality for discrete-state Markovian systems. This inequality relates cycle affinity to *cross-correlation asymmetry*, the asymmetry of time-lagged cross-correlations between any pair of observables a and b in stationarity. Remarkably, our inequality can be understood as a thermodynamic version of the isoperimetric inequality, which relates the area and perimeter of regular polygons. As one illustration of our result, we prove a previously-conjectured bound on the coherence of noisy oscillations [2]. As another illustration, we derive a thermodynamic bound on directed information flow in a model of biochemical signal transduction [3]. This last example is illustrated below in Figure 1.

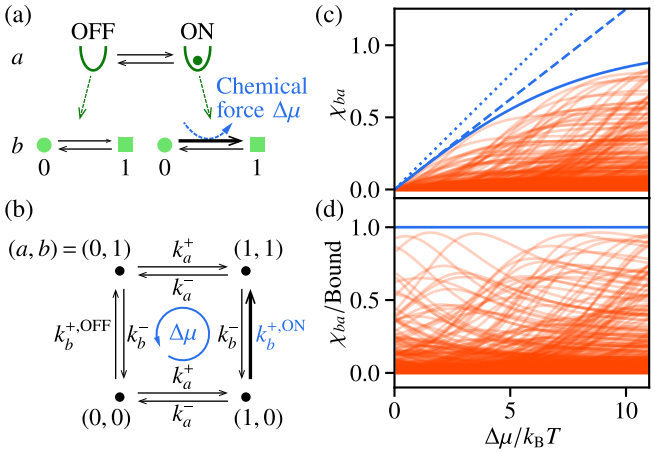

Figure 1: (a) Simple model of biological signal transduction from [3]. (b) Formulation as a Markov jump system with a nonequilibrium cycle. (c) Illustration of the bounds reported in Ref. [1]. Orange indicates (normalized) cross-correlation asymmetry χ_{ab} as a function of the cycle affinity $\Delta\mu$, which determines the rate of the transition $k_b^{+,\mathrm{ON}}$ (other kinetic rates set to random but fixed values). χ_{ba} is nonnegative for $\Delta\mu \geq 0$ in this model. Blue indicates three upper bounds on χ_{ab} in terms of cycle affinity [1]. (d) The ratio between χ_{ba} and the tightest bound $\tanh(\Delta\mu/8k_BT)$.

Keywords: stochastic thermodynamics, cycle affinity, thermodynamic inference, cross-correlations

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MOVING WITH MINIMUM EFFORT - OPTIMAL WORK PROTOCOLS FOR SYSTEMS WITH HIDDEN DEGREES OF FREEDOM

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ABSTRACT

The framework of stochastic thermodynamics provides powerful tools to quantify entropy flows, dissipation, and efficiency in small-scale processes as fluctuating quantities. A key open challenge arises when memory effects are introduced by hidden degrees of freedom that evolve on comparable timescales but remain inaccessible to direct measurement or control. Such memory naturally emerges, for instance, when the system of interest is coupled to a complex fluid with internal relaxation dynamics.

In this talk, we address the impact of memory on thermodynamically optimal control. As a paradigmatic case, we consider the problem of dragging a particle in a harmonic trap through a fluid, over a prescribed distance within a fixed time, while minimizing the average work input. For passive particles in viscous media, the optimal protocol is known to consist of two symmetric jumps at the beginning and end of the trajectory [1]. We analytically demonstrate—and experimentally confirm using colloids in optical tweezers in both viscous and viscoelastic fluids—that this feature originates from an underlying time-reversal symmetry of the optimal control problem [2]. Strikingly, we can show that symmetry holds universally for all media described by a linear generalized Langevin equation, irrespective of the specific memory kernel or noise correlations, encompassing glassy, granular, and active systems [3; 4]. Our findings thus provide both a general criterion for identifying optimal protocols and a practical strategy for constructing them.

Keywords: stochastic thermodynamics, optimal control, non-Markovian dynamics, generalized Langevin equations

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MINI-SYMPOSIUM

Thermodynamics in High-Energy Physics

Organisers:

Trambak Bhattacharyya (Poland)
Airton Deppman (Brazil)

Invited panelists:

Maciej Rybczyński (Poland)
Leonardo Tinti (Poland)
Sushanta Tripathy (Sweden)

UNREASONABLE EFFECTIVENESS OF STATISTICAL APPROACHES TO HIGH-ENERGY COLLISIONS

Maciej Rybczyński, Zbigniew Włodarczyk
Institute of Physics, Jan Kochanowski University, Kielce, Poland

ABSTRACT

This talk addresses the longstanding question of how statistical physics applies at the nano(femto) scale, a topic that emerged following the discovery of nucleation reactions in the early 1930s and was formalized by the introduction of "nano(femto)thermodynamics" as early as 2000. We examine the thermodynamic properties of small systems created in relativistic ion collisions, emphasizing the relevance of non-extensive statistics (as a special form of superstatistics) in describing multiparticle production in hadronic and nuclear interactions where fluctuations cannot be neglected. Finally, the connection between the nonextensivity parameter q and particle number fluctuations is explored, highlighting its significance in understanding these high-energy processes.

Keywords: high-energy collisions, multiparticle production processes, multiplicity fluctuations

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THE PUZZLE OF HYDRODYNAMICS IN HEAVY-ION COLLISIONS

Leonardo Tinti
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ABSTRACT

The use of relativistic hydrodynamics in Heavy-Ion Collisions is puzzling. The classical requirements of small gradients and pressure corrections are often significantly violated. The classical expectations are subverted [1], a free quantum gas has the entropy flow of a perfect fluid, despite having pressure correction, and entropy is produced, despite being a non-interacting gas. In general the quantum corrections are large with respect to the kinetic limit [2]. It is questionable then any direct derivation of hydrodynamics from the relativistic Boltzmann equation. The method of moments, on the other hand can be generalized to the full off-shell (quantum) regime [3].

Keywords: relativistic hydrodynamics, entropy flux, non-equilibrium density operator.

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KEY EXPERIMENTAL FEATURES OF QUARK-GLUON PLASMA IN HEAVY-ION COLLISIONS

Sushanta Tripathy
Division of Nuclear and Particle Physics, Lund University, Sweden

ABSTRACT

Experiments at the Large Hadron Collider (LHC) and Relativistic Heavy-ion collider (RHIC) are designed to detect, track, and identify particles in proton-proton, proton-ion, and ion-ion collisions up to the largest particle multiplicities. The core of heavy-ion collisions physics program is to study the hot and dense medium formed in heavy-ion collisions, the quark-gluon plasma (QGP), through several observables. In addition, these studies can also provide crucial input to the study of quantum chromodynamics and of the strong interaction even outside of the deconfinement regime. In this talk, the measurement of a key set of global observables mostly in the soft sector and their physics implications are discussed. Observables related to the thermal particle production and collectively expanding medium will be highlighted [1-4].

Keywords: heavy-ion collisions, quark-gluon plasma, strong interactions

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MINI-SYMPOSIUM

Thermodynamics of Learning

Organisers:

Beatriz Seoane (Spain)
Aurélien Decelle (Spain)

Invited panelists:

Dinis O. Abranches (Portugal)
Cyril Furtlehner (France)
Christian Maes (Belgium)
Pietro Rotondo (Italy)

STOCHASTIC MACHINE LEARNING: APPLICATIONS FOR MATERIALS DESIGN

Dinis O. Abranches
CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Portugal

ABSTRACT

Gaussian processes (GPs) are a class of stochastic, non-parametric machine learning models. Owing to their characteristics, GPs can be trained with small and scarce datasets. They also provide uncertainty estimates for their own predictions. As such, GPs can accelerate and optimize the discovery and design of novel materials, particularly in data-scarce scientific domains where experimental trial-and-error approaches are commonplace.

Active learning strategies are a natural extension of GPs, leveraging uncertainty quantification to select the most informative data points for subsequent evaluation. This approach enables substantial reductions in the number of experiments or simulations required to achieve accurate models of complex physicochemical systems.

This work illustrates the usage of GPs in a variety of case studies, from solvent composition optimization to molecular design. Emphasis was placed on how GPs provide not only predictive means but also quantified uncertainties, making them ideal surrogates for guiding efficient experimental or computational campaigns.

Overall, this work highlights how stochastic machine learning frameworks, anchored by Gaussian Processes and active learning, offer a principled, data-efficient route to materials discovery. By combining uncertainty-aware modelling with iterative data acquisition, these approaches can significantly reduce cost and time while improving predictive performance in materials informatics and chemical engineering.

Keywords: artificial intelligence, chemical engineering, green solvents, phase diagrams.

TRAINING RESTRICTED BOLTZMANN MACHINES DESPITE PHASE TRANSITIONS

Cyril Furtlehner
Paris-Saclay University, France

ABSTRACT

Restricted Boltzmann Machine (RBM) is an old, simple but fundamental Energy based model still widely used to analyze and generate structured data of medium size. RBM are notoriously difficult to train and require advanced sampling techniques to obtain the actual equilibrium distribution of the data. In this talk we discuss the distinction to be made between equilibrium vs non-equilibrium models and the various hurdles to overcome in order to obtain interpretable equilibrium model of high quality. These hurdles are related to the presence of first and second order phase transition present all along the learning process that can be analyzed in details. Based on this analysis an innovative approach based on a low rank initialization and a parallel tempering procedure along the learning trajectory is presented that addressed efficiently the problem in difficult cases of interest.

NON-THERMODYNAMIC LEARNING

Christian Maes
Department of Physics and Astronomy, KU Leuven, Belgium

ABSTRACT

The traditional approach to modeling associative memory is variational: e.g. via steepest entropy ascent; that is a gradient flow toward local minima using a (thermodynamic) cost function. On the other hand, it appears that nature learns by solving problems via selection, adaptability,... leading to evolution and not following variational (detailed balance) principles.

We know indeed that the brain possesses a far-from-equilibrium dynamics, essentially not-governed by free energies, having no gradient dynamics. We propose an alternative which we term a "nonequilibrium-enabled frenetic steering." There, strong dissipation is not avoided at all, but is essential to enable the use of the time-symmetric dynamical fluctuation sector. An important role is played by Landauer's blowtorch theorem to select population and current statistics. In that way we propose to re-think learning as a non-thermodynamic process, where dissipation has its role in harnessing time-symmetric fluctuations, enabling frenetic steering. We hope that may offer a viable alternative leading to models of natural intelligence.

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STATISTICAL PHYSICS OF DEEP LEARNING

Pietro Rotondo
University of Parma, Italy

ABSTRACT

Understanding how and why Deep Learning works is considered a major challenge in Mathematics, Computer Science and Theoretical Physics. In this talk, I will present recent advances in Deep Learning Theory, focusing on the so-called proportional regime (which is formally defined as the thermodynamic limit where both the size of the trainset and the size of the hidden layers are taken to infinity keeping their ratio finite).

I will show that this regime is suitable to rationalise the behaviour of realistic finite width deep neural networks. In particular, I will show that an effective statistical physics description based on "kernel renormalization" captures feature learning in finite architectures and identifies different forms of representation learning that strongly depend on the topology and weight-sharing properties of the architecture.

MINI-SYMPOSIUM

New Horizons in Continuum Mechanics

Organizers:

Antonio Sellitto (Italy)
Vito Antonio Cimmelli (Italy)

Invited panelists:

Arkadi Berezovski (Estonia)
Paolo Maria Mariano (Italy)
Francesco Oliveri (Italy)
Vittorio Romano (Italy)
Michele Sciacca (Italy)
Federico Zullo (Italy)

ON THE VELOCITY OF TWIN BOUNDARY

Arkadi Berezovski
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ABSTRACT

One of the most essential features of twins is their ability to move in response to external forces, which results in growth of one of the differently oriented lattices and carries a macroscopic deformation of the material. Twin boundary motion is especially essential in shape memory alloys [1],[2], where the twins appear between different variants of martensite. The reversible reorientation of martensite via twins motion is the key mechanism of pseudoplastic straining of shape memory alloys, and the speed of this process can be decisive for the overall mechanical performance of the alloy.

Twin boundary velocity is a macroscopic characteristic of the twinning process. The velocity is measurable, but experimental results range from near-zero up to sound velocity of a material. The diversity of experimental data related to the motion of twin boundaries cannot be explained within the context of classical continuum description. The extension of the continuum description of twin boundary motion by internal variables allows for the theoretical distinction between twin slow and fast dynamics. Internal variables serve as order parameters indicating the difference in twin variants. This makes it possible to use them to identify twin boundaries. Equations of motion are coupled to evolution equations of internal variables.

The simplest possible scenario (uniaxial motion with only two twin variants) was chosen to explain the experimentally observed discrepancies in twin boundary velocities. A diffusional slow motion of twin boundaries is reproduced in the case of a single internal variable [3], and the gradient of the internal variable serves as an order parameter. In contrast, the dual internal variable approach [4] leads to a hyperbolic evolution equation for the evolution of the primary internal variable and provides fast dynamics of a twin boundary.

Keywords: thermodynamics with internal variables, twin boundary dynamics, macroscopic description

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A REVISITATION OF THE PRINCIPLE OF MATERIAL OBJECTIVITY: A LIE SYMMETRY APPROACH

Matteo Gorgone, Francesco Oliveri, Patrizia Rogolino
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ABSTRACT

In continuum mechanics and thermodynamics, the principle of material frame-indifference, also referred to as the principle of material objectivity, is a fundamental postulate introduced by Truesdell and Noll in 1965 [1]. It represents the main requirement for assigning constitutive relations and identifying objective quantities.

Roughly speaking, the principle states that the constitutive relations must be invariant with respect to a change of the observer, namely by a transformation like

$$\mathbf{x}^\star = Q(t)\mathbf{x} + \mathbf{c}(t), \qquad t^\star = t + t_0$$

where Q is an arbitrary time dependent orthogonal matrix, and $\mathbf{c}$ an arbitrary time dependent vector. This principle implies, the invariance of scalar functions, and suitable transformations for vectors and tensors, say

$$f(\mathbf{x}^\star) = f(\mathbf{x}), \qquad \mathbf{v}(\mathbf{x}^\star) = Q\mathbf{v}(\mathbf{x}), \qquad T(\mathbf{x}^\star) = Q^T T(\mathbf{x}) Q.$$

A long series of strong disputes accompanied this principle; a historical view (at least, until 2008) can be found in [2].

We exploit the transformations for scalar, vectorial and tensorial functions in order a *principle of material frame indifference* is fulfilled by using the infinitesimal invariance with respect to the so called fundamental group of mechanics [3], *i.e.*, the ten–parameter Lie goup made of isometries, time translation and Galilean transformations. So doing we can provide a suitable framework for identifying objective quantities, providing the desired transformation rules for scalars, vectors and tensors, and giving the representation for isotropic constitutive functions. This approach provides the same results obtainable by the Truesdell and Noll principle in most of the cases, but not all. The differences are discussed.

Keywords: frame–indifference principle, Lie symmetries, invariance

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SEMICLASSICAL AND QUANTUM TRANSPORT OF PHONONS

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ABSTRACT

Thermal effects in micro and nano electronic and mechanical devices has acquired an increasingly relevant importance [2; 3; 4] and their description requires accurate physical models beyond the standard Fourier law. At kinetic level a good model can be formulated by introducing the phonons, which are bosonic quasi particles, whose dynamic in the semiclassical case (mean-free path greater or equal the characteristic length of the phenomenum) is described by the Peierls-Boltzmann equation for each phonon branch. In the case of typical lengths smaller than the phonon mean-free path quantum effects must be taken into account as well (see [5]). A natural extension of the Peierls-Boltzmann equation is the Wigner one that better reveals the wave nature of phonons and still keeps the structure of a kinetic formulation. However, in the literature an almost standard approximation is to consider the Wigner equation with quadratic dispersion relation. We focus on the inclusion of general dispersion relation into the Wigner equation and then we consider as particular cases the group velocity of acoustic and optical phonons.

The approach is based on Weyl quantization and Moyal's calculus [6]. In order to get asymptotic expression for the heat flux the pseudo-differential operators are expanded up to the second order in $\hbar$ while the phonon-phonon collision operators are modelled in a relaxation form depending on a local equilibrium temperature which is definite according to [2].

An energy transport model is obtained by using the moment method with closures based on a quantum version of the Maximum Entropy Principle [7; 8; 9; 10; 11; 12; 13]. An explicit form of the thermal conductivity with quantum correction is obtained under a suitable scaling. Numerical results are presented in the semiclassical limit for thermal effects in graphene.

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NONLINEARITY IN THE HEAT TRANSPORT MODELS

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ABSTRACT

The growing possibilities of heat transfer control in solids, and in particular in nanosystems, has stimulated the research of thermal transfer modeling. In those systems where the relaxation time of the heat flux is not neglegible, the Fourier law has been generalized by the so-called Maxwell-Cattaneo (MC) equation. Additionally, in those systems with size comparable to the mean free path of heat carriers, nonlocal contributions are required to be considered, and the heat flux satisfies the so-called Guyer–Krumhansl (GK) equation (also related to phonon hydrodynamics) [1]. These models are linear differential equations for the heat flux field, and they have led to some interesting results in the propagation of thermal waves and in the hydrodynamics of heat transport. There is a recent interest to investigate the nonlinear contribution to these models, in order to analyzed similarities and differences with other well-known physical systems. In this talk I will introduce some recent results we have found by considering the nonlinear contributions to the MC equation [2] and to the GK equation [3; 4]. In the former we have shown a parallelism with optical communications which has led to solitons. The other two papers instead are related to phonon hydrodynamics and they take into account a possible non-Newtonian generalization of the GK and the contribution (linear or nonlinear) of the walls.

