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Book of Abstracts

Contents

Session 6 / **57**

q-Neighbor Majority-Vote Model on Complex Networks

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A q-neighbor majority-vote model for the opinion formation is introduced in which agents represented by two-state spins update their opinions on the basis of the opinions of randomly chosen subsets of q their neighbors (q-lobbies). The agents with probability $(1-2p)$, $0 \leq p \leq 1/2$, obey the majority-vote rule in which the probability of the opinion flip depends only on the sign of the resultant opinion of the q-lobby, and with probability $2p$ act independently and change opinion or remain in the actual state with equal probabilities. Thus, the parameter p controls the degree of stochasticity in the model. In the model under study the agents are located in the nodes of complex networks, e.g., Erd\"os-R\'enyi graphs or scale-free networks, and the neighborhood of each agent consists of all agents connected with him/her by edges, out of which the q-lobby is chosen randomly at each step of the Monte Carlo simulation. This model is related to a recently introduced q-neighbor Ising model [A.\ J\c{e}drzejewski et al., Phys.\ Rev.\ E 92, 052105 (2015); A.\ Chmiel et al., Int.\ J.\ Modern Phys.\ C 29, 1850041 (2018)], with agents obeying Metropolis opinion update rule, in which, in particular, first-order ferromagnetic transition was reported, with the width of the hysteresis loop oscillating with q. In contrast, in the q-neighbor majority vote model only second-order ferromagnetic transition is observed. Theory for this transition is presented both in the mean-field approximation, valid for large mean degrees of nodes and large q, and in a more elaborate pair approximation. In the latter case the predicted location of the critical point p_c agrees quantitatively with that obtained from Monte Carlo simulations for various complex networks with broad range of mean degrees of nodes and sizes of the q-lobby. Finite size scaling analysis shows that in the vicinity of the critical point the magnetization shows scalin typical for the mean-field Ising model, with the critical exponent $\beta = 1/2$, but other critical exponents depend on the topology of the underlying complex network.

Summary:

Session 8 / **63**

A particle's transport and absorption modelling in a system consisting of two media separated by a thin membrane

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We study a system which consists of two media divided by a thin partially permeable membrane. One of these media is diffusive. The second one is subdiffusive. Moreover, transported particles can be absorbed in the subdiffusive medium. In order to find methematical description of a transport process we use a new, universal model that is presented in details in \textit{T. Koszto\l{}owicz, Phys. Rev. E \textbf{99}, 022127 (2019)}. This new model leads to the general (sub)diffusion–absorption equations, Green's functions and boundary conditions at a thin partially permeable membrane for a system consisting of two media separated by a thin membrane. We find concentration profiles and the other functions which describe the time evolution of an amount of transported substance between media, as well as the amount of substance that will be absorbed depending on time in the

subdiffusive medium. We also compare our results with the experimental data found in the scientific literature.

Summary:

Session 2 / **48**

Active Interface Equations

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In this work we consider the role of active inclusions in a growing interface, for example membrane binding proteins which catalyse growth in the plasma membrane of eukaryotic cells. The interface is thus rendered active and is described by two coupled fields: the height field of the interface and the density of the inclusions. The equations generalise to active interface growth the Kardar Parisi Zhang equation which descibes nonequilibrium growth and also represents many other systems driven out of out of equilibrium. In our model inclusions gravitate towards minima of the height field and then catalyse growth which generates interface waves. This leads to complex kinematic waves and pattern formation and the proteins are able to surf the waves they create. The interface width displays a novel superposition of scaling and sustained oscillations distinct from KPZ physics.

F Cagnetta, M. R. Evans and D Marenduzzo Phys. Rev. Lett. 120, 258001 (2018)
F Cagnetta, M. R. Evans and D Marenduzzo Phys. Rev. E 99, 042124 (2019)

Summary:

Session 7 / **7**

Classification of diffusion modes in single particle tracking data: feature based vs. deep learning approach

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Single-particle trajectories measured in microscopy experiments contain important information about dynamic processes undergoing in a range of materials including living cells and tissues. However, extracting that information is not a trivial task due to the stochastic nature of particles' movement and the sampling noise. It usually starts with the detection of a corresponding motion type of a molecule, because this information may already provide insight into mechanical properties of the molecule's surrounding.

The most common analysis method uses mean square displacement (MSD) curves. Within this approach, one fits the theoretical curves for various physical models to the data and then selects the best fit with statistical analysis. However, in many cases, the actual trajectories are too short for extracting meaningful information from the time-averaged MSDs. Moreover, the finite localization precision adds a term to the MSD, which can limit the interpretation of the data.

Classification of trajectories with machine learning (ML) algorithms is one of the possible approaches to overcome the problems of the MSD method. It is rooted in computer science and statistics. And it

is very appealing because it would enable automated analysis of many hundreds or even thousands of trajectories with a reduced amount of manual intervention and initial data curation.

Several attempts to analyze SPT trajectories with the traditional ML methods have been already carried out. However, the methods that have been used for that purpose (e.g. Bayesian approach, random forest and a simple back-propagation neural network) belong to the class of so-called feature-based methods. Each trajectory within this approach is described by a set of human-engineered features and only those features are provided as input to a classifier model. Thus, similarly to the MSD based methods, they require the preprocessing of raw data and their interpretability may be limited for short and noisy trajectories.

In the talk, we will present a novel classification method based on convolutional neural networks (CNN). CNNs is one of the most popular deep learning algorithms, which excels in image classification. Using them is very appealing because they operate on raw data. They do not require any feature selection and extraction carried out by a human expert. Instead, they use a cascade of multiple layers of nonlinear processing units for feature identification, extraction and transformation in order to learn multiple levels of data representations. The performance of the CNN classifier trained on artificial trajectories will be compared with two popular feature based methods (random forest and gradient boosting).

References:
1. Patrycja Kowalek, Hanna Loch-Olszewska, **Janusz Szwabiński**, *Classification of diffusion modes in single particle tracking data: feature based vs. deep learning approach*, arXiv:1902.07942, submitted to Phys. Rev. E

Summary:

Session 8 / **21**

Clustering of dynamic node states in an adaptive network model

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We investigate an adaptive network model describing human smoking behavior incorporating the social processes homophily and induction introduced by Schleussner et al. (Sci Rep 2016). Upon social transition, the smoking prevalence in the model decreases, leaving remaining smokers clustered and marginalized in the network. Intriguingly, the model qualitatively resembles empirical findings. Employing a new measure for the clustering of dynamic node states in networks we study the influence of the locality of node interactions, of the complex contagion process of the node update, and of the homophily during network evolution on the clustering and marginalization of smokers in the network. We find that homophily is the dominant process bringing about clustering.

Summary:

Session 2 / **4**

Competition between cancer and immune system cells in an inhomogeneous system: A thermostatted kinetic theory approach

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The treatment of cancer by boosting the immune system is a recent and promising therapeutic strategy. During interactions, the immune system cells learn to recognize cancer cells. Analogously, the cancer cells can develop the ability to blend into the surrounding tissue and mislead the immune system cells.

I will present a model of cell interactions in the framework of thermostatted kinetic theory [1,2]. Cell activation, learning processes, and memory loss due to cell death are reproduced by regulating the cell activity introduced in the model. By analogy with energy dissipation in a mechanical system, the control of the activity fluctuations is achieved by a so-called thermostat. Proliferation of cancer cells is reproduced by autocatalytic processes. For each cell type, I will write down the thermostatted kinetic equations for the distribution functions of position, velocity, and activity and explain how the direct simulation Monte Carlo (DSMC) method has been adapted to solve them.

The numbers and activities of cancer cells and immune system cells are followed for different initial distributions of cells. The effect of the thermostat on cancer evolution will be compared to unexplained clinical observations. I will show that the model is able to reproduce an apparent elimination of the tumor preceding a long period of equilibrium, eventually followed by the proliferation of the cancer cells, according to a process identified as “the three E’s” of immunoediting, for “Elimination, Equilibrium and Escape” [3,4].

