



PROGRAMA DE  
PÓS-GRADUAÇÃO  
EM FÍSICA



## Book of Abstracts

# Workshop on Quantum Thermodynamics

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Universidade Federal do Paraná  
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Programa de Pós-Graduação em Física

## TALKS

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2. Roberto Serra, UFABC (Maxwell's demons and the control of the thermodynamic arrow of time in quantum systems).
3. Paulo Souto-Ribeiro, UFSC (Classical and quantum optics for quantum thermodynamics).
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5. Domingos Salazar, UFRPE (Heat distribution in open quantum systems: thermal relaxation of bosonic and fermionic modes).
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## POSTERS

1. Adriane Leal, IFSC-USP (Probability analysis of the PQ quantum game).
2. Arthur Faria, UNICAMP (Study on the fluctuations induced by finite thermal baths).
3. Pierre Nazé, UNICAMP (Compatibility of linear response theory with the second law of thermodynamics).
4. Fabiano Andrade, UEPG (Unitary equivalence between the Green’s function and Schrödinger approaches for quantum graphs).

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## Efficiency of harmonic quantum Otto engines at maximal power

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Recent experimental breakthroughs produced the first nano heat engines that have the potential to harness quantum resources. An instrumental question is how their performance measures up against the efficiency of classical engines. For single ion engines undergoing quantum Otto cycles it has been found that the efficiency at maximal power is given by the Curzon-Ahlborn efficiency. This is rather remarkable as the Curzon-Ahlborn efficiency was originally derived for endoreversible Carnot cycles. Here, we analyze two examples of endoreversible Otto engines within the same conceptual framework as Curzon and Ahlborn’s original treatment. We find that for endoreversible Otto cycles in classical harmonic oscillators the efficiency at maximal power is, indeed, given by the Curzon-Ahlborn efficiency. However, we also find that the efficiency of Otto engines made of quantum harmonic oscillators is significantly larger. This work has been published recently<sup>2</sup>.

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<sup>2</sup>S. Deffner, *Efficiency of harmonic quantum otto engines at maximal power*, Entropy 20, 875 (2018).

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## Maxwell's demons and the control of the thermodynamic arrow of time in quantum system

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Entropy production is a ubiquitous fact of nature; invariably happens in a diversity of circumstances, imposing limits for technological applications, biological processes, and information processing. This phenomenon is even more provocative to our intuition about irreversibility in contexts that involve quantum mechanics and are far from equilibrium. The development of coherent control techniques associated with Quantum Information Science and Technology allows us to access energy fluctuations and to test its consequences in the laboratory. We can now implement true Maxwell Demons, which challenge the second law of thermodynamics, in actual experiments. In addition, we can still use quantum features as non-classical correlations to reverse the so-called “thermodynamic arrow of time” (at least in a certain time interval). In this talk, we will present recent experiments involving quantum systems where Maxwell's Demons and nanoscopic machines are tested. We will show how to control and mitigate irreversibility on a quantum scale.

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## Classical and quantum optics for quantum thermodynamics

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Recent attempts to extend concepts from Thermodynamics to Quantum systems are based on fluctuation relations that connect equilibrium and out-of-equilibrium quantities. One of the most prominent example is the Jarzynski's relation connecting work and free energy. It was extended to a quantum version, which brings a discussion about the definition of work for quantum systems and can be viewed as an alternative version of the second law of Thermodynamics. We discuss experimental platforms based on linear optics that can be used to experimentally approach the problem of measuring work distributions and testing fluctuation relations. In particular, we show that it is possible to use Gaussian beams to emulate quantum harmonic oscillators and implement processes in the context of Jarzynski's two-measurement protocol. We also discuss versions of this type of experiments involving entanglement and the potential consequences for the fluctuation relations.

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## Genuine quantum signatures in non-equilibrium states

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Extending the laws of physics beyond the paradigms of thermal equilibrium constitutes one of the main challenges in modern physics. In this regard, substantial effort is being made in identifying what are the genuine quantum mechanical features that may exist in non-equilibrium states. In this talk I will present recent theoretical results from our group which help to shed light on this difficult question. In particular, we focus on the scenario of non-equilibrium relaxation, where a system is prepared in a non-equilibrium state and allowed to relax in contact to one or multiple heat baths. In this case, the relevant question is how the quantumness of the initial state is washed away by the presence of the environments. We answer this from a resource theoretic point of view. We show that the entropy production, which measures the irreversibility of a process, can be divided into a hierarchy of terms quantifying the loss of different resources. The first term is a classical contribution related to changes in population. This is followed by a term representing the loss of local coherence in each subsystem. Afterwards, there is the loss of bipartite correlations, then tripartite correlations and so on, up to genuine  $N$ -partite correlations. Hence, the entropy production may be used as a universal quantifier of irreversibility, encompassing both classical and quantum resources. On the one hand, these results help to shed light on the foundations of the emergence of time-symmetry breaking entailed by irreversibility. On the other, they may be of use in the design of thermodynamically efficient quantum technologies.