Keywords: heat transport, Maxwell-Cattaneo equation, Guyer-Krumhansl equation, phonon hydrodynamics, solitons, thermal waves[†]

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MODLES OF HEAT CONDUCTION THROUGH RATE EQUATIONS

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[2]INFN, Milano Bicocca, Milano, Italy
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ABSTRACT

In this talk we present a general constitutive scheme within continuum thermodynamics to describe the behavior of heat flow in deformable media. The rate-type constitutive equations are defined in the material (Lagrangian) description where the standard time derivative satisfies the principle of objectivity. All constitutive functions are required to depend on a common set of independent variables and to be consistent with thermodynamics. The statement of the Second Law is formulated in a general nonlocal form, where the entropy production rate is prescribed by a non-negative constitutive function and the extra entropy flux obeys a no-flow boundary condition. The thermodynamic response is then developed based on Coleman-Noll procedure. In the local formulation, the free energy potential and the rate of entropy production function are assumed to depend on temperature, temperature gradient and heat-flux vector along with their time derivatives. This approach results in rate-type constitutive equations for the heat-flux vector that are intrinsically consistent with the Second Law and easily amenable to analysis. A huge class of linear and nonlinear models of the rate type are recovered (e.g., Cattaneo-Maxwell's, Jeffreys-like, Green-Naghdi's, Quintanilla's and Burgers-like heat conductors). For each of these models some comments about the properties of the solutions of the corresponding temperature equation will be given. In particular, the stability of the solutions will be derermined by the classical Routh-Hurwitz criterion. In the (weakly) nonlocal formulation of the second law, both the entropy production rate and an entropy extra-flux vector are assumed to depend on temperature, temperature gradient and heat-flux vector along with their spatial gradients and time derivatives. Within this classical thermodynamic framework the nonlocal Guyer-Krumhansl model and some nonlinear generalizations are obtained. This scheme allows the formulation of new models of heat transport that are likely to apply also in nanosystems.

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SPECIAL SESSION

Nonequilibrium Thermodynamics

Invited speaker:
Péter Ván (Hungary)

Presenting authors:
Christian Maes (Belgium)
Frédéric Barbaresco (France)

CHALLENGES OF NONEQUILIBRIUM THERMODYNAMICS

Peter Ván[1,2,3]

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ABSTRACT

The presentation critically reviews some general theories (constructal, constructor, Verlinde's gravity, extended thermodynamics, GENERIC, variational methods, etc..) in which thermodynamics, and in particular nonequilibrium thermodynamics, plays an important role. It is then argued that all such attempts of a general theory face the challenge of validation and must pay attention to the following means and measures of performance and validity:

– Prediction of new experiments.
– Resolution of existing paradoxes.
– Theoretical compatibility, in particular the explanation of universality.

These measures of validity may differ for different theoretical approaches, but one aspect deserves special attention: any proposal must demonstrate compatibility with classical theories: classical thermodynamics and continuum physics, including heat conduction, continuum mechanics and electrodynamics. A consistent connection to the classical background can validate the theory with an enormous amount of empirical facts (observations, experiments and engineering experience), and it is also a source of paradoxes, possible new experiments that can be solved, further increasing the credibility of any theory.

There are two types of approaches. If the mechanical principles of a perfect world are extended to thermodynamics, then the origin of dissipation must be explained. On the other hand, if the thermodynamic principles of an imperfect world are primary, then the laws of perfect mechanics must be explained and validated.

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NOETHER'S THEOREM IN IRREVERSIBLE THERMODYNAMICS

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ABSTRACT

After Helmholtz, the mechanical foundation of thermodynamics included the First Law $dE = \delta Q + \delta W$, and the first part of the Clausius heat theorem $\delta Q_{rev}/T = dS$. The resulting invariance of the entropy S for quasistatic changes in thermally isolated systems invites a connection with Noether's theorem (only established later). In this quest, we continue an idea, first brought up by Wald in black hole thermodynamics and by Sasa et al. in various contexts. We follow both Lagrangian and Hamiltonian frameworks, and emphasize the role of Killing equations for deriving a First Law for thermodynamically consistent trajectories, to end up with an expression of "heat over temperature" as an exact differential of a Noether charge. We extend that scheme to a continuous symmetry for the dynamical fluctuations around (nonlinear) gradient flow. The latter connects macroscopic equilibrium conditions upon introducing a quasistatic protocol of control parameters. The entropy state function becomes the Noether charge.

Keywords: Noether theorem, gradient flow, Helmholtz theorem

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JEAN-MARIE SOURIAU LIE GROUPS THERMODYNAMICS & KOSZUL INFORMATION GEOMETRY STRUCTURES FOR THERMODYNAMICS-INFORMED NEURAL NETWORKS (TINN) AND LIE GROUPS MACHINE LEARNING

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ABSTRACT

The symplectic model of statistical mechanics developed by Jean-Marie Souriau—termed the "Thermodynamics of Lie Groups"—extends the structures of information geometry to the realm of Lie groups. This framework enables the definition of Maximum Entropy Gibbs densities possessing the property of covariance under the action of the group operating on the system. Moreover, it generalises the Fisher-Rao-Fréchet metric to Lie groups, rendering it invariant under the group's action. Crucially, Shannon's axiomatic definition of entropy is supplanted by a purely geometric construction, wherein entropy emerges as a Casimir invariant function defined on the leaves of the foliation induced by coadjoint orbits through the moment map associated with the group action (the moment map being the geometric counterpart of Noether's theorem). Souriau's thermodynamics of Lie groups introduces a web-like geometric structure composed of two transverse foliations: a symplectic foliation generated by coadjoint orbits (corresponding to the level sets of entropy) and a transverse Riemannian foliation (corresponding to the level sets of energy). The dynamics on each foliation make it possible to distinguish between non-dissipative phenomena (with constant entropy) and dissipative phenomena (with constant energy). This dynamic behaviour is governed by a metriplectic flow that encapsulates the first law of thermodynamics through Poisson bracket (quantitative conservation of energy) and the second law through metric flow bracket (qualitative degradation of energy and generation of entropy). We shall explore the connections between TINNs (Thermodynamics-Informed Neural Networks), metriplectic flows, and the Lie groups thermodynamics. The overarching aim is for TINNs not merely to learn from data, but also to adhere to thermodynamic constraints, thereby enabling more accurate predictions and a deeper understanding of physical systems—particularly those characterised by dissipative phenomena. Souriau Lie Groups Thermodynamics is studied in the framework of two european action, European CaLISTA COST action and European CaLIGOLA MSCA action.

Keywords: thermodynamics, transverse symplectic foliation, Lie groups machine learning, thermodynamics-informed machine learning

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SPECIAL SESSION

Thermodynamics of Small Systems

Invited speakers:

Gian Paolo Beretta (Italy)
Jan Korbel (Austria)

Presenting authors:

Alhun Aydin (Turkey & USA)
Ralph V. Chamberlin (USA)

DEFINING THE EULER FREE ENERGY (OR SHOULD WE CALL IT HILL FREE ENERGY?): A GENERAL STABLE-EQUILIBRIUM PROPERTY, NON-TRIVIAL FOR SMALL-SYSTEMS

Gian Paolo Beretta
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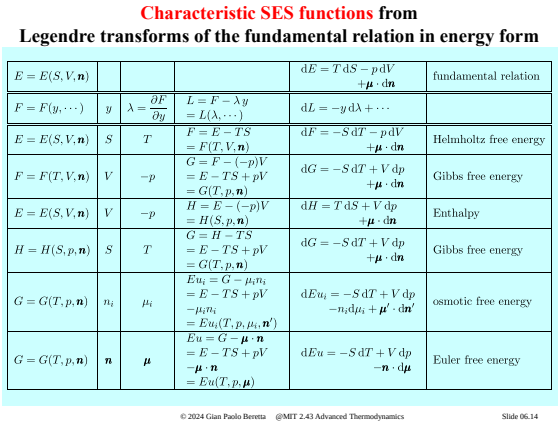
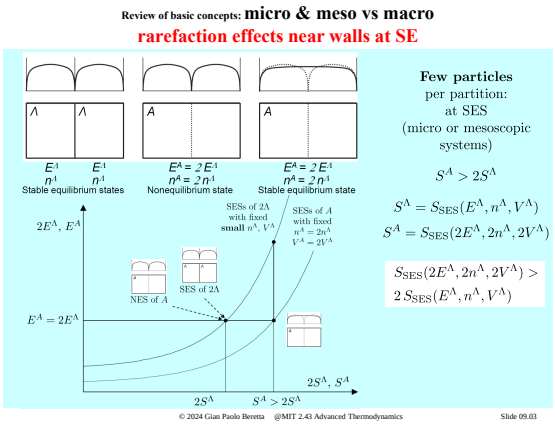
ABSTRACT

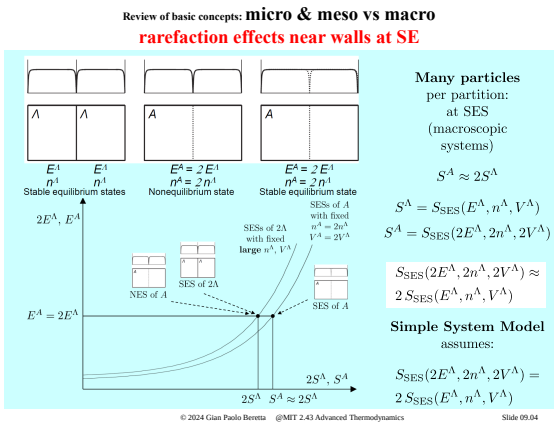
In thermodynamics, the state principle [1, Ch. 8] implies for all confined systems, large and small, the existence of the relation $S = S(E,V,N_1,\dots,N_r)$. Its Legendre transform with respect to all its variables, is the stable-equilibrium characteristic function $Eu = E - TS + pV - \sum_i \mu_i N_i = Eu(T,p,\mu_1,\dots,\mu_r)$ that in Ref. [2, Slide 06 v s 14], I decided to name "Euler Free Energy." In [1, Ch. 17] and [2, Slides 09 v s 03 and 09 v s 04], we show that this function does not vanish for small systems due to rarefaction effects near boundaries and partitions. As a consequence, properties like energy E, entropy S, enthalpy H, Helmholtz and Gibbs free energy, F and G, which are extensive in the macroscopic limit $N \to \infty$, are not extensive for small N's. Indeed, for the respective specific properties we proved the following general relations (see [1, Eqs. (17.19) and (17.22)] and [2, Slide 09 v s 09])

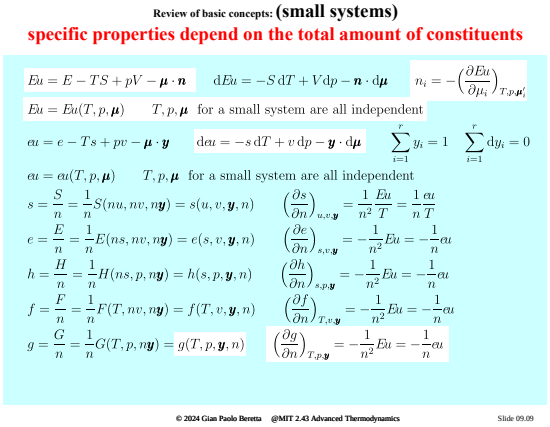
$$\left(\frac{\partial e}{\partial N}\right)_{s,v,\mathbf{y}} = \left(\frac{\partial h}{\partial N}\right)_{s,p,\mathbf{y}} = \left(\frac{\partial f}{\partial N}\right)_{T,v,\mathbf{y}} = \left(\frac{\partial g}{\partial N}\right)_{T,p,\mathbf{y}} = -T\left(\frac{\partial s}{\partial N}\right)_{u,v,\mathbf{y}} = -\frac{1}{N^2}Eu\,.$$

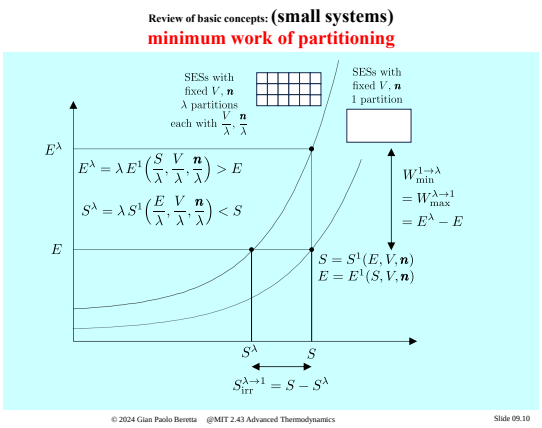
In this presentation, like in [2, Slides 09 v s 10 and 09 v s 11], I explain how the Euler free energy is also related to the minimum work required to increase (maximum work extractable by decreasing) the number of partitions by one. This can be illustrated very effectively by means of the representation of equilibrium and nonequilibrium states on energy–entropy diagrams we developed in [1, Ch. 13], as shown in the slides reproduced below.

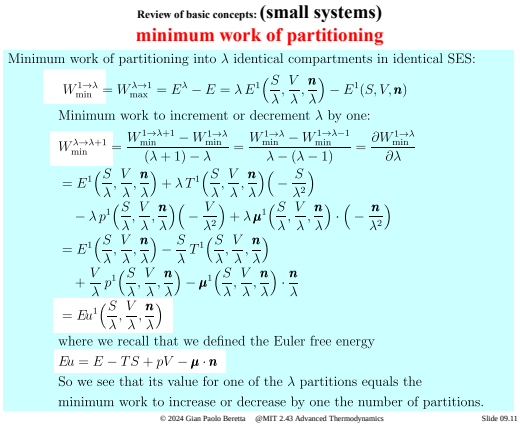












I hope my presentation will inspire further exploration of the connections between these general thermodynamic concepts applied to small systems and both classical and recent formulations of equilibrium thermodynamics for small systems [3] and nanothermodyamics [4], based on Hill's ensemble procedure, which we did not invoke to derive the presented relations and results and which, therefore, appears conceptually unnecessary. So, one question is: Does the Euler free energy coincide with Hill's subdivision potential? If so, I would agree to call *Eu* the "Hill Free Energy."

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THERMODYNAMICS OF STRUCTURE-FORMING SYSTEMS

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Complexity Science Hub, Vienna, Austria

ABSTRACT

Many natural and social systems exhibit self-organization, where particles or agents aggregate into clusters while the total number of entities remains fixed. To describe such structure-forming systems, we introduce a canonical ensemble framework that generalizes Boltzmann's entropy by accounting for both microscopic states and mesoscopic cluster configurations. This leads to new combinatorial expressions for multiplicity and entropy, which satisfy most information-theoretic and thermodynamic axioms but reflect the specific constraints of structured systems.

From this entropy, we derive equilibrium distributions via a MaxEnt principle, characterize free energy, and obtain cluster size distributions. Extending the framework to stochastic thermodynamics, we generalize fluctuation theorems for structure-forming systems.

Applications range from self-assembly of Janus particles to opinion dynamics in social systems and network models of phase transitions, demonstrating how the approach captures both continuous and discontinuous transitions. The results show that a canonical thermodynamic treatment provides a unifying description of clustering phenomena across physics and complex systems.

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UNCONVENTIONAL THERMODYNAMIC SPONTANEITY DUE TO NONUNIFORM LEVEL SCALING

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[2]Department of Physics, Harvard University, Cambridge, Massachusetts, USA

ABSTRACT

Thermodynamics of quantum confined systems is different than their classical counterparts due to quantum size and shape effects. While quantum size effects cause effects like loss of extensivity of thermodynamic properties, the quantum shape effects cause even more unconventional effects including classically inconceivable thermodynamic behaviours, such as spontaneous transitions into lower entropy states, temperature-dependent work exchanges, cooling by adiabatic compression or heating by adiabatic expansion, and net work extraction occurring at the cold side (as opposed to the hot side) in thermodynamic cycles [1,2].

Here we consider a quantum particle confined in a nested domain (red and blue regions) like the one shown in Figure 1a. Both outer and inner square boundaries are impenetrable for the particle. The inner square is free to rotate, which allows one to control the shape of the domain with the shape parameter θ rotation angle, without changing the sizes (volume, area, etc.) of the domain. This technique of generating a specific type of geometric coupling between the energy levels of a quantum system called the size-invariant shape transformation [3]. Unlike global transformations of the system parameters, which affect all energy levels uniformly, local transformations, such as shape, can modulate specific regions of the spectrum in a nonuniform manner.

We investigate the variations of thermodynamic quantities, such as free energy, entropy and internal energy, under quantum shape effects. We observe that entropy of the system decreases spontaneously due to the nonuniform level scaling. We explain the fundamental reason behind this phenomenon by introducing a novel effect called the quantum thermal avalanche [3]. Furthermore, we explore the possibility of leveraging the effect in a two-level quantum systems and show that it is possible to exploit the nonuniform level scaling even in the simplest nontrivial quantum systems [4].

