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Dipartimento di Fisica - Università di Bari ”Aldo Moro”

Book of Abstracts

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Prova

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Prova

Session 3 B / 63

Active semiflexible polymer under shear flow

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The dynamic behavior of a self-propelled semiflexible filament of length L is considered under the action of a linear shear flow. The system is studied by using Brownian multi-particle collision dynamics. The system can be characterized in terms of the persistence length Lp of the chain, of the Peclet number, and of the Weissenberg number. The quantity Lp/L measures the bending rigidity of the polymer, the Peclet number Pe is the ratio of active force times L to thermal energy, and the Weissenberg number Wi characterizes the flow strength over thermal effects. In this presentation we will focus our attention to intermediate values of Pe corresponding to the weak spiral regime when no external flow is applied. The numerical results allow us to outline the main features of the physics underlying the considered system:

- At low values of Wi, polymer is stretched by activity and aligned by shear along the flow direction. This effect is more marked in the case of more flexible chains.
- At the intermediate values of Wi, polymer is prone to tumble due to shear and this promotes a contraction of the chain.
- At very high values of Wi, activity sums up to shear enhancing polymer stretching and deformation.

Session 2 / 64

A condensation transition at equilibrium and out-of-equilibrium

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Several lattice models display a condensation transition in real space when the density of a suitable order parameter exceeds a critical value. At equilibrium there are well established results and we discuss different scenarios of the condensation trantition.

In the out-of-equilibrium setup we consider one of such models with two conservation laws, attached to two external reservoirs, R_1 and R_2. Both reservoirs impose subcritical boundary conditions: when R_1=R_2 the system is in equilibrium below the localization threshold and no condensate appears. Instead, when R_1 differs from R_2 localization may arise in an internal portion of the lattice.
This phenomenon is due to the coupled transport of two conserved quantities.

Session 3 / 65

Elementary particle mass generation without Higgs

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We discuss how a recently discovered non-perturbative field-theoretical mechanism giving mass to elementary fermions can be extended to generate a mass for the electro-weak bosons, when weak interactions are introduced, and can thus be used as a viable alternative to the Higgs scenario. We will show that this new scheme, tested in extensive lattice simulations, offers a solution of the mass naturalness problem, an understanding of the fermion mass hierarchy and a physical interpretation of the electro-weak scale.

Session 7 / 66

Understanding the non-Gaussianities in the Hubble-Lemaitre diagram

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I will present the theoretical framework to understand the non-Gaussianities in the Hubble-Lemaître diagram, namely the distance-redshift relation, emerging from relativistic cosmological simulations, such as *gevolution*. With these analytic results, I will discuss which kind of non-Gaussianities can be addressed to intrinsic non-linear effects, such as post-Born corrections and higher-order statistic, against spurious effects introduced by the binning in redshift along the data analysis. Moreover, the numerical shortcuts introduced to account for the matter bispectrum will be discussed, especially in regard of the choice of the appropriate UV-cutoff to be chosen for a well-posed comparison with the above-mentioned relativistic simulations.

Session 6 / 67

Binary Neutron Stars: from macroscopic collisions to microphysics

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I will argue that if black holes represent one the most fascinating implications of Einstein's theory of gravity, neutron stars in binary system are arguably its richest laboratory, where gravity blends with astrophysics and particle physics. I will discuss the rapid recent progress made in modelling these systems and show how the gravitational signal can provide tight constraints on the equation of state and sound speed for matter at nuclear densities, as well as on one of the most important consequences of general relativity for compact stars: the existence of a maximum mass. Finally, I will discuss how the merger may lead to a phase transition from hadronic to quark matter. Such a process would lead to a signature in the post-merger gravitational-wave signal and open an observational window on the production of quark matter in the present Universe.

Session 5 / 68

Using machine learning in geophysical data assimilation (some of the issues and some ideas)

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In recent years, data assimilation, and more generally the climate science modelling enterprise have been influenced by the rapid advent of artificial intelligence, in particular machine learning (ML), opening the path to various form of ML-based methodology.
In this talk we will schematically show how ML can be included in the prediction and DA workflow in three different ways. First, in a so-called "non-intrusive"ML, we will show the use of supervised learning to estimate the local Lyapunov exponents (LLEs) based exclusively on the system's state [1]. In this approach, ML is used as a supplementary tool, added to the given physical model. Our results prove ML is successful in retrieving the correct LLEs, although the skill is itself dependent on the degree of local homogeneity of the LLEs on the system's attractor.
In the second and third approach, ML is used to substitute fully [4] or partly [5]a physical model with a surrogate one reconstructed from data. Nevertheless, for high-dimensional chaotic dynamics such as geophysical flows this reconstruction is hampered by (i) the partial and noisy observations that can realistically be gathered, (ii) the need to learn from long time series of data, and (iii) the unstable nature of the dynamics. To achieve such inference successfully we have suggested to combine DA and ML in several ways. We will show how to unify these approaches from a Bayesian perspective, together with a description of the numerous similarities between them [2,3]. We will show that the use of DA in the combined approach is pivotal to extract much information from the sparse, noisy, data. The full surrogate model achieves prediction skill up to 4 to 5 Lyapunov time, and its power spectra density is almost identical to that of the original data, except for the high-frequency modes which are not well captured [4]. The ML-based parametrization of the unresolved scales in the third approach [5] is also extremely skilful. This has been studied using a coupled atmosphere-ocean model and again the use of coupled DA [6] in the combined DA-ML method makes possible to exploit the data information from one model compartment (e.g., the ocean) to the other (e.g., the atmosphere).

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Session 3 / 69

Finite temperature BKT phase transition in the planar psi^4 model with a strongly modulating potential

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We employ analytical as well as numerical Monte Carlo methods to
discuss the BKT phase transition in the finite-temperature psi^4 model over a square lattice in the presence of a strong modulation of the chemical potential. By going through a systematic mapping over the anisotropic planar XY model with modulated spin interaction strengths, we show that the strength of the modulation only affects the effective anisotropy of the XY model and that the BKT phase transition is present even at very large values of the modulation, thus evidencing the persistence of the two-dimensional critical behavior of the system even in that limit.

Session 2 / 70

Laplacian Renormalization Group for heterogeneous networks: information core and entropic transitions

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Complex networks usually exhibit a rich architecture organized over multiple intertwined scales. Information pathways are expected to pervade these scales reflecting structural insights that are not manifest from analyses of the network topology. Moreover, small-world effects correlate the different network hierarchies complicating the identification of coexisting mesoscopic structures and functional cores. We present a communicability analysis of effective information pathways throughout complex networks based on information diffusion to shed further light on these issues [1]. This will lead us to a formulation of a new and general renormalization group scheme for heterogeneous networks. The renormalization group is the cornerstone of the modern theory of universality and phase transitions, a powerful tool to scrutinize symmetries and organizational scales in dynamical

systems. However, its network counterpart is particularly challenging due to correlations between intertwined scales. To date, the explorations are based on hidden geometries hypotheses. Here, we propose a Laplacian RG diffusion-based picture for complex networks, defining both the Kadanoff supernodes' concept, the momentum space procedure and applying this RG scheme to real networks in a natural and parsimonious way [2].

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Session 7 B / 71

Data-driven emergence of convolutional structure in neural networks

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Exploiting invariances in the inputs is crucial for constructing efficient representations and accurate predictions in neural circuits. In neuroscience, translation invariance is at the heart of models of the visual system, while convolutional neural networks designed to exploit translation invariance triggered the first wave of deep learning successes. While the hallmark of convolutions, namely localised receptive fields that tile the input space, can be implemented with fully-connected neural networks, learning convolutions directly from inputs in a fully-connected network has so far proven elusive. In this talk, I will show how initially fully-connected neural networks solving a discrimination task can learn a convolutional structure directly from their inputs, resulting in localised, space-tiling receptive fields. Both translation invariance and non-trivial higher-order statistics are needed to learn convolutions from scratch. I will provide an analytical and numerical characterisation of the pattern-formation mechanism responsible for this phenomenon in a simple model, which results in an unexpected link between receptive field formation and the tensor decomposition of higher-order input correlations.