1. C. Bianca and A. Lemarchand, Commun. Nonlinear Sci. Numer. Simul. 20, 14 (2015).
2. C. Bianca, C. Dogbe, and A. Lemarchand, Acta Appl. Math. 189, 1 (2015).
3. C. Bianca and A. Lemarchand, J. Chem. Phys. 145, 154108 (2016).
4. L. Masurel, C. Bianca, and A. Lemarchand, Physica A 506, 462 (2018).

Summary:

Session 8 / **22**

Continuous-time random walk with correlated waiting times - activity clustering description

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Continuous-time random walk (CTRW) is a stochastic process with continuous and fluctuating waiting (inter-event) time. It was first introduced to physics by Montroll and Weiss. Since then it has been used in many areas of science [1]. CTRW is also successfully applied in econophysics [2], for example, it is used to describe stock price dynamics. We can consider the stock price as the price of the last transaction, so the value of a process represents the stock price and waiting times correspond to times between transactions.
Our latest results [3] suggest that dependencies between inter-trade times are the key element to explain long-term memory in financial time-series, even when taking into account intraday seasonality (so-called „lunch effect”). We introduce the new CTRW model with long-term memory in waiting

times, able to successfully describe power-law decaying time autocorrelation of the absolute values of price changes. We compare our model with empirical data from the Polish stock market.

[1] Kutner, R., Masoliver, J. (2017), The continuous time random walk, still trendy: fifty-year history, state of art and outlook, Eur. Phys. J. B, 90(3), 50
[2] Scalas, E. (2006), Five years of continuous-time random walks in econophysics, In The complex networks of economic interactions (pp. 3-16), Springer, Berlin, Heidelberg.
[3] Klamut, J. & Gubiec, T. (2019), Directed continuous-time random walk with memory, Eur. Phys. J. B 92:69.

Summary:

Session 3 / **5**

Cross-diffusion in concentrated reactive systems revealed by perturbation of FKPP wave front

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The sensitivity to perturbations of the Fisher, Kolmogorov, Petrovskii, and Piskunov (FKPP) wave front is used to find a quantity revealing the perturbation of diffusion in a concentrated solution. We consider two chemical species A and B engaged in the reaction A + B $\rightarrow$ 2A. When A and B have different diffusivities D_A and D_B, the deterministic dynamics includes cross-diffusion terms due to the deviation from the dilution limit [1].

The behaviors of the front speed, the shift between the concentration profiles of the two species, and the width of the reactive zone are investigated, both analytically and numerically. The analytic results are deduced from a perturbation approach in the limit of small diffusion terms with respect to reaction terms. The shift between the two profiles turns out to be a well-adapted criterion presenting noticeable variations with the deviation from the dilution limit in a wide range of parameter values. In particular, the difference between the shifts obtained in a dilute system and a concentrated system increases as D_B differs from D_A, especially in the case $D_B > D_A$ [2].

[1] L. Signon, B. Nowakowski, and A. Lemarchand, Phys. Rev. E **93**, 042402 (2016).
[2] G. Morgado, B. Nowakowski, and A. Lemarchand, Phys. Rev. E **99**, 022205 (2019).

Summary:

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Deterministic and randomized motions in single-well potentials

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We study the Newtonian, undamped motion in single-well potentials. We investigate and compare long-time properties of fully deterministic motions in single-well potentials with analogous randomized systems. As a special special type of energy conserving randomization process we consider hard velocity reversals: $\vec{v}(t_i) \rightarrow -\vec{v}(t_i)$ at random time instants t_i. On the one hand, in the 1D case, for fixed initial conditions, the differences in probability distributions disappear in the long-time limit making asymptotic densities insensitive to the selection of random time instants when velocity is reversed. On the other hand, randomization of initial conditions (on the constant energy curve) produces densities which significantly differ from the ones recorded for fixed initial conditions. The former 1D model is extended to the 2D setup, in case of which the analysis is accompanied with the exploration of the recurrence time distributions.

M. Mandrysz and B. Dybiec, Deterministic and randomized motions in single-well potentials, J. Phys. A (in print) arXiv:1908.00586.

Summary:

Session 8 / **17**

Diffusion in a system with a membrane that can change the state of the particles passing through it.

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Using a new method, time evolution of the probability distribution of the number of particle passes through a thin membrane will be derived. As far as we know, a distribution of the number of particle's passes between selected points of the system (membrane surfaces) have not been determined yet.
We assume that a passage of a particle through the membrane may cause a change in particle's state or vanishing (absorption) of the particle. These processes will be included in the model of particle diffusion in a system with a thin, partially permeable membrane that separates different media in which normal diffusion, subdiffusion or slow subdiffusion can occur [1]. The probability distributions (Green's functions) and other functions characterizing the process, such as the first passage time distributions, will be shown.

[1] T. Kosztołowicz, Phys. Rev. E 99, 022127 (2019)

Summary:

Session 8 / **54**

Discliantion formation in two-dimensional dense systems of hard and soft disks

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Hard objects can behave differently from the objects/particles that are interacting through soft potential. The main difference is that soft interacting particles can store potential energy accomodating

at the same time their positions. Hard interacting particles possess no potential energy and their arrangement is fully according to the entropic and geometry conditions. The excluded volume wich is determined by the shape of the particles play here a decisive role. Still all the consequences of these conditions are not fully examined. In this presentation we show the behavior of the very dense system of hard disks in comparison to the system made of soft disks. Using Event Driven molecular dynamics we observe in an initially perfect hexagonal arrangement a strong tendency of disclination formation, which we also call as minicracks. Minicracks are the places in the system where particles close to each other are situated on the square lattice. This concerns only two rows of particles. Beyond this areas the arrangement is hexagonal. Upon evolution the free space initially present in between particles diffusess to the minicraks areas, although some part must be still present, otherwise the system will be blocked. At the same time the average distance between particles diminishes. This is puerely an entropic effect which is not observed in soft interacting particles. We argue that such a free space diffusion into disclinations in harder objects systems can tell on the formation of large cracks, since the minicracks play the role of the seeds for larger crevices. Cracking is a big technological problem. In thin film, for instance, cracking spoils surface properties. It has been already observed that under electron or ion bombardment, even if such the interaction at the surface is rather point like, a large crack develop which ruins the regularity of the surface. We speculate whether the free space diffusion mechanism can be the driving force for spoiling such films. The possible physical reasons why free spaces diffuse to minicracks have been also discussed.

Summary:

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Dynamical mean field theory of neural networks with power-law disorder

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Transitions to chaos have been previously extensively studied in different setups of randomly connected networks. The prevailing assumption is that, due to the central limit theorem, synaptic input can be modeled as a Gaussian random variable. In this scenario, a continuous transition has been found in rate models with smooth activation functions. However, these models do not take into account that neurons feature thresholds that cut off small inputs. With such thresholds, the transition to chaos in Gaussian networks becomes discontinuous, making it impossible for the network to stay close to the edge of chaos and to reproduce biologically relevant low activity states.

Here we introduce a model with biologically motivated, heavy-tailed distribution of synaptic weights and analytically show that it exhibits a continuous transition to chaos. Notably, in this model the edge of chaos is associated with well-known avalanches. We validate our predictions in simulations of networks of binary as well as leaky integrate and fire neurons. Our results uncover an important functional role of non-Gaussian distributions of synaptic efficacy and suggest that their heavy tails may form a weak sparsity prior that can be useful in biological and artificial adaptive systems.

Summary:

Session 8 / **13**

Dynamical properties of confined hard-sphere glasses

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The structural relaxation of dense liquids displays a drastic slowing down upon compression or cooling, a phenomenon which is commonly identified with the glass transition. Many dynamical properties of the glass transition in bulk liquids have been successfully described by mode-coupling theory (MCT [1]). Even more involved is the description of confined liquids since they already exhibit interesting phenomena, like layering and gradients in the diffusivity, below the glass transition due to the breaking of the translational symmetry. In recent years, a MCT for confined hard-sphere liquids has been derived and its static properties have been compared to results from computer simulations [2,3]. Most importantly, it was discovered that the confinement induces a multiple reentrant glass transition. This could lead to the coexistence of glass and liquid in a wedge geometry [3].