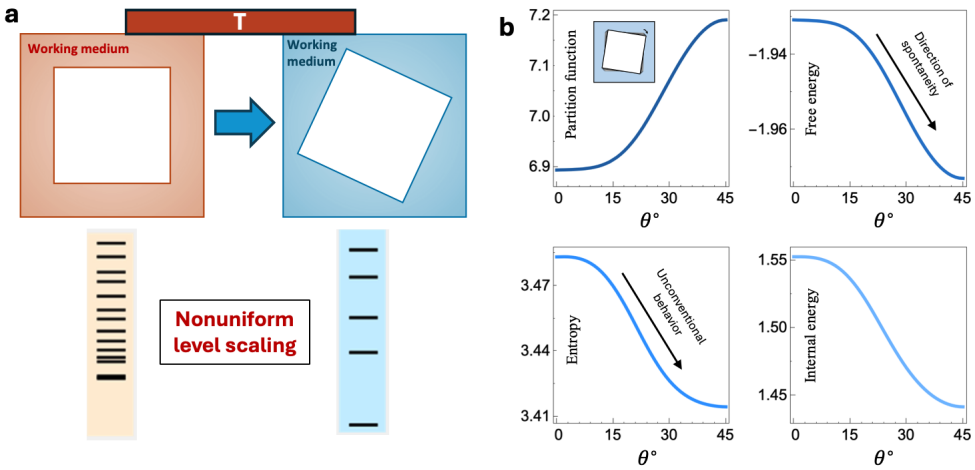

Figure 1: (a) Size-invariant shape transformation causes a nonuniform level scaling in the energy spectrum of the quantum particle confined in the working medium. Rotation angle of the inner object determines the shape of the confinement domain by keeping the sizes fixed. (b) Variation of the thermodynamic quantities under a quasistatic and isothermal size-invariant shape transformation. Entropy of the system reduces in the direction of thermodynamic spontaneity, which is a hallmark of the quantum shape effect.

Keywords: nanoscale thermodynamics, quantum confinement, entropy, thermodynamic spontaneity

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SMALL AND SIMPLE SYSTEMS THAT FAVOR THE ARROW OF TIME

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ABSTRACT

The second law of thermodynamics is the source of the irreversibility that we experience in everyday life. One formulation of this 2nd law states that the entropy of an isolated system increases irreversibly until it reaches its maximum value. Then the entropy stays at this maximum, which stabilizes the thermal equilibrium and helps to define the temperature (T) needed for Boltzmann's factor ($e^{-J/kT}$) to give the probability that a system has energy J. A common claim is that the 2nd law is not microscopic, instead applying only to large and complex systems that are unlikely to return to their initial state, while small and simple systems are routinely reversible. Another claim is that the 2nd law applies only to most initial states, while entropy may decrease from some states (that are extremely rare for large systems). I will present evidence that such claims are false, at least for computer simulations of standard models $[1-3]$. In other words, we find that the 2nd law of thermodynamics is a fundamental physical law, not just a statistical rule of thumb. I will then speculate about a microscopic mechanism that may provide a common source of irreversibility in nature.

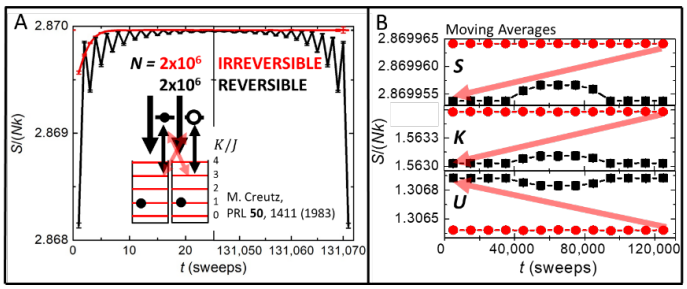

Figure 1: A) Inset: the Creutz model is a closed system that can be as small as two Ising spins coupled to a bath of two Einstein oscillators. Main figure: time-dependent entropies of two large systems having irreversible dynamics (red) or reversible dynamics (black). The dynamics is reversed at the midpoint of each simulation, but (of course) only reversible dynamics shows Loschmidt's paradox for entropy reduction that violates the 2nd law of thermodynamics. B) High-resolution values of the entropies of the spins U, the bath K, and the total S. Arrows show how the onset of reversible dynamics always reduces the total entropy, due to the bath.

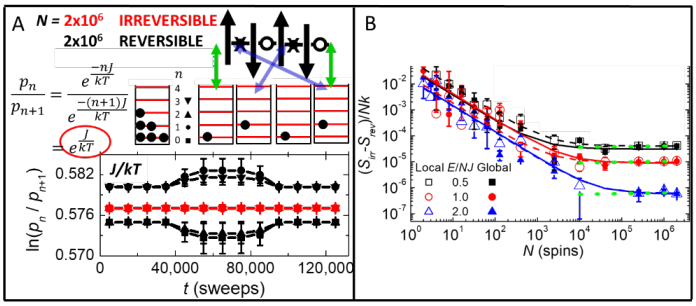

Figure 2: A) Top: the occupation of energy levels in the bath of Einstein oscillators should obey Boltzmann statistics. Bottom: logarithm of the ratio of occupation probabilities yields a well-defined temperature only for irreversible dynamics in large systems. B) Log-log plot of the difference between entropies of irreversible and reversible dynamics as a function of system size.

Keywords: irreversible thermodynamics, second law, Loschmidt's paradox, statistical fluctuations, Ising model

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SPECIAL SESSION

Physics of Life

Invited speaker:

Mohammad Reza Ejtehadi (Iran)

Presenting authors:

Artemy Kolchinsky (Spain & Japan)
Dimitrios Fessas (Italy)
Vítor A. F. Costa (Portugal)

CROSSING THE POTENTIAL BARRIERS

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ABSTRACT

Free energy calculations are important for our understanding of physical, chemical, and biological processes on an atomic scale. Provides information on the various mechanisms; computational methods to find interactions and reactions in such systems are very helpful. However, they are limited to timescales typically much shorter than in nature. In particular, the time scales of reactions depend on the high of the free energy barrier between the states, typically are far from the feasible time scales of atomistic simulations. Even coarse graining of the systems and application of semi-classical force fields cannot help to follow reactions of the machines.

In principle, finding the free-energy landscape is straightforward from the probability distribution of the states of the system. The problem is that to find the barriers, we need to calculate the free energy at points in the phase space that are usually very unlikely to be visited by the system during the simulation time.

Over the years, many computational methods have been developed to calculate free energy barriers by forcing the system to meet rare events. Jarzynski's equality enables free energy calculations for both experimental and computational works as a bridge between equilibrium statistical mechanics and non-equilibrium systems [1]. Instead, it could be more accurate to calculate the equilibrium free energy with an equilibrated method, such as umbrella sampling [2]. However, the presence of non-conservative forces in the out-of-equilibrium method and the need of considering environmental dependencies of the force fields during transitions (in both non-equilibrium and equilibrium ones) could affect the efficiency as well as the accuracy of the methods. Here we will propose some simple modifications to solve these problems without drastically increasing the computational cost [3] [4].

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GENERALIZED FREE ENERGY AND EXCESS ENTROPY PRODUCTION FOR ACTIVE SYSTEMS

Artemy Kolchinsky[1,2] , Andreas Dechant[3,*], Kohei Yoshimura[4], Sosuke Ito[2,4]

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[2]Universal Biology Institute, The University of Tokyo, Tokyo, Japan
[3]Department of Physics, Kyoto University, Kyoto, Japan
[4]Department of Physics, The University of Tokyo, Tokyo, Japan

ABSTRACT

In thermodynamics, the free energy potential is typically defined as the relative entropy between the system's actual state and the equilibrium state. This potential governs many important thermodynamic and statistical properties, but by definition it is restricted to detailed-balanced systems that relax toward equilibrium.

Recently, however, nonequilibrium thermodynamics has focused on active systems that undergo continuous driving. Such "genuine nonequilibrium" systems violate detailed balance and relax toward nonequilibrium steady states, oscillations and/or chaos. Because such system lack equilibrium states, they do not possess a free energy potential as usually defined.

In our recent work [1], we propose a *generalized free energy potential* appropriate for active systems, including both stochastic master equations and deterministic nonlinear chemical reaction networks (possibly without steady states). Our potential is defined variationally as the "most irreversible" state observable. This variational principle is motivated from several perspectives, including large deviations theory, thermodynamic uncertainty relations, and optimal transport. Our approach leads to a universal definition of the excess entropy production, the nonstationary contribution to dissipation that vanishes in steady-state. The remaining "housekeeping" term quantifies the magnitude of cyclic fluxes and nonconservative forces. We derive thermodynamic speed limits for excess entropy production for both linear and nonlinear systems.

We also show that our approach overcomes several limitations of the steady-state potential and the Hatano-Sasa (adiabatic/nonadiabatic) decomposition.

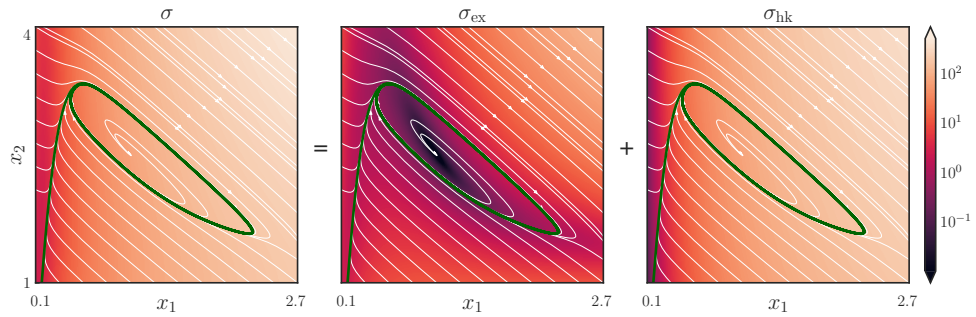

Figure 1: Using our potential, entropy production rate σ is decomposed into excess σ_{ex} and housekeeping σ_{hk} for the Brusselator (a nonlinear chemical oscillator). Colors indicate entropy production rate as a function of concentration of the two species. The green line indicates an example trajectory that approaches the limit cycle.

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PROTEIN CONFORMATIONAL STABILITY AND INTERACTIONS: THERMODYNAMIC EXPLOITATION OF CALORIMETRIC DATA

Dimitrios Fessas, Marco Signorelli, Francesca Saitta
Department of Food, Environmental and Nutritional Sciences, University of Milan, Milan, Italy

ABSTRACT

Calorimetry is widely used for the characterization of bio-systems. The rather well defined general picture of the field implies the use of techniques and theoretical approaches that depend not only on the chemical peculiarities but mainly on the status of the system with respect to the aqueous medium and the co-solutes.

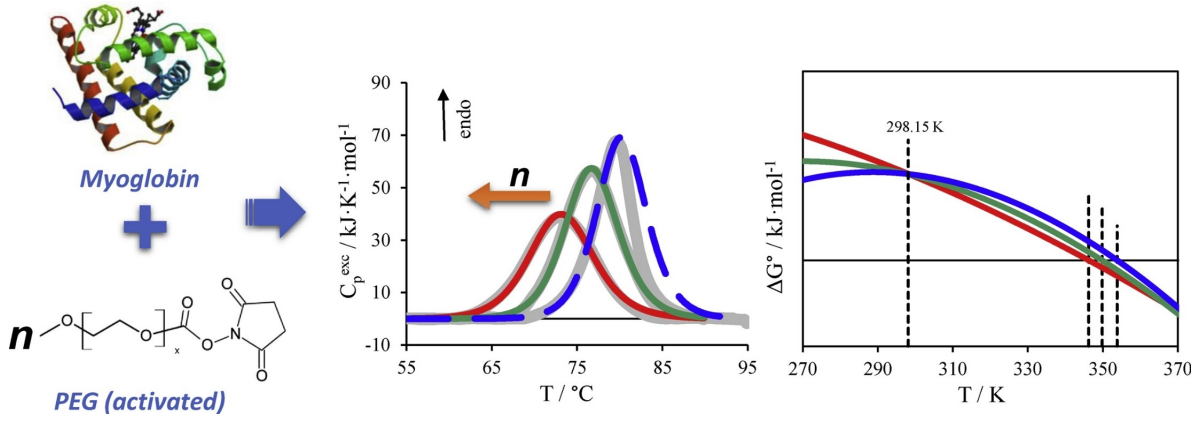

Figure 1: Protein thermodynamic stability evaluated from DSC data (graphical abstract, [1]).

In the frame of biological and pharmaceutical research, particular interest is devoted to the study the thermodynamic properties of globular proteins in diluted solution (mimicking physiological conditions) to be correlated with the structural information (crystallography, MD Simulations, NMR, etc). In this context, calorimetric data, once treated according to the formal expressions of thermodynamics and statistical mechanics, allow evaluation of the partition function of the system which includes all the thermodynamic information about the accessible states and their stability, singling out enthalpic from entropic contributions. More specifically, the HS-DSC (High Sensitive Differential Scanning Calorimetry) provides quantitative information about the mechanisms of the conformational transitions and the thermal stability of the energetic domains of the macromolecules, allowing one to separate the contributions relevant to either the solvent or the co-solutes that are responsible for specific interactions [2-3]. Further details about the thermodynamics of this kind of interaction (affinity constant, interaction enthalpy and entropy, cooperativity, allosteric effects, etc.) can be drawn from ITC (isothermal titration calorimetry) investigations [4,5].

However, despite the principles of equilibrium thermodynamics for these systems are well consolidated, they present a vast range of peculiarities that requires the implementation of specific thermodynamic models for a full experimental data exploitation that are often beyond the approaches offered by the common instrumental software.

In this frame we present some case studies on these biological systems investigated in our laboratory to highlight the methodologic approach for a suitable thermodynamic analysis.

Keywords: proteins, DSC, ITC, thermodynamics

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A THERMODYNAMIC APPROACH OF ECONOMICS

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ABSTRACT

Thermodynamics and Economics analogies are not new [1]. However, only recently has a new approach been introduced to explore this analogy [1,2]. The economic analog of the First Law is expressed through the units of merchandise and money balance equations, similar to the First Law of Thermodynamics expressed through the energy balance equation [1]. Taking as the analog of spontaneous heat transfer in the decreasing temperature direction, driven by a temperature difference, the spontaneous merchandise transfer in the increasing unit price difference, driven by a unit price difference, allows setting the Economics analog of entropy and of the Second Law. Entropy is defined through the differential expression as $dS \equiv (\delta Q/T)_{\text{intrev}}$, and the economic entropy is defined similarly through the differential expression as $dS_E \equiv (\delta M/T_E)_{\text{int rev}} = (\delta M \cdot p)_{\text{int rev}}$.

Entropy is generated in heat transfer Q through a finite temperature difference $(T_1 - T_2) > 0$, and it is $S_g = Q(1/T_2 - 1/T_1) > 0$. Similarly, economic entropy (financial value) is generated in merchandise transfer M through a finite unit price difference $(p_2 - p_1) > 0$, and it is $S_{E,g} = M(1/T_{E,2} - 1/T_{E,1}) = M(p_2 - p_1) > 0$, easily identified as the profit generation (financial value generation) in the trading operation of merchandise M, purchased at unit price p_1 and sold at the unit price $p_2 > p_1$. Defining the economic temperature as the inverse of the merchandise unit price $T_E = 1/p$, merchandise transfer occurs spontaneously in the decreasing economic temperature direction. With that in mind, developments can be made starting from the first principles which are the economic analogs of the Kelvin-Planck and Clausious statements of the Second Law, to set a Four Laws structure for Economics similar to that well-established in Thermodynamics [2].

The economic analog of the Carnot cycle, and cycles arbitrary in terms of reversibility can be introduced in Economics, as illustrated in Fig. 1 (right), which allows obtaining merchandise wealth W_M (merchandise at an infinite economic temperature, or a null unit price), the reversible economic operation having null economic entropy generation (null financial value generation). This similarly to what is made in Thermodynamics, the Carnot cycle, and cycles arbitrary in terms of reversibility as illustrated in Fig. 1 (left), allowing obtaining mechanical work W (which can be seen as heat at an infinite), the reversible operation having null economic generation.

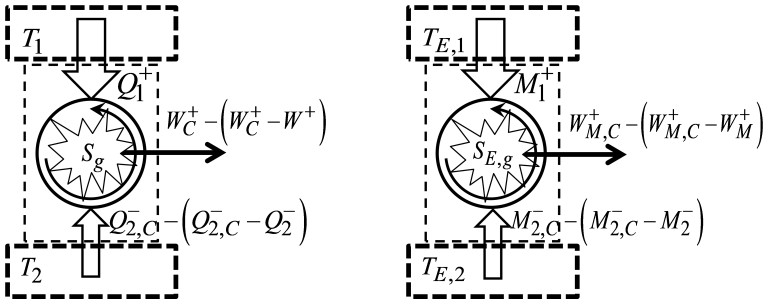

Figure 1: Cycles arbitrary in terms of reversibility: (left) In Thermodynamics; and (right) In Economics.