Session 7 / 72

A new first-order formulation of the Einstein equations exploiting analogies with electrodynamics

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The Einstein and Maxwell equations are both systems of hyperbolic equations which need to satisfy a set of elliptic constraints throughout evolution. However, while EM and MHD have benefited from a large number of evolution schemes that are able to enforce these constraints and are easily applicable to curvilinear coordinates, unstructured meshes, or N-body simulations, many of these techniques cannot be straightforwardly applied to existing formulations of the Einstein equations. We develop a 3+1 a formulation of the Einstein equations which shows a striking resemblance to the equations of relativistic MHD and to EM in material media. The fundamental variables of this formulation are the frame fields, their exterior derivatives, and the Nester-Witten and Sparling forms. These mirror the roles of the electromagnetic 4-potential, the electromagnetic field strengths, the field excitations and the electric current. The role of the lapse function and shift vector, corresponds exactly to that of the scalar electric potential. The formulation, that we name **dGREM** (for differential forms, General Relativity and Electro-Magnetism), is manifestly first order and flux-conservative, which makes it suitable for high-resolution shock capturing schemes and finite-element methods. Being derived as a system of equations in exterior derivatives, it is directly applicable to any coordinate system and to unstructured meshes, and leads to a natural discretisation potentially suitable for the use of machine-precision constraint propagation techniques such as the Yee algorithm and constrained transport. Due to these properties, we expect this new formulation to be beneficial in simulations of many astrophysical systems, such as binary compact objects and core-collapse supernovae as well as cosmological simulations of the early universe. In this talk I also comment on the hyperbolicity of the formulation and its application in the context of high performance computing.

Session 5 / **73**

Statistically validated hypergraphs

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In many real-world systems, successfully represented as networks, interactions are not limited to dyads, but often involve three or more nodes at a time. Under this condition, a better description of the system is given by hypergraphs, where hyperlinks encode higher-order interactions among a group of nodes. We discuss an analytic and computational approach to filter hypergraphs by identifying those hyperlinks that are over-expressed with respect to a random null hypothesis and represent the most relevant higher-order connections [1]. We apply our method to a class of synthetic benchmarks and to several datasets, showing that the method highlights hyperlinks that are more informative than those extracted with pairwise approaches. We also discuss a method for the detection of Statistically Validated Simplices. Statistically validated simplices represent the maximal sets of nodes of any size that consistently interact collectively and do not include co-interacting nodes that appears only occasionally [2].

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Joint work with Federico Musciotto and Federico Battiston

Session 3 / **74**

On the origin of the correspondence between quantum integrable system and classical models

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I will discuss a non-perturbative procedure on how to derive a classical systems, in the form of a Lax pair, from a quantum integrable model. I will exemplify the method by starting from the quantum sine-Gordon model and deriving a Lax pair containing the solution of the classical sinh-Gordon equation. The link between quantum and classical theory is provided by a Marchenko-like equation, which descends from the quantum TQ-system and is the basis for deriving the Lax pair. This construction reverses and justifies the usual construction in the Ordinary Differential Equation/Integrable Model correspondence.
The talk is based on paper arXiv: 2106.07600 with D.Fioravanti.

Session 1 / 75

Linking hubs, embryonic neurogenesis, transcriptomics and diseases in human brain networks

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Linking hubs, embryonic neurogenesis, transcriptomics and diseases in human brain networks
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The most characteristic anatomical property of brain networks is their organization across multiple spatial scales. A key challenge is to decipher the rules of connectivity that shape brain networks in order to understand how the brain works and how traumatic or neurological damage may affect brain functionality[1]. The general structure and function of the human brain, and its internal connectivity are all the result of its developmental history, which is at the same time the product of evolution[2].
Small-world, scale-free or heavy-tailed distribution network organizations have been identified at the structural-functional level in microcircuits, and in meso- and macro-scale networks[3].
Inspired by the Barabasi-Albert model [4] which showed that the principle "the rich gets richer" (a.k.a. "preferential attachment") led to scale-free networks and hubs in real-world networks, in this work we test the hypothesis that the topology of brain networks could be shaped according to the rule that "the older gets richer", i.e. the evolutionary older circuits or those generated earlier in embryogenesis are most central in the organization of the adult brain network[5].
As a consequence, we expect that quantification of the hubness of brain nodes (i.e. circuits) based on metrics of centrality from complex networks should be correlated with circuits'embryogenic age.
We identified eighteen macro-circuits (MACs) according to their first (i.e. earliest) neurogenic time (FirsT) during embryogenesis. Since MACs'volumes span across multiple scales, we studied the brain

networks with two different spatial resolutions: a low resolution parcellation corresponding to the eighteen MACs, and a high resolution parcellation composed of approximately two and half thousand regions of interest (ROI) of similar volumes.
Structural and functional brain networks were obtained using 7 Tesla MRI images acquired within the Human Connectome Project[6]. At high resolution level, we observed that FirsT reversely shaped the nodes'centrality in the structural and functional networks, where highly central nodes displayed respectively early and late FirsT. Distinctly, the structural and functional nodes'centrality of the low-resolution MACs similarly correlated with FirsT, with higher centrality displayed in the early born MACs. In addition, we observed that FirsT-lags reversely correlated with wiring probability and connection weight, so ROIs and MACs connected more and stronger with those at similar age. Finally, brain transcriptomic analysis revealed also high association between genes'expression, FirsT and nodes'centrality, in respect to physiological nervous system development and synapse regulation, and to neuropathological conditions. Notably, a significant rate of genes involved in major neurological diseases such as epilepsy, Parkinson's, Alzheimers'and autism spectrum disorder displays extreme correlation values with nodes'centrality (we especially mention high correlation for highly studied genes such as SCN1A, SNCA and APOE). The results [7] provide a new multi-scale evidence on how neurogenesis time shapes structural and functional networks, brain nodes'centrality and their transcriptomics in patho-physiological conditions and underlie two main neurogenesis preferential wiring principles: "the older gets richer"and "preferential age attachment".

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Session 7 B / 76

Territorial bias in university rankings: a complex network approach

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University rankings are increasingly adopted for academic comparison and success quantification, even to establish performance-based criteria for funding assignment. However, rankings are not neutral tools, and their use frequently overlooks disparities in the starting conditions of institutions. In this research, we detect and measure structural biases that affect in inhomogeneous ways the ranking outcomes of universities from diversified territorial and educational contexts. Moreover, we develop a fairer rating system based on a fully data-driven debiasing strategy that returns an equity-oriented redefinition of the achieved scores. The key idea consists in partitioning universities in

similarity groups, determined from multifaceted data using complex network analysis, and referring the performance of each institution to an expectation based on its peers. Significant evidence of territorial biases emerges for official rankings concerning both the OECD and Italian university systems, hence debiasing provides relevant insights suggesting the design of fairer strategies for performance-based funding allocations.

Session 3 / 77

Lattice Gauge Theories at finite density with Tensor Networks

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Gauge theories are of paramount importance in our understanding of fundamental constituents of matter and their interactions, ranging from high-energy particle physics to low-temperature quantum many-body physics. However, the complete characterization of their phase diagrams and the full understanding of non-perturbative effects are still debated, especially at finite charge density, mostly due to the sign-problem affecting Monte Carlo numerical simulations. In recent years, a complementary numerical approach, Tensor Networks (TN) methods, in strict connection with emerging quantum technologies, have found increasing applications for studying Lattice Gauge Theories (LGTs) in low-dimensional systems. In this talk, I will present some recent results concerning the extension of TN algorithms to high-dimensional LGTs including dynamical matter. In particular, I will focus on their application to a compact Quantum Electrodynamics at zero and finite charge densities, addressing questions such as the characterization of collective phases of the model, the presence of confining phases at large gauge coupling, and the study of charge-screening effects.