Here we go further and investigate the dynamical properties of confined glass-forming liquids. By applying the standard scaling analysis [4], we find that the multiple decay channels (parallel and perpendicular to the walls) lead to additional, non-trivial contributions to the asymptotic solutions of the MCT. This qualitatively changes the connection between the bifurcation of the nonergodicity parameter and the long-time behavior of the coherent scattering function. Additionally, we present a detailed comparison of the dynamical properties predicted by MCT to results from computer simulations of hard-spheres (using event-driven molecular dynamics simulations). This includes the investigation of the coherent and incoherent scattering functions as well as an analysis of the α and β relaxation processes.

[1] Götze, W.; *Complex Dynamics of Glass-Forming Liquids, Oxford University Press*, 2009.
[2] Lang, S. *et al.*; *Phys. Rev. Let.* 2010, **105**, 125701.
[3] Mandal, S. *et al.*; *Nat. Comm.* 2014, **5**, 4435.
[4] Franosch, T. *et al.*; *Phys. Rev. E* 1997, **55**, 7153.

Summary:

Session 8 / **53**

Effective Medium Theory for an ultra thin liquid crystalline films and its consequences for the ellipsometric modeling -

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Technological applications of liquid crystals (LC) have been for many decades a continous driving force for investigating properties of this fascinating state of matter by theorists as well as by experimentalists. Still many questions about LC properties need to be answered. Special attention is paid to the optical characteristics of liquid crystalline thin films. In the current presentation we show an Effective Medium Theory for an ultrathin film of nematic liquid crystals that is based on the capacitor connection rule. This theory provides the effective dielectric tensor for a continuosly changing order of the liquid crystal which emerges from the interaction of molecules with the substrate which causes different degree of ordering with respect to the distance from the substrate. The needed order tensor has been obtained on the basis of the density functional theory. The resultant spatial changes of the particles ordering will influence the overall dielectric and optical properties. The changes of the dielectric properties due to the influence of the walls are shown to be as strong as several percent with respect to the bulk properties. The proposed EMA theory allows to calculate changes of polarisation in the light reflected or trasmitted through the sample and finds its application to ellipsometric modeling of optical properties.

Summary:

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Energy landscape in polymer translocation

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The passage of long biochemical structures through nano-channels from one side to the other side of a membrane is a normal process in biology. Drug absorption, protein and DNA/RNA passage through cell membranes and nuclear pores, DNA packaging by phage viruses are a few known examples.

After Kasianowick work on 1996, both theoretical and experimental investigations have been developed to understand the basic physics involved in this process. Moreover, the technological advances have now permitted to manipulate single molecules and to study the translocation through artificial channels also under time dependent driving exerted by molecular motors.

The study of polymer translocation is conveniently achieved by using coarse grained models to describe the process in affordable conditions, and to better control the contribution of specific parameters involved in the dynamics.
The bead-spring-based polymer here introduced is driven by an end-pulled force applied at different velocities opens a new way to investigate translocation[1]. In fact, the assisted velocity-dependent force registered at the translocation can be analysed with a spectroscopic approach similar to the one used in the folding/unfolding of macromolecules, so permitting a new perspective in the study of the translocation phenomenon which has the goal to characterise the energy landscape in the polymer translocation.

Summary:

Session 6 / **18**

Entropy Production in Open Systems: The Predominant Role of Intra-Environment Correlations

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We show that the entropy production in small open systems coupled to environments made of extended baths is predominantly caused by the displacement of the environment from equilibrium rather than, as often assumed, the mutual information between the system and the environment. The latter contribution is strongly bounded from above by the Araki-Lieb inequality, and therefore is not time-extensive, in contrast to the entropy production itself. Furthermore, we show that in the thermodynamic limit the entropy production is associated mainly with generation of the mutual information between initially uncorrelated environmental degrees of freedom. We confirm our results with exact numerical calculations of the system-environment dynamics.

Summary:

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Evolutionary paths in affinity maturation

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The humoral response to an infection relies on the process of affinity maturation. In order to develop antibodies with good binding properties, B cells gather in germinal centers where they proliferate and acquire mutations. The best mutants are selected to further proliferate. This evolutionary process is fueled by somatic hypermutations (SHM) which occur at a very high frequency. We propose a repertoire-wide approach to study the properties of mutations on evolutionary trees. We find that the mutation rate is position-dependent and that subsequent mutations colocalize. Our results help to understand the mutational landscape of SHM and assert the relevance of a phylogenetic approach.

Summary:

Session 4 / **55**

Exact resuts on Quantum Walks

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Quantum analogs of classical random walks have been defined in quantum information theory as a useful concept to implement algorithms. Due to interference effects, statistical properties of quantum walks can drastically differ from their classical counterparts, leading to much faster computations.

We shall present various statistical properties of continuous-time quantum walks on a lattice, such as: survival properties of quantum particles in the presence of traps (i.e. a quantum generalization of the Donsker-Varadhan stretched exponential law), the growth of a quantum population in the presence of a source, quantum return probabilities and Loschmidt echoes.

Summary:

Session 2 / **60**

Fluctuation Theorems for Systems without Stationary PDF: KPZ case

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We analyze a couple of simple systems, without stationary probability distribution, in order to show how to proceed for obtaining detailed as well as integral fluctuation theorems in such a kind of

systems. To reach such a goal, we exploit a path integral approach that adequately fits to this kind of study. This methodology, together with the variational approach, are also exploited to analize fluctuation theorems in the paradigmatic KPZ equation, as well as to determine a Large Deviation Function. This lead us to conjecture that a higher critical dimension does not exists for the KPZ system.

Summary:

Session 4 / **10**

Fundamental limitations of the step quantum heat engine

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The model of a step quantum heat engine (SQHE) is defined as a working body, given by the two-level system (TLS), acting separately (i.e. in steps) with the heat baths and the energy storage system (a battery). A single step of the engine is defined as the unitary and energy conserving operation. For the general SQHE we prove the fundamental attainable efficiency, given as a function of a cold and hot temperature, which is below the Carnot efficiency. The reason is that the engine is quasi-autonomous, i.e. there is no extra external control like fields commonly used in a non-autonomous setting, but in contrary the SQHE is realised by a unique physical process of the TLS population inversion via a strong coupling with the heat bath. For our model of the SQHE we additionally discuss the problem of the work definition for the fully quantum systems. So far one of the reasonable definition of the work (consistent with the fluctuation theorems) is given by the change in a mean energy of the battery which has additionally a translational symmetry, i.e. these changes do not depend on how much energy is currently stored in the battery. However, this symmetry impose a nonphysical property that the battery cannot have a ground state. We solve this problem showing that the battery with a ground state can be used as a proper energy storage system only if the work is defined as a change of the ergotropy instead of a mean energy.

Summary:

Session 8 / **28**

Generation of prototype membranes with prescribed structure and diffusion properties comparable to real hybrid polymer membranes

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This work aims to create prototype structures of hybrid polymeric membranes with the desired quantity, size and distribution of obstacles, which corresponds to the given amount of magnetite in the hybrid alginate membrane. The membrane is represented by a black and white image where the black regions corresponds to polymer matrix and are available for diffusive particles and the white ones are obstacles, which cannot be penetrated by tracer particle. The work describes two algorithms used to generate prototype membranes. The first method (algorithm A) subdivides the

whole membrane into multiple square blocks, each of size z by z pixels. Each block can independently become an obstacle with probability equal to the given ratio of obstacles. The second method (algorithm B) accounts for the possibility of irregular, differently shaped obstacles. They are grown around randomly distributed seeds until desired amount of polymer matrix is reached. The membranes are characterized by the following characteristics: the amount of polymer matrix, the fractal dimension of polymer matrix, the average size of polymer matrix domains, the average number of obstacles in the proximity of each polymer matrix pixel. For both presented algorithms, generated membranes possessing specific parameters are comparable to the real hybrid alginate membranes filled with magnetite.

[1] G. Dudek, M. Krasowska, R. Turczyn, M. Gnus, A. Strzelewicz, Structure, morphology and separation efficiency of hybrid Alg/Fe3O4 membranes in pervaporative dehydration of ethanol, Separation and Purification Technology 182 (2017) 101–109.
[2] M. Krasowska, A. Strzelewicz, G. Dudek, M. Cieśla, Structure-diffusion relationship of polymer membranes with different texture, Physical Review E 95, 012155 (2017).