Relevant and challenging results can be obtained and reflections made, allowing different and innovative approaches to both, Economics and Thermodynamics. In Thermodynamics, the first analyses are based on First Law (balance) principles, and the Second Law results are a consequence of that. In Economics, the first analyses are based on Second Law (financial value) principles, and actions, of First Law nature, are a consequence of that. Only *specialists* are prepared to conduct Thermodynamics Second Law analyses, but everyone has experience and expertise and is thus a specialist, in conducting Economics Second Law analyses (financial analyses, and mental calculation of the economic entropy flows and economic entropy generation). A natural (Physics) law states that heat flows spontaneously in the decreasing temperature direction, and government laws state that merchandises (must!) flow *spontaneously* in the decreasing economic temperature direction (in the increasing unit price direction) in trading operations.

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SPECIAL SESSION

Stochastic and Information Thermodynamics

Invited speaker:

Édgar Roldán (Italy)

Presenting authors:

Shiling Liang (Germany)
Kristian Olsen (Germany)
Rajeshree Chakraborty (India)
Petr Jizba (Czech Republic)

GAMBLING CARNOT ENGINE

Édgar Roldán
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ABSTRACT

We propose a theoretical model for a colloidal heat engine driven by a feedback protocol that is able to fully convert the net heat absorbed by the hot bath into extracted work. The feedback protocol, inspired by gambling strategies, executes a sudden quench at zero work cost when the particle position satisfies a specific first-passage condition. As a result, the engine enhances both power and efficiency with respect to a standard Carnot cycle, surpassing Carnot's efficiency at maximum power. Using first-passage and martingale theory, we derive analytical expressions for the power and efficiency far beyond the quasistatic limit and provide scaling arguments for their dependency with the cycle duration. Numerical simulations are in perfect agreement with our theoretical findings, and illustrate the impact of the data acquisition rate on the engine's performance.

Keywords: stochastic thermodynamics, feedback control, first passage times, heat engines

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NON-EQUILIBRIUM RESPONSE RELATIONS: INSIGHTS FOR BIOLOGICAL INFORMATION PROCESSING

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[1] Department of Physics, Graduate School of Science, The University of Tokyo, Tokyo, Japan
[2] Center for Systems Biology Dresden, Dresden, Germany
[3] Max Planck Institute for the Physics of Complex Systems, Dresden, Germany
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ABSTRACT

We uncover fundamental physical constraints on information processing in nonequilibrium networks through rigorous analysis of response relations of Markov chains. Our work establishes two key principles: a universal precision bound of 1/2 for state observable responses to single edge/vertex perturbation that cannot be overcome by increasing network complexity of the unperturbed parts, and exact identities and bounds describing system responses to strong perturbations. These results provide physical insights into why simple network architectures - as illustrated with a push-pull motif - can be optimal despite evolutionary pressure for precision. By bridging statistical physics and information theory, our framework reveals how thermodynamic and structural constraints shape the design of nonequilibrium markov networks, with implications for biological sensing and information processing systems.

Keywords: Markov chain, response theory, information processing, nonequilibrium thermodynamics, stochastic thermodynamics

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HARNESSING NON-EQUILIBRIUM FORCES TO OPTIMIZE WORK EXTRACTION

Kristian Olsen[1], Rémi Goerlich[2], Yael Roichman[2], Hartmut Löwen[1]
[1]Institute for Theoretical Physics II - Soft Matter, Heinrich Heine University Düsseldorf, Düsseldorf, Germany
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ABSTRACT

Optimization of work extraction from non-equilibrium environments not only raises intriguing questions in thermodynamics and control, but also holds the potential to advance microscopic bio-inspired technologies. In this work, we explore optimal protocols for harmonically trapped particles driven out of equilibrium by arbitrary time-dependent internal or external forces. Beyond minimizing thermodynamic work, our protocols leverage the non-equilibrium driving forces to actively extract work, transforming transient dynamics into a source of energy.

We present exact solutions for the optimal protocol and the associated work valid for arbitrary driving forces and protocol durations. Additionally, we derive a quasistatic bound on the work, determined solely by coarse-grained time-integrated properties of the forces. The quasistatic work naturally decomposes into three contributions; i) an information-geometric term representing how the information contained in an initial non-equilibrium state can be converted to work, ii) the work associated with slowly dragging a particle in the presence of time-averaged forces, and iii) additional work extraction facilitated by protocols responding to fast dynamical modes. Our results show how non-equilibrium forces can be strategically harnessed, with the protocols effectively acting as automatic information engines.

Recently, increased attention has been given to active matter in the context of both optimal control problems and stochastic engine designs. Using our framework, we consider a range of examples from active matter, including particles with correlated reorientations, chiral particles, and particles with algebraic rather than exponential correlations. In all cases, work extraction is compared to the base case of simple two-dimensional active Brownian motion.

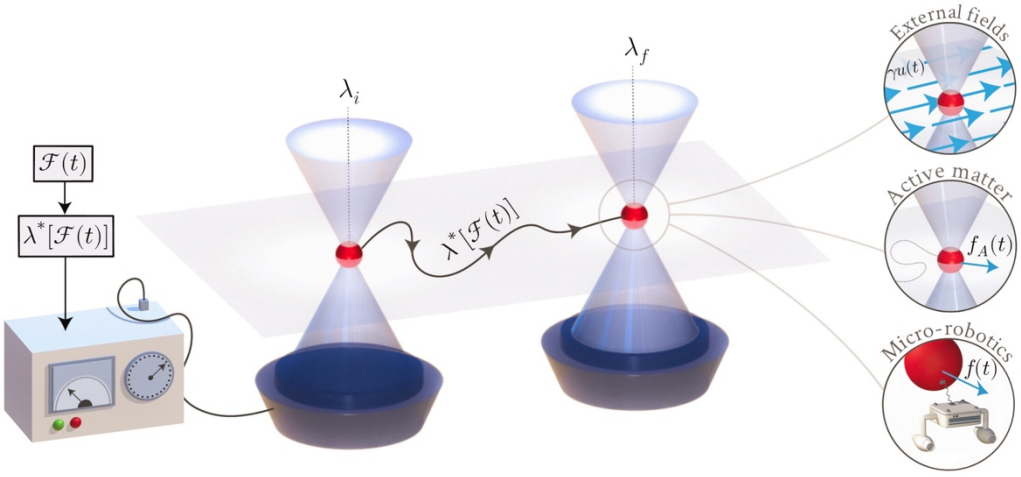

Figure 1: Optimal protocols for particle transport are derived for particles under the influence of arbitrary time-dependent forces. Given knowledge about these forces, a harmonic trap with a movable center $\lambda(t)$ is tuned by the controller, at the cost of thermodynamic work. The forces may represent external drives such as applied fields or flows, or internally general forces such as in active matter. The optimal transport problem can also be interpreted in terms of micro-robotics and cargo transport, where $\lambda(t)$ represents the trajectory of a micro-robot transporting a cargo that is exposed to non-equilibrium conditions.

Keywords: stochastic thermodynamics, energy harvesting, active matter

OPTIMAL PERFORMANCE OF THERMOELECTRIC DEVICES WITH SMALL EXTERNAL IRREVERSIBILITY

Rajeshree Chakraborty, Ramandeep S. Johal
Indian Institute of Science Education and Research Mohali, Punjab, India

ABSTRACT

In thermodynamic analysis of thermoelectric devices, understanding and mitigating irreversibilities is key to optimizing performance. Two primary irreversibilities affect device performance: internal (e.g., Joule heating and heat leakage) and external (due to heat transfer through heat exchangers) [1,2]. Traditional analyses focus on these separately, leading to efficiency expressions, such as those derived by Curzon-Ahlborn and Schmiedl-Seifert for endoreversible and exoreversible models, respectively. However, real-world devices experience both types, with internal irreversibilities linked to the material's figure of merit and external ones arising from heat exchanger conductance. We address this by formulating a scenario within the Constant Properties model [3,4] that accounts for both simultaneously.

Our study introduces the symmetric and small external irreversibility (SEI) model [5], where external irreversibilities are confined to the regime of large external conductance relative to the internal thermal conductance of the thermoelectric material. By incorporating this approximation, we derive a generalized expression for the efficiency at maximum power (EMP) that depends not only on the thermoelectric figure of merit and the temperature ratio but also on the ratio of internal to external conductance. This approach bridges the gap between simple idealized models and more realistic scenarios, enabling a more comprehensive understanding of thermoelectric device performance.

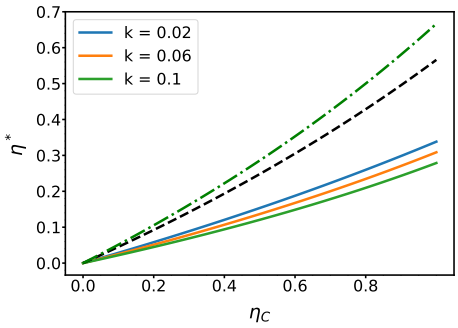

Figure 1: Efficiency at maximum power (EMP) vs. Carnot efficiency, η_C.

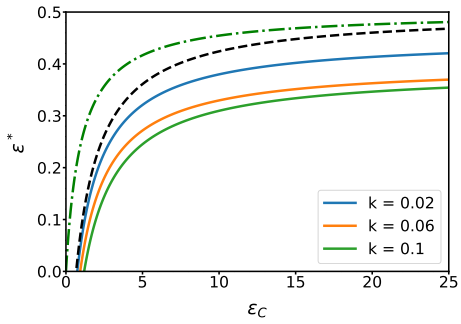

Figure 2: Efficiency at maximum cooling power vs. coefficient of performance of a Carnot refrigerator, ε_C.

We also extend our analysis to thermoelectric refrigerators, exploring efficiency at maximum cooling power. While previous studies suggest optimization is only feasible for the exoreversible model [6], our analysis shows that even with small external irreversibilities, valuable insights into cooling power performance can be gained.

This study highlights the SEI model as a key benchmark for thermoelectric devices where heat exchanger conductance exceeds that of the material. By integrating internal and external irreversibilities, it offers insight into the interplay between external and internal irreversibilities, which may guide their practical design.

Keywords: thermoelectric devices, irreversibilities, efficiency at maximum power (EMP), thermoelectric materials, thermoelectric refrigerators.

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DECOHERENCE MEETS TSALLIS: A NEW TAKE ON QUANTUM THERMOSTATISTICS

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[2]Dipartimento di Fisica, Università di Salerno, Fisciano (SA), Italy

ABSTRACT

Generalized Uncertainty Principle (GUP) is a phenomenological framework designed to incorporate a *minimal length scale* — such as the Planck scale or a characteristic inverse-mass scale in effective quantum theories — into quantum mechanics. In this talk, I will explore potential *observable consequences* of GUP in the *decoherence regime*. First, I construct *coherent states* associated with GUP and demonstrate that, in the momentum representation, these states coincide with *Tsallis-type probability amplitudes*, where the *non-extensivity parameter* q increases monotonically with the GUP deformation parameter β. Second, in the regime $\beta < 0$ (i.e., $q < 1$), I show — using the *Beckner–Babenko inequality* — that GUP becomes *fully equivalent* to *information-theoretic uncertainty relations* based on *Tsallis entropy power*. Finally, I apply the *Maximum Entropy Principle* from estimation theory to uncover a connection between the *quasi-classical (decoherence) limit* of GUP-based quantum theory and the *nonextensive thermostatistics* of Tsallis. This connection suggests a potentially rich and unifying paradigm, bridging quantum theory and analog gravity. Notably, in certain quantum gravity models — such as *conformal gravity*—the quasi-classical regime shaped by this framework may have *observable implications*. I will conclude with a discussion of some of these implications.

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TOPICAL SESSION

Quantum Thermodynamics

Presenting authors:

Miloš Milovanović (Serbia)
José A. Almanza-Marrero (Spain)
Beyza Aslanbaş (Turkey)
Grazia Di Bello (Italy)

THE MEASUREMENT PROBLEM OF A CONSCIOUS OBSERVATION

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ABSTRACT

The measurement problem is defined by von Neumann to be a discrepancy between reversible evolution by the Schrödinger equation and an irreversibility characterizing the measurement process [1]. In that respect, it fits well to the time operator formalism of complex systems which is aimed to unify reversible and irreversible theories in physics [2]. Von Neumann moreover indicated a relation to the principle of psychophysical parallelism which had already been mentioned by Bohr [3]. He referred to the Fechner psychophysics which was termed the identity view, since the observer is not considered a conglomeration of two substances but one single entity [4]. Fechner still distinguished the outer psychophysics which is a link between sensation and stimulation from the inner psychophysics which is a link between sensation and consciousness [5]. The problem is therefore related to a discernment of the conscious observation from a crude perception [6].

The time operator formalism developed by the Brussels school of thermodynamics concerns a change in representation linking reversible and irreversible evolution of a system [2]. Von Neumann has also remarked significance of the time operator for resolution of the measurement problem [1]. The change in representation that corresponds to an operator function of time should relate the outer to an inner psychophysics which is denoising the crude perception [5]. In that regard, an observation is about the optimal base which is aimed to denoise a signal [6]. It is an eigenbase of the time operator that has characterized a process which the signal originates from [7]. The process refers to measurement which is a reason to be presented by the Euclidean algorithm that is automorphous to a time series of binary digits [5]. The evolution is concerned by a shift in the binary code, which relates an eigenbase of the time operator to wavelets [8]. A step towards the general measurement involves as well wavelet frames which are redundant dictionaries that should warrant a stable reconstruction of the signal [9]. Duality in frame theory has tied the psychophysical parallelism to a relation between states and devices of the measurement process [5].

Keywords: general measurement, psychophysical parallelism, time operator, wavelet frames, optimal decomposition

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REASSESSING QUANTUM-THERMODYNAMIC ENHANCEMENTS IN CONTINUOUS THERMAL MACHINES

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Institute for Cross-Disciplinary Physics and Complex Systems IFISC (UIB-CSIC), Palma de Mallorca, Spain

ABSTRACT

The role of quantum coherence in thermodynamic processes has been a subject of intense debate in quantum thermodynamics. While coherence is often claimed to enhance the performance of quantum thermal machines, the precise conditions under which it leads to a genuine thermodynamic advantage remain unclear. In this talk, we present a systematic reassessment of coherence-induced enhancements in steady-state quantum thermal machines, including both autonomous and externally driven systems operating in the weak-coupling regime. Our work critically examines different sources of coherence—whether induced by the system's Hamiltonian or generated by noise—and evaluates their respective contributions to thermodynamic performance.

We begin by distinguishing between Hamiltonian-induced coherence, which arises due to perturbations in the machine's energy structure, and noise-induced coherence, which emerges from collective dissipation effects. By constructing classical thermodynamic-equivalent models, we establish a robust criterion for assessing whether coherence provides a genuine quantum advantage beyond classical stochastic machines. Our findings reveal that Hamiltonian-induced coherence systematically improves the stability and precision of thermodynamic outputs—reducing fluctuations while maintaining efficiency and power. On the other hand, noise-induced coherence does not universally yield advantages; in many cases, we show that it leads to no net benefit or even worsens performance when compared to an equivalent classical counterpart.

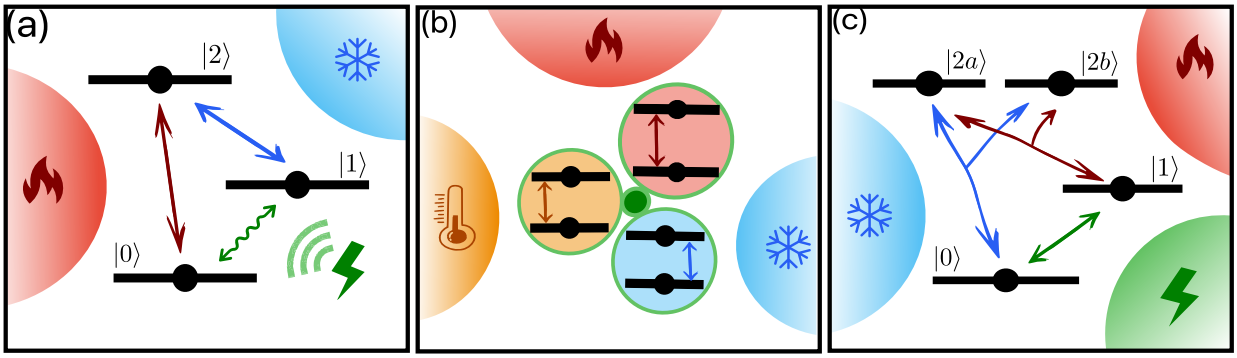

Figure 1: Schematic representation of three quantum thermal machine models. (a) The coherent three-level amplifier with couplings to baths at hot β_h(red) and cold β_c(blue) temperatures, as well as coherent external driving (green thunderbolt), (b) the three-qubit autonomous (absorption) refrigerator where each qubit is locally coupled to baths at hot (red), cold (blue), and intermediate (yellow) temperatures β_m, and (c) the noise-induced-coherence machine showing collective jumps induced by the baths at hot (red) and cold (blue) temperatures, together with a classical work source given by an infinite-temperature bath (green).

To illustrate these insights, we analyze three prototypical models of continuous quantum thermal machines: a coherent three-level amplifier, a three-qubit autonomous refrigerator, and a noise-induced coherence engine. Through multi-objective optimization techniques, we identify operational regimes where quantum coherence yields an unambiguous advantage, surpassing the classical thermodynamic limits set by the thermodynamic uncertainty relation (TUR). We also highlight cases where coherence provides no benefit, challenging previous claims of universal enhancements.