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- G. Magnifico, T. Felser, P. Silvi, and S. Montangero, Nature Communications 12, 3600 (2021).
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Session 1 / 78

Challenges in Programming Recent HPC Processors

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Recent processors commonly used for HPC applications heavily rely on multi-threading and vectorization design to deliver high performance computing throughput. Exploiting these features efficiently in applications is not however an easy task, and several programming strategies have to be put in place to be able to exploit at best the computing performance. The aim of this talk is then to highlight the issues that programmers may encounter in programming recent processors, focusing on discussing the most relevant strategies and methodologies to program recent multi- and many-core architectures for lattice-based applications. Using codes based on Lattice Boltzmann Methods, the talk will present the major programming issues that are relevant to exploit a large fraction of available peak performance of the target processors, giving various programming solutions to get high efficiency of execution. The talk takes into account multi-core processors based on "traditional" core-architecture, as well as many-core systems such as GP-GPUs and Intel Xeon-Phi. It also considers several memory data-layouts to store the lattice domain, that meet the conflicting computing

requirements of distinct parts of the application, and sustain a large fraction of peak performance both in terms of computing and memory throughput.

Session 6 / 79

Computational Physics for Theoretical Cosmology

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In my talk, I will review the use of HPC resources in the field of theoretical cosmology, focusing on the research activity carried on within the INFN "Iniziativa specifica" InDark (Inflation, Dark Matter, Large Scale Structure of the Universe). Advanced computing allows to tackle different classes of problems of great importance for current cosmological research, including structure formation, higher-order statistics of cosmological fields, and inference problems in a large number of dimensions.

Session 8 B / 80

Morphology and dynamics of phase separation in two-dimensional active systems

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Active (or self-propelled) particles constantly consume internal energy to move in the environment, constantly preventing the system to reach equilibrium. This allows for a variety of fascinating phenomena to appear, such as the phase separation into a dense and a dilute phase in the complete absence of attractive interactions, known as motility-induced phase separation (MIPS) [1]. Although MIPS retains many aspects of gas-liquid demixing at equilibrium, its inherent non-equilibrium origin leads to a new physical phenomenology. Here we illustrate some of the peculiar features of the MIPS dynamics in numerical simulations of 2d self-propelled disks [2].
We show the presence of another ordering mechanism beyond the equilibrium-like phase separation, namely the micro-phase separation of hexatic domains and vapor bubbles within dense clusters of particles [3]. We studied the steady-state size of these structures and found that it can be directly controlled by tuning the self-propulsion strength of the individual particles.
We also provide a detailed analysis of the dynamics of individual clusters during the phase separation process [4]. We show that active clusters have diffusive behavior that is enhanced by the self-propulsion strength and that the diffusion coefficient depends in a non-trivial way on the total mass of the cluster, which is a pure non-equilibrium effect induced by self-propulsion. Finally, we show that cluster diffusion controls the phase separation process of the system and leads to the formation of larger structures characterized by a fractal geometry.

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Session 7 B / 81

Defect-Mediated Morphogenesis

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It has been a long-standing mystery how complex biological structures emerge during embryonic development from such seemingly uncoordinated building blocks as cells and tissues without guidance. Recent experiments have suggested that misalignment in the collective structure of tissues – the so called topological defects–could play a fundamental guiding role in morphogenesis. Inspired by tentacle development in the Hydra and using a combination of linear stability analysis and computational fluid dynamics we demonstrate that active layers, such as cell monolayers, are unstable to the formation of protrusions in the presence of disclinations. To this aim, we considered a thin layer of active polar gel [1] confined at the interface between two passive and isotropic fluids in a cylindrical geometry to stabilize a +1 topological defect. Under the effect of the active stress, the system generates in-plane vortical flow, consistently with a classic result by Kruse et al. [2]. Importantly, this active flow yet plays a crucial role in driving the active membrane out of its flat configuration and buckle out of plane. Indeed, the buckling instability, analytically predicted here, originates from the interplay between the focusing of the elastic forces, mediated by defects, and the renormalization of the system's surface tension due to the active vortical flow. Finally, to make progress beyond analytical predictions, we support our findings with 3D numerical simulations. First, we recover the predicted instabilities, then we focus on the post-transitional scenario and we find a plethora of complex morphodynamical processes, such as oscillatory deformations, droplet nucleation, and active turbulence [3,4].

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Session 3 B / 82

Microscopic theory for the diffusion of an active particle in a crowded environment

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We study the diffusion coefficient of an active tracer in a schematic crowded environment, represented as a lattice gas of passive particles with hardcore interactions. Starting from the Master Equation of the problem, we put forward a closure approximation that goes beyond trivial mean field and provides the diffusion coefficient for arbitrary density. The approximation is accurate for a wide range of parameters and correctly captures numerous nonequilibrium effects, which are the signature of the activity in the system. Preliminary results on the phenomenon of absolute negative mobility when the tracer is driven by an external force are also discussed.

Session 8 B / 83

Thermalization with a multibath: an investigation in simple models

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We study analytically and numerically a couple of paradigmatic spin models, each described in terms of two sets of variables attached to two different thermal baths with characteristic timescales T and τ and inverse temperatures B and β.
In the limit in which one bath becomes extremely slow ($\tau \to \infty$), such models amount to a paramagnet and to a one-dimensional ferromagnet, in contact with a single bath. We show that these systems reach a stationary state in a finite time for any choice of B and β. We determine the non-equilibrium fluctuation-dissipation relation between the autocorrelation and the response function in such state and, from that, we discuss if and how thermalization with the two baths occurs and the emergence of a non-trivial fluctuation-dissipation ratio.

Session 4 B / 84

A dynamic-Immersed Boundary approach for blood-borne cells transport

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Here a numerical framework for computing the vascular journey of microsized particles is presented. The incompressible Navier–Stokes equation is modeled through an incompressible BGK-Lattice Boltzmann scheme. The discrete Boltzmann equation is endowed with a forcing term accounting for the presence of immersed geometries. Dirichlet boundary conditions are imposed on moving deformable or rigid geometries through a dynamic-Immersed Boundary method, while, on fixed immersed geometries a second-order bounce–back technique is adopted. The proposed computational framework is employed to detail transport, dynamic, and deformation of micrometric capsules into a microfluidic bifurcation. This journey is characterized in terms of: i) the capsule/bifurcation interaction depending on the sharpness of the bifurcation junction; ii) daughter branches aperture angle; iii) occlusion ratio, ratio between capsule size and main channel diameter; iv) flowing capsules stiffness; v) number of flowing particles.

Session 7 / 85

Entanglement entropy from non-equilibrium lattice simulations

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The entanglement entropy is a quantity encoding important features of strongly interacting quantum many-body systems and gauge theories, but its analytical study is still limited to systems with high level of symmetry. This motivates the search for efficient techniques to investigate this quantity numerically, by means of Monte Carlo calculations on the lattice.
In this talk, we present a lattice determination of the entropic c-function by means of a novel algorithm based on Jarzynskis equality: an exact theorem from non-equilibrium statistical mechanics. After presenting benchmark results for the Ising model in two dimensions, where our algorithm successfully reproduces the analytical predictions from conformal field theory, we discuss its generalization to three dimensions and comment on potential future applications to gauge theories.

