

5th Workshop on Statistical Physics / 5ta Escuela de Física Estadística

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Universidad Nacional de Colombia / Universidad de los Andes



Libro de resúmenes

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Tutorial courses / 101**Disordered systems out of equilibrium****Autor:** Leticia F. Cugliandolo¹¹ *Sorbonne Université, Paris***Corresponding Author:** leticia@lpthe.jussieu.fr

1. Introduction. Quenched and configurational disorder. Coarsening. Glassiness and active matter. Models and methods.
2. Equilibrium analysis. Free-energy landscapes (extensions of Ginzburg-Landau).
3. Out of equilibrium dynamics. Dynamic mean-field theory.

Invited Talks / 67**Do Lyapunov exponents measure chaos?****Autor:** Jorge Kurchan¹¹ *ENS Paris*

The solar system has a relatively large Lyapunov exponent, and yet has been stable for much longer than the inverse Lyapunov time. Similarly, almost integrable systems like the low energy Fermi-Pasta-Ulam chain take much longer to thermalize than one would expect from their Lyapunov exponent.

This phenomenon has more recently been studied in quantum systems.

El sistema solar tiene un exponente de Lyapunov relativamente grande y, sin embargo, ha permanecido estable durante mucho más tiempo que el inverso del tiempo de Lyapunov. De manera similar, sistemas casi integrables como la cadena de Fermi-Pasta-Ulam a baja energía tardan mucho más en termalizar de lo que cabría esperar a partir de su exponente de Lyapunov. Este fenómeno ha sido estudiado más recientemente en sistemas cuánticos.

Contributed talks / 63**Very persistent random walkers reveal transitions in landscape topology****Autor:** Jaron Kent-Dobias¹¹ *ICTP-SAIJR & IFT-UNESP***Corresponding Author:** jaron@ictp-saifr.org

In large random systems, certain behaviors are reliably predicted, like the energy density of the ground state. The long-time behavior of many physical and algorithmic dynamics is likewise predictable, through DMFT and related approaches. But can these behaviors be connected to static structures of the problem at hand, like its energy landscape? Recently, development of the Overlap Gap Property, which depends on the existence of a system-spanning component of the energy level set, suggests that static topological properties can predict the performance of the best algorithms.

Here, I will describe progress towards predicting the performance of the mediocre but simple algorithms we usually use. We use the ergodicity of a random walker to probe whether typical configurations belong to a system-spanning component of the energy level set. Passive random walkers lose ergodicity at a depth associated with the glass transition, but active random walkers remain ergodic to greater depth. We argue that in the limit of infinite persistence time, the ergodicity-breaking transition coincides with the point at which system-spanning components become atypical, and discuss connections with gradient descent dynamics.

Contributed talks / 85

Fast thermal equilibration using machine learning

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Fast thermal equilibration, also known as a shortcut to adiabaticity, is an external control technique employed to expedite operations beyond the system's natural timescale. In this talk, we will introduce a machine learning technique, specifically automatic differentiation, to identify control protocols that accelerate the equilibration process in stochastic systems modeled by the overdamped Langevin equation.

Tutorial courses / 102

Threeway out of equilibrium many body dynamics

Autor: Frédéric van Wijland^{None}

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These three lectures will focus on three manners to fall out of equilibrium, and on the many-body effects that arise from the nonequilibrium nature of the dynamics. We will begin with systems harboring a macroscopic current (leading to long range correlations). Then we shall stop by systems that should be relaxing towards equilibrium, but that fail to do so for reasons that are still under investigation. And the final lecture will concern systems with no macroscopic current that are nevertheless maintained out of equilibrium by a constant input of energy that drives the individual motion of the particles.

1. Out of equilibrium with a macroscopic current: Driven Systems
 - Macroscopic Fluctuation Theory
 - The possibility of phase transitions in one dimension
2. Out of equilibrium, but lost on the way to equilibrium: Glasses
 - Mode-coupling approach
 - Infinite-dimensional insight
3. Out of equilibrium, because that's life: Active Matter
 - From one particle to many
 - Field theories for active matter

Invited Talks / 59**Antifragility of stochastic transport on networks with damage****Autor:** Leidy Katherin Eraso Hernandez¹¹ *Universidad Nacional Autónoma de México***Corresponding Author:** erasoleidy@estudiantes.fisica.unam.mx

A system is called antifragile when damage acts as a constructive element improving the performance of a global function. In this work, we analyze the emergence of antifragility in the movement of random walkers on networks with modular structures or communities. The random walker hops considering the capacity of transport of each link, whereas the links are susceptible to random damage that accumulates over time. We show that in networks with communities and high modularity, the localization of damage in specific groups of nodes leads to a global antifragile response of the system improving the capacity of stochastic transport to more easily reach the nodes of a network. Our findings give evidence of the mechanisms behind antifragile response in complex systems and pave the way for their quantitative exploration in different fields.

Contributed talks / 57**From motifs to Lévy flights: modeling urban mobility in Bogotá's public transport system****Autores:** Juan Felipe Alayón Martínez¹; Alejandro Pérez Riascos¹¹ *Universidad Nacional de Colombia***Corresponding Author:** jalayonm@unal.edu.co

Paper published in 2026: we study two years of access card validation records from Bogotá's multi-modal public transport system, comprising over 2.3 billion trips across bus rapid transit, feeder buses, dual-service buses, and an aerial cable network. From user trajectories constructed exclusively from access records, we derive motifs that reveal recurrent mobility patterns extending beyond simple two-location visits. This approach enables the construction of an integrated origin–destination (OD) matrix covering 2828 urban zones. Similarity analysis using the Jensen–Shannon divergence confirms the temporal stability of mobility structures across semesters, despite infrastructure changes and fare policy adjustments. From the obtained OD matrices, we derive transition probabilities between zones and uncover a robust power-law relationship with geographical distance, consistent with Lévy flight dynamics. We validate our model using Monte Carlo simulations showing that reproduces both local and long-range displacements, with similar scaling exponents across time. These findings demonstrate that Bogotá's public transport mobility can be effectively modeled through Lévy processes, providing a novel framework for analyzing complex transportation systems based solely on user access records.

