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05 Jul 2025 - 10 Jul 2025
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P01

Emergent Behaviours in AI-Human Systems: Insights from Statistical Mechanics

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As artificial intelligence (AI) becomes an integral part of our daily lives, understanding the dynamics between humans and AI is critical. In this paper, we explore the interactions within an AI-human ecosystem through a novel mathematical model inspired by statistical mechanics (quartic mean field Ising model). By simulating various group scenarios such as teams of humans working alongside or against AI agents, we investigate how the proportion of AI participants can impact the overall behaviour of the system. Our results show that even small shifts in the ratio of AI to human agents can lead to major changes in outcomes, pushing the system towards extreme polarization or leaving it in a delicate state of uncertainty. This study provides valuable insights into the tipping points where AI begins to take a dominant role in decision-making, with significant implications for fields like healthcare, education, and public policy. The findings emphasize the need for careful management of AI's role in human collaborations to maintain balanced, ethical outcomes. Beyond identifying challenges in integrating AI into human-centred environments, this research also opens up new pathways for exploring the evolving relationship between humans and intelligent machines.

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P02

Abstract template for Statistical Physics-Driven AI Methods for Drug Design: A Review of Emerging Frameworks

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The convergence of statistical physics and artificial intelligence (AI) is fundamentally reshaping computational drug discovery, providing innovative solutions to address the high-dimensional complexity inherent in molecular systems. This synthesis work examines cutting-edge methodologies emerging from this interdisciplinary synergy, focusing on their theoretical underpinnings, practical implementations, and transformative potential in global health applications.

Contemporary approaches bridge statistical mechanics with machine learning through three principal paradigms. First, **diffusion models** rooted in non-equilibrium thermodynamics [1] employ stochastic noise-reversal processes to iteratively refine molecular structures. As demonstrated by [2] and extended in pharmaceutically relevant applications by [3], these models leverage equivariant neural architectures to preserve essential 3D biochemical constraints during ligand generation. Second, **Boltzmann Generators** [4] combine energy-based sampling with deep learning to efficiently explore conformational landscapes, achieving order-of-magnitude reductions in computational cost compared to traditional molecular dynamics. Third, **energy-based models (EBMs)** [5] establish direct connections between statistical mechanical principles and machine learning through explicit energy functions, enabling precise prediction of protein-ligand binding thermodynamics.

In practical drug discovery pipelines, these methods enable: (1) generation of chemically diverse ligand libraries via diffusion processes, (2) prediction of equilibrium binding poses through Boltzmann sampling, and (3) free energy calculations using physics-informed EBMs. Recent successes include antiviral [3] and antimalarial [4] compound development. However, critical challenges persist: maintaining physical interpretability in black-box AI systems requires integration of domain knowledge (e.g., entropy maximization principles and spin-glass theory), while scaling these methods for resource-constrained African settings demands novel algorithms optimized for sparse datasets and limited computing infrastructure.

Emerging directions focus on hybrid architectures combining spin-glass inspired networks for multi-target drug design with active learning strategies prioritizing synthetically feasible molecules. The development of fragment-based approaches compatible with African pharmaceutical manufacturing capabilities could dramatically accelerate local drug development cycles. Strengthening North-South research collaborations through initiatives like this workshop will be crucial to tailor these technologies for combating neglected tropical diseases, aligning with Sustainable Development Goal 3 (Good Health and Well-being).

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P03

Multiscale nonlinear integration drives accurate encoding of input information

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Biological and artificial systems encode information through several complex nonlinear operations, making their exact study a formidable challenge. These internal mechanisms often take place across multiple timescales and process external signals to enable functional output responses. In this work, we focus on two widely implemented paradigms: nonlinear summation, where signals are first processed independently and then combined; and nonlinear integration, where they are combined first and then processed. We study a general model where the input signal is propagated to an output unit through a processing layer via nonlinear activation functions. Further, we distinguish between the two cases of fast and slow processing timescales. We demonstrate that integration and fast-processing capabilities systematically enhance input-output mutual information over a wide range of parameters and system sizes, while simultaneously enabling tunable input discrimination. Moreover, we reveal that high-dimensional embeddings and low-dimensional projections emerge naturally as optimal competing strategies. Our results uncover the foundational features of nonlinear information processing with profound implications for both biological and artificial systems.