Session 10 / 86

On fits to correlated and auto-correlated data

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Observables in particle physics and specifically in lattice QCD calculations are often extracted from fits. Standard chi^2 tests require a reliable determination of the covariance matrix and its inverse from correlated and auto-correlated data, a challenging task often leading to close-to-singular estimates. These motivate modifications of the definition of chi^2 such as uncorrelated fits. We show how the goodness-of-fit measured by their p-value can still be estimated robustly for a broad class of such fits.

Session 5 / 87

Computational Challenges in Lattice QCD

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In this talk I will review recent progress and open challenges of nonperturbative calculations on the lattice. I will discuss novel mathematical approaches, improved numerical algorithms, and unresolved issues covering several aspects of the strong interaction phenomenology.

Session 7 B / 88

Work fluctuations in the harmonic Active Ornstein–Uhlenbeck particle model

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Over the past few years great interest arose in providing a thermodynamic description of Active Matter Systems, a class of non-equilibrium systems in which the single components are able to transform energy into self-propelled motion. A measure of the transformation efficiency is provided by the Active Work performed by active particles. The distribution of such an observable has been object of recent research [1] as possible singularities signal the occurrence of Dynamical Phase Transitions (DPTs) [2,3], in turn related to peculiar trajectory realisations.

In light of this scenario, we focus on a single overdamped harmonically trapped Active Ornstein-Uhlenbeck Particle and provide the analytic expression for the scaled cumulant generating function (SCGF) of the Active Work obtained using the large deviation theory recently developed for quadratic functionals of stable Gauss-Markov chains [4]. Interestingly, we find the SCGF to be non-steep in many physical situations and we provide insight on the effect of relevant system parameters, such as the Peclet number, on the SCGF steepness trough a phase diagram in the system parameter space. Through Legendre-Fenchel transform, the SCGF steepness is shown to lead to singular rate functions with linear tails, and ultimately to the occurrence of DPTs also in this system. We also investigate on the role of initial and final condition in producing the consequent anomalous trajectories.

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Session 5 / 89

Turbulent Inverse cascade in quantum fluids of light

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We study the turbulent dynamics of a 2D quantum fluid of exciton-polaritons, hybrid light-matter quasiparticles, by measuring the kinetic energy spectrum and the onset of vortex clustering. We demonstrate that the formation of clusters of quantum vortices is triggered by the increase of the incompressible kinetic energy per vortex, showing the tendency of the vortex-gas towards highly excited configurations despite the dissipative nature of our system. Our results lay the basis for the investigation of quantum turbulence in two-dimensional fluids of light.

Session 7 / 90

Stochastic normalizing flows as non-equilibrium transformations

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Normalizing Flows are a class of deep generative models recently proposed as a promising alternative to conventional Markov Chain Monte Carlo simulations to sample lattice field theory configurations, since they provide a unique approach to potentially avoid the large autocorrelations that characterize Monte Carlo simulations close to the continuum limit. In this talk we explore the novel concept of Stochastic Normalizing Flows (SNFs), in which neural-network layers are combined with traditional Monte Carlo updates: in particular, we show how SNFs share the same theoretical framework of out-of-equilibrium simulations based on Jarzynski's equality. We discuss how this connection can be exploited to optimize the efficiency of this extended class of generative models and we present some numerical results in the 2d ϕ^4 scalar field theory.

Session 3 B / 91

A predictive model for the thermomechanical melting transition of double stranded DNA

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By extending the classical Peyrard-Bishop model, we are able to obtain a fully analytical description for the mechanical response of DNA under stretching at variable values of temperature, number of base pairs and intrachains and interchains bonds stiffness. In order to compare elasticity and temperature effects, we first analyze the system in the zero temperature mechanical limit, important to describe several experimental effects including possible hysteresis. We then analyze temperature effects in the framework of equilibrium statistical mechanics. In particular, we obtain an analytical expression for the temperature-dependent melting force and unzipping assigned displacement in the thermodynamical limit, also depending on the relative stability of intra vs inter molecular bonds. Such results coincide with the purely mechanical model in the limit of zero temperature and with the denaturation temperature that we obtain with the classical transfer integral method. Based on our analytical results, explicit analysis of the phase diagrams and cooperativity parameters are obtained, where also discreteness effect can be accounted for. The obtained results are successfully applied in reproducing the thermomechanical experimental melting of DNA and the response of DNA hairpins. Due to the generality of the model, exemplified in the proposed analysis of both overstretching and unzipping experiments, we argue that the proposed approach can be extended to other thermomechanically induced molecular melting phenomena.

Session 7 B / 92

Long-range quenched disorder in the bidimensional Potts model.

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In collaboration with M. Picco and Raoul Santachiara, we tackled the problem of weak disordered bi-dimensional Potts model at criticality.
The aim of this study is to understand how the critical properties of the pure (P) model are modified by the addition of long-range-correlated disorder on the spin-couplings, i.e. the random-bond Potts model.
For uncorrelated or short range (SR) disorder the answer is given by the Harris criterion, [5].
We, instead, analysed the case where the couplings, $J(x) \geq 0$, are drawn from an isotropic-long-range-correlated-bimodal probability distribution, whose second cumulant, decreases as a power-law for large distances, $g(|x|) \sim |x|^{-a}$. The extended Harris criterion, [6], determine in which region of the parameters (q, a) the disorder is relevant.
When $a > d = 2$, the critical behavior of the system is expected to be the same as the one with SR disorder.
The behavior of the Potts model when the long-range (LR) is dominant over the SR is much less understood.
We studied the SR-LR crossover for $q \in \{1, 2, 3\}$ on the self-dual critical line. These q values are representative for all q, since the SR disorder is respectively irrelevant, marginal and relevant .
By tuning the range of the correlation, the strength of the disorder, and by measuring the fractal dimension of the Fortuin-Kasteleyn (FK) clusters, d_f, we gained information about the fixed-points stability in different phases of the renormalisation group (RG) flow. We established the existence of an LR fixed point for all values of $q > 1$. Also, for $q = 1$, a 1-loop RG computation, done above the upper critical dimension, predicted the existence of a Long Range percolation (LRp) point. This is in agreement with our study in $d = 2$.
Furthermore, we built a unifying phase diagram a vs. q describing the crossover among LR-SR, LR-P and LR-LRp physics.

Session 2 / 93

Trapping active particles up to the limiting case: bacteria enclosed in a biofilm

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Active matter systems are composed of constituents, each one in nonequilibrium, that consume energy in order
to move [1]. A characteristic feature of active matter is collective motion leading to nonequilibrium phase
transitions or large scale directed motion [2]. A number of recent works have featured active particles interacting with obstacles, either moving or fixed [3,4,5]. When an active particle encounters an asymmetric obstacle, different behaviours are detected
depending on the nature of its active motion. On the one side, rectification effects arise in a suspension of run-and-tumble particles interacting with a wall of funnelled-shaped openings, caused by particles persistence length [6]. The same trapping mechanism could be responsible for the intake

of microorganisms in the underground leaves [7] of Carnivorous plants [8].
On the other side, for aligning particles [9] interacting with a wall of funnelled-shaped openings, trapping
happens on the (opposite) wider opening side of the funnels [10,11]. Interestingly, when funnels are located on a circular array, trapping is more localised and depends on the nature of the Vicsek model. Active particles can be synthetic (such as synthetic active colloids) or alive (such as living bacteria). A prototypical model to study living microswimmers is P. fluorescens, a rod shaped and biofilm forming bacterium. Biofilms are microbial communities self-assembled onto external interfaces. Biofilms can be described within the Soft Matter physics framework [12] as a viscoelastic material consisting of colloids
(bacterial cells) embedded in a cross-linked polymer gel (polysaccharides cross-linked via proteins/multivalent cations), whose water content vary depending on the environmental conditions. Bacteria embedded in the
polymeric matrix control biofilm structure and mechanical properties by regulating its matrix composition. We
have recently monitored structural features of Pseudomonas fluorescens biofilms grown with and without
hydrodynamic stress [13,14]. We have demonstrated that bacteria are capable of self-adapting to hostile
hydrodynamic stress by tailoring the biofilm chemical composition, thus affecting both the mesoscale structure
of the matrix and its viscoelastic properties that ultimately regulate the bacteria-polymer interactions.