Summary:

Session 5 / **64**

How is information decoded in developmental systems?

Marcin Zagórski[1]

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The development of multicellular organisms is a dynamic process in which cells divide, rearrange, and interpret molecular signals to adopt specific cell fates. Despite the intrinsic stochasticity of cellular events, the cells identify their position within the tissue with striking precision of one cell diameter in fruit fly or three cell diameters in vertebrate spinal cord. How do cells acquire this positional information? Where is this information encoded and how do cells decode it to achieve the observed level of cell fate reproducibility? These are fundamental questions in biology that are still poorly understood. In this talk, I will combine both information theory methods and mechanistic models to address these questions. I will investigate to what extent the level of noise in the input signals affects precision of the resulting gene expression pattern. I will present data-driven analysis of gene regulatory network that interprets two positional cues in the developing spinal cord. Interestingly, the observed precision of gene expression pattern is close to the theoretical limit of precision of decoding of noisy signals.

Summary:

Session 8 / **32**

Influence of molecular conformations on formation of nematic phases on a surface

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Bent-shaped particles gain more and more interest nowadays
due to the formation of novel liquid crystalline structures. Here, we investigate impact of molecular shape and conformational degrees of freedom on stabilization of nematic phases in two dimensional systems. Analyzed particles are composed of two and three arms built of either hard disks or hard

needles. Additionally, they have infinite amount of possible conformations. We compare hard disks and hard needles models, analyze impact of molecular shape, conformations and barrier between conformers on phase transition density, order parameters, probability distribution functions of different conformers and radial distribution functions.

Summary:

Session 8 / **41**

Information processing in biological molecular machines

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Biological molecular machines are enzymes that simultaneously catalyze two processes, one donating free energy and second accepting it. Recent studies show that most native protein enzymes have a rich stochastic dynamics that often manifests in fluctuating rates of the calatyzed processes and the presence of short-term memory resulting from transient non-ergodicity. For such dynamics, we prove the generalized fluctuation theorem predicting a possible reduction of energy dissipation at the expence of creating some information stored in memory. The theoretical relationships are verified in computer simulations of random walk on a model critical complex network. The transient utilization of memory turns out to be crucial for the movement of protein motors and the reason for most protein machines to operate as dimers or higher organized assemblies. Our conclusions are based on analysis of the simulated time course of the catalyzed processes expressed by the strings of discrete jumps at random moments of time. Since similar signals can be registered in the experiments, all the theses of our studies are open for experimental verification.

Summary:

No summary

Session 1 / **43**

Introduction to the quantum first detection problem

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We consider quantum dynamics on a graph, with repeated strong measurements performed locally at a fixed time interval τ. For example a particle starting on node x and measurements performed on another node x'. From the basic postulates of quantum mechanics the string of measurements yields a sequence no,no,no, $\cdots$ and finally in the n-th attempt a yes, i.e. the particle is detected. Statistics of the first detection time $n\tau$ are investigated, and compared with the corresponding classical first passage problem. Dark states, Zeno physics, a quantum renewal equation, winding number for the first return problem (work of A. Grunbaum et al.), total detection probability, detection time operators and time wave functions are discussed.

Summary:

Session 8 / **59**

Kinetic equation for the pair distribution function \\ in the Boltzmanns gas

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We report on a new kinetic equation for an auxiliary two-particle distribution function $f(\mathbf{k_1}, \mathbf{v_1}, \mathbf{k_2}, \mathbf{v_2}, t)$.
Its general form reads
\begin{equation}
\begin{array}{l}
\displaystyle
\left(\frac{\partial}{\partial t} \, + \, {\rm i} \, {\bf k_1} {v_1} \, + \, {\rm i} \ {\bf k_2} {v_2} \right)
f({\bf k_1}, {\bf v_1}, {\bf k_2}, {\bf v_2}, t) \, =
\\
\displaystyle
\hspace{5cm}
\int_0^t {\rm d} \tau \, {\cal G}(({\bf k_1}, {\bf k_2}, \tau) \, f({\bf k_1}, {\bf v_1}, {\bf k_2}, {\bf v_2}, t - \tau)
\end{array}
\end{equation}
with
\begin{equation}
\begin{array}{l}
\displaystyle
{\cal G}(({\bf k_1}, {\bf k_2}, \tau) \, \equiv \,
\\
\displaystyle
\hspace{2cm}
\int
{\rm d} {\bf v}^{N-2} \, {\rm d} {\bf r}^N \, {\rm e}^{- \,{\rm i} {\bf k_1}{\bf r_1}} \, {\rm e}^{- \,{\rm i} {\bf k_2}{\bf r_2}} \,
{\cal P} K_N \,
\\
\displaystyle
\hspace{3.5cm}
{\rm e}^{- \, \tau \, (1 - {\cal P}) K_N } \,
{\rm e}^{{\rm i} {\bf k_1}{\bf r_1}} \, {\rm e}^{{\rm i} {\bf k_2}{\bf r_2}} \,
\frac{f^0_N ({\bf v}^N, {\bf r}^N)}{\varphi_{\rm M}(v_1) \, \varphi_{\rm M}(v_2)}
\end{array}
\end{equation}
which is the scattering operator for our problem.
We have applied to this problem the technique of projection operators.
We find that $calG(t)$ is finite at $t = 0$ and can be readily expanded in Taylor series about $t = 0$. This is a distinct feature which is not present usually in other kinetic equations. Therefore the kinetic equation (1) with tne kernel (2) is not only valid for long times but for arbitrarily short times, including $t = 0$, as well.

Next we set the distance between particles 1 and 2, $|\mathbf{r}_1 - \mathbf{r}_2| = a$ = constant. This creates a dumbbell model of molecule, the diffusion of which is being studied.

Summary:

Session 5 / **19**

Levy walk with rests: Escape from bounded domain

Agnieszka Kamińska[None] ; Tomasz Srokowski[None]

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The Levy walk processes with rests restricted to a region bounded by two absorbing barriers are discussed. The waiting time between the jumps is given by an exponential distribution with a constant jumping rate and with a position-dependent jumping rate. The time of flight for both ranges of α: lower $(0, 1)$ and higher $(1, 2)$, is considered.
For constant jumping rate two limits are taken into account: of short waiting time that corresponds to Levy walks without rests, and long waiting time which exhibits properties of Levy flights model. The quantities describing the escape process: first passage time distribution, mean first passage time are analysed. The analytical results are compared with Monte Carlo trajectory simulations.

Summary:

Session 8 / **8**

Light-driven resonance of concentration oscillations in fluorescent proteins

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Selective imaging is a challenge in Biology. Out-of-Phase Imaging after Optical Modulation (OPIOM) [1] exploits reversibly photoswitchable fluorophores to selectively detect a target species in the presence of spectrally interfering fluorescent species. The method combines optimized periodic illumination and phase-sensitive detection, which matches the dynamics of the targeted photoreactive protein.

Increasing the complexity of the reaction network improves the multiplexing capacity of the discriminating method, i.e. the number of different objects that can be simultaneously detected. I have investigated a chemical mechanism involving the competition between the complexation of a protein tag and a fluorogen and the photoisomerization of the fluorogen [2]. The kinetics of association between the fluorophore and the protein tag provides discriminating factors for its selective detection. I will explore the multiplexing possibilities offered by coupling the photoisomerization of the fluorogen with the competitive complexation for multiple protein tags.

I will show that for a fluorogen-protein couple the out-of-phase amplitude of the concentration oscillations of the fluorescent complex displays a maximum [3] when the radial frequency ω and the average intensity I^0 of the illumination take singular values which depends on the kinetics of both isomerization and complexation reactions: The maximum is reached for a resonant species which have a particular set of rate constants. Hence, I will show how the experimentalist can tune the control parameters ω and I^0 to optimize the out-of-phase amplitude response for the targeted protein tag only.

[1] J. Querard et al., Nat. Commun. **8**, 1 (2017).
[2] M.-A. Plamont et al., Proc. Natl. Acad. Sci. U.S.A. **113**, 3 (2016).
[3] A. Pellissier-Tanon, R. Chouket, T. Le Saux, L. Jullien, and A. Lemarchand, Phys. Chem. Chem. Phys. **20**, 23998 (2018).