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## Heat distribution in open quantum systems: thermal relaxation of bosonic modes

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We analyze a stochastic parametrization of phase space for a thermal relaxation of a bosonic mode. In the case of a sudden change of thermal baths, we show how this parametrization allows the deduction of a law of cooling and a closed form propagator for the Wigner function that results in the nonequilibrium heat distribution in a two point measurement scheme. We connect the stochastic parametrization of bosonic modes to the highly underdamped limit of a classic oscillator in a single-well potential, where the introduction of classic thermodynamic work is straightforward and it allows the computation of optimal protocols.

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## Entropy production as tool for characterizing nonequilibrium phase transitions

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Nonequilibrium phase transitions can be typified in a similar way to equilibrium systems, for instance, by the use of the order parameter. However, this characterization hides the irreversible character of the dynamics as well as its influence on the phase transition properties. Entropy production has revealed to be an important concept for filling this gap since it vanishes identically for equilibrium systems and is positive for the nonequilibrium case. Based on general arguments, we present distinct scenarios for the characterization of phase transitions in terms of entropy production. A full analysis is reported for discontinuous and continuous phase transitions; regular and complex topologies within the framework of mean field theory (MFT) and beyond the MFT.

Our predictions will be exemplified by an icon system, perhaps the simplest nonequilibrium model presenting an order-disorder phase transition and spontaneous symmetry breaking: the majority vote model. Its dynamics is ruled by the misalignment and inertia parameters whose phase transition is continuous or discontinuous depending on symmetry, connectivity and inertia. Our work paves the way to a systematic description and classification of nonequilibrium phase transitions through a key indicator of system irreversibility.

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## Entropy evolution in the electronic transport in strongly coupled mesoscopic systems

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We develop a Landauer-Büttiker theory of entropy evolution in time-dependent strongly coupled electron systems<sup>2</sup>. In distinction to the standard non-equilibrium Green's function approach, our formalism is partition free and naturally avoids the problem of system-bath distinction – a pressing problem in the strong coupling regime – by defining the entropy current in the attached leads. This current can then be used to infer changes of the entropy of the system which we refer to as inside-outside duality. We show that this approach gives the entropy production rate predicted by the standard thermoelectric theory for stationary processes. We then carry out our proposed program in an adiabatic expansion up to first order beyond the quasi-static limit. When combined with particle and energy currents as well as the work required to change an external potential, our formalism provides a full thermodynamic description, applicable to arbitrary non-interacting electron systems in contact to reservoirs. This provides a clear understanding of the relation between heat and entropy currents generated by time-dependent potentials and their connection with the occurring dissipation. We conclude by establishing the contact of our formalism with principle of minimum entropy production in steady state currents.

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<sup>2</sup>Anton Bruch, Caio Lewenkopf, Felix von Oppen, *Landauer-Büttiker Approach to Strongly Coupled Quantum Thermodynamics: Inside-Outside Duality of Entropy Evolution*, Phys. Rev. Lett. 120, 107701 (2018).

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## Advances in quantum transport

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Modern quantum thermodynamics is greatly interested in out-of-thermal equilibrium scenarios. Heat transport is maybe the most natural problem where thermal equilibrium is clearly not desired. If the whole system is at equilibrium, meaning that all its points are found at the same temperature, no transport will take place. In this work, we will be presenting the transport problem from the point of view of quantum information. This means that we want to investigate propagation of energy or heat taking into account aspects which are traditionally seem as resources in quantum information. Examples include quantum correlations such as entanglement and also superposition effects generically known as quantum coherence.

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## System-environment correlations for dephasing two-qubit states coupled to thermal baths

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Based on the exact dynamics of a two-qubit system and environment, we investigate system-environment (SE) quantum and classical correlations<sup>2</sup>. The coupling is chosen to represent a dephasing channel for one of the qubits and the environment is a proper thermal bath. Based on the usual thermal bath of harmonic oscillators, we derive criteria of separability and entanglement between an initial X-state and the environment. Applying these criteria to initial Werner states, we find that entanglement between the system and environment is built up in time for temperatures below a certain critical temperature  $T_{\text{crit}}$ . On the other hand, the total state remains separable during those shorter times that are relevant for decoherence and loss of entanglement in the two-qubit state. During these times and close to  $T_{\text{crit}}$  the SE correlations oscillate between separable and entangled. Even though these oscillations are also observed in the entanglement between the two qubits, no simple relation between the loss of entanglement in the two-qubit system and the build-up of entanglement between the system and environment is found.