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Session 2 / 94

Quantum Simulations of Abelian Gauge Theories

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We propose an implementation of a two-dimensional Z2 lattice gauge theory model on a shallow quantum circuit, involving a number of single- and two-qubit gates comparable to what can be achieved with present-day and near-future technologies. The ground-state preparation is numerically analyzed on a small lattice with a variational quantum algorithm, which requires a small number of parameters to reach high fidelities and can be efficiently scaled up on larger systems. Despite the reduced size of the lattice we consider, a transition between confined and deconfined regimes can be detected by measuring expectation values of Wilson loop operators or the topological entropy. At the end we will discuss extensions to ZN aas well as non-abelian theories with finite group.

Session 3 B / 95

Ordering kinetics with long-range interactions

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We discuss the phenomenon of phase-ordering after a temperature quench in systems with long-range interactions decaying with distance r as $r^{-\alpha}$, focusing mainly on the Ising model in $d = 1$. For $\alpha > d$ one observes formation and growth of ordered domains, with scaling exponents continuously depending on
α. For $\alpha = 0$ one has mean field, where the system coherently orders without domains formation. For $\alpha \leq d$
there is an hybrid situation where both mean-field like and coarsening like behaviors are observed as different statistical realizations of the process are considered.

Session 3 B / 96

Localization, negative temperatures and ensemble inequivalence in the discrete nonlinear Schrodinger equation: a large deviations approach.

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We present a detailed account of a first-order localization transition in the discrete nonlinear Schrödinger equation, where the localized phase is associated with the high energy region in parameter space [1,2]. We show that, due to ensemble inequivalence, this phase is thermodynamically stable only in the microcanonical ensemble. In particular, we obtain an explicit expression of the microcanonical entropy close to the transition line, located at infinite temperature. This task is accomplished by making use of large-deviation techniques, that allow us to compute, in the limit of large system size, also the subleading corrections to the microcanonical entropy. These subleading terms are crucial ingredients to account for the first-order mechanism of the transition, to compute its order parameter and to predict the existence of negative temperatures in the localized phase.

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Session 10 / 97

Flux tubes and quark confinement in QCD

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The quark confinement in QCD is well established both experimentally and by the numerical lattice simulations showing a linearly growing quark-antiquark potential. The confinement is further evidenced by the chromoelectric field between a static quark-antiquark pair concentrating in a tube-like structure called a flux tube.
This talk is a review of the recent results establishing the spatial structure of the flux tubes both in pure gauge theories and in QCD with dynamical quarks and the insights that these results can bring to understanding confinement.

Session 4 / 98

Dynamical quantum phase transitions of the Schwinger model: real-time dynamics on IBM Quantum

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A striking quest for quantum computing applications in available platforms is spanning across a wide range of topics. The framework of lattice gauge theories in the Hamiltonian formulation is tested through a simple quantum system. Limitations in the simulation capabilities are imposed by noise affecting the gates elaboration of quantum states, combined in the decomposition of Trotter evolution according to single and double qubit gates to implement real-time dynamics. Experimental results collected on IBM Quantum are compared with noise models to identify most characterizing parameters, in the absence of any error correction or mitigation. Proposed simulations of the Schwinger model quenched dynamics represent a paradigmatic use case scenario, based on input states preparation, evolution and measurement in a noisy environment, well suited to test quantum hardware capabilities.

Session 8 / 99

QCD phase diagram in strong magnetic background

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A background magnetic field is able to alter the confinement and chiral properties of QCD. We study the effects of two extremely strong magnetic background intensities, namely $eB = 4$ and 9 GeV^2, on the phase structure of the QCD with $2+1$ flavors at the physical point, by means of lattice simulations. We find evidences for a first order phase transition in the stronger magnetic field, occurring at an unexpected low temperature: about 60 MeV. Then, we provide the updated phase diagram of the QCD in a background magnetic field.

Session 4 / 100

Topological susceptibility in high-T $N_f = 2+1$ QCD via staggered spectral projectors

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We focus on the computation of the topological susceptibility of $N_f = 2 + 1$ QCD at the physical point for some temperatures above $T_c \simeq 155$ MeV. Topological fluctuations are enhanced by using a multicanonical approach and the susceptibility is computed by adopting the spectral projectors over the eigenmodes of the staggered Dirac operator. This method allows to reduce lattice artifacts affecting the standard gluonic definition, making the continuum limit extrapolation more reliable and providing a better control on the systematics.

Session 9 / 101

Thermodynamic limits of sperm swimming precision.

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I will briefly review the simplest thermodynamic uncertainty relation (TUR) and then I will show how it applies to the beating of a sperm's flagellum. Experiments show that the maximum precision is 10^(-2) s^(-1) which is of the same order of the maximum precision of each of the N \sim 10^5 dynein molecular motors that actuate the flagellum. For a molecular motor the TUR bound is almost saturated, this means that for the whole flagellum, that consumes N times the power of a single

motor, the TUR largely overestimate the precision. Additional experiments however demonstrate that when the power consumption decays (e.g. under oxygen deprivation) the precision decays according to the TUR. These observations suggest a scenario where the dynamics of the N motors is highly coordinated, the motors fluctuations are correlated and the whole flagellum inherits their low precision. I will conclude showing how a well established model for active flagellar beating can be modified to incorporate the correlation ingredient, reproducing the observed experimental behavior.

Session 5 / 102

Identifying informative distance measures in high-dimensional feature spaces

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Real-world data in physical chemistry, material science and beyond typically contain a large number of features that are often heterogeneous in nature, relevance, and also units of measure.
When assessing the similarity between data points, one can build various distance measures using subsets of these features.
Finding a small set of features that still retains sufficient information about the dataset is important for the successful application of many statistical learning approaches. We introduce a statistical test that can assess the relative information retained when using two different distance measures, and determine if they are equivalent, independent, or if one is more informative than the other. This ranking can in turn be used to identify the most informative distance measure and, therefore, the most informative set of features, out of a pool of candidates. The approach is applied to find the most relevant policy variables for controlling the Covid-19 epidemic and to identify compact yet informative descriptors for atomic structures.
We further provide evidence that the information asymmetry measured by the proposed test can be used to infer relationships of causality between the features of a dataset.

Session 4 / 103

From classical to quantum Markov chains: known and new results

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Since the first years of the 20th century, classical Markov chains have been a standard theoretical tool to model the statistics of a huge plethora of phenomena in physics, economics, biology, etc. Also, they are intensively used for Monte Carlo simulations [1]. The mathematical properties of these stochastic processes have been still studied over the last years because of their broad interest [2].

In this talk we will focus our attention on quantum Markov chains, the quantum counterpart of classical ones, commonly used in quantum information theory but also employed to describe neural networks [3]. Specifically, we will discuss known and new results about the asymptotics of these chains [4], comparing them with the analogous findings in the classical setting.
Joint work with P. Facchi and A. Konderak.

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Session 4 / 104

Lattice determination of the topological susceptibility slope χ' of $2d$ CP^{N-1} models at large N

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We compute the topological susceptibility slope χ', related to the second moment of the two-point correlator of the topological charge density, of $2d$ CP^{N-1} models for $N = 5, 11, 21$ and 31 from lattice Monte Carlo simulations. Our strategy consists in performing a double limit: first, we take the continuum limit of χ' at fixed smoothing radius in physical units; then, we take the zero-smoothing-radius limit. Since the same strategy can also be applied to $4d$ gauge theories and full QCD, where χ' plays an intriguing theoretical and phenomenological role, this work constitutes a step towards the lattice investigation of this quantity in such models.

Session 7 / 105

Lindblad master equation approach to the topological phase transition in the disordered Su-Schrieffer-Heeger model

Authors: Andrea Nava[1]; Gabriele Campagnano[None]; Pasquale Sodano[2]; Domenico Giuliano[1]

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We use the Lindblad equation method to investigate the onset of a mobility edge and the topological phase transition in the disordered Su-Schrieffer-Heeger chain connected to two external baths in the large bias limit. From the scaling properties of the nonequilibrium stationary current flowing across the system, we recover the localization/delocalization in the disordered chain.
To probe the topological phase transition in the presence of disorder, we use the even-odd differential occupancy as a mean to discriminate topologically trivial from topologically nontrival phases in the out-of-equilibirum system.

Session 1 / 106

Nonequilibrium thermodynamics of DNA nanopore unzipping

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We report on the systematic characterization of DNA unzipping via nanopore translocation. We show that at intermediate forces (20-60pN range) the unzipping process is drift-diffusive and can be modelled as a one-dimensional stochastic process in a tilted periodic potential. With a suitable and transferable theoretical analysis of the driven translocation trajectories we recover the effectuve potential and demonstrate that it corresponds to the free-energy landscape of the unzipping process. The results imply that the the DNA-unzipping thermodynamics can be recovered from out-of-equilibrium translocation trajectories, paving the way for broader uses of the method in single-molecule contexts.

Session 6 / 107

Topology in Lattice QCD

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We discuss methods and results on QCD topological studies on the lattice.
We review the interrelation of topology with chiral and axial symmetries,
and the effects on the meson spectrum in the different phases of QCD. We comment
on topological aspects of dense matter, and we discuss the high temperature
limit. We discuss the extrapolations needed to reach the regime of cosmological
relevance, and the resulting constraints on the QCD axion mass.

Session 8 / 108

Quantum computing algorithms for the investigation of the thermodynamic properties of physical systems

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Co-authors: Claudio Bonati [2]; Giuseppe Clemente [2]; Massimo D'Elia [3]; Lorenzo Maio [4]; Pariente Ruben [5]

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Quantum computing is a promising approach to avoid the sign problem that hinders the numerical simulation of many interesting physical systems. Here we report some progress on the application of quantum computing algorithms to the study of the thermodynamics for the one-dimensional Hubbard model, which can be regarded as a prototype for more complex theories having non-trivial fermionic degrees of freedom. We also explore the effectiveness of different quantum error mitigation strategies for simulating the real time evolution on IBM quantum computers.

Session 4 / 109

Lattice study of electromagnetic conductivity of quark-gluon plasma at finite baryon density and magnetic field

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In this talk we present our study of the electromagnetic conductivity in dense quark-gluon plasma obtained within lattice simulations with $N_f = 2 + 1$ dynamical quarks. We employ stout improved rooted staggered quarks at the physical point and the tree-level Symanzik improved gauge action. To reconstruct electromagnetic conductivity from current-current correlators, we employ the modified Backus-Gilbert, computing the convolution of the spectral density with the target function. The computation of the conductivity is performed both in presence of non zero chemical potential and in presence of strong magnetic field. In the first case, the simulations are performed at imaginary chemical potential. Then, the results are analytically continued to real values of baryon chemical potential. Our study indicates that electromagnetic conductivity of quark-gluon plasma rapidly grows with the real baryon density. In the second case, we studied the conductivity of QGP in presence of two large values of the magnetic field, namely $eB = 4, 9\ GeV^2$. Our results may indicate a manifestation of the Chiral Magnetic Effect (CME). The conductivity is also studied at different values of the temperature for both the values of the magnetic fields. This allows us to extract the temperature dependence of the relaxation time related to the decrease of chirality due to the chirality-changing processes.

Session 3 B / 110

Towards learning a Lattice Boltzmann collisional operator

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In this work we explore the possibility of learning a collisional operator
for the Lattice Boltzmann Method from data using a deep learning approach.
We present results where a Neural Network is successfully trained as a surrogate of the single relaxation time BGK operator.
We show that only by embedding in the Neural Network physical properties such as
conservation laws and symmetries, it is possible to correctly reproduce
the short and long time dynamics of standard fluid flows.

Session 7 B / 111

A novel methodology for epidemic risk assessment of COVID-19 outbreak

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We propose a novel data-driven framework for assessing the a-priori epidemic risk of a geographical area and for identifying high-risk areas within a country [1]. Our risk index is evaluated as a function of three different components: the hazard of the disease, the exposure of the area and the vulnerability of its inhabitants. As an application, we discuss the case of COVID-19 outbreak in Italy. We characterize each of the twenty Italian regions by using available historical data on air pollution, human mobility, winter temperature, housing concentration, health care density, population size and age. We find that the epidemic risk is higher in some of the Northern regions with respect to Central and Southern Italy.

The corresponding risk index shows correlations with the available official data on the number of infected individuals, patients in intensive care and deceased patients, and can help explaining why regions such as Lombardia, Emilia-Romagna, Piemonte and Veneto have suffered much more than the rest of the country.

Although the COVID-19 outbreak started in both North (Lombardia) and Central Italy (Lazio) almost at the same time, when the first cases were officially certified at the beginning of 2020, the disease has spread faster and with heavier consequences in regions with higher epidemic risk. Our framework can be extended and tested on other epidemic data, such as those on seasonal flu, and applied to other countries.

Session 8 / 112

Effect of the N3LO three-nucleon contact interaction on p-d scattering observables

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In nuclear physics the so-called *ab initio* methods allow to solve the full Schroedinger equation, for few-body systems, with realistic potentials. From the theoretical point of view, chiral effective field theory provides a solid basis with interactions organized according to the importance of their contribution in powers of Q, the typical nucleon momentum, on the cutoff $\Lambda_\chi \sim 1$ GeV.
In this work we analyze the effect of the next-to-next-to-next-to leading order (N3LO) terms of the chiral three-body contact potential on the scattering variables for the p-d system.
Through the use of a unitary transformation five terms of the N4LO three-body contact potential are promoted to N3LO, implying the existence of five LECs for the three-body force at this order. Preliminary investigations carried out in this work suggest that the long standing N-d puzzle can be fixed by these terms.

Session 3 / 113

Quantum Computing Algorithms for Thermal Averages Estimation: an Analysis of Sources of Systematical Error

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In this talk we first present an overview of quantum computing algorithms for estimating the average of observables in a thermal ensamble, focussing in particular on two: the Quantum Metropolis Sampling algorithm and the Quantum-Quantum Metropolis Algorithm. We then analyze the effects systematical errors in the results for both algorithms under quantum noiseless conditions and using a system of frustrated spins as testbed.

Session 8 B / 114

From smeared spectral functions to the lattice calculation of inclusive semileptonic decays

Authors: Antonio Smecca[1]; Francesco Sanfilippo[2]; Marco Panero[1]; Nazario Tantalo[3]; Sandro Mächler[4]; Shoji Hashimoto[5]; Silvano Simula[2]; Paolo Gambino[1]

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Hadronic spectral functions are important objects as they can be used to calculate several phenomenologically relevant quantities. However, in order to extract these quantities from Euclidean correlation functions it is necessary to solve an ill-posed inverse problem of the Laplace type.
In this talk we discuss one of the recently proposed method for the extraction of spectral densities based on the Backus-Gilbert algorithm.
Furthermore, we show one of the many possible application of the method which is the lattice calculation of inclusive semileptonic decays of heavy mesons.

Session 4 B / 115

Emulsions in homogeneous and isotropic turbulence

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Emulsions are a major class of multiphase flows, crucial in industrial process (e.g. food and drug production) and ubiquitous in environmental flows (e.g. oil spilling in maritime environment). Already at volume fractions of few precents, the dispersed phase interacts with pre-existing turbulence

created at large scale, yet the interaction between phases and the turbulent energy transport across scales is not yet fully understood.
In this work, we use Direct Numerical Simulation to study emulsions in homogeneous and isotropic turbulence, where the Volume of Fluid (VOF) method is used to represent the complex features of the liquid-liquid interface.
We consider a mixture of two matching-density phases under various conditions, aiming to understand the turbulence modulation and the observed droplet size distributions. We observe the -10/3 and -3/2 scaling on droplet size distributions, suggesting that the dimensional arguments which led to their derivation are verified in HIT conditions and denser conditions. Finally, we discuss the highly intermittent behaviour of the multiphase flow, which can be directly related to the polydisperse nature of the flow.

Session 8 / 116

Estimation of the Nambu-Goto string thickness using continuous normalizing flows

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The explosive growth of machine learning provides a novel approach to study quantum field theories on the lattice. One intriguing class of algorithms recently proposed are Normalizing Flows, deep generative models able to learn highy expressive transformations between distributions. In lattice field theory, Normalizing Flows can sample uncorrelated configurations from Boltzmann distributions; moreover, they can infer the exact partition function of the target. In this talk, we present preliminary numerical computations of the thickness of the Nambu-Goto string. We sample the configurations using Continuous Normalizing Flows and validate our results using numerical and analytical studies of the Nambu-Goto action as benchmarks.

Session 4 B / 117

Slow round-trip variations across quantum and classical critical points

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We address the out-of-equilibrium dynamics of many-body systems subject to time-dependent round-trip protocols across quantum and classical (thermal) phase transitions.

They are realized by slowly changing one relevant parameter w across its critical point $w_c = 0$, linearly in time with a large time scale t_s , from $w_i < 0$ to $w_f > 0$ and then back to $w_i < 0$, thus entailing multiple passages through the critical point.

Analogously to the one-way Kibble-Zurek protocols across a critical point, round-trip protocols develop dynamic scaling behaviors at both classical and quantum transitions, put forward within

renormalization-group frameworks. The scaling scenario is analyzed within some paradigmatic models undergoing quantum and classical transitions belonging to the two-dimensional Ising universality class, such as one-dimensional quantum Ising models and fermionic wires, and two-dimensional classical Ising models (supplemented with a purely relaxational dynamics).

While the dynamic scaling frameworks are similar for classical and quantum systems, substantial differences emerge due to the different nature of their dynamics, which is purely relaxational for classical systems (implying thermalization in the large-time limit at fixed model parameters), and unitary in the case of quantum systems.

In particular, when the critical point separates two gapped (short-ranged) phases and the extreme value $w_f > 0$ is kept fixed in the large-ts limit of the round-trip protocol, we observe hysteresis-like scenarios in classical systems, while quantum systems do not apparently develop a sufficiently robust scaling limit along the return way, due to the presence of rapidly oscillating relative phases among the relevant quantum states.

Session 10 / 118

Random Field Ising model, dimensional reduction and supersymmetry

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I will present recent results for the study of the Random Field Ising model in various dimensions. Using results of large scale numerical simulations, I will argue that dimensional reduction is valid at D=5 and that we observe the consequences of supersymmetry.
Next, I will discuss recent analytical results in D=4 which argued that there should also exist a fixed point with dimensional reduction but hidden by the presence of relevant interactions.

Session 4 / 119

Color-flavor reflection in the continuum limit of two-dimensional lattice gauge theories

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We present and discuss the interplay between local and global symmetries in determining the continuum limit of two-dimensional lattice scalar theories characterized by SO(N_c) gauge symmetry and non-abelian O(N_f) global invariance. We argue that, when a quartic interaction is present, the continuum limit of these models may correspond to a gauged non-linear σ model field theory associated with the real Grassmannian manifold SO(N_f)/(SO(N_c)×SO(N_f−N_c)), which is characterized by *color-flavor* reflection invariance under $N_c \leftrightarrow N_f - N_c$.

Session 4 B / 120

Entropy of quantum states

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In a theory with superselections rules, a state can be represented by different density matrices. As a result, different von Neumann entropies can be associated with the same state. Motivated by a minimality property of the von Neumann entropy of a density matrix with respect to its possible decompositions into pure states, we give a purely algebraic definition of entropy for states of an algebra of observables, thus solving the above ambiguity. The entropy so defined satisfies all the desirable thermodynamic properties, and reduces to the von Neumann entropy in the quantum mechanical case. Moreover, it can be shown to be equal to the von Neumann entropy of the unique representative density matrix belonging to the operator algebra of a multiplicity-free Hilbert-space representation.

Session 8 B / 121

Fluctuations of arctic curves and the Tracy Widom distribution

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Arctic curves in two-dimensional lattice models separate disordered regions from others whose degrees of freedom are frozen. A celebrated example is the so-called arctic circle in the six-vertex model. In this talk, I will analyze numerically fluctuations of the arctic curves in the six-vertex model and discuss their relation with the Tracy-Widom distribution. The latter arises in the context of random matrices theory when studying statistics of extrema. This is joint work with V. Korepin and I. Lyberg.

Session 8 / 122

Quantum computing to witness nonclassicality

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We take the existence of a generalized-noncontextual model as a notion of classical explainability, an idea that has been previously shown to have solid foundational motivations (subsuming many other popular notions of classicality), broad applicability (unlike Bell's notion of locality), and a track record of being able to account for quantum-over-classical advantages in information processing. Through cloud quantum computing, we study quantum interference, one of the most characteristic features of quantum theory, to answer the question of which aspects resist explanation within the classical worldview. We found that, even though the basic phenomenology of quantum interference can be explained in a noncontextual model, we identify an aspect of interference that goes beyond the basic phenomenology and that can witness the failure of noncontextuality, namely, the functional form of wave-particle duality relation.
This, therefore, constitutes an aspect of interference that is nonclassical in a rigorous sense. Crucial for proving our result is to show that the wave-particle duality relations that we consider are

an instance of uncertainty relations, thus establishing a connection with another main feature in quantum theory.

Session 1 / 123

A tribute to Raffaele Tripiccione: 1956-2021

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It is almost one year that Raffaele Tripiccione is no longer with us. He was a colleague , a very deep thinker and, above all, a friend.

In this short talk, I will review his figure and some of his scientific work.

Session 3 / 124

A quantum optimization algorithm for deriving e ective shell model Hamiltonians

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In the recent years, theoretical methods for calculating the two body matrix elements of shell-model e ective Hamiltonians starting from realistic interactions have evolved considerably. However, these methods, usually rooted in the framework of many-body perturbation theory, present several sources of inaccuracies: 1) the convergence of the perturbation expansion; 2) the oscillator basis used for matrix elements and energy denominators is an approximation; 3) three-body force are required.
Thus, to obtain realistic wave functions there is a need to modify the e ective interactions based on constraints from experimental data, or, alternatively, to determine them from scratch. Usually, these kind of analysis are performed resorting to least squares approach. Notable examples are the Cohen and Kurath [1] and the USD interactions [2] for the p- and sd-shell nuclei, respectively. However, this approach starts to be demanding once the dimension of the model space and/or the number of experimental data increases.
Here, we propose an alternative approach, to our knowledge never used for this purpose, based on the use of an evolutionary algorithm, the Genetic Algorithm (GA). It is inspired by the process of natural selection and commonly used to generate high-quality solutions to optimization and search problems by relying on biologically inspired operators such as mutation, crossover and selection. The quantum version of the GA algorithm for the binary encoding case can be found in Ref. [3]. Its quantum version for the real encoding case is under development and we are using the derivation of an effective interaction for p-shell nuclei as possible application. I will discuss preliminary results obtained on a classical computer demonstrating the possibility to use GA to derive e ective

shell-model Hamiltonians capable to give a description of p-shell nuclei better or comparable to well-established Hamiltonians like the Cohen and Kurath one.

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Session 9 / 125

Non-perturbative thermal QCD at very high temperatures: the case of mesonic screening masses

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We present a strategy based on the step-scaling technique to study non-perturbatively thermal QCD up to very high temperatures. As a first concrete application, we compute the flavour non-singlet meson screening masses in the temperature range from approximatively 1 GeV up to the electroweak scale in the theory with three massless quarks. On the one side, chiral symmetry restoration manifests itself in our results through the degeneracy of the vector and the axial vector channels and of the scalar and the pseudoscalar ones. On the other side, we observe a clear splitting between the vector and the pseudoscalar screening masses up to the highest temperature investigated. A comparison with the high-temperature effective theory shows that the known one-loop perturbative matching with QCD does not provide a satisfactory description of the non-perturbative data up to the highest temperature considered.

Session 4 B / 126

A multicolour polymer model for the prediction of 3D structure and transcription in human chromatin

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Within each human cell, three types of RNA polymerases and a panoply of different types of transcription factors bind chromatin to simultaneously determine 3D chromosome structure and transcriptional programme. Experiments suggest that, in some cases, different types of proteins segregate to form specialised transcription factories, while in others they mix and gather together, binding the same chromatin regions. Here, we use coarse grained molecular dynamics simulations to study the coupled 3D structure and transcriptional dynamics of chromatin fibers and whole human chromosomes, via a polymer model which accounts for multiple types – or "colours" – of DNA-binding proteins, mimicking complexes containing RNA polymerase I, II, and III, or cell-type-invariant and cell-type-specific transcription factors.
Our simulations show the appearance of both segregated and mixed clusters, depending on their size, with larger clusters being more likely mixed: this is suggestive a transition between the two types of clusters based on simple biophysical parameters. Second, the model leads to non-trivial spatio-temporal correlations between different transcription units, dependent on the underlying

chromosome structure. Finally, it predicts transcriptional data better than previously considered models.

Session 7 / 127

The Exodus to GPU. The case of scientific analysis for the Euclid mission.

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All the main HPC facilities in the world rely on GPUs for their new computational systems. CINECA' s Leonardo powerful computing capabilities are rooted on GPU performances. Missions like Euclid that make a lot of use of computing power to perform scientific analysis with their data will now need to produce and optimize codes that adapt to the GPU in a short timescale.
In this presentation I will show how the Julia programming language could be the game changer in the updates of scientific analysis codes with GPU for the Euclid mission.

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The Equation of State from Lattice QCD

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The equation of state of the quark gluon plasma at finite density from first principle lattice QCD simulations has been a challenge for many years due to the infamous sign problem. This talk will discuss recent developments and results which allow access to the equation of state up to μ/T 3.5.

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OPTIMIZING [FEFE]-HYDROGENASE

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[FeFe]-hydrogenase is an iron-sulfur protein that catalyzes the chemical reduction of protons into the H2 molecule [1]. This enzyme can be found in cyanobacteria and microalgae organisms. HydA1 enzyme of the unicellular alga Chlamydomonas Rheinhardt is very efficient in reducing protons in water to molecular hydrogen, but it is very sensitive to dioxygen (O2), which irreversibly degrades the enzyme. When O2 becomes concentrated enough, like in intensive photosynthesis, the hydrogenase protein is attacked in the most oxygen sensitive points and the protein becomes non-functioning,

unfolded, and suited for degradation pathways. On the other hand, other microalgae strains showed higher resistance to O2. The molecular engineering of hydrogenase has been proposed as a possible workaround to the problem of O2 sensitivity. With this work, we aim at understanding how the hydrogenase (Hyd) variants expressed by these strains can better sustain hydrogen production in the presence of O2. As already performed by other groups, the project begins mapping sequences of hydrogenase expressed in the latter strains to the structure of cyanobacteria Clostridium Pasteurianum H-domain of [FeFe]-hydrogenase. The latter is the unique known structure of Hyd including the position of all atoms in the H-cluster. [FeFe]-hydrogenase is made by two domains: H-domain, within H-cluster principal active site, and F-domain, within secondary active sites. In some microalgae organisms, the evolutionary process guided [FeFe]-hydrogenase protein to lose F-domain and replace it with a smaller disordered domain of variable sequence.
We are focusing on the possible effect of the disordered N-terminal segment of Hyd on the accessibility of dioxygen to the H-cluster [2].

[1] James A. Birrell et al., Coordination Chemistry Reviews 449 (2021) 214191.
[2] Giovanni La Penna, NIC Symposium Proceedings, G. Munster, D. Wolf, M. Kremer 2010

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Pattern capacity of a single quantum perceptron

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Artificial neural networks have proven to be an extremely efficient computational model in specific tasks such as pattern recognition or image classification and have revolutionized the field of data analysis on classical computers. At the same time, the advent of quantum computation has shown that purely quantum mechanical features such as coherence and entanglement allow for addressing hard computational tasks with an exponential improvement of the performances compared to classical computation. The great success achieved in these two fields has motivated a surge of interest in quantum machine learning, with the aim to understand whether the two fields can benefit from each other. Recent developments in this field have seen the introduction of several models to generalize the classical perceptron to the quantum regime. The capabilities of these quantum models need to be determined precisely in order to establish if a quantum advantage is achievable. Here we use a statistical physics approach to compute the pattern capacity of a particular model of quantum perceptron realized by means of a continuous variable quantum system.

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Mixing of a Buoyant Jet in a Crossflow with the Lattice Boltzmann Method

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The Lattice Boltzmann Method (LBM) is a numerical approach for the study of fluid flows. It is based on a discretized version of the Boltzmann equation, and employs a mesoscopic approach where macroscopic flow quantities such as flow density and velocity are recovered as zero-th and first order moments of probability density functions. This method is, at its core, very simple, versatile and highly parallelizable; because of this, during the last few decades it has been used to investigate fluid flows in an increasing number of different fields of research. The aim of this talk is to describe how the LBM can be used to study mixing phenomena, as they are very common and play a fundamental role in a great number of processes. The dilution and diffusion of contaminants with negatively buoyant jets in a crossflow (JICF), in particular, is investigated carrying out large eddy simulations in a LBM framework, and it is shown how this method is able to capture some of the fundamental characteristics of JICF.

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Confinement in Lattice QCD

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QCD provides the fundamental description of the strong force and is a key component of the Standard Model. QCD is a quantum gauge field theory with local SU(3) symmetry that describes the interactions of coloured quarks and gluons. These are observed to be confined inside hadronic states, such as the protons, neutrons and pions. Colour confinement is among the most important and fascinating phenomena in fundamental physics. A characteristic feature of confinement is the formation of chromo-electric flux tubes, usually called QCD strings, that connect a quark with an antiquark. These strings have been observed in numerical Lattice QCD calculations and found that they behave to an adequate extent as bosonic Nambu-Goto strings. I would thus, present a general overview of confinement and I will then focus on the behaviour of flux-tubes as bosonic strings by focussing on our new findings on the spectrum of closed flux-tubes. Namely, our calculations demonstrate that most flux tube states exhibit a spectrum which can be approximated adequately by Nambu-Goto and in addition there is strong evidence for the existence of a massive axion on the world-sheet of the QCD flux-tube as well as a bound state of two such axions.

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New governance of INFN Scientific computing management and overview of PNRR activities in the context National Scientific Computing infrastructure

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The new governance of INFN Scientific computing management and an overview of PNRR activities in the context National Scientific Computing infrastructure will be presented in this talk.