Contributed talks / 72**Thermostatistical study of the opinion formation phenomenon in the DNAW model****Autores:** Jefferson Rubiano Forero¹; Carlos José Quimbay Herrera²¹ *Universidad Nacional DE Colombia*

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The model proposed by Default, Neau, Amblard, and Weisbuch (DNAW) is relevant in sociophysics for studying the phenomenon of opinion formation in social systems composed of agents that interact in a binary manner. Its relevance lies in the fact that, through the formulation of an opinion exchange rule between pairs of agents whose opinion differences are smaller than a bounded confidence threshold (d), and which is expressed in terms of a convergence parameter (μ), it is possible to reproduce collective phenomena observed in social systems such as consensus, fragmentation, and polarization. Within the framework of this model, by establishing an analogy between a system of social agents and an ideal gas of free particles, we present a novel thermostistical study of the opinion formation phenomenon based on the definition of the following macroscopic variables: social temperature (T_s), social entropy (S_s), and social chemical potential (P_s). In particular, we define T_s as the first absolute moment of the opinions of all agents in the system with respect to the average opinion (Op) per agent. Through numerical simulations that systematically explore the parameter space (d, μ), we first identify the equilibrium state as the state for which S_s stabilizes and estimate the convergence time as the elapsed time required to reach equilibrium. Subsequently, we study the opinion formation process by analyzing the temporal evolution of the macroscopic variables Op , T_s , S_s , and P_s . In this way, we observe that d can be interpreted as a measure of social tolerance to interact with differing opinions, while μ quantifies the degree of mutual influence between a pair of agents during an interaction.

Contributed talks / 75

Exploration mechanisms intrinsic to semantic networks and the nuanced appraisal of lexical repetition occurrences

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Semantic memory is responsible for storing knowledge of concepts or meanings in the long term. Based on the semantic network from the study by Goñi et al. (2011), we study the efficiency and performance of the network using the switching random walker model for different transition biases between nodes. Diffusion in the network is described by Markov chains, a process that allows the calculation of descriptive random variables such as average first-pass time and entropy rate. The MFPT and the entropy rate are very useful measures because they provide information about how reachable a node is on average from any other node, and the rate at which information can spread through the network. In addition, we designed a fluency test simulation model based on the changing random walker (SRW) where the relationship between short-term memory (STM), the number of repetitions and the flexibility of change is analyzed. STM was found to play an important role in verbal fluency performance, at least as it relates to verbal fluency tests.

Invited Talks / 66

Sobreviviendo la era de LLMs

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Si bien los LLMs han irrumpido con excepcional fuerza en el campo de la IA con una percepción de un potencial de impacto y cambio enorme, su adopción para resolver problemas en la práctica

sigue planteando muchísimos retos. Su naturaleza como modelos estadísticos del lenguaje es la causa principal de estas dificultades y, en ese contexto se han creado muchas técnicas que permiten abordar parte de estos retos en distintas circunstancias. Esto incluye técnicas como grounding, continual pretraining, thinking models, etc. En esta charla revisaremos algunos casos en la industria y en la investigación donde relucen estas limitaciones y las aproximaciones que con las que estamos intentando explotar ese potencial prometido.

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Centro Nacional de Consultoría

Poster session / 58

Critical time-dependent phenomena in diffusion generative models

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In recent years, diffusion generative models have become state-of-the-art for tasks such as image, video, and audio generation, among others. More recently, there has been growing interest in studying the statistical mechanics of these models, driven by the observation of apparent phase transitions during the sampling process. More specifically, a symmetry breaking that resembles the one encountered in the Ising model. In this proposal, a theoretical description of the diffusion models is presented, explaining what diffusion models are, how they can be studied from perspective of equilibrium statistical mechanics, and how critical phenomena emerge in a simple case. Additionally, a simple simulation using a feed forward network and two delta functions as the initial distributions provides some insight into the model's behavior near the critical point. The main objectives include a deeper investigation of this critical phenomenon, with particular focus on questions concerning the relationship between data dimensionality and the number of spins in the Ising model, as well as the emergence of scaling-free properties. Furthermore, the development of new models is proposed to allow for a more detailed observation and analysis of these critical behaviors.

Poster session / 62

Encounter times of random walkers with simultaneous resetting on networks

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In this work, we study the dynamics of multiple random walkers on networks subject to a simultaneous resetting protocol, whereby all walkers are synchronously returned to their respective initial nodes. For this collective Markovian process, we derive exact analytical expressions for the mean first-encounter time, defined as the average time required for all walkers to meet for the first time at a given node. These results are formulated in terms of the eigenvalues and eigenvectors of the transition matrices governing the dynamics without resetting, providing a clear spectral interpretation of the impact of resetting on encounter processes. We further establish a general criterion for finite networks that determines when the introduction of a nonzero resetting probability reduces the mean first-encounter time and leads to an optimal resetting strategy. The theoretical predictions are illustrated through numerical results on regular and heterogeneous networks, for encounters involving two or more walkers, and for combinations of local and nonlocal dynamics. Our findings demonstrate that simultaneous resetting can significantly reduce encounter times for specific targets and initial conditions, while becoming ineffective for highly exploratory dynamics or distant targets. The framework provides a unified approach to collective search and encounter problems on networks with resetting.

Poster session / 64

Inducing synchronization in complex networks via stochastic resetting in the Kuramoto model

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Collective synchronization is an emergent phenomenon in physical, biological, and technological systems, where local interactions enable dynamical adjustment among oscillators. In complex networks, the Kuramoto model provides a fundamental framework to study the transition between incoherent and synchronized states; however, synchronization typically requires sufficiently strong coupling, which limits its controllability in subcritical regimes. In this work, we investigate an extension based on the stochastic resetting of subsystems, defined as random interruptions that restore the phase of a fraction of nodes to a reference value. We analyze this dynamics on different network topologies using numerical simulations and a mean-field theoretical approach, evaluating the role of the resetting rate, the fraction of reset nodes, and structural heterogeneity in the synchronization transition.

Our main result shows that stochastic resetting can induce synchronization even in regimes where the original dynamics remains incoherent. This mechanism acts as a local realignment process that counteracts phase dispersion and reduces the effective coupling threshold. These findings identify resetting as an effective strategy to promote and control collective coherence in complex oscillator networks.

Poster session / 69

Dynamics of correlations in a Werner state weakly coupled to a thermal bath

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Quantum thermodynamics aims to understand how thermodynamic processes emerge in quantum systems, particularly in relation to information and entanglement. In this work we study the dynamics of correlations of a Werner state composed of two qubits weakly coupled to a thermal bath. The system is described using a Lindblad master equation, modelling the environment as a thermal reservoir that induces transitions between the qubit energy levels according to Boltzmann statistics. Within this framework we analyze the evolution of thermodynamic and informational quantities, such as entropy and mutual information, as functions of temperature and of the Werner-state parameter. Finally, we discuss mechanisms governing the transformation between different Werner states and the thermodynamic aspects associated with these changes.

Poster session / 70

Scale invariance in heavy tails of the S&P 500 stock index using the fractional Laskin model

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In this work, we study the time scale invariance for the heavy tails of the minute log returns time series of the S&P 500 stock index for three different time periods (January 2011 – October 2015, November 2015 – December 2019, January 2020 – October 2023), considering minute, hour, and day time series for each case. Using the symmetric fractional Laskin model, which describes the dissipative effects of the financial market through a shot noise type stochastic dissipative force that is similar for positive and negative log returns, we calculate the fitting parameters of the heavy tails for each of the considered time periods and for each of the studied time scales. We contrast these fitting parameters with the power law exponents calculated for the high log returns time series (data above a certain threshold), for both positive and negative log returns, showing the existence of asymmetry for each of the cases. The asymmetries found in the heavy tails are consistent with those observed through the Lévy distribution fitting parameters of the low and medium time series log returns.

Poster session / 71

Scaling of ensemble fluctuation and Pareto laws in the distributions of average property prices per block in Bogotá

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An econophysical study of datasets on cadastral and commercial values of average prices per property per block in Bogotá leads us to identify the existence of ensemble fluctuation scaling. This scaling, which is a property of complex systems observed in a variety of natural scenarios and is characterized by a power-law relationship between the variance and the mean of the data, is found for the first time in data on average urban property prices. Furthermore, we find that the scaling of ensemble fluctuations exhibit spatial scale invariance when considering average property prices per block at the following spatial scales: blocks, neighborhoods, zoning planning units, and localities. Finally, for low and medium average price values, we find that the probability distribution fits a lognormal distribution, while the distribution above a certain price threshold follows a Pareto law for heavy tails.

Poster session / 73

Random Walks on Networks: Effective Distance, Entropy, and Fractional Dynamics

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We develop a path-integral formulation of first-passage random walks on networks and extend it to fractional transport dynamics. In this framework, the random-walk effective distance is defined from the ensemble of all first-passage trajectories connecting a source to a target, weighted by both their probabilities and their lengths. This construction naturally introduces a trajectory partition function, an effective action, and a free-energy-like interpretation of transport on networks. We further define the Shannon entropy of the first-passage trajectory ensemble and node-level indicators based on total shortest-path and total random-walk effective distances.

The formalism is first analyzed in simple benchmark topologies, where it captures symmetry, boundary effects, hub dominance, and hierarchy. It is then generalized to the fractional case by replacing local random-walk dynamics with nonlocal transport induced by the fractional network operator. The results show that fractional dynamics reshapes effective distances, trajectory diversity, and node accessibility by enhancing long-range exploration across the network. Altogether, the framework provides a unified description of local and nonlocal spreading on networks and offers a basis for future applications to complex systems.

Poster session / 74

Stability of Nonrelativistic Matter

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The stability of matter is often assumed without question. We typically believe that established physical theories can easily predict that atoms and molecules will not collapse or that the total energy of matter scales linearly with the number of particles. However, these questions remained unresolved when quantum theory was first established, and it actually took several decades before any proof was provided. In this talk, we present Lieb's proof of the stability of non-relativistic matter. By modeling matter as a system of N particles interacting under Coulomb forces, we show how to derive a linear bound for the total energy of the system as a function of N ; that is, to find a constant k such that $\mathcal{E}(\psi) > kN$ for every wave function ψ of the system. To achieve this, we apply the Lieb-Thirring inequalities in the context of Schrödinger operators and use a semiclassical approximation of the Coulomb energy. Finally, we discuss how this linear bound for the total energy leads to the conclusion that matter is extensive and bosonic matter is unstable.

Poster session / 77

Non-Extensive Statistical Mechanics and Heavy Tails in Financial Log>Returns: Stocks, FX, and Cryptocurrencies

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Non-extensive statistical mechanics, introduced by Tsallis, provides a robust theoretical framework for describing complex systems characterized by long-range correlations and extreme events. In the context of financial markets, the q-Gaussian distributions that emerge from this formalism constitute a natural generalization of Gaussian approaches, as they are capable of capturing the heavy tails that characterize empirical log-returns, which standard Gaussian models fail to reproduce. In this work, we present a comprehensive empirical validation of a hybrid model that integrates non-extensive statistical mechanics with a microscopic agent-based dynamics characterized by herding behavior. The simulated log-returns are compared with high-frequency data from stocks in developed and emerging markets, revealing that the q-Gaussian model reproduces the heavy tails of liquid markets with remarkable accuracy, whereas the Gaussian model better captures the statistical structure of assets such as oil and exchange rates, additionally exhibiting a surprising degree of temporal scale invariance. An additional finding is the identification of an intrinsic limit to the validity of the hybrid model, arising from its own dynamics without the need for externally imposed criteria. The analysis is further extended to high-frequency cryptocurrency and foreign exchange pairs, where the systematic variation of the parameter q enables the quantification of the degree of non-extensivity inherent to each market. The results indicate that the Tsallis formalism not only successfully captures the heavy tails of the assets considered, but also that the parameter q serves as a quantitative indicator of the degree of statistical complexity inherent in each asset class, raising the question of the potential universality of this approach across financial markets as diverse as digital and traditional ones.

Poster session / 78

Topological Edge States and Nonequilibrium Quantum Transport in One-Dimensional Topological Models: A Green's Function Approach

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This work presents an analytical Green's function study of one-dimensional topological models aimed at connecting their equilibrium spectral properties to nonequilibrium quantum transport. Working in the continuum limit, we derive exact expressions for the retarded Green's function of the bulk, the semi-infinite chain, and the finite chain, computing the Local Density of States (LDOS) in each geometry and tracing the progressive emergence of topologically protected boundary states, which are absent in the bulk spectrum. By this framework, we model a two-terminal junction consisting of a finite topological chain contacted by two normal metallic leads and using the Keldysh Non-Equilibrium Green Function formalism, we compute the transmission function and analyze the nonequilibrium transport properties of the junction. This work provides a fully analytical and unified framework connecting bulk topology, boundary spectral properties, and out-of-equilibrium current statistics in topological junctions.