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<sup>2</sup>A. C. S. Costa, M. W. Beims, W. T. Strunz, *System-environment correlations for dephasing two-qubit states coupled to thermal baths*, Phys. Rev. A 93, 052316 (2016).

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## Optimal thermodynamic work in finite-time isothermal processes: a linear-response approach

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The finite-time manipulation of thermodynamic systems demands an energetic cost whose quantification has practical and scientific importance. In particular, it is of extreme interest to predict which finite-time processes lead to the minimal cost given the thermodynamic boundary conditions. Motivated by these issues, we present a theoretical formulation of this optimization problem based on linear response theory. We show that this approach can be applied to a wide class of systems and discuss its advantages over other formulations. Finally, we show how it helps to understand the origin of negative entropy production rates in the close-to-equilibrium regime.

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## Work on a quantum dipole by a single-photon pulse: energy exchange and entropic analysis

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The work performed by a classical electromagnetic field on a quantum dipole is well known in quantum optics, where the absorbed power linearly depends on the time derivative of the average dipole moment. However, the problem concerning the work performed by a single-photon state on a quantum dipole still lacks an answer. As a matter of fact, the average quantum dipole moment exactly vanishes in such a scenario. In this talk, we address this problem. For that, quantum work is defined as the unitary contribution to the energy variation of the quantum dipole. It is shown that this definition furnishes a correspondence with the energy spent by the photon pulse to dynamically Stark shift the dipole. On the other hand, the non-unitary contribution to the dipole energy is defined here as a generalized quantum heat. It is shown that this generalized quantum heat is the energy corresponding to out-of-equilibrium photon absorption and emission. By providing physical means for being accessed, such connections for quantum work and generalized heat represent a step forward for such definitions. Finally, the system description allows a complete entropic analysis, where standard Thermodynamics equilibrium states can be reached, as well as non-thermal states can be investigated.

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## A definition of quantum mechanical work

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Work and heat are two of the most fundamental concepts related to the new emerging physics area frequently called Quantum Thermodynamics. Widely accepted definitions of these concepts were introduced by Alicki in his 1979 seminal work. Although such definitions have been successfully applied to many contexts, there seems to be deep foundational questions to be answered. In fact, alternative definitions have been proposed with basis on analogies with Classical Thermodynamics. In the present approach, a definition of quantum mechanical work is introduced which preserves the mathematical structure of the Classical Mechanics concept of work without, however, in any way invoking the notion of trajectory. By use of Gaussian states and the Caldirola-Kanai model, a case study is conducted through which the proposed quantum work is compared with Alicki's definition, both in quantum and semiclassical regimes, showing promising results. Conceptual inadequacies of Alicki's model are found in the classical limit and possible interpretations are discussed for the presently introduced notion of work.

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## Quantum theory of hierarchical systems

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A novel formalism, called quantum H-theory (QHT), is introduced to describe the statistical equilibrium of hierarchical quantum complex systems with multiple time and length scales. The formalism builds from a related classical H-theory (HT), which has been successfully applied to the description of statistical equilibrium of multiscale classical hierarchical complex systems. In QHT, the system is formally treated as being composed of a small subsystem in contact with a set of hierarchical organized bosonic reservoirs. The temperatures of the reservoirs are allowed to fluctuate at different scales by virtue of complex interactions among underlying bosonic degrees of freedom. The Wigner distribution function of the reservoir at a given scale is conditioned on the temperature of the reservoir at the next largest scale in the hierarchy and can be determined from a maximum entropy principle subject to appropriate constraints. The Wigner function of the relevant subsystem, obtained by averaging the local Wigner distribution over the distribution function of the innermost reservoir, is expressed in terms of Meijer  $G$ -functions. Possible connections with experimental results include atoms trapped on dissipative optical lattices and multicharged vortices in trapped atomic Bose-Einstein condensates.