Summary:

Session 5 / **2**

Lévy flights in steep potential wells: Langevin modeling versus direct reponse to energy landscapes

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The Eliazar-Klafter targeted stochasticity concept , together and that of the reverse engineering (reconstruction of the stochastic process once a target pdf is a priori given), has been originally devised for Lévy-driven Langevin systems. Its generalization, discussed in [PRE 84, 011142, (2011)], involves a non-Langevin alternative which associates with the sam Levy driver and the same target pdf, another (Feynman-Kac formula related) confinement mechanism for Lévy flights, based on a direct reponse to energy (potential) landscapes, instead of that to conservative forces. We revisit the problem of Lévy motion in steep potential wells, addressed in [A.A. Kharcheva et al., J. Stat Mech., (2016), 054029] and [B. Dybiec et al. , PRE 95, 05201, (2017)] and discuss the alternative semigroup (Feynman-Kac) motion scenario. Our focus is on a link with the problem of boundary data (Dirichlet versus Neumann, or absorbing versus reflecting) for the Lévy motion and its generator on the interval (or bounded domain, in general).

Summary:

Session 7 / **56**

Machine learning methods in estimates of heart rate variability

Danuta Makowiec[1] ; Joanna Wdowczyk[2]

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Enormous progress in machine learning achievements, going together with their excellent implementations on user-friendly platforms, have pushed many of us towards this
methodology. Can we get better explanations for studied data? Can we get the explanation easier? In the following we deal with data formed from recordings on healthy people with different age and sex. The problem is how the age and/or sex influence the normal rhythm of a healthy heart.

The healthy human heart remains under the permanent influence of both branches of the autonomic neural system (ANS): the parasympathetic (considered to slow down heart rate) and the sympathetic (considered to speed up heart rate). Many measures estimating heart rate variability (HRV) have been proposed in order to quantify the regulatory function of the ANS. Intensive studies on healthy population have found a correlation between an increase in age and a decrease in many HRV indices. Therefore higher values of HRV have been attributed to better organization of feedback reflexes driving an organism's response to actual body needs. However, there are observations suggesting that abnormal levels of some indices should be related to erratic rhythms, i.e., rhythms resulting from remodeling of the cardiac tissue due to disease or aging. We hypothesize that increase of measures of dynamical patterns in elderly indicates at unhealthy autonomic activity, or possible erratic rhythm associated with degradation of cardiac tissue, or both. Such erratic rhythms might be the first stage of developing silently arrhythmogenesis.

The task of separating different cardiac patient groups on the basis of HRV parameters is an urgent problem. If there are differences, it might be possible to find noninvasive marker for specific cardiac

diseases. Answering to these questions demands wide knowledge about the way in which information hidden in heart rate variability displays the actual state of the heart regulatory system.

Summary:

Session 6 / **3**

Maxwell demons in phase space

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Although there is not a complete "proof" of the second law of thermodynamics based on microscopic dynamics, two properties of Hamiltonian systems have been used to prove the impossibility of work extraction from a single thermal reservoir: Liouville's theorem and the adiabatic invariance of the volume enclosed by an energy shell (Helmholtz's theorem). In this talk, I will review these two properties and analyze the dynamics of isothermal and microcanonical Szilard engines in the phase space. In particular, we will see that ergodicity breaking plays a crucial role in all these variants of the Maxwell demon because the enclosed volume is no longer an adiabatic invariant in non-ergodic systems.

Summary:

Session 3 / **50**

Mimicking heterogeneous diffusion with time dependent random diffusivity.

Author(s): Vittoria Sposini[1]

Co-author(s): Gianni Pagnini [2] ; Ralf Metzler [3] ; Aleksei Chechkin [4]

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[3] *University of Potsdam*

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A considerable number of systems have recently been reported in which Brownian yet non-Gaussian dynamics was observed. These are processes characterised by a linear growth in time of the mean squared displacement, yet the probability density function of the particle displacement is distinctly non-Gaussian, and often of exponential (Laplace) shape. This behaviour has been interpreted as resulting from diffusion in inhomogeneous environments and mathematically represented through a variable, stochastic diffusion coefficient. Indeed different models describing a fluctuating diffusivity have been studied. In particular, we focus on the theory of diffusing diffusivity and consider the very generic class of the generalised Gamma distribution for the random diffusion coefficient. Moreover, addressing the first passage problem for a specific diffusing diffusivity model, we emphasize that even when the non-Gaussian character appears for certain regimes only and in the tails of the distributions (thus with low probability), it may be essential for those systems in which rare events dominate triggered actions.

Summary:

67

Modeling of living cell's mechanical properties

Agnieszka Kurek[1] ; Leszek Krzemień[2] ; Jakub Barbasz[1]

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Cell's mechanical and physical properties such as elasticity or adhesion are significant parameters determining cell behaviour [1].
Changes in mechanical properties of cells can be connected with diseases such as cancer or blood diseases. Quantification of mechanical properties, analysis and comparison of collected data, can allow understanding the mechanism of disease formation and development [2].
Many technique can be used to measure single cells or tissues properties. One of commonly used technique is Atomic Force Microscopy. Thought interaction between sample surface and tip measurement, AFM allow to create single living cell mapping [2].
Another way to understand cell behaviour is computer modelling of cell response in indentation experiments [3]. In literature many authors describe variety of models, which base on divers physical lows and for this reason have different restrictions [4]. In our poster we present a few models which are commonly used to description and modelling of cell properties.

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3. Liu, Y., Mollaeian, K. & Ren, J. Finite element modeling of living cells for AFM indentation-based biomechanical characterization. Micron 116, 108–115 (2019).
4. Guz, N., Dokukin, M., Kalaparthi, V. & Sokolov, I. If Cell Mechanics Can Be Described by Elastic Modulus: Study of Different Models and Probes Used in Indentation Experiments. Biophys. J. 107, 564–575 (2014).

Summary:

Session 8 / **65**

Molecular arrest in binary mixtures induced by spatially correlated stochastic dynamics

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Binary mixtures, i.e. the systems composed of two different species of particles, exhibit a huge variety of dynamical modes and phase transitions. This includes demixing effects and several combinations of mobility and arrest, e.g. the collective critical slow-down of the bigger particles mediated by the presence of the smaller molecules. It was recently realized that the interactions in such system could be effectively mapped on the Spatially Correlated Noise (SCN), i.e. the thermal noise that affects neighboring particles in a similar manner[1,2]. Following this idea, the over-damped SCN-driven Langevin dynamics was investigated as an effective, one-component model of dynamics in a dense binary mixture. It was found that the thermodynamically consistent Fluctuation-Dissipation Relation for such system provides a novel insight into the arrest effects [3]. I will show that the mechanism of singular dissipation is embedded in the dissipation matrix, accompanying SCN. The

characteristic length of collective dissipation, which diverges at the critical packing is also identified. This is a new quantity, which conveniently grasps the difference between the ergodic and non-ergodic dynamics and is a measure of cooperativity in the system. The model is fully analytically solvable, one-dimensional and admits arbitrary interactions between particles. The transition is controlled by the interplay between the packing fraction and the noise correlation length, representing the packing fraction of smaller particles. As a practical example, both the hard spheres and the system of ultra-soft particles were studied. The framework of this model makes it is possible to discuss e.g. the re-entrant arrest.

Bibliography:
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[3] M. Majka, P.F. Góra, Molecular arrest induced by spatially correlated stochastic dynamics https://arxiv.org/abs/1707.07076

Summary:

Session 8 / **47**

Multi-branchness and the phase transitions in time series of inter-event times

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We develop an extended multifractal analysis based on the Legendre-Fenchel transform (some- times referred to as Legendre multi-branched one) rather than the routinely used canonical Legendre transform. In our variant of coarse-graining pre-processing, the local detrending of time series has been replaced by an appropriate averaging over days combined with properly-suited detrending on a daily time scale. This new approach is devoid of troublesome artifacts in the form of innumer- able faults of these local trends that can deform the hierarchy of fluctuations and hence the final multifractality. Notably, our analysis is sensitive to the change of time scale as it should be. This analysis has developed, e.g., for empirical time series of inter-event or waiting times, which are an essential element of the popular continuous-time random walk formalism. The core of this extended multifractal analysis is the non-monotonic behavior of the generalized Hurst exponent – the funda- mental exponent of the study – and hence a multi-branched spectrum of dimensions, which for our case is additionally of the left-sided one. We examine the main thermodynamic consequences of the existence of this type of multifractality. They can be expressed directly in the language of thermally stable, metastable, and unstable phases, and phase transitions between them as well. These phase transitions are of the first and second orders according to the modified Ehrenfest classification, sometimes called the Mandelbrot one.