Keywords: quantum thermodynamics, quantum thermal machines, coherence-induced enhancement, thermodynamic uncertainty relation (TUR), multi-objective optimisation

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FINITE-TIME QUANTUM SZILARD ENGINE UNDER QUANTUM SHAPE EFFECTS

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ABSTRACT

The quantum Szilard engine provides a profound example establishing a rigorous link between quantum thermodynamics and quantum information. A single particle Szilard engine in a quantum domain with quantum measurements has been initially carried out by Zurek, demonstrating the consistency of measurement cost with the second law of thermodynamics [1]. The validity of Landauer's principle in a quantum Szilard engine in the absence of an explicit Maxwell's demon has also later been demonstrated [2]. While quasistatic variations give us maximum limits for work and heat exchanges, the finite-time analysis is important to capture the effect of quantum coherences. Recently, a finite-time quantum Szilard engine has been proposed to investigate the trade-off between power and efficiency, using a spin-1/2 particle as a working medium, with Maxwell's demon performing non-ideal quantum measurement to extract work [3]. The redistribution of energy levels during a time-dependent potential barrier insertion governed by a Markovian LGKS master equation is also analyzed through a finite-time Stirling engine [4]. Building upon these recent works, here we study the work extraction process of a quantum Szilard engine in finite time under size-invariant shape transformations [5]. Size-invariant shape transformation is a geometric technique of continuously changing the shape of an object without altering its sizes. It allows one to separate the influences of quantum size and shape effects and to examine the pure quantum shape effects in confined systems with quantized energy levels.

By altering the shape of the working medium without changing its sizes, we inspect the influences in the spectrum and the work output of the engine. We also explore the effect of localization due to weak measurement and its thermodynamic manifestation in comparison with the projective measurement. The system is assumed to be in contact with a thermal bath, which is modeled by a collection of harmonic oscillators. Dynamics of the Szilard engine, for the conditions that we outlined, is governed by a Markovian LGKS master equation. To perform a finite-time thermodynamic analysis of the engine, we solve the master equation numerically. The relevant thermodynamic quantities such as changes in internal energy due to heat and work contributions and changes in entropy are also calculated. Our work links the role of finite-time Markovian evolution on measurement-based heat engines with the unique contribution of operating it under the quantum shape effect.

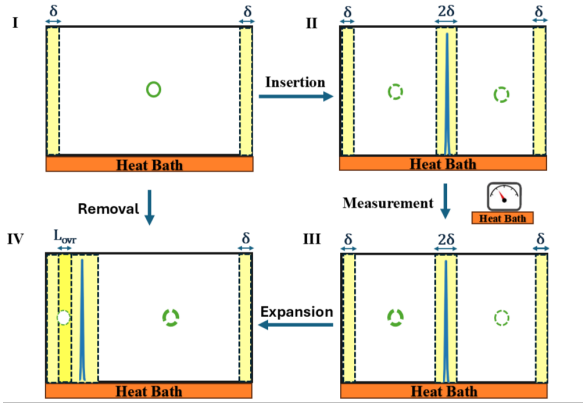

Figure 1: Representation of a quantum Szilard engine setup with boundary layers. I → II the insertion of a finite δ-function potential partition, II → III weak measurement is applied, and the particle is localized partially to each compartment with different probability density. III → IV the partition expands. IV → I the system returns to its initial state.

Keywords: open quantum systems, quantum confinement, quantum Szilard engine, quantum measurement

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WORK EXTRACTION VIA LOCAL GATES AND PHASE TRANSITIONS IN OPEN QUANTUM SYSTEMS

Grazia Di Bello[1], Vittorio Cataudella[2,3], Giulio De Filippis[2,3], Donato Farina[1], Francesco Formicola[1], David Jansen[4], Carmine Antonio Perroni[2,3]

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[4]ICFO-Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, Barcelona, Spain

ABSTRACT

We investigate the dynamical and thermodynamic properties of an open two-qubit Rabi model [1; 2] and a disordered XXZ Heisenberg spin chain using advanced numerical methods, including the density-matrix renormalization group (DMRG) and time-dependent variational principle (TDVP). These techniques describe open quantum systems states as matrix product states (MPSs). Our focus is on work extraction from a subsystem treated as an open quantum battery, particularly its relation to quantum phase transitions. We analyze ergotropy, the maximum extractable work, in the context of many-body phenomena such as quantum phase transitions. Local ergotropy [3], which quantifies work extraction in an uncontrollable environment, is studied across a Berezinskii-Kosterlitz-Thouless phase transition in the Rabi model, compared with its "switch-off" counterpart, where the energy cost of decoupling the subsystem from the environment is included in the work calculation. We propose a protocol for charging, storage, and work extraction optimized via Bayesian methods [4], revealing that strong system-bath coupling nearly doubles local ergotropy. Furthermore, ergotropy fluctuations serve as signatures of equilibrium quantum phase transitions (see Fig. 1).

Extending this framework, we examine the disordered XXZ Heisenberg spin chain, where the first two spins function as a quantum battery coupled to a spin bath [5]. Using the Néel state as an initial condition, we compute ergotropic quantities to identify transitions between many-body localized (MBL), Anderson localized (AL), and ergodic phases. Long-time behavior varies across these phases, with AL exhibiting saturation, MBL showing logarithmic decay, and the ergodic phase experiencing rapid decay of extractable work (see Fig. 2). Our results demonstrate that ergotropic quantities witness MBL-AL-ergodic transitions and that localized quantum batteries discharge more slowly and store more work, offering a pathway for experimental validation using two-qubit operations and energy measurements.

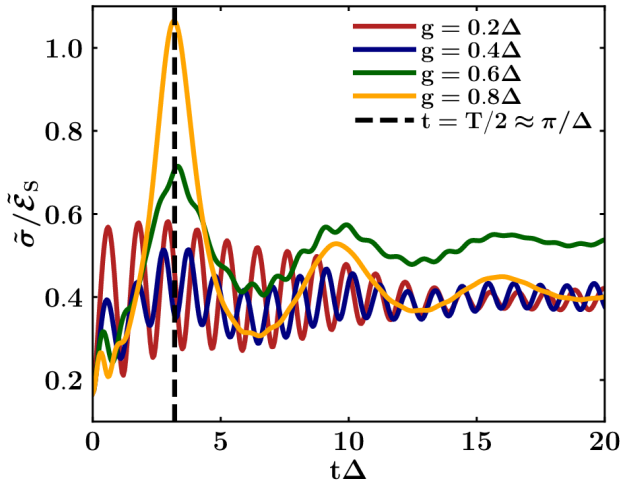

Figure 1: Relative fluctuations of the lower bound of local ergotropy (solid lines) as a function of dimensionless time for increasing system-environment coupling g/Δ (from red to orange). The vertical dashed black line is the time when the bath is in counterphase, farthest from initial state.

Keywords: open quantum systems, quantum batteries, ergotropy, quantum phase transitions, many-body localization

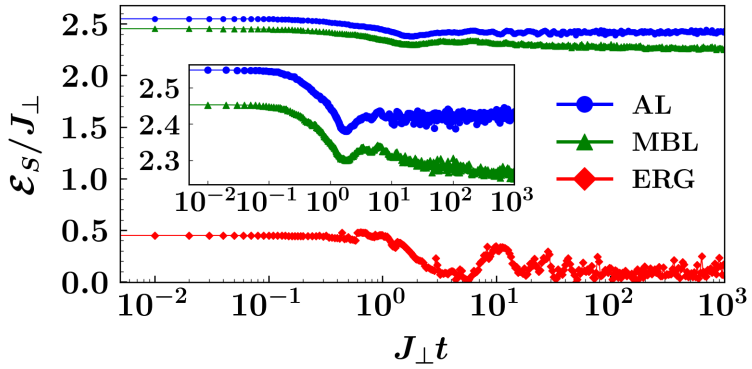

Figure 2: Local ergotropy as a function of dimensionless time for AL (blue circles), MBL (green triangles) and ergodic (red diamonds) phases. The inset provides a zoomed-in view of the local ergotropy as a function of time for the two localized phases.

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TOPICAL SESSION

Heat Conduction 1

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ON THE POSSIBILITY OF SPATIAL INTERACTIONS IN HIGHER-GRADE MATERIALS

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ABSTRACT

An elastic material of grade N is a deformable continuous system in which, in order to model the effects of complex spatial interactions, the constitutive quantities are permitted to depend not only on the first gradient of the deformation, the strain, but also on all gradients of the deformation less than or equal to the integer N. A heat conducting elastic material of grade N is said thermoelastic material of grade N. More complex systems with respect to the thermoelastic ones are the elastic solids of grade N with heat conduction and viscosity, which are said thermo-viscoelastic solids of grade N. Classically, for thermo-viscoelastic solids of grade N, the higher-order gradients of the deformation represent the elastic properties, while the viscosity is accounted by the presence in the state space of the time derivative of the deformation tensor. A troubling aspect higher-grade materials is that they are, in general, incompatible with second law of thermodynamics [1], unless some modifications of the basic field equations of Rational Thermodynamics [2] is made. Accordingly to this last point of view, in 1986 Dunn and Serrin [1], postulated the following new form of the local balance of energy

$$\rho\dot{\varepsilon}_I + q_{I,I} - T_{iL}\dot{F}_{iL} - \rho r = u_{I,I}, \tag{1}$$

wherein ρ is the referential mass density, T_{iL} are the components of the first Piola-Kirchhoff stress tensor, ε is the referential specific internal energy, q_I are the components of the referential heat flux, r is the local heat supply, and u_I are the components of an additional flux of mechanical energy, the interstitial working, engendered by long-range spatial interactions [1]. In this way they succeeded in proving the thermodynamic compatibility of such materials, with some severe restrictions. In particular, they showed that second law of thermodynamics requires that for elastic materials of grade 3 the free energy, the entropy and the internal energy cannot depend on the second gradient of the deformation tensor. As a consequence, the materials for which such a dependency is evident from the experimental point of view, from a theoretical point of view are not compatible with thermodynamics. In a series of papers we proposed an alternative approach to the above problem that does not modify the basic thermodynamic laws, but generalizes the classical Coleman-Noll procedure for the exploitation of the entropy principle [2]. The basic idea is to consider as additional equations to be substituted into the dissipation inequality the spatial differential consequences (gradients) of the balance laws, up to the order of the gradients entering the state space [3; 4; 5; 6; 7]. Here we present a complete thermodynamic analysis of thermo-viscoelastic solids of grade 3 based on the above mathematical procedure, and show that such a class of materials is fully compatible with the classical formulations of the field equations and of the second law of thermodynamics postulated in [2]. For homogeneous and isotropic bodies, under the validity for the heat flux of a generalized Maxwell-Cattaneo equation [8] which depends on the deformation too, we study the propagation of small-amplitude thermomechanical waves [6].

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ANALYTICAL SOLUTION OF MAXWELL-CATTANEO HEAT EQUATION WITH NON-HOMEGENEOUS BOUNDARY CONDITIONS

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ABSTRACT

The classical Fourier law is no longer applicable when studying thermal transient problems at the nanoscale or when describing heat transfer phenomena in heterogeneous materials. Non-Fourier models are of great interest in the engineering field, particularly due to the use of heat sources in many applications. In this paper, we provide an analitycal solution to the Maxwell-Cattaneo heat equation with homogeneous initial conditions and non-homogeneous time-dependent boundary conditions, restricting ourselves to the linear regime and a one-dimensional situation. Thus, the model solved analitycally is the following:

$$\rho c_v \partial_t T + \partial_x q = 0$$
$$\tau \partial_t q + q = -\lambda \partial_x T$$

with the following initial and boundary conditions

$$T(x=0) = 0; \qquad q(x,0) = 0$$
$$q(0,t) = f(t); \qquad q(1,t) = 0$$

respectively. In particular, by combining the temperature evolution equation and internal energy balance, an analytical solution of the heat wave-type equation is derived. This is achieved by substituting the time-dependent heating function acting on the boundary with a time- and space-dependent heat source. To solve the thermal equation, we apply Duhamel's theorem, considering the problem initially at zero temperature. An exact solution is obtained using the method of superposition, combining the homogeneous transient case and the inhomogeneous steady state.

Finally, the time evolution of the temperature history and the heat flux profile with time is represented for both the original problem and the one approximated with a space- and time-dependent heat source, thus validating the solution method.

Keywords: Maxwell-Cattaneo equation, heat conduction, analytical solution

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NONLINEAR EFFECTS IN THE MICROSTRUCTURE-INDUCED FINITE SPEED HEAT PROPAGATION

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ABSTRACT

In condensed matter, the time variation of active microstructures that directly depend on temperature may induce finite speed heat propagation. Such a property is independent of the type of microstructures [1], so that the picture of the phenomenon can be considered in this sense universal.

The adjective 'active' refers to bodies with microstructure endowed with inner (but observable) degrees of freedom with pertinent interactions not directly associated with those kinematic mechanisms that determine the standard stress (namely, the crowding and shearing of material elements merely considered as black boxes). A physically significant case is the one of materials showing pyroelectric effects. They occur in different phases, even those in which strain can be negligible.

With respect to this last circumstance (one that could be ideally referred to rigid bodies with active microstructure), we can derive a hyperbolic equation for the temperature propagation, although we accept the Fourier law for the heat flux [1]. Its linear form can be solved in closed form at least in one-dimensional case; the result show wave-type temperature propagation with velocity that is obviously *different* from the thermal conductivity [2]. Here and always in one-dimensional setting, we discuss the first nonlinear version of that equation, namely

$$c_v\theta_t + \zeta\theta_{xt} - \kappa\theta_{xx} + \gamma\lambda^2(\theta_t\theta_x)_x = 0\,,$$

where c_v is the specific heat, κ the conductivity coefficient, while ζ, γ and λ are constitutive coefficients. Finally, the subscript indicate derivatives with respect to the space variable x and time t.

For Neumann's type problems (prescribed heat flux at the boundary) we find a closed form solution with propagation velocity

$$\theta_t = \frac{\kappa q_1}{c_v + \gamma\lambda^2 q_1}$$

when we consider an external heat flux q_1 applied to the boundary, besides, considering, we repeat, the Fourier law within the body. We also discuss relevant numerical schemes and simulations.

Keywords: hyperbolic heat conduction, active microstructures, multi-field theories, numerical methods, continuum mechanics

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VORTICITY IN HYPERBOLIC HEAT CONDUCTION

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ABSTRACT

Transport of heat in a crystal can be formulated within the kinetic theory of phonons, phonon hydrodynamics, or within the usual Fourier heat conduction theory. These various levels of description are linked by thermodynamic reductions. While the reductions typically involve linearization in both reversible and irreversible parts of the evolution, we reduce the Poisson brackets (generating the reversible part) without any linearization. Then, we obtain a new phonon hydrodynamics that contains convective terms dependent on vorticity of the heat flux, missing in the standard theories of phonon hydrodynamics.

The new vorticity-dependent terms violate the alignment of the heat flux with the temperature gradient even in the stationary state, which is expressed by a Fourier-Crocco equation, illustrated in Figure 1. With those terms, temperature plays a similar role in heat transport as pressure does in aerodynamics. This is illustrated on numerical simulations of flow past a cylinder, Figure 2. The vorticity-dependent terms lead to a colder spot just behind the cylinder, and for high-enough Reynolds numbers they lead to the von Kármán vortex street, Figure 3. See [1] for more details.

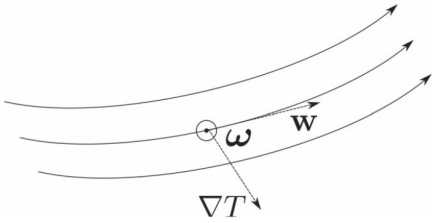

Figure 1: In the presence of heat flux vorticity $\omega = \nabla \times \mathbf{w}$, the heat flux $\mathbf{w}$ does not align with the temperature gradient ∇T.

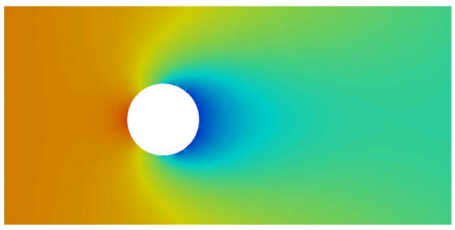

Figure 2: Temperature field when heat flows past an insulated cylinder.

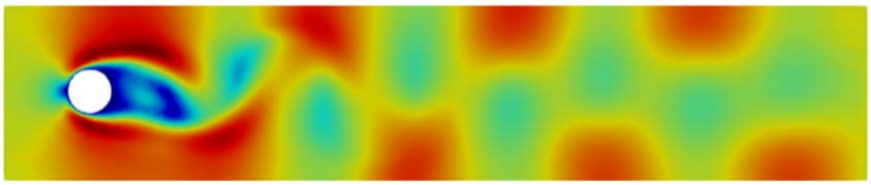

Figure 3: When the analogue of the Reynolds number grows (here $Re = 150$), the heat flux becomes unstable and produces an analogue of the von Kármán vortex street.