Poster session / 90

Bosonisation of one-dimensional fermion systems and applications to spin chains

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Bosonisation is a technique to solve one-dimensional fermion models by transforming them to bosonic systems. S. Coleman (1975) showed that the correlators of the massive Thirring model, a one-dimensional Dirac fermion with self-interactions, coincide with those of the Sine-Gordon boson, and later, S. Mandelstam (1975) found the explicit map between these two systems. The identities found by Mandelstam generalise to a broader set of one-dimensional fermion models, that is, those that can be associated to a boson, and whose properties can hence be studied in an often simpler way by means of this mapping.

The transformation between fermions and bosons, however, is but a particular case of seeking equivalent models to a particular system in order to examine its behaviour in a potentially simpler way. Another example of such transformations is that of Jordan and Wigner (1928), who developed a way to map quantum spin lattices to fermions. This project seeks to examine quantum spin chains under the light of the Jordan-Wigner transformation and a subsequent bosonisation, which in many ways simplify the study of the statistical and thermodynamic behaviour of the chain.

Poster session / 89

Active Paths and Effective Stochastic Dynamics in Small Neural Networks

Autor: Cristian Pena^{None}**Corresponding Author:** cpenav@unal.edu.co

This project proposes to study a small neural network trained on a simple supervised learning task from a perspective inspired by statistical mechanics. The central idea is to identify the active paths connecting the input and output layers, analyze how they contribute to the represented function before and after training, and investigate whether their collective behavior admits an effective macroscopic description. To do this, the network output will be decomposed into contributions associated with active paths, and several collective observables will be introduced, including the number of active paths, the distribution of their effective contributions, and their temporal evolution during learning. Using multiple random initializations and training trajectories under stochastic gradient descent, the project will examine whether the evolution of the learned output can be approximated by an effective stochastic differential equation of the form $df_t(x) = A_t(x)dt + B_t(x)dW_t$, where $A_t(x)$ represents an average learning drift and $B_t(x)$ a fluctuation term induced by the stochastic nature of training. The main goal is to explore whether active paths can be interpreted as mesoscopic variables linking the microscopic dynamics of the weights with the macroscopic evolution of the learned function, providing a more structured description of supervised learning.

Poster session / 104

Structural and magnetic characterization of $Pr_{0.5}Ca_{0.09}Sr_{0.41}MnO_3$ manganites

Autor: Gabriela Rodríguez¹**Co-autores:** Daniel Hernández²; Juan Gabriel Ramírez²; Diego Carranza²¹ *Los Andes University*² *Universidad de Los Andes***Corresponding Author:** g.rodriguez1123@uniandes.edu.co

Manganites with a $CaMnO_3$ -type structure are generally antiferromagnetic and insulating at low temperatures. However, chemical substitution with rare-earth elements induces strong competition

between coexisting antiferromagnetic (AFM) and ferromagnetic (FM) phases, often leading to phase separation and field-induced metamagnetic transitions. These transitions can be understood as percolation events, where FM metallic clusters grow within an AFM insulating matrix until a conducting network spans the system at the percolation threshold, driving the metal-insulator transition. Despite extensive research, the coupling between structural distortions and magnetic ordering in these systems remains not fully understood.

Here, we present a structural and compositional characterization of $Pr_{0.5}Ca_{0.09}Sr_{0.41}MnO_3$ (PC-SMO) powder. The crystal structure and phase purity were examined by X-ray diffraction (XRD) and Raman spectroscopy, while the elemental composition was analyzed using energy-dispersive X-ray spectroscopy (EDX). Magnetic characterization was done through vibrating sample magnetometry (VSM) measurements performed at different temperatures to evaluate magnetic transitions. Our results suggest potential applications in neuromorphic computing as well as in magnetic and thermal sensing devices.

Poster session / 93

Modeling Invasion Percolation in Granular Media with Evolving Rheology: The Case of Rice Cooking.

Autor: Braithier Diaz^{None}

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The rice cooking process represents a complex physical system where phase transition thermodynamics, biopolymer leaching, and granular media mechanics converge. In this work, we present a cellular automaton model based on the Invasion Percolation (IP) algorithm to simulate the dynamics of nucleation and water vapor transport through a grain bed. Unlike standard IP models, our approach incorporates a thermo-rheological coupling: the heat flux at the base induces a thermal gradient that governs starch gelatinization kinetics via an Arrhenius-type relationship. The subsequent leaching of amylose and amylopectin modifies the viscosity of the continuous phase following the Quemada model, leading to a viscosity divergence as the solvent is depleted. Simultaneously, the mechanical transition of the grains is modeled through a critical invasion radius (R_c), which discriminates between the physical displacement of the grains (piston-like regime with geometric memory) and capillary flow (channeling). Preliminary results suggest that the competition between bubble buoyancy and the hardening of the polymeric gel defines the morphology of the vapor channels, explaining the formation of the tubular structures ("rice holes") observed macroscopically during cooking. This model provides a framework to understand how local heterogeneities in friction and dynamic surface tension dictate the final transport state in saturated granular systems.

Poster session / 97

Estudio Monte Carlo de la Entropía Residual en Redes de Ising Frustradas

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Este trabajo analiza cómo las modificaciones topológicas afectan la entropía residual y la degeneración del estado base en sistemas frustrados del modelo de Ising. Tomando como referencia las redes triangular y kagome antiferromagnéticas, se emplea un enfoque computacional basado en simulaciones de Monte Carlo e integración termodinámica.

Se estudian tanto defectos aleatorios como modificaciones periódicas de la red. Los resultados muestran que la dilución de sitios y enlaces reduce la entropía residual al aliviar la frustración, mientras

que las estructuras tipo stitched kagome permiten modificar la degeneración de forma controlada. Estos resultados muestran que la conectividad de la red modifica la degeneración del estado base y la entropía residual en estos sistemas.

Tutorial courses / 103

A statistical physics perspective on the theory of machine learning

Autor: Bruno Loureiro¹

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The past decade has witnessed a surge in the development and adoption of machine learning algorithms to solve day-a-day computational tasks. Yet, a solid theoretical understanding of even the most basic tools used in practice is still lacking, as traditional statistical learning methods are unfit to deal with the modern regime in which the number of model parameters are of the same order as the quantity of data – a problem known as the curse of dimensionality. Curiously, this is precisely the regime studied by Physicists since the mid 19th century in the context of interacting many-particle systems. This connection, which was first established in the seminal work of Elisabeth Gardner and Bernard Derrida in the 80s, is the basis of a long and fruitful marriage between these two fields.

The goal of this mini-course is to provide an in-depth overview of these connections and a good vision of the different tools available in the statistical physics toolbox, as well as their scope and limitations.

Syllabus:

- Historical overview of the connections between Statistical Physics and Computer Science.
- Mean-Field Models 101: Curie-Weiss Model
- Statistical-to-Computational Gaps
- The double-descent phenomena and benign overfitting (time permitting)

Bibliography:

The mini-course will be based on the following lectures notes: https://brloureiro.github.io/assets/pdf/NotesPrinceton_

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Preisach-percolation dynamics of multilevel resistive switching in phase-separated LPCMO

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We investigate the complex interplay of competing phases in bulk $\text{La}_{5/8-x}\text{Pr}_x\text{Ca}_3/8\text{MnO}_3$ (LPCMO) to demonstrate the coexistence of volatile and non-volatile multilevel resistive switching (RS) within a single device. In this system, ferromagnetic metallic (FM-M) and charge-ordered insulating (COI) phases spatially coexist across a broad ~ 160 K temperature window. While volatile RS is driven

by a reversible, electrically induced metal-insulator transition, the non-volatile RS is governed by the thermal history of the FM volume fraction. Specifically, voltage pulses that heat the device into a critical 90–210 K window permanently alter the phase fraction, modulating the resistance by up to seven orders of magnitude ($\sim 300 \Omega$ to $\sim 109 \Omega$). The metallic state is fully recoverable by cycling the temperature above the charge-ordering threshold (~ 210 K). To quantitatively capture this phase-fraction control, we implement a Preisach–percolation framework. Calibrated directly from experimental R–T hysteresis loops without free parameters, the model extracts domain switching distributions and utilizes a percolation threshold of $p_c = 0.65$ to successfully predict both macroscopic resistance at 2 K and magnetization at 5 K following specific thermal pathways. Ultimately, we demonstrate the stabilization of three distinct, highly reproducible resistance states over 25 cycles with ratios exceeding 10^3 , showcasing phase-fraction engineering as a robust mechanism for multilevel memory in correlated oxides.

Keywords: resistive switching, phase separation, Preisach model, percolation theory, LPCMO, neuromorphic computing.

Acknowledgements

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From ferrimagnetic to spin glass behavior and back in lamellar Mn oxides undoped and doped with Co

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In this work we describe magnetization measurements on lamellar Mn oxides un-doped and doped with Co. They show that the magnetic structure of this oxides system is extremely sensitivity to the (Co/Mn) ratio. Special emphasis is given to the inverse susceptibility and the temperature derivative of the magnetic susceptibility. Interestingly, the magnetic order changes from a typical ferrimagnetic one with two sublattices (sample with Co/Mn = 0) to an unconventional ferrimagnetic one with many sublattices (sample with Co/Mn = 0.014) and, subsequently, to a possible spin glass-type structure (sample with Co/Mn = 0.037), before finally back to a predominant typical ferrimagnetic order taking place at intermediate temperatures (sample with Co/Mn = 0.096) with increasing the (Co/Mn) ratio. The behavior of the susceptibility is described by means of its association with the spatial range of correlations between the spins of the system. The possible mechanisms leading to such unusual changes of magnetic ordering are discussed, including the super exchange interaction, double exchange interaction, and the frustration associated to such magnetic interactions.

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Defect-induced ferroic states in solid solutions of layered van der Waals

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Solid solutions of transition-metal dichalcogenides (TMDs), a family of quasi-2D van der Waals materials, provide a powerful platform to explore how composition, structural symmetry, and defect chemistry collectively determine electronic and ferroic properties in layered materials. In particular, the ability to independently tune substitutional disorder and intrinsic defect populations offers a route to stabilize emergent phases that are absent in stoichiometric compounds. These materials therefore offer a versatile framework to investigate how compositional engineering and defect-mediated symmetry breaking can generate new functional states.

In this talk, I will discuss how alloying different TMDs can be a general strategy to control structural symmetry and electronic instabilities that give rise to multiple ferroic orders. Within this framework, chemical substitution primarily modifies lattice parameters, bonding geometry, and spin-orbit coupling, while deviations from ideal stoichiometry introduce defect populations that can locally break inversion symmetry and generate magnetic moments or electric dipoles. The interplay between these two control parameters provides a pathway to stabilize magnetic, polar, and multiferroic states in otherwise non-ferroic layered materials.

I will illustrate these ideas with experimental examples from the alloy families WSe₂-WTe₂ and WS₂-WTe₂, synthesized as bulk single crystals and characterized through structural, magnetic, piezoresponse and transport measurements. In particular, the WSe₂-WTe₂ system reveals a systematic evolution of lattice symmetry and unit cell volume with tellurium substitution and the emergence of defect-stabilized magnetic and polar responses as the chalcogen vacancy density increases. By correlating substitution and defect concentration, a configurational ferroic phase diagram can be constructed that separates paramagnetic-ferromagnetic, paraelectric-ferroelectric, and multiferroic regimes. These results highlight how solid-solution engineering in layered van der Waals materials provides a general route to stabilize emergent ferroic phases through the coupled control of composition and defects.

Contributed talks / 61

Spin Glass Dynamics on Complex Hardware Topologies: A Bond-Correlated Percolation Approach

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Understanding how frustration and disorder shape relaxation in complex systems is a central challenge in statistical physics and directly relevant to quantum annealing. Spin-glass models provide a natural setting to address this problem, as their energy landscapes are governed by competing interactions and constrained network topologies. In this talk, I explore the non-exponential relaxation dynamics of spin glasses defined on hardware-relevant graphs such as Chimera, Pegasus and Zephyr. These architectures impose finite connectivity and embedding constraints that strongly influence how correlations propagate and how metastable states are organized. Using the Fortuin-Kasteleyn-Coniglio-Klein (FKCK) cluster framework, I show that even in the absence of a conventional finite-temperature spin-glass transition, frustration and disorder generate multiple dynamical time scales. The emergence and fragmentation of large-scale clusters provide a geometric interpretation of slow relaxation and reveal how topology controls the onset of collective dynamics. This perspective offers a physically transparent way to characterize energy landscapes on realistic annealing hardware and provides quantitative insight into how graph connectivity and frustration jointly determine the performance and limitations of quantum annealing architectures.

Keynote / 99

Active Quantum Particles from Engineered Dissipation

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While the physics of classical active particles—such as bacteria, synthetic Janus colloids, and bird flocks—is well-established via models like Active Brownian Motion (ABM), the extension of these principles to the quantum regime has only recently gained traction. This talk will first review the fundamental principles of classical self-propulsion, highlighting unique features of individual particle dynamics. We will then transition to new frameworks for Quantum Active Matter from Engineered Dissipation, presenting three specific models and demonstrating that they all recover the hallmark features of active motion.

Talk based on the preprint with the same title, by Jeanne Gipouloux, Matteo Brunelli, Leticia Cugliandolo, Rosario Fazio, Marco Schirò
arXiv:2603.19094
<https://arxiv.org/abs/2603.19094>

Invited Talks / 82

The complex evolution of chess openings

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Chess is a board game that demands deep positional understanding from the very first move of the opening to the end of the game. The initial moves, by both White and Black, contain information at the individual level about each player's strengths, knowledge of the adversary, and personal preferences, as well as broader insights into the state of the art of the game itself. The evolution of chess can be traced back to the fifteenth century, with major transformations linked to the formal establishment of rules—such as Ruy López's treatise—, the beginning of organized tournaments in London, the formation of FIDE—Fédération Internationale des Échecs or International Chess Federation, and the establishment of the Chess Olympiads. Several tournaments have been reserved for high-level players, with selection processes ranging from direct invitations, such as the Hastings call, to eliminatory systems like the Chess Olympiads and the World Championship Candidates Tournament. Participants in these events bring well-established strategies and techniques, and innovations that emerge from the global practice of chess.

In this study, we analyze the development of chess openings over the course of a century, using the complete dataset of matches played in the Olympiads from 1924 to 2024. We combine two theoretical and methodological approaches: on one hand, we represent matches and tournaments using graphs; on the other, we apply entropy measures and complexity indices to explore and trace the organizational processes underlying the evolution of the game. Graphs are constructed by adding directed dyads corresponding to the first move of each match, with nodes representing Black's responses to White's moves using Descriptive Notation (e.g., Pawn to King 4 as PK4), recorded in a 20×20 matrix. We compute the following measures of complexity: Shannon entropy, Tsallis entropy, the Shiner-Davison-Landsberg complexity index, and the López-Ruiz-Mancini complexity index—based on both degree and strength of the nodes. These are analyzed across three match outcomes: White wins, Black wins and draws. In- and out-degree and strength are associated with the player's perspective (White or Black), while outcomes are treated as subsystems to estimate Tsallis entropy. Our results show that chess has evolved towards increasing diversity, due to broader explorations and preferences for rare strategies, reflecting both innovation and adaptation to evolving winning patterns: While Shannon entropy captures the growing dispersion of opening choices and shifts in player's preferences, and complexity indices highlight rising interdependence between moves, assuming superadditivity Tsallis entropy parameter (q), ranges from 1.1 to 3.0, signals a transition toward correlated structures.

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El escalamiento temporal de la temperatura de los sistemas complejos: Una nueva propiedad en la naturaleza

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Los sistemas complejos presentan diferentes tipos de escalamiento, tales como el escalamiento de la fluctuación temporal caracterizada por el hecho de que la dispersión de los datos en una serie de tiempo no estacionaria (cuantificada mediante la variancia) satisface una relación de ley de potencia con respecto al promedio de los datos, o el escalamiento del Theil temporal en el que la dispersión de los datos en una serie de tiempo de trayectoria difusiva (cuantificada mediante el índice de Theil) satisface una relación de ley de potencia con respecto al promedio de los datos mediante una expresión que tiene cierta similitud con la existente en las transiciones de fase de segundo orden. El objetivo principal de esta charla es mostrar la existencia en la naturaleza de una nueva relación de escalamiento, en la que la temperatura de los sistemas complejos definida como el primer momento central absoluto se relaciona mediante una ley de potencia con respecto al promedio de los datos. La anterior relación de ley de potencia, que es denominada escalamiento temporal de la temperatura de los sistemas complejos, está presente en diferentes tipos de sistemas complejos de naturaleza económica, social, financiera, meteorológica, epidemiológica, etc.

Contributed talks / 76

Temporal fluctuation scaling and thermostistical study of the per capita gross domestic products of 105 countries of the world during the period 1960-2023

Autor: Alejandro Riascos Ochoa¹

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We perform an econophysics study of the gross domestic product per capita (GDPP) data from $N = 105$ countries worldwide, which have annual records in the World Bank database for every year between 1960 and 2023.

Starting from the time series of annual values of the average GDPP per country and the variance of the GDPP for the period 1960-2023, we find that the variance presents a power law relationship with respect to the average, that is, the existence of the scaling of the temporal fluctuation in this economic system is verified.

Subsequently, after verifying that there is also scaling of the time fluctuation for 15-year observation windows, we studied the annual evolution of the values of the proportionality constant and the exponent of the scaling of the time fluctuation during the period 1974-2023, observing the existence of anticorrelated cycles for these two quantities.

Finally, defining the economic temperature (T_e) as the first absolute moment of the 105 GDPP values with respect to the average GDPP per country, the economic entropy (S_e) as the average Shannon entropy per country multiplied by N , and the economic chemical potential (P_e) by establishing an analogy with the first law of thermodynamics, we study the temporal evolution of the macroscopic variables T_e , S_e , and P_e over the period 1960-2023.

We find that, in terms of these macroscopic variables, it is possible to identify historical periods in which different economic factors led to growth or decline dynamics in the annual values of both the average GDPP per country and the variance of GDPP.

Keynote / 106

Scaling Laws and Spectra of Shallow Neural Networks in the Feature-Learning Regime

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Neural scaling laws underlie many of the recent advances in deep learning, yet their theoretical understanding remains largely confined to linear models. In this work, we present a systematic analysis of scaling laws for quadratic and diagonal neural networks in the feature learning regime. Leveraging connections with matrix compressed sensing and LASSO, we derive a detailed phase diagram for the scaling exponents of the excess risk as a function of sample complexity and weight decay. This analysis uncovers crossovers between distinct scaling regimes and plateau behaviours, mirroring phenomena widely reported in the empirical neural scaling literature. Furthermore, we establish a precise link between these regimes and the spectral properties of the trained network weights, which we characterize in detail. Consequently, we provide a theoretical validation of recent empirical observations connecting the emergence of power-law tails in the weight spectrum with network generalization performance, yielding an interpretation from first principles.

<https://arxiv.org/abs/2509.24882>

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La Relación de Crooks aplicada a sistemas de dos osciladores armónicos acoplados simulados bajo movimiento browniano

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La Relación de Crooks [1], uno de los teoremas de fluctuación, es hoy en día un método estándar para calcular diferencias de energía libre entre dos estados de un sistema utilizando procesos fuera del equilibrio. En el presente trabajo construimos un sistema de dos osciladores armónicos de masa y resorte en un baño térmico acoplados por un tercer resorte, y simulamos mediante dinámica browniana el proceso directo por el cual separamos los osciladores hasta que el enlace entre ellos se rompe, para luego volver a juntarlos en un proceso reverso durante el cual el enlace entre ellos se restablece. En un segundo sistema, el resorte de acople vuelve a aparecer al final del proceso de estirado. Al trazar las curvas de fuerza vs. elongación y medir para muchas repeticiones los histogramas de los trabajos realizados en los procesos directo y reverso, es posible usar la Relación de Crooks para calcular la diferencia de energía libre entre los estados inicial y final. Nuestros resultados evidencian que la Relación de Crooks es capaz de predecir con exactitud del 1% la diferencia de energía libre entre los ensambles canónicos inicial y final, incluso al ejecutar el protocolo con velocidades tres órdenes de magnitud mayores que las de la evolución cuasi-estacionaria. Además, las curvas obtenidas de fuerza vs elongación se asemejan a las obtenidas en experimentos con horquillas de ARN [3]. Los sistemas propuestos no sólo ilustran el funcionamiento y significado conceptual de la Relación de Crooks, sino que también podrían usarse como punto de partida para construir modelos simplificados de moléculas biológicas.

[1] Crooks, G. E. Phys. Rev. E 60, 2721-2726 (1999).

[2] Julián David Jiménez Paz, “La relación de Crooks: trabajo y energía libre en osciladores acoplados fuera del equilibrio”, Trabajo de Grado, Físico. Director Prof. José Daniel Muñoz, Universidad

Nacional de Colombia, Bogotá (2024).

[3] D. Collin et. al, Bustamante, C. et al. Nature 437, 231-234 (2005).

Contributed talks / 92

Feedback control and the Second Law of thermodynamics in a ratchet physical system

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We simulate a realization of Maxwell's demon based on the experimental setup developed in \textit{Bayesian Information Engine that Optimally Exploits Noisy Measurements}, in which a heavy bead, immersed in water at room temperature, is trapped by an optical tweezer and lifted through rapid feedback control without net work expenditure. This system functions as an information engine, harnessing favorable thermal fluctuations to increase the bead's gravitational potential energy while keeping the trap's potential energy unchanged. Our simulations successfully reproduce key experimental findings regarding the engine's performance across a range of noisy measurements and verify the Generalized Jarzynski Inequality. In contrast to previous works that employ a Langevin dynamics approach, we implement a molecular dynamics algorithm to model the system. Our results confirm that the Generalized Jarzynski Inequality holds for all tested cases, by a significant margin. This study contributes to the theoretical understanding of the thermodynamics of mesoscopic systems under feedback control and further reinforces the fundamental connection between information and thermodynamics.

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Monte Carlo modeling of asphalt surface wear under studded-tire traffic

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This study investigates the evolution of asphalt pavement surface damage caused by studded-tire traffic using a combined experimental and stochastic modeling approach. Laboratory tests on six asphalt mixtures were integrated into a Monte Carlo simulation framework that models rutting as the cumulative effect of random stud impacts. The model incorporates parameters describing cumulative damage, particle detachment energy thresholds, and material susceptibility to wear. The simulations successfully reproduce the transition from an initial nonlinear damage phase to a stabilized linear rutting regime observed experimentally. A strong linear relationship was identified between the stochastic detachment parameter, the laboratory rutting rate, and the abrasion resistance of the mixtures. These results confirm the model's capacity to reproduce measurable material behavior. By linking mixture characteristics to probabilistic descriptions of surface deterioration, the proposed framework provides a predictive tool to support the design of more wear-resistant pavements in cold-climate regions.

Contributed talks / 60

Criticality and non-reciprocity of catastrophic phase inversion in emulsions

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The production of concentrated emulsions involves high-shear flows and it is well known that at a critical volume fraction the emulsion loses stability, undergoing an extremely rapid process where the continuous and dispersed phases in the emulsion exchange roles. This process, called catastrophic phase inversion, which resembles in several respects a dynamical phase transition, has remained widely elusive from an experimental and theoretical point of view. We present state-of-the-art experimental and numerical data to support a dynamical-system framework capable of precisely highlighting the dynamics occurring in the system as it approaches the catastrophic phase inversion. The study clearly highlights that at high volume fractions, dynamical changes in the emulsion morphology, due to coalescence and breakup of droplets, play a critical role in determining the emulsion rheology and stability. Additionally, we show that at approaching the critical volume fraction, the dynamics can be simplified as being controlled by the dynamics of a correlation length represented, in our systems, by the size of the largest droplet. This dynamics shares a close connection with non-reciprocal phase transition where two different physical mechanisms, coalescence and breakups, can get out of balance leading to large non-symmetric periodic excursions in phase space. We clarify the phenomenology observed and quantitatively explain the essential aspect of the highly complex dynamics of stabilized emulsions undergoing catastrophic phase inversion.

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Field-theoretic Formulation of Ion Correlations with Explicit Hard-Core Size in Aqueous and Non-Aqueous Electrolytes

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The accurate formulation of ion correlations in charged solutions is a critical task for the control of various biological and industrial processes ranging from ion transport through cells to water purification procedures. The theoretical tools enabling the comprehension of these systems is based on 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 of aqueous and non-aqueous electrolytes up to molar salt concentrations.

[1] P. Debye and E. Hückel, “The theory of electrolytes. I. Lowering of freezing point and related phenomena”, *Zur Theorie der Elektrolyte*. Phys. Z. 24, 185 (1923).

[2] S. Buyukdagli, “Self-consistent electrostatic formalism of bulk electrolytes based on the asymmetric treatment of the short- and long-range ion interactions”, *Soft Matter* 20, 9104 (2024).

[3] S. Buyukdagli, “Unified theory of equilibrium thermodynamics and ion association in aqueous and non-aqueous electrolytes with explicit hard-core size”, *J. Chem. Theory Comput.* 22, 831 (2026).

Contributed talks / 88**Two-Point Correlation in Dyson Gases Out-of-Equilibrium****Autor:** John Fredy Mateus Rubio¹**Co-autor:** Gabriel Téllez¹¹ *Universidad de los Andes***Corresponding Author:** jf.mateusr@uniandes.edu.co

We study the dynamics of a Log-Coulomb gas consisting of N charged particles confined to a unitary circle and coupled to a thermal bath characterized by a dimensionless effective parameter $\beta = q_0^2/(k_B T)$ with q_0 the charge per particle, T the bath temperature, and k_B the Boltzmann's constant. The use of a circular domain eliminates boundary effects and ensures exact rotational invariance, leading to an uniform equilibrium density without external confinement. This geometry isolates universal collective properties and greatly simplifies both static and dynamical analyses of logarithmic Coulomb gases particularly, for $\beta = 2$, the system can be treated as a free-fermion model, for which we can obtain an analytical expression for the two-point correlation function in the simplest case $N = 2$, and then extend our analysis to $N > 2$ both numerically and analytically. By varying β , we show that a logarithmic time-law scaling governs the time evolution of this process, and we verify the validity of the probability distribution of spacings between consecutive particles (levels), called Wigner's surmise, for $\beta \geq 1$ by comparison with the corresponding Gaussian ensembles for times larger than the relaxation time, $\tau \geq \tau_{\text{Eq}}$, i.e., once the system has reached thermal equilibrium.

Keynote / 100**Wetting by active fluids****Autor:** Frédéric van Wijland^{None}**Corresponding Author:** frederic.van-wijland@u-paris.fr

In equilibrium fluids, wetting is controlled by the competition of three surface tensions between the three phases (liquid, gas, solid). When the particles comprising the fluid become self-propelled, the question of wetting begins with a proper definition of surface tension (which may not be unique out of equilibrium). I will present a robust mechanics-based definition for surface tension. I will use this definition to explore the properties of a droplet at contact with a solid. It will appear that the angle of contact of an active droplet is no more governed by the Young-Dupré equation.

With Y. Zhao, J. Tailleur, A. Daerr, R. Zakine, Y. Kafri

Invited Talks / 107**TBA****Autor:** John Reina¹¹ *Universidad del Valle***Corresponding Author:** john.reina@correounivalle.edu.co**Invited Talks / 98**

Interplay of quantum resources: magic-protected entanglement

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Entanglement and magic (non-stabilizerness) are widely regarded as necessary for quantum universality and potential advantage. Yet the form in which they must appear within a quantum state remains unclear. We introduce an operational diagnostic of their interplay: *magic-protected entanglement*, defined as entanglement remaining after optimal stabilizer (Clifford) processing. This reframes the heuristic “entanglement~+~magic” as a sharp operational question: how much entanglement is intrinsically linked to magic. This perspective endows the state space with structure, distinguishing *T-magic*-type states, where magic is injected locally and entanglement can often be removed by stabilizer processing, from *W-magic*-type states (including Dicke and non-stabilizer hypergraph families), whose entanglement cannot be completely undone by Clifford circuits. The resulting separation enables a principled discussion of nonlocal quantum resources.

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Decoherence-assisted quantum key distribution

Autor: Alejandra Valencia¹

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In the development of quantum technologies, the interaction between a quantum system and its environment, that leads to decoherence, is traditionally viewed as a fundamental obstacle. In Quantum Key Distribution (QKD) protocols like BB84, environmental noise inevitably degrades state purity, increases the Quantum Bit Error Rate (QBER), and ultimately compromises the security of the communication channel.

In this talk, we challenge this standard paradigm by presenting a theoretical and experimental study of a controllable decoherence-assisted QKD scheme [1]. Rather than attempting to isolate the quantum system from environmental noise, we demonstrate how decoherence can be actively harnessed as a tool to enhance security against specific eavesdropping strategies, such as the entangling probe attack.

We will discuss our method of introducing tunable decoherence to polarization qubits by coupling them to the spatial degree of freedom of light. By treating the transverse momentum of the light as a controllable environment, the sender and receiver (Alice and Bob) can dynamically coordinate and vary the induced dephasing during transmission. When incorporated into a modified key reconciliation stage, this shared, controlled decoherence effectively limits the amount of information an eavesdropper can extract.

Finally, we will share the results of our experimental implementation, demonstrating that Alice and Bob can cancel out the dephasing effects to recover a low QBER of approximately 7.38%. Ultimately, this work adds to the effort of a different perspective on open quantum systems: proving

that system-environment interactions can be strategically managed to our advantage rather than merely mitigated.

[1] Sci. Rep. 15, 31258 (2025).

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TBA

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Invited Talks / 91

StatMech Insights on Na⁺/I⁻ Symporter transport cycle

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The intrinsic transmembrane protein known as sodium iodide symporter (NIS) facilitates the active transport of iodide across the basolateral membrane of thyroid follicular cells. Iodine is an essential molecule that is used to produce the classical thyroid hormones.

To perform a molecular dynamics (MD) simulation, we used structures of apo-NIS and NIS with I⁻ and an oxyanion (ReO4⁻) bound to it.

The goal of our computational study was to explore the conformational space of NIS and gain insights into the conformations it assumes over the course of its transport cycle.

We prepared a realistic simulation system that included NIS Na⁺ + I⁻ / Na⁺ + ReO4⁻ complexes embedded in a central membrane with the mammalian lipid composition, with two half-membrane leaflets on either side. We simulated the membrane potential by applying a constant external electrical field to the system, thereby bringing about the equivalent of a membrane potential. We are using this system to conduct unbiased and enhanced dynamics (metadynamics, Deep-Tica), a NPT statistical ensemble, with the program GROMACS (2023.3) and a modified CHARMM36 force-field, to include non-bonded interactions between I⁻ and the oxyanion ReO4⁻. In order to determine the effects of the potential on the outwardly open NIS events, simulations were conducted with three different membrane potentials (0, -70, and -140 mV) using the wild-type NIS with the anion and oxyanion bound to it, and using a double mutant with interesting transport characteristics.

The resulting MD trajectories are currently being analyzed using a Python 3.11 script and some public libraries such as mdtraj (v1.9), MDanalysis (v2.7), Pyemma (v2.5.12), mlcolvs and pytorch for deep-learning analysis. Metadynamics calculations of the transport of I⁻/ReO4⁻ free energy along the transport path are currently being done for the different membrane potentials, using funnel bias metadynamics.

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Scaling limits of random curves via Schramm–Loewner evolution

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The Schramm–Loewner Evolution (SLE) provides a rigorous framework for characterizing the scaling limits of fractal curves, encoding their geometric properties through the diffusion parameter of a Brownian motion and enabling a universal classification of stochastic growth processes. In this talk, we introduce the basic ideas behind SLE and discuss its role in understanding conformally invariant scaling limits of critical lattice models, such as coastlines and invasion percolation trees. We also discuss some limitations of this description and suggest possible directions for generalizations.