Summary:

Session 8 / **46**

Multimodal stationary states in symmetric single-well potentials driven by Cauchy noise

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Stationary states for a particle moving in a single-well, steeper than parabolic, potential driven by Lévy noise can be bimodal. We explore in details conditions required to induce multimodal stationary states with a modality higher than two and provide phenomenological arguments determining necessary conditions for emergence of stationary states with an anticipated multimodality. The poster presents results of this consideration using sample symmetric single-well potentials, for which phenomenological arguments were verified using numerical methods.

Capała, K., & Dybiec, B. (2019). Multimodal stationary states in symmetric single-well potentials driven by Cauchy noise. J Stat. Mech., 2019 (3), 033206.

Summary:

Session 8 / **14**

Negative differential response in chemical reactions

Gianmaria Falasco[1] ; Tommaso Cossetto[1] ; Emanuele Penocchio[1] ; Massimiliano Esposito[1]

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Reaction currents in chemical networks can decrease when increasing their driving affinities. Such negative differential response (NDR), a hallmark of nonequilibrium physics, is found in reaction schemes of major biological relevance, namely, substrate inhibition and autocatalysis. We display it by deriving the full counting statistics of two minimal representative models by large deviation methods. We explore the consequences of NDR for biochemical networks in terms of precision-dissipation tradeoff and stability against external perturbations. Furthermore, we go beyond the realm of biochemistry and examine the relevance of NDR in artificial applications, showing how it limits the performance of dissipative self-assembly.

Summary:

Session 4 / **49**

Non-Hermitean and Zeno limit of the quantum first detection problem

Author(s): Felix Thiel[1]

Co-author(s): Eli Barkai [1] ; David A. Kessler [1]

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The classical first-passage theory for random walks is generalized to quantum systems by using repeated attempts with a fixed frequency $1/\tau$ to find the system in the detection state $|\psi_{\mathrm{d}}\rangle$. The first successful of these attempts defines the time $T = N\tau$ of first *detected* arrival. Here, the Zeno limit $\tau \to 0$ of diverging detection frequency is investigated. The repeated detection setup is compared

with a non-Hermitean Schrödinger equation. Using an electrostatic analogy we can determine all absorbtion modes in the Zeno limit and find the pdf as well as all moments of T for systems with a discrete energy spectrum. The pdf has a scaling form in τ. Applying known results from the repeated detection setup to the non-Hermitean equation shows that the mean dissipation time in the latter system is quantized.

Summary:

Session 8 / **58**

Non-diffusive Fluxes in Brownian System with Lorentz Force

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The Fokker-Planck equation provides complete statistical description of a particle undergoing random motion in a solvent. In the presence of Lorentz force due to an external magnetic field, the Fokker-Planck equation picks up a tensorial coefficient, which reflects the anisotropy of the particle motion. This tensor, however, can not be interpreted as a diffusion tensor; there are antisymmetric off-diagonal terms which give rise to fluxes perpendicular to the density gradients. Here, we show that for an inhomogeneous magnetic field these non-diffusive fluxes have finite divergence and therefore affect the density evolution of the system. Only in the special cases of the uniform magnetic field or carefully chosen initial condition with the same symmetry as the magnetic field, can these fluxes be ignored in the density. These non-diffusive fluxes are reminiscent of the Corbino effect in solid-state systems.

Summary:

Session 8 / **33**

Non-equilibrium thermodynamics and coarse-grained models of polymers.

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Polymers are a group of molecules that presents various physicochemical properties. Some of these properties result from specific chemical groups in the polymer. Another properties are universal, they result from the fact of the chain structure of the molecule. To describe these universal properties of polymers, there are coarse-grained models, which represents this molecule as a chain. Such representation allows study these universal dynamic properties of polymer in a large scale.

Dynamics of polymer chain is due to thermal energy, which is a reason a transitions between polymer's conformational states. Polymers often operate under non-equilibrium conditions (for example

in a living systems), therefore dynamics of transitions has to fulfil laws of nonequilibrium thermodynamics. Using this theory kinetic equation of polymer chain in conformational space can be obtained. According some assumptions fractional equation can appear.

In the framework of non-equilibrium thermodynamics, polymers can be seen as a free enthalpy and free energy transducers, where the entropy production takes place. In this approach I will present a generalization of entropy production to the entropy production in a subdiffusive environment.

Summary:

Session 3 / **9**

Of Brains and Markets

Jonathan Khedair[1] ; Reimer Kuehn[2]

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In this talk, we explore an approach to understanding price fluctuations within a market via considerations of functional dependencies between asset prices. Interestingly, this approach suggests a class of models of a type used earlier to describe the dynamics of real and artificial neural networks. Statistical physics approaches turn out to be suitable for an analysis of their collective properties. We first motivate the basic phenomenology and modeling arguments before moving on to discussing some major issues with inference and empirical verification. In particular, we focus on the natural creation of market states through the inclusion of interactions and how these then interfere with inference. This is primarily addressed in a synthetic setting. Finally we investigate real data to test the ability of our approach to capture some key features of the behavior of financial markets.

Summary:

Session 8 / **29**

Option pricing under the Generalized Geometric Brownian Motion

Viktor Stojkoski[1] ; Trifce Sandev[1] ; Kocarev Ljupco[1] ; Lasko Basnarkov[1]

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Classical option pricing schemes assume that the value of a financial asset follows a geometric Brownian motion (GBM). However, a growing body of studies suggest that a simple GBM trajectory is not an adequate representation for the dynamics of an asset due to the fat-tailed properties found in empirical distributions of the asset returns. To capture this phenomenon three approaches have been proposed: i) stochastic volatility, where the amplitude of the noise itself is a stochastic process; ii) utilizing fat-tailed distributions for the noise; and iii) generalizations of GBM based on subdiffusion. Here, we turn our attention to the last approach and develop a generalization of GBM where the introduction of a memory kernel critically determines the behavior of the stochastic process. We utilize the resulting generalized GBM to examine the empirical performance of a selected group of memory kernels in pricing European call options. Our results indicate that the performance of kernel ultimately depends on the maturity of the option and its moneyness. This yields novel inights to both finance theory and stochastic processes in general.

Summary:

Session 7 / **52**

Problems in creating adequate stochastic model of memristors

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Currently, the investigations of resistive switching have attracted much attention. Electronic devices, the functioning of which is based on the resistive switching, are called memristors. The memristor as a new fundamental element of the electrical circuit that dissipates energy and has memory was theoretically predicted by Chua in 1971, but found its hardware implementation only in 2008. It represents a thin (from several nanometers to several tens nanometers in thickness) dielectric film sandwiched between two conductive electrodes. The switching of a memristor from the low resistance state (LRS) to the high resistance state (HRS) is achieved by the rapture of the filament by a voltage pulse (so-called RESET process). The filament can be restored by a voltage pulse of the opposite polarity that results in the switching from the HRS back to LRS (so-called SET process). As a result, its current-voltage characteristic is nonlinear and takes the form of hysteresis. At present, memristors have found application in diverse areas of science and technology ranging from information processing to biologically inspired systems. In particular, they are considered to be promising for application in the next generation non-volatile computer memory (Resistive Random Access Memory, ReRAM), in the neuromorphic computer systems, etc.
All previous theoretical and experimental studies have neglected the important effect of noise on the memory properties of these elements. As a result, an adequate stochastic model of memristor, taking into account many different factors as well as internal and external noises, is still far from being constructed. Difficulties in creating an adequate model associated with complex physico-chemical reactions occurring inside the film under the action of an applied electric field, the structure of the conducting filament, setting the right conditions at the boundaries with contacts, various memristor materials, etc. It has already become clear that to create a real model of the device, the ideal memristor models proposed by Chua are not enough and it is necessary to consider the system as multistable in terms of statistical physics approach.
In this report after a brief overview of previous achievements in this area the new results both theoretical and experimental studies of memristors performed in the "Laboratory of stochastic multistable systems" of National Research Lobachevsky State University of Nizhni Novgorod would be presented. Among them, experimental investigations of the resistive switching in a memristor based on a thin film ZrO2(Y)/Ta2O5 stack under a random noise voltage in the form of white Gaussian noise signal with certain parameters, measurements of the activation energies of oxygen ion diffusion in yttria stabilized zirconia by flicker-noise spectroscopy, probabilistic analysis of the voltage-controlled and the current-controlled ideal memristor under the action of the external voltage in the form of Gaussian noise, non-stationary distributions and relaxation times in a stochastic model of memristor.