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P04

Multistability emergence, dynamical analysis and the stochastic D-bifurcation through the tristate electronic circuit and its microcontroller-based experiment.

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Most of the studies in the field of particles are modeled by physical systems having a varying shape potential. Nevertheless, these systems in majority with periodic structures, although interesting, describe realistic system only with some approximations. To obtain a physically more realistic trapped particles, the effects of physical parameter such as temperature, amplitude, should be take into account. It then appears necessary to consider the multiple character of the medium in multistable particles. It is highlighted that multistability [1, 2] means the fact that multiple stable states coexist for the similar set of parameters by starting model development from different initial conditions or different rank of parameters. In connection with multistability effects in a system, the dynamics of the stochastic tristate circuit [3] is studied. The circuit [3] shows the dynamic behavior and the stochastic D-bifurcation of the tristate electronic circuit [3], according to the system parameters. The D-Bifurcation is an important quantity to explore the stability domains of many systems. It is also known as dynamical bifurcation, which is based on the sudden sign change of the largest Lyapunov exponent (LLE) when the intensity of the noise varies. We investigated the various dynamics occurred in the circuit[3] composed of two AC generator and one noise generator. A wide spectrum of non-linear behavior triggered with sensitivity to initial conditions and the noise effect is showcased. The stochastic circuit[3] shows the changes according to four control parameters: the applied voltage amplitude, the frequency, the circuit[3] damping and the multistability parameters (resistors). The system's behavior is studied numerically and by Pspice Simulation. subsequently, the Pspice estimates match with numerical simulations. We start by studying numerically the stability of the circuit [3] taking into account the multistability effects as well as the damping term effects. Then we propose several bifurcation features along with the corresponding maximal Lyapunov exponent forms. With the help of some phase portraits and some basins of attractions, we further investigate the different behaviors encountered in the circuit [3]. The D-bifurcation of the system [3] versus the noise intensity D, is study through the largest Lyapunov exponent calculations, for different parameters. Interestingly, the variation of resistance of resistors greatly influences the system's behavior as well as the D-bifurcation. A microcontroller-based implementation for digital engineering applications is presented to confirm the feasibility of the circuit.

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P05

Abstract template for Advanced School and Workshop: StatPhys in Kigali

Modulational Instability in nonlinear coupled nerve fibers

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The nerve signal conduction, and particularly in myelinated nerve fibers, is a highly dynamic phenomenon that is affected by various biological and physical factors. Delving and displaying modulation instability regions may seemingly help to elucidate the mechanisms underlying normal and abnormal behavior. Additional insights into the processes of nerve conduction is highlighted. Mathematical modelling of the dynamical behavior of the signal pulse along the nerve fiber displays a critical biological function within living systems[1,2,3]. We perform the modulational instability (MI)[2,4] plots in the nonlinear coupled nerve fibers equations[1,2,3]. Through numerical simulations and analysis we exhibit and provide significant regions of equilibrium and modulational instability showing that the behavior of the nerve fibers is more dynamic and interesting. Furthermore, we apply the fixed points theory to establish some equilibrium points and the Jacobian matrix [1,5,6,7]. In future research, we expect to delve novel and interesting solitary waves including fractional derivatives.

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P06

Title: Multisolitons-like patterns in a one-dimensional MARCKS protein cyclic model

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ABSTRACT

The **M**yristoylated **A**lanine-**R**ich **C**-kinase **S**ubstrate (**MARCKS**) have a wide range of functions, ranging from roles in embryonic development to adult brain plasticity and the inflammatory response. Recently, this protein has also been identified as important players in regeneration [1]. MARCKS is expressed at the highest levels in the brain during embryonic development and ubiquitous expression persists throughout adulthood. In neurons, MARCKS is heterogeneously distributed and enriched in axons and dendrites. During early development, MARCKS is broadly expressed in the cells surrounding the neural tube, and later, throughout the forebrain with particular enrichment at the apical membranes of ventricular zone neural progenitor cells. Alonso and Bär proposed a model which describes the patio-temporal evolution of the concentration of the MARCKS protein at the bio membrane involving: binding, phosphorylation and dephosphorylation of the MARCKS protein. The pioneers have shown by using numerical simulations that the model presents two qualitatively different mechanisms of protein domain formation [2]. Base on this result, we performed the modulational instability (MI) phenomenon. We find the domains of some parameter space where nonlinear patterns are expected in the model. The analytical results on the MI growth rate predict that phosphorylation and binding rates affect MARCKS dynamics in opposite way: while the phosphorylation rate tends to support highly localized structures of MARCKS, the binding rate in turn tends to slow down such features. On the other hand, self-diffusion process always amplifies the MI phenomenon. These predictions are confirmed by numerical simulations. As a result, the cyclic transport of MARCKS protein from membrane to cytosol may be done by means of multisolitons-like patterns [3].

Keywords: MARCKS protein, Long wavelength instability, Patterns formation, Multisolitons

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P07

Abstract template for poster Activity on the Title Effects of Periodic force on stabilisation of turbulence regime in subcritical systems

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Abstract

We study the dynamic regimes observed in two dimensional cubic-quintic Ginzburg-Landau equation by adding an external periodic force. We show that the external periodic force can change deeply the structure of the systems.

By considering a turbulence defect regime, our study revealed that even small nonlinear gradient termswhich appear at the same order as the quintic term can cause dramatic changes in the behavior of the solution. Chaos regime can be suppressed progressively, and new regimes like weak turbulence or phase turbulence are observed until the laminar state. Then, a fully developped turbulence can be completely annihilated by injecting a periodic signal into the domain.

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P08

Spectral and dynamical characters of 1D incommensurate optical lattices with PT-symmetry.

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In this paper, we investigate the spectral and dynamical properties of a 1D incommensurate optical lattice, which displays a Parity-time (PT) symmetry described by the Non-Hermitian Aubry–André potential. We show through the spectral analysis of the eigenvalues and the associated Eigen functions that, taking into account a non-Hermitian variant of the site energy modulated by a cosine form, leads the system to undergo a transition from the unbroken- PT phase to the broken- PT phase, which corresponds here to the delocalized-to-localized phase transition. Our findings also indicate that the critical point of transition can be selectively adjusted and consequently, the single-particle eigenstates taken in the metallic regime of the original Aubry–André model thus move from a conducting state to an insulating one upon an increase of the complex phase parameter. Furthermore, we also investigate the dynamical features of the system’s wave function according to different parameters.

P09

Abstract for the advanced School and workshop: StatPhys in Kigali, Rwanda.: Delayed swarmalator systems in Fluidic Environment

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This paper introduces a novel approach to studying swarmalator systems [1, 2, 3], which replicate the complex dynamics of many real-world systems by observing how their dynamical states evolve within a fluid-based environment [4].

Despite the rapidly growing interest in research involving swarmalators, the role of the environment has not yet been adequately addressed. This oversight should be rectified, as accounting for the environment brings these systems closer to real-world scenarios. Moreover, the internal phase dynamics of swarmalators, coupled with delays, have been scarcely studied. This study bridges the gap, as both delay and the environment are crucial in interactions between communicating entities.

The inclusion of delay [5] and fluid dynamics [6] introduces new phenomena in the transition to synchronisation, particularly within the active phase wave domain. These phenomena are characteristic of the motion of sperm cells and the aggregation of starfish. This research lays the foundation for expanding the field of swarmalators by exploring the influence of their environment and sheds further light on the mechanisms of synchronisation and communication.

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P10

Corrected Thermodynamics of Nonlinear Magnetic-Charged Black Hole Surrounded by Perfect Fluid Dark Matter

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In this work, we investigate the influence of perfect fluid dark matter and quantum corrections on the thermodynamics of nonlinear magnetic-charged black hole. We consider the metric of the static nonlinear magnetic-charged black hole in the background of perfect fluid dark matter. Starting with the black hole temperature and the corrected entropy, we use the event horizon propriety in order to find the temperature, and based on the surface gravity definition, we find the uncorrected entropy. However, using the definition of the corrected entropy due to thermal fluctuation, we find and plot the entropy of the black hole. We find that the entropy is affected for smaller nonlinear magnetic-charged black holes. Afterwards, we study the thermodynamic stability of the black hole by computing and plotting the evolution of heat capacity. The results show that second-order phase transition occurs, which appears more later as the dark matter parameter decreases, and leads the black hole to move from the stable phase to the unstable phase. Furthermore, we show that the heat capacity for smaller black holes are also affected, since it appears not being only an increasing function. We also find that the behavior of Gibbs energy is modified when taking into account quantum corrections.

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P11

Data-Driven Discovery of the Origins of UV Absorption in Alpha-3C Protein

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Over the last decade, there has been a growing body of experimental work showing that proteins devoid of aromatic and conjugated groups can absorb light in the near-UV beyond 300 nm and emit visible light. Understanding the origins of this phenomena offers the possibility of designing non-invasive spectroscopic probes for local interactions in biological systems. It was recently found that the synthetic protein α_3C displays UV-vis absorption between 250-800 nm which was shown to arise from charge-transfer excitations between charged amino acids. In this work, we use data-driven approach to re-examine the origins of these features using a combination of molecular dynamics and excited-state simulations. Specifically, an unsupervised learning approach beginning with encoding protein environments with local atomic descriptors, is employed to automatically detect relevant structural motifs. We identify three main motifs corresponding to different hydrogen-bonding patterns that are subsequently used to perform QM/MM simulations including the entire protein and solvent bath with the density-functional tight-binding (DFTB) approach. Hydrogen-bonding structures involving arginine and carboxylate groups appear to be the most prone to near-UV absorption. We show that magnitude of the UV-vis absorption predicted from the simulations is rather sensitive to the size of the QM region employed as well as to the inclusion of explicit solvation.

P12

Get rich or go extinct trying: Finding optimal sizes of wagers in betting games using species dynamics in stochastic environments

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The Kelly criterion [1] holds a central place in the world of investing, as it provides a formula for the optimal size of a bet (or a series of bets) given the chance of winning the bet and the payoff on winning. Kelly proved in his seminal paper [1] that this formula maximizes the winnings at infinite time. However, since neither time nor money is actually infinite, the recommendation for the optimal betting size that the Kelly criterion makes can be too risky for real investors. To address this problem various less risky strategies have been developed based on Kelly's work, including, most notably, fractional Kelly, under which investors bet only a fraction of the amount that the Kelly criterion suggests [2].

In this work we provide an alternative recommendation for the optimal betting size, which takes into account the minimum wealth that the investor is willing to go down to. This is based on a correspondence between investments in noisy markets and the populations of species in ecosystems under fluctuating environments. Kelly's criterion considers the change in the logarithm of the wealth size, which is analogous to the invasion growth rate for measuring the growth of species populations which also is the expected value of the change in the logarithm of the population size. In recent work we have developed analytical formulae which quantify the chance of a species to grow to a target value without first going extinct, and these formulae perform much better in predicting this chance than the invasion growth rate [3,4]. Informed by these formulae, we improve the recommendation for the betting size that Kelly makes, making the bets significantly more resistant to wealth drawdown and ruin.

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Advanced School and Workshop: StatPhys in Kigali | (smr 4085)

Title: Refining Thermodynamic Models: Quantum and relativistic Corrections to Classical Gas Descriptions

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The aim of this study is to explore quantum and relativistic corrections to ideal gas models, including ideal Fermi and Bose gases, by considering the quantum nature of phase space [1]. This approach extends beyond the classical considerations of bosonic and fermionic particles and incorporates quantum size and shape effects into thermodynamic properties.

The study improves the partition function for ideal gases through phase space representations that account for the uncertainty principle. The thermodynamic properties of these gases are derived using quantum mechanical phase space formulations, considering both non-relativistic and relativistic quantum regimes.

The results show that quantum corrections are especially significant at low temperatures and in confined spaces, leading to deviations from the Maxwell–Boltzmann distribution. Thermodynamic quantities such as entropy, internal energy, and free energy are modified by these corrections, which also highlight quantum size and shape effects [2].

These quantum corrections significantly alter the thermodynamic equations of state and functions, providing a more accurate description of ideal gases at low temperatures and small volumes. Classical limits are recovered at high temperatures and large volumes [3].

This work introduces a novel approach by incorporating quantum phase space effects into the models of ideal gases, extending the scope of existing models and improving their accuracy in quantum regimes.

By addressing the corrections and their thermodynamic implications, this work provides a foundation for further applications in nanoscale systems, quantum gases, low-temperature physics, ultra-cold physics and astrophysics.

Keywords : Quantum mechanics, Relativity, Thermodynamics, Quantum gases, Quantum phase space, Quantum statistical physics.

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P14

Fractional kinetic equations and truncated L ´evy stable distributions in frameworks of statistical physics

P15

We report numerical observations of scattering process of moving multibreathers by isolated impurities in the discrete nonlinear Schrödinger lattice representing the vibrational energy transport along the protein chain. It is found that, except for the multibreather passing, internal collision phenomenon support all types of scattering outcomes for both attractive and repulsive impurities. Furthermore, for large strength of attractive impurity the scattering of two-hump soliton can give rise to a trapping on a site other than the one containing the impurity. As concerns three-hump soliton, the passing, trapping and reflection are simultaneously carried out for some parameters. In the case of three-hump soliton introduced between two repulsive impurity sites, back and forth are observed as well as increasingly individualistic behavior of humps over time. Nonetheless, two-hump soliton launched under the same conditions results in large stationary single breather.

P16

Undeniable role of rogue waves in the dynamics of pulses in DNA

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We show that the short-lived variety of rogue wave (RW), the Peregrine soliton (PS) that plays a pivotal role in the local and short excitation of DNA [1, 2, 3] can become the typical long-lived breather-like modes, the Akhmediev breathers (ABs) that can propagate along the helix protein of biological molecules. Through the modified Hamiltonian of the Peyrard-Bishop model [4], a nonparaxial cubic-quintic nonlinear Schrodinger equation is derived in the continuous media from the discrete equation motion of DNA base pairs. The rogue wave solutions are constructed with the symmetry reduction method and represented in the strain variable formulation, to detect the presence of propagating structures. We found that the classic breather that is, the ABs is qualitatively interesting in DNA biological systems. Moreover, we have shown that for a specific set of parameters of the system, the short-lived RW can become a typical long-lived breather-like modes which can match experimentally, the observed bubbles that propagate along the helix [5]. The richness and good stability of rogue waves in the dynamics of pulses show that they are physically relevant for DNA.

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P17

Nonequilibrium Phase Transitionins in Ferromagnetic systems under Effective Interactions

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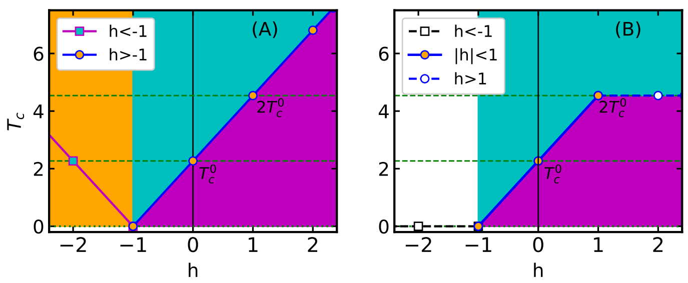
The study of nonequilibrium steady-state (NESS) in the Ising model offers rich insights into the properties of complex systems. The poster aims to explore the nature of NESS phase transitions in a 2D ferromagnetic Ising model on a square lattice under effective interactions using Monte Carlo (MC) algorithms. It requires extensive MC simulations using the modified Metropolis and Glauber update rules. An appropriate definition of an effective parameter h helps to qualify the modified update rules. For $|h| > 1$, the analytical solution shows that the nature of the phase transition (including the critical temperature) is independent of h. Furthermore, for $-1 < h < 1$, we study the steady-state properties of phase transitions using numerical methods. Therefore we performed simulations for different lattice sizes and measured relevant physical quantities. From the data, we determined the numerical results of the transition temperature and relevant critical exponents for various values of h by applying finite-size scaling (FSS). We found that the FSS analysis of the exponents is consistent with the analytical values of the equilibrium 2D Ising model, Reference [1].



- Two models (A) and (B) are corresponding to equilibrium and nonequilibrium, respectively.
- The critical temperature for the usual equilibrium model [2] is

$$T_c^0 = \frac{2}{\ln(1+\sqrt{2})}$$

Figure 1: Plot of T_c vs h for two models (A) and (B). The horizontal dashed lines represent T_c^0 and $2T_c^0$.

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P18

Linearisation of nonlinear stochastic processes and observable.

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Abstract

Large deviation techniques have been widely used in physics to study the fluctuations of nonequilibrium systems, which are often modelled using Markov processes, including Markov diffusion describe by stochastic differential equations (SDEs). Large deviation theory allows for the calculation of the probability distribution of time integrate of the state, which can represent observables such the work done on a Brownian particle or the heat exchanged with the environment. In many cases, obtaining exact analytical solutions of large deviation functions requires solving complex spectral or optimization problems [1, 2]. This same complexity arises when trying to understand how fluctuations arise in effective or driven processes. In these systems, fluctuations are viewed as optimal modifications to the stationary density or as an effective diffusion process that adjusts the original force or drift of the diffusion [2, 3, 4].

I will present in this talk, a novel approach that combines large deviation theory and linearization techniques to analyze fluctuations and rare events in nonlinear Markov diffusion processes. Our method focuses on deriving approximations for the scaled cumulant generating function (SCGF) and the large deviation function. These approximations offer valuable insights into the long-term behavior of the systems observables, enabling us to characterize fluctuations and identify the underlying effective processes or paths responsible for driving these rare events. To validate this approach, we apply it to a specific nonlinear diffusion system and compare the large deviation functions obtained through our linearization methods with exact results derived from numerical spectral techniques. This comparison will allow us to assess the effectiveness of the linearization approach in capturing rare event behavior within the nonlinear regime.

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P19

Title: Using a thin grey soliton to learn and impact the nonlinear dynamics of quantum systems

Abstract: Grey solitons, which are a type of localized excitation characterized by a dip in a continuous wave, play an important role in nonlinear systems, particularly in optics, low-temperature physics and fluid dynamics. Despite the reduction in intensity, grey solitons maintain their shape and speed as they propagate, due to a delicate balance between nonlinear effects and dispersion. Such a speed is a measure of the grayness of the soliton, yielding dark solitons as a special case with zero speed. In this poster, using two examples, we show that a thin grey soliton can be used to change or learn about the dynamics of nonlinear systems. In the first example, taking the case of an ultracold quantum gas, we show that a grey soliton can allow us to track the breakdown of adiabaticity at different scales in a system that undergoes a strong ramp of interparticle interaction. The second example is devoted to an atomic cloud that is continuously bombarded by a well controlled electron beam. We show that the presence of a grey soliton in the system may lead, on one hand, to the quantum Zeno effect, a phenomenon where a quantum system's evolution can be slowed or even halted by frequent measurements. Such a slowdown occurs, for instance, in the decay of the condensate density. On the other hand, a grey soliton may induce the backflow paradox, a phenomenon where the flow of information or particles appears to reverse direction in certain physical systems.