Keywords: phonon hydrodynamics, vorticity, heat conduction, GENERIC

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BEYOND THE CARNOT LIMIT: PERPETUAL HEAT FLOW IN GRAVITATIONAL AND ROTATIONAL NON-EQUILIBRIUM SYSTEMS

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ABSTRACT

The Carnot limit defines the theoretical maximum efficiency a heat engine can achieve when operating between two temperatures. Exceeding this limit would enable a system to function as a perpetual motion machine of the second kind, which is commonly assumed to be impossible [1]. In 1867, Maxwell claimed that gravity could not produce a temperature gradient in a column of gas, as such a gradient would enable a perpetual motion machine of the second kind [2], where two mediums with differing temperature gradients connected at different heights would result in a continual non-equilibrium state within the system, allowing for perpetual heat flow through the system with work extracted as heat flows via heat engines between each column. This view was widely supported by Clausius, Thomson, and Boltzmann, who concluded that gravity could not induce a temperature gradient in a gas column, maintaining that the Carnot limit was unbreakable [3], and while others, like Loschmidt disagreed [4], they failed to provide compelling evidence to the contrary.

However, recent experimental findings have measured gravitational temperature gradients in practically insulated solid, liquid and gas mediums including 0.04 $\mathrm{K{\cdot}m^{-1}}$ in water [5], 2.2 $\mathrm{K{\cdot}m^{-1}}$ in an air-sawdust mixture [6], and 0.02 $\mathrm{K{\cdot}m^{-1}}$ in an iron rod when under gravitational or rotational acceleration [7].

Despite these findings, little effort has been made to evaluate the feasibility of such non-equilibrium systems as a method to extract work from heat.

This study demonstrates that systems utilising temperature gradients induced by gravitational or rotational acceleration can achieve perpetual heat flow enabling the system to exceed the Carnot limit, without requiring the heat engines within the system to exceed the Carnot limit. A gravitational system employing both conductive and radiative heat transfer methods is shown to achieve greater temperature differentials over shorter heights than conduction-only systems, with power output in gravitational systems found to be constrained by the medium's thermal conductivity. Rotational system concepts were shown to overcome these material limitations by using rotational acceleration instead of gravity to achieve higher power outputs and efficiencies than gravity systems.

These findings and concepts aim to inspire interdisciplinary research into extracting work from perpetual heat flow within non-equilibrium systems, leading to a greater understanding of energy and potentially redefining the feasibility of perpetual motion systems of the second kind.

Keywords: perpetual non-equilibrium heat engine system

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GRAVITY-INDUCED SYMMETRY BREAKING IN CHEMICAL GARDENS

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ABSTRACT

Chemical gardens are hollow precipitates with a plant-like appearance (Figure 1) formed when a metal salt seed is immersed in an alkaline aqueous solution containing silicate, phosphate, or carbonate ions.

Figure 1: Silicate chemical gardens grown under normal gravity conditions. The morphological aspect observed is typical of chemical gardens obtained by the seed growth method.

While interest in chemical gardens was previously restricted mainly to science fair projects, nowadays they have become a hot research topic with direct applications in the development of new materials and technologies and in the understanding of life's emergence on Earth and Mars. Notwithstanding the increasing interest in the formation and growth of chemical gardens under micro and normal gravity conditions, very little is known about the subject. In fact, there are only a few publications [1; 2] in the literature that report the formation and growth of metal silicate precipitates under microgravity conditions. According to these papers, when compared with the precipitates formed under normal gravity, the precipitates obtained in a microgravity environment grow randomly, and their formation is much slower, suggesting that gravity plays an important role in the selection of dissipative structures.

Hence, in this work, the influence of the gravitational field on the formation and growth of chemical gardens formed via the seed growth method is examined through the nonequilibrium sensitivity theory [3; 4]. To this end, the chemical garden is regarded as a chemical system sufficiently far from equilibrium whose spatio-temporal evolution is described by a solution-diffuusion model with reaction. The results obtained from the non-equilibrium sensitivity analysis show that the gravitational field plays a role that goes beyond forming a concentration gradient in the medium. Under microgravity conditions, thermal fluctuations are predominant near the critical point, making the system insensitive to the gravitational field. However, under normal gravity conditions, the strength of the gravitational field is sufficient to favor the upward growth pattern. To quantify these conclusions, the degree of asymmetry between the bifurcating states that emerge as the system passes through a critical point is numerically evaluated. This quantity, also called the non-equilibrium sensitivity of the chemical garden to gravitational fields, indicates that the upward growth pattern will be the most probable dissipative structure as long as the gravitational field magnitude is larger than $\sim 10^{-5}\,\mathrm{m\,s^{-2}}$.

Keywords: chemical gardens, self-organization, symmetry breaking, gravity

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TOPICAL SESSION

Heat Conduction 2

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ELECTRON AND PHONON TEMPERATURES: APPLICATION TO THE THERMAL-SHOCK PROPAGATION IN NANO-SYSTEMS

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ABSTRACT

The rapid progress in nano-technology and its very huge impact in modern life have stimulated a true revolution in the heat-transfer phenomenon, spreading its domain of applicability and discovering new regimes and phenomenologies wherein the Fourier law and some classical theories are no longer applicable, if one aims at the correct modeling and interpretation of the experimental data.

A better understanding of the physical mechanisms governing the heat transfer at nano-scale may lead to a more accurate thermal management of optoelectronic devices, as well as to a better design of advanced materials (characterized by novel thermal-transport features) which could enhance the ability of the energy conversion.

In order to correctly describe the heat transport at nano-scale one should properly split the non-equilibrium temperature T into two different contributions: the electron temperature T^e and the phonon temperature T^p.

For this reason in literature some very interesting models of heat transfer involving those two different temperatures can be found.

As a possible alternative to those models, in this talk we propose a theoretical two-temperature model which fully agrees with the well-known Maxwell-Cattaneo theory for the description of the heat transport in a rigid body [1].

The aforementioned theoretical model is then used to study the propagation of thermal shock in nano-systems [2].

Keywords: phonon temperature, electron temperature, thermal-shock propagation, nano-systems, extended irreversible thermodynamics, second law of thermodynamics

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COUPLING OF NON-FOURIER THERMAL AND MECHANICAL EFFECTS IN 2D ISOTROPIC MATERIALS

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ABSTRACT

In this work, we investigate the mechanical effects in two-dimensional isotropic thermo-elastic materials, focusing on the interaction between the thermal and mechanical fields [1]. We present a model that analyze the thermo-mechanical behavior by coupling the generalized hyperbolic heat equation for the heat flux—known as the Maxwell–Cattaneo–Vernotte (MCV) equation—with a mechanical model that accounts for thermal expansion and stress in the material. This approach improves upon the classical model, where, in the case of the Duhamel-Neumann body, thermal expansion appears only in the pressure tensor. Here, we strengthen the coupling by adding mechanical effects to the internal energy, so that mechanical motion affects the temperature field, creating a two-way (strong) coupling between the thermal and mechanical fields. However, this classical approach still does not account for the second sound phenomenon.

To overcome this limitation, the Maxwell-Cattaneo-Vernotte equation is introduced as the first generalization of Fourier's law [2; 3; 4]. This equation addresses the shortcomings of the classical approach, and by incorporating temperature-dependent coefficients, it becomes necessary to include the effects of thermal expansion and, consequently, the coupling with mechanical effects. This is why we aim to study the effects of this mechanical coupling on the temperature distribution during a thermal pulse experiment and investigate whether it is possible to reproduce the longitudinal waves observed in McNelly's experiments [5; 6; 7; 8].

Using this model, we can more accurately predict the material's response under varying thermal conditions. To solve the governing equations for the heat pulse problem, we have developed a numerical solution using the staggered finite difference method and/or finite elements, ensuring precise results for the coupled thermo-mechanical interactions [9; 10].

Keywords: thermoelasticity, thermal expansion, mechanical effects, Duhamel-Neumann body, Cattaneo equation, non-Fourier heat conduction

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A NEW ADDITIONAL ROLE FOR THE CLAUSIUS-DUHEM INEQUALITY

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ABSTRACT

Traditionally, the role of being a source of constitutive restrictions and compatibility or stability conditions is attributed to the second law of thermodynamics written as the Clausius-Duhem inequality. We show that another fundamental role pertains to it. Specifically, we prove that the basic structures of phase-field models for phase-transitions in non-isothermal setting and (in general) bodies with 'active' microstructures can be derived all together from a unique principle requiring structure invariance of the second law of thermodynamics, written as a Clausius-Duhem inequality, under orientation-preserving diffeomorphism-based changes of observer and standard regularity conditions [1]. We show also that the microstructural behavior can be responsible of effects leading to wave-type heat propagation. When we consider a body with evolving macroscopic defect and a version of the Clausius-Duhem inequality that includes a power written with respect to a virtually varying reference configuration (a choice that is appropriate for a virtual representation over the reference configuration of the defect evolution), the above invariance requirement allows one to get directly the above results but also the local balances of configurational actions [2].

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EFFECTIVE GRAND-CANONICAL DESCRIPTION OF CONDENSATION IN NEGATIVE-TEMPERATURE REGIMES

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ABSTRACT

The observation of negative-temperature states in the localized phase of the Discrete Nonlinear Schrödinger (DNLS) equation has challenged statistical mechanics for a long time. This model has applications in several physical setups involving propagation of nonlinear waves in discrete media, from ultracold gases in optical lattices to arrays of optical waveguides. Negative temperatures are formally unstable in grand-canonical setups, being associated to an unlimited growth of the condensed fraction. Dynamically, the condensate is realized by a tall discrete breather, i.e. a spatially localized nonlinear excitation. Here, we show that negative-temperature states in open setups are metastable and their lifetime is exponentially long with the absolute value of temperature. The presence of an adiabatic invariant makes the instability mechanism even weaker than the thermodynamic prediction because of the resulting freezing of the breather dynamics.

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GRAHAME EQUATION GENERALIZED TO STUDY IONIC THERMOELECTRIC SUPERCAPACITORS

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ABSTRACT

Recently, ionic thermoelectric supercapacitors have gained attention owing to its high electromotive force (EMF) of 10 mV/K. In ionic thermoelectric supercapacitors, the high EMF has been achieved using redox-inactive ions in an open circuit condition. Herein, we theoretically estimated EMF generated in the Stern layer, and the diffuse layer by taking into account the temperature gradient and the Eastman entropy of transfer. The EMF is obtained by solving self-consistent equations using the adsorption isotherm as schematically shown in Fig. 1. The Grahame equation has been generalized to consider the parts in the dotted line in Fig. 1.

The current density of cations (j_+) can be expressed using the cation concentration(n_+), diffusion constant of cations (D_+), electric field (E), the valency of cations (z) and the elementary charge (q) as

$$j_+ = -D_+ \left(\frac{\partial}{\partial x} n_+ - \frac{z_+ q E n_+}{k_\mathrm{B} T} + \frac{\hat{S}_+}{k_\mathrm{B} T} n_+ \frac{\partial}{\partial x} T \right), \tag{1}$$

where $\hat{S}_+ = \alpha_+ k_\mathrm{B}$ indicates the Eastman entropy of transfer and α_+ is the dimensionless Eastman entropy of transfer. Using $E(x) = -\partial\psi(x)/(\partial x)$, Eq. (1) can be integrated. As the boundary condition, we consider the surface charge density (σ).

The generalized Grahame equation is obtained as

$$\left| \frac{z_+ q \Psi_\mathrm{i}}{k_\mathrm{B} T_\mathrm{i}} - \frac{z_+ q \psi_\mathrm{m}}{k_\mathrm{B} T_\mathrm{m}} \right| \approx \cosh^{-1} \left[\left(\frac{T_\mathrm{i}}{T_\mathrm{m}} \right)^{\alpha - 1} \left(1 + \frac{\sigma^2}{4 \varepsilon_\mathrm{r} \varepsilon_0 n_\mathrm{m} k_\mathrm{B} T_\mathrm{m}} \right) \right], \tag{2}$$

where ε_r and ε_0 are the relative and vacuum dielectric constant of electrolyte, respectively; we used $\cosh^{-1}(x) = \ln(x + \sqrt{x^2 - 1})$ if $x \geq 0$. The quantities with the subscript i are those at the closest distance to the electrode. The quantities with the subscript m are those at distances away from the electrode so that the charge neutrality can be assumed in the electrolyte. The EMF of $2 - 3$ mV/K is estimated after solving the self-consistent equations.

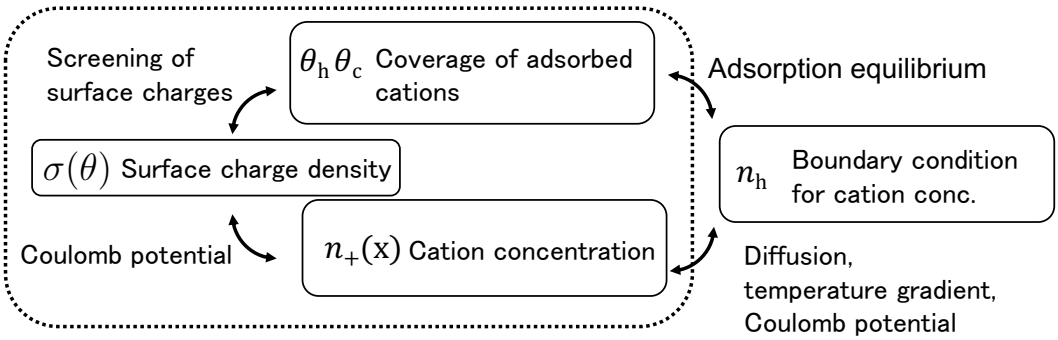

Figure 1: Theoretical formulation of thermoelectric supercapacitors: Grahame equation is generalized for the parts in the dotted line.

Keywords: Seebeck coefficient, Grahame equation, Eastman entropy of transfer

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TOPICAL SESSION

Thermodynamics of Fluids

Presenting authors:

Dennis Alt (Germany)
Xueqi Zhang (Germany)
Domenico Giordano (Netherlands)
Chiara Pezzotti (Italy)
Máté Pszota (Hungary)
Sahin Buyukdagli (Turkey)

THERMOPHYSICAL PROPERTIES AT EXTREME CONDITIONS

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ABSTRACT

Lubricated contacts between machine elements are subject to extreme pressures of up to 4 GPa. To model tribo-contacts at the macroscale, reliable models of the thermophysical properties of the lubricant fluids are required. The density and the viscosity are of particular significance. At such conditions, thermophysical properties of lubricants are challenging to measure experimentally. In this work, a variety of model lubricants were studied, including n-alkanes, squalane, and 1-octanol by combining experiments, molecular dynamics simulation, and molecular-based models. In a first step, high pressure experiments were carried out for determining the viscosity and density of the model lubricants at pressures up to 1 GPa for the viscosity and up to 120 MPa for the density and in the temperature range 298 – 373 K. Molecular dynamics simulations were used to identify the most accurate and reliable transferable force field for modelling branched alkanes [1], which turned out to be the Potoff united-atom force field. This force field evaluation was carried out by comparing MD predictions to available experimental data. Then, molecular dynamics simulations based on the Potoff force field were carried out for predicting thermophysical properties at extreme conditions, where no experimental data were available. The hybrid data set, comprising both experimental and molecular simulation data, was used for the parameterisation of a molecular-based equation of state model, based on the SAFT-VR Mie equation. For modeling transport properties, such as the viscosity and thermal conductivity, entropy scaling [2] was used. The model describes the hybrid data set very well. The model's performance is further demonstrated by its ability to extrapolate well to extreme pressures and temperatures, as well as mixtures. Finally, the model was used for describing thermophysical properties in tribological elastohydrodynamic simulations [3].

Keywords: extreme conditions, measurements, MD-simulation, equation of state modeling, entropy scaling

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COUPLING MOLECULAR THERMODYNAMICS MODELS WITH CFD SIMULATION ENGINES

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ABSTRACT

Analytical molecular thermodynamics models are an attractive option for the modeling of thermophysical properties of fluids. The basis of this model class are molecular-based equations of state, e.g. PC-SAFT [1] or SAFT-VR Mie [2]. These models enable the description of static properties. For describing intramolecular thermodynamic properties, a quantum mechanical model is used. Using auxiliary models such as density gradient theory and entropy scaling [3], also interfacial and transport properties, respectively, can be described. These models can be used even when very limited data are available and can be used for extrapolation of extreme conditions. In particular, they can be applied for predicting mixture properties based on the pure component models alone. We have developed a software package, called MicTherm, that contains a large library of such molecular thermodynamics models. MicTherm comprises an application programming interface (API) for the coupling to other simulation engines – especially Computational Fluid Dynamics (CFD) simulation packages. A schematic representation of the coupling is shown in Figure 1. CFD simulations typically require the specification of several thermodynamic properties, such as the viscosity, thermal conductivity, phase equilibrium properties, heat capacity, speed of sound and density at a given temperature and pressure and eventually composition if mixtures are considered. In CFD simulations, traditionally very simple models for the thermodynamic properties are employed, e.g. the ideal gas model or a constant density model. However, fluid properties play a crucial role in ensuring accurate simulation outcomes. We demonstrate the feasibility of coupling MicTherm with CFD simulations by using OpenFOAM. Also, results are presented for coupling MicTherm with elastohydrodynamic fluid simulations [4]. This general concept can be used for various CFD engines for the modeling of various thermophysical fluid properties. This enables the modeling of thermodynamic properties and transport properties using thermodynamically consistent frameworks that are applicable also in metastable states, across large ranges of pressures and temperatures, for mixtures, and phase equilibria.