Summary:

Session 8 / **20**

Quantum boomerang effect in disordered interacting systems

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Anderson localization (AL), the absence of diffusion, is one of the most famous phenomena occurring in disordered systems. Since the original Anderson's paper [1], AL was thoroughly investigated theoretically and observed in numerous experimental setups including light, classical waves and quantum systems. Presence of localization leads to many surprising phenomena. One of them is the *quantum boomerang effect* [2]. Due to AL, a wave packet moving with an initial velocity undergoes a retroreflection and returns to its initial position. On the other side, an inclusion of interactions to disordered systems, and more importantly, understanding of their impact on interference phenomena, was always undergoing intense studies. Through many years it was established that interactions may destroy the localization but also a new phenomenon emerged, dubbed *many-body localization* [3]. In our study we focus on the influence of interactions on the boomerang effect, in both the mean field theory approach and many-body simulations. As in other studies, which included nonlinearities to disordered systems, we observe a partial destruction of AL. Due to this, the boomerang effect is lessened, as the interactions act as an effective decoherence mechanism. Additionally, we compare results from the mean field theory with simulations of many-body systems.

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Summary:

Session 8 / **26**

Random sequential adsorption kinetics for several two-dimensional shapes placed on a one-dimensional line

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Random sequential adsorption (RSA) is a protocol to generate random packing in the following way:

- a virtual particle position and orientation in case of anisotropic shapes is selected randomly inside the packing;
- if the virtual particle does not intersect with any object on the plane, it is added to the packing. Otherwise, it is removed from the system and abandoned.

One of is's key feature is the observed algebraic time dependence of the asymptotic jamming coverage:
$\theta_{max} - \theta(t)\ t^{-d}$ when $t \to \infty$. Recent, theoretical study of A. Baule suggests that the scaling exponent observed for objects placed on a one-dimensional line depends on their shape, contrary to the original conjecture and, remarkably, falls into two universality classes.
Here we check this experimentally using new algorithms that allow generating strictly saturated RSA packings for ellipses, spherocylinders and rectangles. Additionally, we also study other properties of obtained packing.

Summary:

Session 8 / **37**

Role of thermal fluctuations in gene expression

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The role of thermal fluctuations is crucial in certain important biological processes, such as, transcription, translation, replication mechanisms, as they take place in very small scale systems.
We propose paradigmatic models for the transcription, i.e., DNA to m-RNA formation and DNA replication to see the effect of the environment on these important biological processes. We consider these processes as the copying of biological memory, where information is transferred from the parent DNA to its predecessor. We suggest that the sequence of bases in the strand of the parent DNA which is being copied to serve as the input signal for the process. The output is the base that binds to the parent DNA strand. Now, there are four possible outcomes as there are four conjugate bases present in the system. We consider these outputs to correspond to the minima of a four-stable potential. Thermal fluctuations have an important role when we consider systems of this scale. So, we propose that the output is described by the dynamics of a Brownian particle moving in a potential well having four stable minima. We consider both one-dimensional stochastic model and a four-state model and suggest that one of the minima gets lowered compared to the others when the system reads a particular signal. This minimum signifies the appropriate conjugate base of the corresponding base in the parent DNA strand. We allow the system to evolve for a finite-time and then examine whether the correct minimum corresponding to the given signal is occupied or not at the end of the process. When the output ends up in the correct minimum, we consider that as a successful process. Interestingly, we have found that this success rate shows a maximum at an intermediate value of temperature, i.e., the biological memory gets copied most efficiently at an optimum temperature. This result is encouraging as it is reported that for certain species, mutation rate which is just opposite to the success rate exhibits minimum at an intermediate temperature. We also intend to investigate the limit of the amount of information transferred from the parent strand to the nascent m-RNA or DNA strand.

Summary:

Session 8 / **25**

Searching for the shape that maximises saturated random sequential adsorption packings

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The problem of packing objects into limited space has an ancient history and is still of great importance from both utilitarian and fundamental point of view. Three-dimensional random packings are especially important due to their potential application in a granular matter and life sciences, while two-dimensional packings can, for example, model adsorption monolayers. These packings are generated using random sequential adsorption (RSA) protocol, which bases on consecutive iterations of the following steps:

- a virtual particle position and orientation in case of anisotropic shapes is selected randomly inside the packing;

- if the virtual particle does not intersect with any object on the plane, it is added to the packing. Otherwise, it is removed from the system and abandoned.

Formally, the process ends when there is no large enough space to place another shape, and such packing is called saturated. However, in general, it is hard to determine if given packing is already saturated. Here, we present recent algorithms that allow to generate saturated RSA packing and use them to find the shape, for which obtained packing is the densest.

Summary:

Session 2 / **6**

Single particle diffusion in periodic potentials

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We calculate the time-dependent probability distribution function (PDF) of an overdamped Brownian particle moving in a one-dimensional periodic potential energy $U(x)$. The PDF is found by solving the corresponding Smoluchowski diffusion equation. We derive the solution for any periodic even function $U(x)$ and demonstrate that it is asymptotically (at large times t) correct up to terms decaying faster than $1/t^{3/2}$. As part of the derivation, we also recover the Lifson-Jackson formula for the effective diffusion coefficient of the dynamics. The derived solution exhibits agreement with Langevin dynamics simulations. The approach is generalized for inhomogeneous systems where, in additional to the periodic potential, the particle also experiences a periodic diffusion coefficient. The application of a one-dimensional (Fick-Jacobs) diffusion equation for describing Brownian dynamics in periodic corrugated channels is also discussed.

Summary:

Session 8 / **40**

Social influence with recurrent mobility and multiple options

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In this presentation, we discuss the possible generalizations of the social influence with recurrent mobility (SIRM) model [Phys. Rev. Lett. 112, 158701 (2014)]. Although the SIRM model worked approximately satisfying when U.S. election was modeled, it has its limits: it has been developed only for two-party systems and can lead to unphysical behavior when one of the parties has extreme vote share close to 0 or 1. We propose here generalizations to the SIRM model by its extension for multiparty systems that are mathematically well-posed in case of extreme vote shares, too, by handling the noise term in a different way. In addition, we show that our method opens alternative applications for the study of elections by using an alternative calibration procedure and makes it possible to analyze the influence of the "free will" (creating a new party) and other local effects for different commuting network topologies.

Summary:

In this presentation, we discuss the possible generalizations of the social influence with recurrent mobility (SIRM) model [Phys. Rev. Lett. 112, 158701 (2014)]. Although the SIRM model worked approximately satisfying when U.S. election was modeled, it has its limits: it has been developed only for two-party systems and can lead to unphysical behavior when one of the parties has extreme vote share close to 0 or 1. We propose here generalizations to the SIRM model by its extension for multiparty systems that are mathematically well-posed in case of extreme vote shares, too, by handling the noise term in a different way. In addition, we show that our method opens alternative applications for the study of elections by using an alternative calibration procedure and makes it possible to analyze the influence of the "free will" (creating a new party) and other local effects for different commuting network topologies.