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## Kolmogorov-Sinai entropy and dissipation in classical Hamiltonian systems

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A central concept in the connection between physics and information theory is entropy, which represents the amount of information extracted from the system by the observer performing measurements in an experiment. Indeed, Jaynes' principle of maximum entropy allows to establish the connection between entropy in statistical mechanics and information entropy. In this sense, the dissipated energy in a classical Hamiltonian process, known as the thermodynamic entropy production, is connected to the relative entropy between the forward and backward probability densities. Recently, it was revealed that energetic inefficiency and model inefficiency, defined as the difference in mutual information that the system state shares with the future and past environmental variables, are equivalent concepts in Markovian processes. As a consequence, the question about a possible connection between model unpredictability and energetic inefficiency in the framework of classical physics emerges. Here, we address this question by connecting the concepts of random behavior of a classical Hamiltonian system, the Kolmogorov-Sinai entropy, with its energetic inefficiency, the dissipated work. This approach allows us to provide meaningful interpretations of information concepts in terms of thermodynamic quantities.

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## Entanglement and identical particles: desymmetrization and generalized “Bell-type” states

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Entanglement measuring of distinguishable bipartite systems is acceptably well performed using von Neumann Entropy. When it comes to identical bipartite systems, some difficulties arise, due to the symmetrization postulate. This paper attempts to develop a desymmetrization method, so that von Neumann Entropy calculation becomes feasible and also relatively simple. Some simulations with identical bosonic and fermionic systems are performed and von Neumann Entropy shows signs of being consistent with expected results. Furthermore, a method for generating maximally entangled pure states is built, which seems to work for any bipartite system, either for identical or distinguishable cases, with any finite dimension.

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### Probability analysis of the PQ quantum game

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This study is developed from the first penny flip game on the quantum version, renamed as PQ game, by D. Meyer<sup>2</sup>. In this sense, the probabilities of the PQ game depend on a general angular parameter, which defines a quantum strategy operator. From these analyses, we observe that Picard can win the game if Q chooses appropriate value parameter  $\theta$ , equal to 0 or  $2\pi$ . However, if Q chooses  $\theta = \pi$  he always wins, regardless which quantum strategy operator Picard applies.

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### Study on the fluctuations induced by finite thermal baths

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The analysis of fluctuations generated by a thermal reservoir has produced many results throughout the history of physics, ranging from the verification of the atomic hypothesis, running through critical phenomena to the most recent advances in the description of non-equilibrium thermodynamic processes. Motivated by recent theoretical and experimental works, we analyze the equilibrium and non-equilibrium fluctuations caused by a finite bath of deterministic and chaotic dynamics when weakly coupled with a system of interest whose total system is approximately ergodic. In particular, in this work we tested the heat theorem and the fluctuation theorem for finite baths considering the mentioned model. In both cases, we verified the agreement between numerical results and analytic estimates.

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## Compatibility of linear response theory with the second law of thermodynamics

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The reliability of physical theories depends on whether they agree with well established physical laws. In this work, we discuss how to make the Hamiltonian formulation of linear response theory compatible with the Second Law of Thermodynamics. In order to do so, we verify three complementary aspects often understood as statements of the Second Law: 1) no dissipation for quasistatic process, 2) dissipation for finite-time processes and 3) positive entropy production rate. Our analysis focus on two classes of nonequilibrium processes: slowly-varying and finite-time but weak ones. For the former, we show that these aspects are easily verified. For the later, we present conditions for the achievement of the first two aspects. We also show that the third one is not always verified comparing exact and linear-response results for an example where negative values of the entropy production rate are observed.

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## Unitary equivalence between the Green’s function and Schrödinger approaches for quantum graphs

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In a previous work<sup>2</sup>, it was shown that the exact Green’s function (GF) for an arbitrarily large (although finite) quantum graph is given as a sum over scattering paths, where local quantum effects are taking into account through the reflection and transmission scattering amplitudes. To deal with general graphs, two simplifying procedures were developed: regrouping of paths into families of paths and the separation of a large graph into subgraphs. However, for less symmetrical graphs with complicated topologies as, for instance, random graphs, it can become cumbersome to choose the subgraphs and the families of paths. In this work, an even more general procedure to construct the energy domain GF for a quantum graph based on its adjacency matrix is presented. This new construction allows us to obtain the secular determinant, unraveling a unitary equivalence between the scattering Schrödinger approach and the Green’s function approach. It also enables us to write a trace formula based on the Green’s function approach. The present construction has the advantage that it can be applied directly for any graph, going from regular to random topologies.

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<sup>2</sup>Fabiano M. Andrade, A. G. M. Schmidt, E. Vicentini, B. K. Cheng, and M. G. E. da Luz, *Green’s function approach for quantum graphs: An overview*, Phys. Rep. 647, 1 (2016)