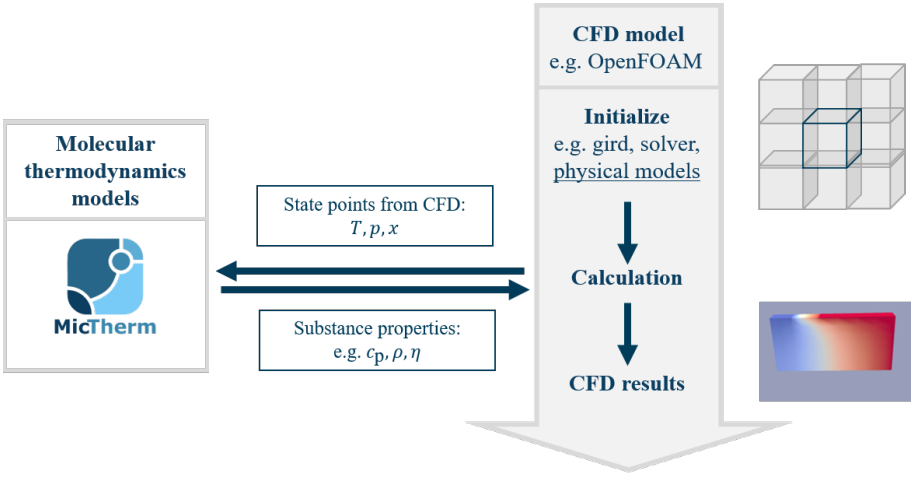

Figure 1: Schematic representation of the coupling of molecular themrodynamics models with CFD simulation engines.

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DOES THE FLUID-STATIC EQUILIBRIUM OF A SELF-GRAVITATING ISOTHERMAL SPHERE OF VAN DER WAALS' GAS PRESENT MULTIPLE SOLUTIONS?

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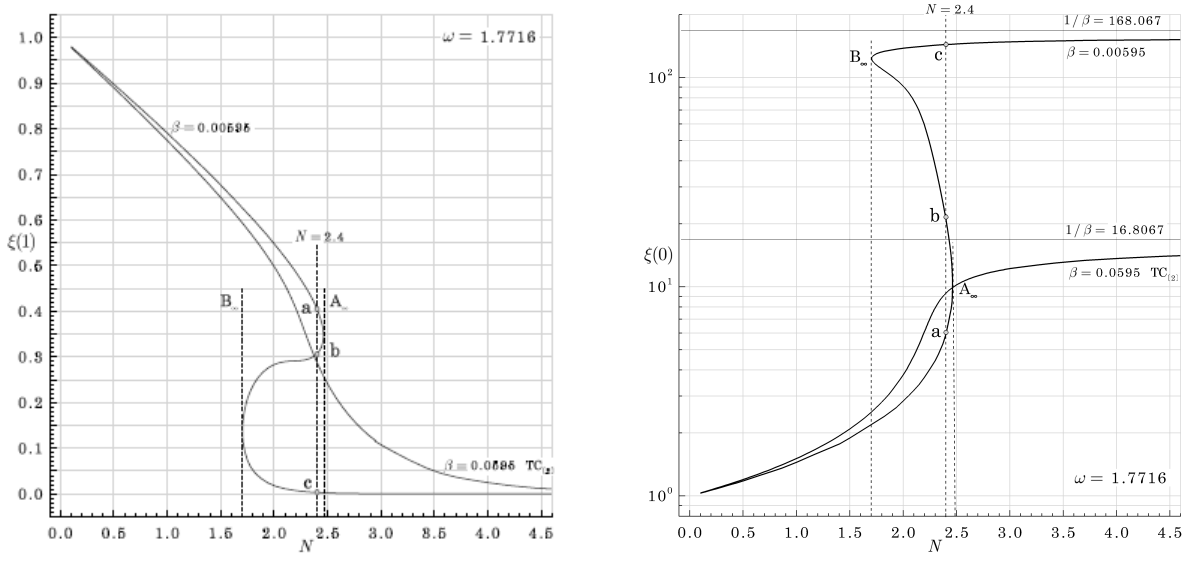
ABSTRACT

We describe the investigation we left in the future-work stack in Giordano et al. [1] in which we pointed out the obvious necessity to inquire about the existence or absence of values of the non-dimensional constants α and β of the van der Waals' equation of state in correspondence to which the perfect-gas model's self gravitational effects, namely, upper boundedness of the gravitational number, spiraling behavior of peripheral density, oscillating behavior of central density, and existence of multiple solutions corresponding to the same value of the gravitational number, appear also for the van der Waals' model.

The development of our investigation brings to the conversion of our M_2 scheme based on a second-order differential equation governing the fluidstatic equilibrium into an equivalent system of two first-order differential equations that incorporates Milne's homology invariant variables [2]. The converted scheme $1oM_2$ turns out to be much more efficacious than the M_2 scheme in terms of numerical calculations' easiness and richness of results.

We use the perfect-gas model as benchmark to test the $1oM_2$ scheme; we re-derive familiar results and put them in a more general and rational perspective that paves the way to deal with the van der Waals' gas model. We introduce variable transformations that turn out to be the key to study (almost) analytically the monotonicity of the peripheral density with respect to variations of the gravitational number.

The investigation brings to the proof that the gravitational number N is not constrained by upper boundedness, the peripheral density $\xi(1)$ does not spiral [Fig. 1(a)], and the central density $\xi(0)$ does not oscillate [Fig. 1(b)] for any couple of values assumed by the non-dimensional constants α and β; however, multiple solutions corresponding to the same value of the gravitational number can exist but their genesis is completely different from that of the perfect-gas model's multiple solutions. As crucial result of our investigation, we provide the boundary between the two regions of solution's uniqueness and multiplicity in the α, β plane.



(a) Peripheral density (b) Central density

Figure 1: Effect of the characteristic number β on the peripheral/central density's dependence on the gravitational number and appearance of multiple solutions ($\omega = \alpha/\beta$).

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HYDROMECHANIC THEORY OF ANOMALOUS TRANSPORT: RELAXATION TOWARDS EQUILIBRIUM IN THE ABSENCE OF DISSIPATION

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ABSTRACT

Motivated by the analysis of particle transport in heterogeneous systems, e.g. hydrogels, we consider the statistical and thermodynamic properties of colloidal particles in fluid possessing memory effects in isothermal conditions. The momentum balance equation for a particle of mass m reads

$$m\frac{dv(t)}{dt} = -\int_0^t h(t-\tau)\,v(\tau)\,d\tau - \int_0^t k(t-\tau)\left(\frac{dv(\tau)}{d\tau} + v(0)\,\delta\tau\right)d\tau \tag{1}$$

where $v(t)$ is the particle velocity, $h(t)$, $k(t)$ are respectively the dissipative and fluid inertial kernels, and $R(t)$ is the fluctuating force the statistical properties of which stem from the fluctuation-dissipation relations [1; 2; 3]. The kernel $h(t)$ accounts for the dissipative viscoelastic effects, while $k(t)$ arises from fluid inertial contributions, and corresponds to the generalization of the Newtonian Basset kernel to generic fluids [4].

The fluid-inertial kernel does not contribute to dissipation, that solely depends on $h(t)$ via its integral

$$\eta_\infty = \int_0^\infty h(t)\,dt \tag{2}$$

Two cases occur: 1) if η_∞ is finite, the particle diffusivity can be defined, since the Stokes-Einstein relation for the particle diffusivity D at constant temperature T holds, $D\eta_\infty\, k_B T$, where k_B is the Boltzmann constant; 2) if η_∞ diverges to infinity, particle motion is anomalous and the Generalized Stokes-Einstein relations applies [5].

From the hydromechanic theory of anomalous motion developed recently in [2], there exists also another case that deserves particular attention from the point of view of the thermodynamics of irreversible phenomena.

This is when no dissipation occurs, i.e. $h(t) = 0$, and particle motion is controlled purely by fluid inertial effects. Physically, this could be the case of a superfluid phase at very low temperature. Also in this case, the integrability of the kernel controls the qualitative properties of the dynamics. If $k(t)$ is summable, i.e. if

$$k_\infty = \int_0^\infty k(t)\,dt \tag{3}$$

is finite, no relaxation towards an equilibrium behaviour in the momentum dynamics occurs, and particle motion is ballistic. Conversely if k_∞ is unbounded, in the meaning that $k(0)$ is finite and

$$k(t) \sim t^{-\xi}, \quad \text{for large } t \tag{4}$$

with $\xi < 1$, relaxation towards an equilibrium velocity distribution occurs, and the motion is superdiffusive, i.e.

$$\langle x^2(t)\rangle \sim t^{1+\xi} \tag{5}$$

where $\langle x^2(t)\rangle$ is the particle's mean square displacement. The slowly relaxing tails in $k(t)$ determine the emergence of an apparently dissipative dynamics, and this can be explained by means of the theory developed in [2].

The aim of this presentation is to address the hydromechanic theory of anomalous diffusion, focusing particularly on the case where $\eta_\infty = 0$ and $k_\infty = \infty$, addressing the mathematical physical origin of the occurrence of an equilibrium behaviour and discussing its thermodynamic implications.

Keywords: Brownian hydromechanics, thermalization, anomalous diffusion, dissipation, fluid inertial effects.

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DERIVATION OF HIGHER ORDER GRADIENT THERMODYNAMIC GRAVITY

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ABSTRACT

In this presentation, the generalised derivation of a gradient modification of Newtonian gravity is presented within a thermodynamic framework. The resulting field equation is compared to the models considered by Franklin [1], Lazar [2] and Ván [3], for a general field-dependent energy contribution to the internal energy in the form of

$$u = e - \varphi - \frac{\varepsilon(\varphi, \nabla\varphi, \nabla^2\varphi, \nabla^3\varphi)}{\rho}. \tag{1}$$

When assuming a cross-coupling (characterised by the parameter K) between the mechanical and gravitational thermodynamic forces and fluxes, the theory results in a dissipative field equation relaxing to a generalised Poisson's equation for gravity:

$$\begin{aligned}\tau\partial_t\varphi = l^2 4\pi G\Bigg(&\nabla\cdot(\partial_{\nabla\varphi}\varepsilon) - \rho - \partial_\varphi\varepsilon - \nabla^2 : \partial_{\nabla^2\varphi}\varepsilon + \nabla^3 \dddot{:} \partial_{\nabla^3\varphi}\varepsilon \\ &+ 2K\left[-3\varepsilon + (\partial_{\nabla\varphi}\varepsilon - \nabla\cdot\partial_{\nabla^2\varphi}\varepsilon + \nabla^2 : \partial_{\nabla^3\varphi}\varepsilon)\cdot(\nabla\varphi) + (\partial_{\nabla^2\varphi}\varepsilon - \nabla\cdot\partial_{\nabla^3\varphi}\varepsilon) : (\nabla^2\varphi) + (\partial_{\nabla^3\varphi}\varepsilon) \dddot{:} (\nabla^3\varphi)\right]\Bigg).\end{aligned} \tag{2}$$

The resulting nonrelativistic modifications of gravity may potentially explain astronomical observations of phenomena usually contributed to dark matter, or help exploring the potential corrections to the results of Solar system-level tests (for example, with Yukawa-like terms).

Keywords: nonequilibrium thermodynamics, modified gravity, dark matter

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THERMODYNAMIC FORMULATION OF CHARGED LIQUIDS BASED ON THE ASYMMETRIC TREATMENT OF DISTINCT IONIC INTERACTION RANGES

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ABSTRACT

The accurate characterization of ion correlations in charged solutions is critical for the control of various biophysical and industrial processes ranging from ion transport through plasma membranes to water purification and desalination procedures. The theoretical tools enabling the comprehension of these systems is based on the the Debye-Hückel (DH) theory suffering from major limitations [1]. Namely, the validity of the DH formalism neglecting the ionic hard-core (HC) size and including exclusively electrostatic weak-coupling-level ion correlations is limited to the characterization of monovalent salts at dilute concentrations.

In this talk, I will present an ion size-augmented self-consistent DH (SCDH) theory of bulk electrolytes exploiting the asymmetric incorporation of the short- and long-range ion interactions via their virial and cumulant-level treatment, respectively [2,3]. The underlying variational splitting of the distinct interaction ranges enables the accurate prediction of ionic activity coefficients, internal energies, osmotic pressures, and radial distribution functions up to molar salt concentrations. Via comparison with simulations and experimental data, I will show that the SCDH formalism can also reproduce accurately the underscreening and overscreening effects occurring in monovalent and multivalent electrolytes. The analytical transparency of the SCDH theory enables the detailed characterization of the ionic association mechanism behind these effects in terms of the close competition between repulsive HC and attractive charge correlations.

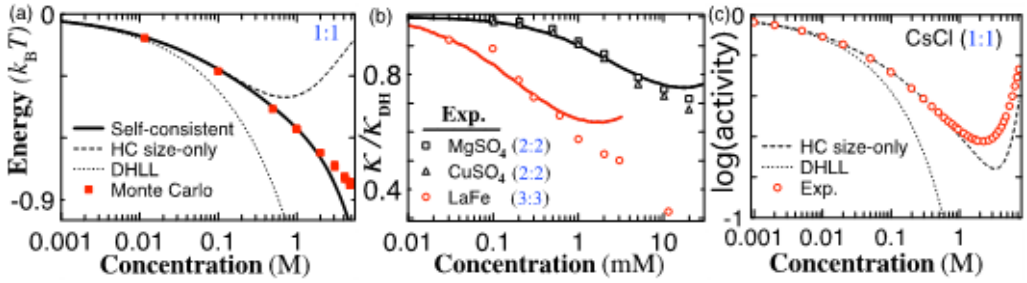

Figure 1: a) Internal energy, (b) reduced screening parameter, and (c) ionic activity.

Keywords: thermodynamics of electrolytes, charge correlations, hard-core interactions, ion size

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POSTER SESSION

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TORQUE BOUNDS OF DUMBBELL-LIKE MOLECULAR MOTORS AT THE INTERFACE OF 2 FLUIDS – BEYOND THE KRAMERS REGIME

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ABSTRACT

We study a dumbbell-like biological rotatory molecular motor whose two ends are separated by a membrane, where each end is in contact with fluids of different viscosity[1]. The motor operates cyclically in the over-damped regime[2]. We compute bounds for τ the torque (maximum and minimum) when the motor operates in the regime of maximum diffusion, beyond the Kramers regime[3]. These bounds are calculated solely on long-time observables and our findings complement the entropy generation bounds offered by the well-known TUR[4]. The cyclic operation of the motor in the overdamped regime is well described by $V_{\rm eq}(\phi) - \tau\phi$ a tilted periodic potential[2] and solutions for the long-time drift velocity and diffusion are known[5]. The entropy generation rate of such a model can be computed as the product of generalized thermodynamic forces and associated current. In the case of a rotatory motor with only one degree of freedom, τ is the thermodynamic force and ω the angular velocity of its associated current. Thus, the rate of entropy production is: $T\sigma = \omega\tau$. When the motor operates either very-close-to or very-far-from equilibrium the TUR provides a tight bound for the rate of entropy generation. However, the TUR bound is very loose close to the regime of maximum diffusion[6]. For the particular system studied here, the TUR bound becomes $T\sigma \geq \omega^2/D_\phi$, where D_ϕ is the rotational diffusion.

The challenges present in most in-vivo experiments with molecular motors: i) direct measurement of the thermodynamic torque (force) applied(generated) is not possible, ii) precise determination of the viscous drag is challenging. Thus, when the TUR is a tight bound, the estimation of this torque(force) based on diffusion and drift values solely is straightforward[6]. However, if the motor operates close to the regime of maximum diffusion, the TUR is a loose bound, and estimating the torque is no longer trivial. Additionally, motors like the bacteria flagellar motor (BFM) operate in a fashion such that the motor's outer and inner parts are of very different sizes and subject to different sources of friction. In the present work, for the vicinity of maximum diffusion, one viscous drag-independent equation between torque(force), ω, D_ϕ, and E_a (the energy barrier at equilibrium corresponding to the underlying $V_{\rm eq}(\phi)$) is found:

$$k_{\rm B}T\frac{\omega}{D_\phi}\left[1+\frac{a_1}{E_a^2}\tau^2+a_2\tau^4\right]-\tau-\frac{a_3}{E_a^2}\tau^5=0. \tag{1}$$

Depending on the E_a value the torque is bound. With the torque estimated, we compute the effective viscous drag using the general relation for current and thermodynamic force[5]. The effective drag computed this way includes the motor's outer and inner parts contribution. In experiments, only the outer part of motors like the BFM is in contact with probes, resulting in several previous studies not accounting for any inner part contribution. The results of our study emphasize that this contribution is not negligible, and that in many circumstances dominates the dynamics of the system.

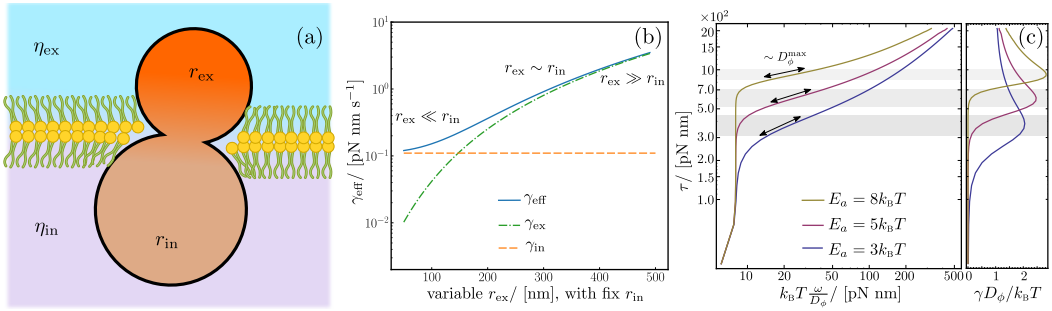

Figure 1: (a) Dumbbell motor scheme. (b) Effective viscous drag as function of motor's external radius. (c) Torque bound according to Eq.(1).

Keywords: Brownian motion, molecular motors, effective viscosity, fluctuation theorems, non-equilibrium processes

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A PATH INTEGRAL APPROACH TO THE LACK-OF-FIT REDUCTION

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ABSTRACT

Even though microscopic dynamics is reversible in time, macroscopic systems show irreversible dynamics. The lack-of-fit reduction, as formulated by Kleeman in [1], gives macroscopic irreversible dynamics as the most probable trajectory, when minimizing the loss of information caused by the transition from a more detailed level of description. This trajectory is then given without any fitting constants, based purely on the minimizing principle. In previous work [2], we focused only on the macroscopic trajectory, generalizing the lack-of-fit reduction for systems described by the GENERIC formalism (General Equation for Non-Equilibrium Reversible-Irreversible Coupling). In our current work, we add also the theory of fluctuations in the form of random noise. The reduction is tested on the Kac-Zwanzig model – large particle in an outside potential surrounded by a bath of N smaller particles. Detailed computer simulation is compared to the reduced dynamics found by the model. To show the emergence of damping from purely reversible dynamics as well as keep calculations explicit, we use harmonic potential as the outside potential.

Keywords: GENERIC, non-equilibrium thermodynamics, multiscale, transitions, Kac-Zwanzig model

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MODELLING ANOMALOUS DYNAMICS IN CLASSICAL AND QUANTUM SYSTEMS

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ABSTRACT

Anomalous dynamics, characterized by deviations from standard Brownian motion, play a crucial role in understanding transport processes in complex classical and quantum systems. In this study, we investigate how non-local interactions influence anomalous diffusion and quantum wave propagation by incorporating fractional calculus and memory effects into classical and quantum models.

In the classical domain, we analyze a generalized diffusion equation with a memory kernel, Lévy-type superdiffusion and a non-local term [1], which accounts for interactions over extended spatial and temporal scales. We derive analytical solutions and explore their impact on transport properties. The results reveal how non-local effects modify the diffusion behavior and influence the probability distribution.

In the quantum domain, we extend our analysis to two non-local modifications of the Schrödinger equation: (1) A fractional Schrödinger equation with a memory kernel, capturing long-range correlations in quantum evolution [2]; (2) A three-dimensional Schrödinger equation incorporating a non-local potential constrained by a Dirac delta function, simulating heterogeneity of the system [3].

Using Green's function methods, we obtain exact solutions and analyze the impact of non-locality on wave packet dynamics and quantum transport. Our findings demonstrate that non-local interactions can significantly alter coherence properties, leading to modified localization effects and anomalous spreading of wave functions [4].

The interplay between fractional diffusion, memory effects, and non-local interactions provides a unifying theoretical framework for describing transport in systems that exhibit deviations from standard diffusive and wave-like behavior. Fractional diffusion equations generalize classical transport laws by incorporating memory and non-locality, allowing for a more comprehensive description of systems with long-range correlations. Memory effects introduce non-Markovian behavior, which plays a fundamental role in systems with strong temporal correlations, such as those governed by spatial geometrical constraints. Meanwhile, spatial non-locality enables the description of transport mechanisms where interactions extend beyond nearest neighbors, leading to correlated motion that cannot be captured by traditional local models. By bringing together these concepts, our approach provides a generalized perspective on transport phenomena, encompassing a broad spectrum of behaviors ranging from constrained subdiffusion to Lévy-type superdiffusion and non-local quantum evolution.

Keywords: anomalous diffusion, non-locality, Lévy flights

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EQUATION OF STATE MODELING AND MOLECULAR SIMULATION OF FLUIDS WITH POLAR INTERACTIONS

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ABSTRACT

The thermodynamic behavior of many fluids is significantly influenced by polar interactions. Molecular-based equation of state (EOS) models describe the Helmholtz energy of fluids based on perturbation theory and account for polar contributions by an additive term. In this work, polar contribution models have been comprehensively evaluated and compared for the first time. Both dipole contribution models and quadrupole interaction models were studied. Therefore, molecular simulations of simple polar model fluids were carried out to establish a database of reference data. The evaluation of the polar models was conducted using model fluids, which consist of a 12-6 Lennard-Jones (LJ) interaction site with a point multipole, i.e. either point dipole or point quadrupole. As the kernel, the LJ EOS of Kolafa and Nezbeda [1] was used in all cases, which is known to describe the LJ fluid very well [2]. A large range of dipole moments and quadrupole moments were studied. Important differences for the different polar models were obtained. Molecular simulations were used to determine pseudo-experimental data, which provide a robust basis for testing the theories. In this study, as shown in Figure 1, a large set of reference data was used to validate the accuracy of the polar contribution, obtained through molecular dynamics (MD) and Monte Carlo (MC) simulations using the ms2 [3] simulation engine. In the simulations, both homogeneous states and vapor-liquid equilibria (VLE) were studied. Additionally, Brown's characteristic curves [4] were determined using a simulation method developed in a previous work of our group [5]. Brown's curves are a tool for the assessment of the extrapolation behavior of thermodynamic models.

The VLE data are described well by most of the studied polar EOS models. However, for homogeneous state points, significant deviations between the data from computer experiments and some EOS models were obtained for many properties. These deviations increase with increasing polar moment, as expected. Most importantly, all studied polar contribution models yield some critical artifacts. Thus, robust new polar contribution models are required. We discuss possible paths for developing such models based on the comprehensive study carried out here.

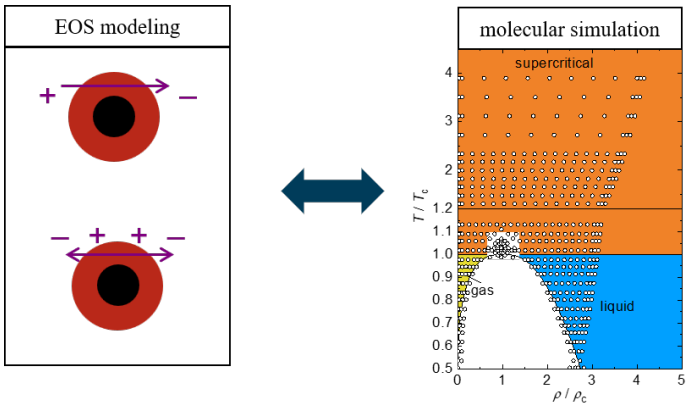

Figure 1: Schematic representation of comparison of the equation of state modeling with reference data obtained from molecular simulations.

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PHENOMENOLOGICAL STUDY OF LIESEGANG RINGS

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ABSTRACT

This work is based on the pre-nucleation model proposed by George et al. [1] to simulate the Liesegang rings phenomenon. There are only three chemical species, which are the outer electrolyte, the inner electrolyte, and the precipitate, and two reactions: precipitation and aggregation. The two electrolytes can diffuse through the gelatinous media, but the precipitate, once formed, stays still. The precipitation phase only occurs if the product of the two reactants is above a critical threshold, whereas the aggregation has an autocatalytic mechanism.

With respect to the three empirical laws — space, time, and width —, according to our simulation results: (i) the rings' position follow a geometric progression; (ii) the time of formation of each ring is proportional to the square of its position; (iii) the width is practically constant across each ring. The first two findings are in agreement with the results generally reported in literature, but the last one is not, and it is probably related to the increase of the average precipitate concentration observed from one ring to another.

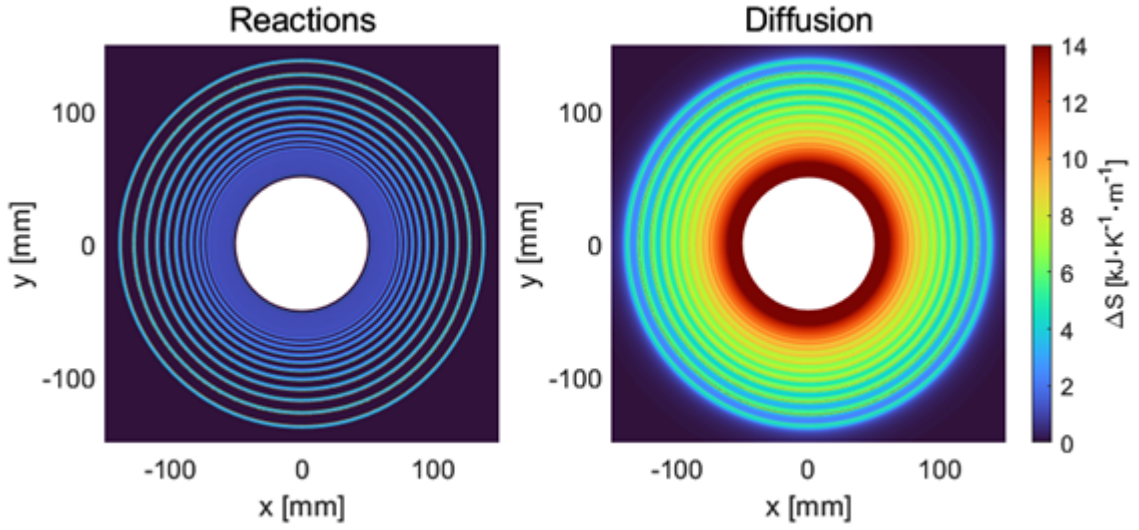

Figure 1: Total entropy production generated by reactions and diffusion processes at $t = 2 \times 10^6 s$. The internal radius is $50mm$, the concentration of the outer electrolyte is constant, at $0.5M$, while the initial concentration of the inner electrolyte is $0.05M$.

It was found that the diffusion is the main driving force for entropy generation. Most diffusion occurs because of the reduction of the concentration of the reagents at the region of the rings, which occurs due to the consumption by the reactions. By increasing the initial concentration of the inner (inside the gel) or the outer electrolyte (outside the gel), the spacing between the rings decreased, which agrees with the Matalon-Packter law. Finally, the findings of this work may be useful for better understanding self-organization chemical processes, especially when diffusive forces are significant within the considered time scales.

Keywords: Liesegang rings, numerical simulation, nonlinear dynamics, pattern formation, reaction-diffusion system

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THERMODYNAMICS OF BLACK HOLES: HAWKING-PAGE TEMPERATURES AND SECOND ORDER PHASE TRANSITIONS

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ABSTRACT

Since black holes lack a straightforward notion of geometrical volume due to their event horizon structure and coordinate dependence [3], various approaches have been proposed to introduce a meaningful geometric and thermodynamic volume [2,4,5]. There is no volume in classical **black hole thermodynamics**, the nonextensivity of black holes is a consequence. Extensivity of such systems can be restored by introducing a new thermodynamic state variable, typically the volume, the mass or the number of particles. Smarr relations show that black hole thermodynamics is nonextensive. However, restored **extensivity** leads to a volume which corresponds to geometric concepts and is also meaningful from a physical point of view. The article examines various volume definitions in the context of Anti-de Sitter (AdS) black holes and their implications for phase transitions, focusing on the **Hawking — Page phase transition in Kerr — AdS** spacetime, including the Christodoulou — Rovelli volume [1]. The goal is to examine the feasibility of integrating volume as a meaningful variable in the thermodynamic framework of different types of black holes.

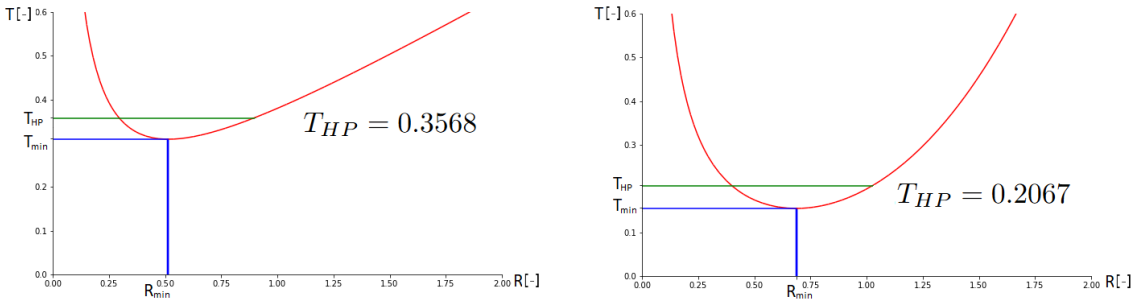

Figure 1: The dimensionless temperature (T) expressed in terms of radius (R) in case of $p = 0.15$. The local minimum remarked with blue and the Hawking – Page temperature with green. Left: For Hawking and Page; Right: with the Christodoulou – Rovelli volume.

Keywords: black hole thermodynamics, Hawking-Page phase transition.

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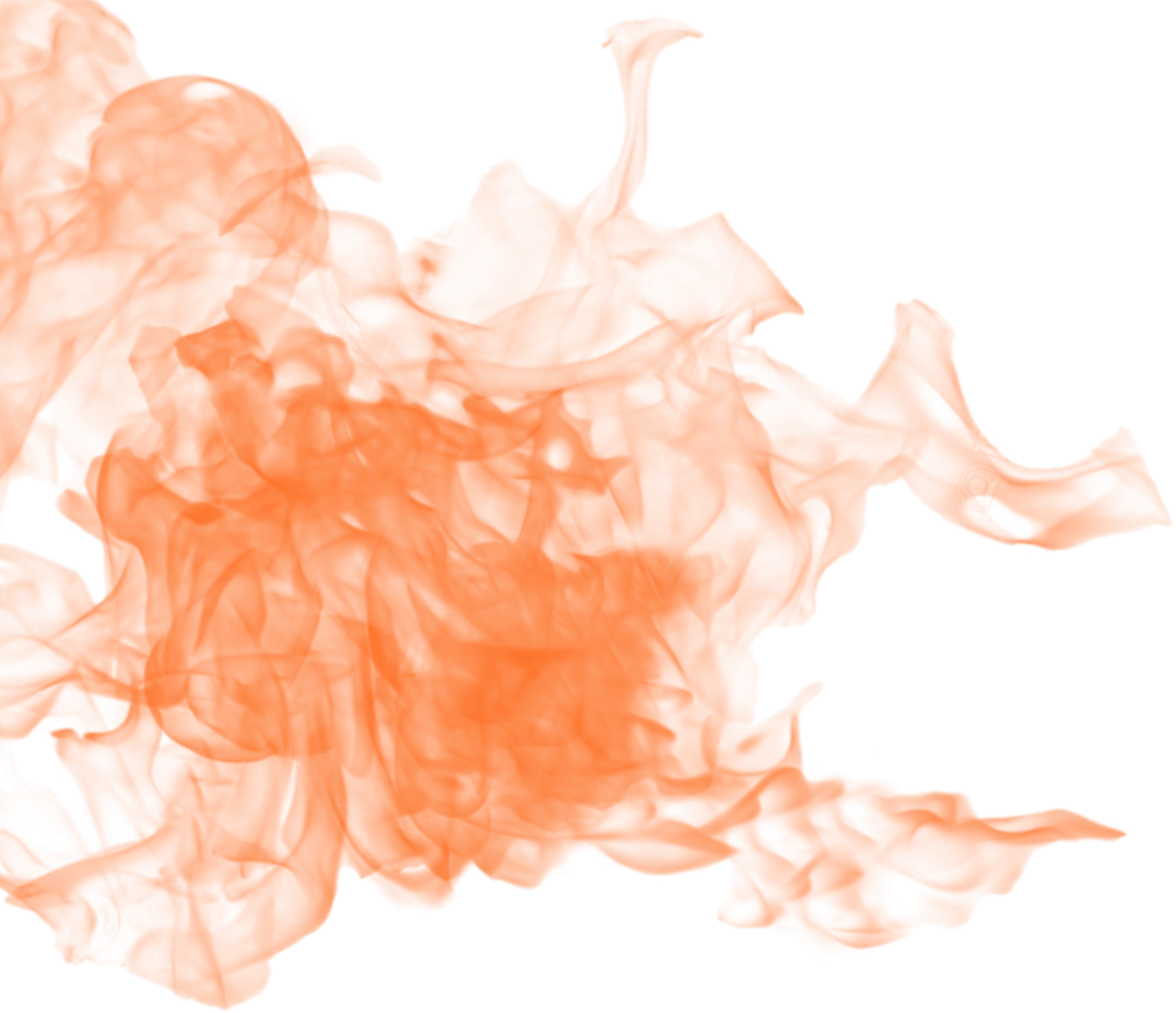

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