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Spectral analysis of electromyographic signals

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This work presents the spectral analysis of electromyography. Electromyographic studies are used to aid in the management and diagnostic of myopathy and neuropathy disease. Using signal analysis techniques to determine the distribution of power into frequency components we indicate that there are significant differences between patients proven healthy, and patients with the myopathy or neuropathy disease. These disparities are particularly noticeable for frequencies below and above 10 Hz, the frequency of the human body vibration.

Summary:

Session 1 / **44**

Stochastic Resetting

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Evolving stochastic process, when interrupted at random epochs and reset to its initial condition, reaches a new nonequilibrium stationary state. The approach to the stationary state is accompanied by an unusual 'dynamical phase transition'. Moreever, the mean first-passage time to a fixed target becomes a minimum at an optimal value of the resetting rate. This makes the diffusive search process rather efficient. Resetting dynamics has been studied intensively in the last few years and is a rapidly emerging field in stochastic processes and nonequilibrium systems. In this talk, I'll give an overview of this evolving field.

Summary:

Session 8 / **23**

Surviving on the edge of instability

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Properties of stochastic dynamics in highly unstable potentials are strongly influenced by divergent trajectories, which quickly leave meta-stable regions and never return there. Using formalism from the theory of Q-processes and quasi-stationary distributions, we discuss distributions of non-diverging trajectories in highly unstable potentials. We focus on two stationary distributions which can be considered as (formal) generalizations of the Gibbs canonical distribution to the case of highly unstable dynamics. Even though the associated effective potentials differ only slightly, properties of the two distributions are fundamentally different for all highly unstable potentials. The distribution of trajectories conditioned to be never divergent is localized and light-tailed. The distribution describing trajectories surviving in the meta-stable region at the instant of conditioning is heavy-tailed. The exponent of the corresponding power-law tail is determined by the leading divergent term of the unstable potential. We also derive properties of the effective force arising in the ensemble of non-diverging trajectories. The presented results are applicable to a broad class of non-linear dynamical models with meta-stable states and fast kinetic transitions.

Summary:

Session 5 / **36**

The Volterra type equation related to the non-Debye relaxation

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I will present the solutions of Volterra equations with the fading memory given by the Prabhakar function with negative upper parameter which is relevant to the standard non-Debye models of dielectric relaxation, namely for the Cole-Cole, Cole-Davidson, and Havriliak-Negami models. These integro-differential equations are solved by using the umbral calculus and Laplace transform method whose results are identically for the same fixed values of the used parameters.

Summary:

Session 8 / **30**

The impact of shape's polyhedral symmetry breaking on packing density

Piotr Kubala[1] ; Michal Ciesla[2]

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When studying packings of objects one observes the depencence of packing density on various factors, the symmetry of particles included. For example, the packings of ellipsoids can be denser than the packings of spheres, which represents the general trend in a transition between two continuous symmetries. Here, our main goal was to check, whether a similar effect can be observed for shapes of polyhedral point symmetries. The packing model chosen was random sequential adsorption of

two-parameter family of polyhedra created by cutting the vertices of a cube, which exposes the transition from tetrahedral to octahedral symmetry. The RSA protocol consists in sequential steps, where:

- position and orientation of a new particle are selected randomly,
- if the paricle does not intersect with any of previously placed objects it is added to the packing; otherwise, it is removed and abandoned.

Moreover, as RSA preserves the non-overlaping criterion, the model allowed us to evaluate how the results correlate with excluded volume effects.

Summary:

Session 3 / **15**

Thermodynamic Efficiency in Dissipative Chemistry

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Chemical processes in closed systems inevitably relax to equilibrium. Living systems avoid this fate and give rise to a much richer diversity of phenomena by operating under nonequilibrium conditions. Recent experiments in dissipative self-assembly also demonstrated that by opening reaction vessels and steering certain concentrations, an ocean of opportunities for artificial synthesis and energy storage emerges. To navigate it, thermodynamic notions of energy, work and dissipation must be established for these open chemical systems. Here, we do so by building upon recent theoretical advances in nonequilibrium statistical physics. As a central outcome, we show how to quantify the efficiency of such chemical operations and lay the foundation for performance analysis of any dissipative chemical process.

Summary:

Session 8 / **24**

Thermodynamic bootstrap program for dynamic correlation functions

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I will address the problem of computing dynamic correlation functions in Integrable QFT's at finite temperature and out of equilibrium. The approach is based on the form-factor expansion of the correlation functions. Thanks to the integrability, the form-factors at finite temperature can be effectively bootstrapped, through a procedure generalizing the Smirnov's bootstrap program for vacuum form factors. The method allows to determine the dynamic correlation functions of strongly interacting systems. The talk is based on the work with A. C. Cubero (JHEP 104 (2019)) and forthcoming publications.

Summary:

Session 8 / **45**

Time-of-flight characteristics of dispersive transport in aligned quantum wires with fractal disorder

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Dispersive transport of photo-injected carriers in arrays of vertically aligned fractal nanowires is considered. The conditions of the time-of-flight experiment are assumed. Photocurrent response after injection of non-equilibrium carriers by the short light pulse is studied. Carriers are injected instantaneously from the left side of the array, then, move along wires under the action of a strong longitudinal electric field. Within the generalized Scher-Montroll model taking the power-law distribution of distances between traps into account, we calculate charge carrier densities and transient current for different cases. The simplest case implies one-sided instantaneous jumps (tunneling) between neighboring localized states. In addition, we consider the role of backscattering, spatial correlations induced by quenching of disorder and spatiotemporal non-locality produced by fractal trap distribution and the finite velocity of motion between localized states. Analyzing power law exponents of transient current decay and dependence of time-of-flight on sample width, we establish criteria which allow determining the fractal dimension of trap distribution along a wire and parameters of waiting time distribution from the characteristics observed in the time-of-flight experiment.

Summary:

Session 8 / **62**

Towards a conformational entropy and viscoelastic properties: molecular dynamic study on mucin example

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We are investigating a conformational entropy of mucin protein to discern its correlation with the viscoelastic properties of the biopolymer system in various thermodynamic conditions. The mucin is believed to be responsible for gel formation inside synovial fluid of joints system which is very sensitive on both temperature and concentration changes[1]. The conformational entropy is computed based on the information about dihedral (Phi-Psi) angles of the mucin during protein self-organization process which in appropriate conditions are prone to network (gel) formation[2]. In turn, the viscoelastic properties are calculated based on information about inter- and intramolecular energies and mean squared displacement of the geometrical centers of the molecules [3]. In our study, we are using molecular dynamic simulation technique with a time duration of up to 50 ns, parameterized by six temperatures ranged between 300-315 K, and six concentrations 10.68-267.1 g/L (thus in the physiological range of the parameters).
We found that the conformational entropy oscillates in time but have a tendency to slightly decrease in a similar way in different concentrations in temperature 310K. There are no significant changes in conformational entropy behavior despite that the system exhibit a transition between c3 and c4

(160 g/L and 214 g/L) where crowding begins affecting the dynamics of the system and network between proteins starts to form changing its dynamic from diffusive to sub-diffusive. For single mucin molecule, the conformational energy trend changes from decreasing in lower temperature (up to 306K) to increasing in higher temperature (above 306K) introducing little more chaotical structures.
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Summary:

Session 8 / **39**

Twist-bend nematic phase in the presence of molecular chirality

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Twist-bend nematic (N_{TB}) [1, 2] is a fifth member of the nematic family, beyond uniaxial (N_{U}) and biaxial (N_{B}) nematics, cholesteric (N^*) and blue phases (BP). Its uniqueness arises from a double degenerate ground-state (ambidextrous chirality) with a periodically modulated heliconical structure possessing a nanoscale pitch, which is formed from achiral bent-shaped molecules [3]. It is a profound example of so-called spontaneous (chiral) symmetry breaking in achiral materials. Despite the short time since the discovery, N_{TB} has already found applications [4].

In this work [5], we present investigations based on Landau-de Gennes theory of chiral nematics, supplemented by terms representing molecular steric polarization [6]. With the helicity mode expansion for the alignment tensor $\mathbf{Q}(\mathbf{r})$ and the polarization $\mathbf{P}(\mathbf{r})$ fields we study relative stability and properties of (N^*) and (N_{TB}) for bent-core materials with chiral centers or dopants.

Acknowledgments
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Summary: