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Book of Abstracts

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Poster session / 55**Mica Surface Properties Investigated by Force Spectroscopy****Author(s):** Agnieszka Kurek¹**Co-author(s):** Beata Cieniawska¹ ; Jakub Barbasz² ; Kamila Sofinska³¹ *Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences*² *Instytut Katalizy i Fizychemii Powierzchni im. Jerzego Habera PAN*³ *Jerzy Haber Institute of Catalysis and Surface Chemistry Polish Academy of Sciences***Corresponding Author(s):** nckurek@cyf-kr.edu.pl

Mica (muscovite) is a substrate commonly used for TEM and AFM imaging because of its atomic flatness, high cleavage and transparency. This aluminosilicate has sheet structure. Crystallographic structure of mica consists of two layers of Si and Al tetrahedrals and one Al octahedral sublayer between them.^{1,2} Force spectroscopy technique was used to determine physicochemical properties such as adhesion between the AFM probe and the surface, Young's Moduli, deformation depth and the surface stiffness.

In this work adhesion forces were measured in different conditions (air or NaCl solution with ionic strengths range of 0.001 – 0.15 M). The velocities of AFM tip withdrawal were in the range of 0.02 – 5 $\mu\text{m s}^{-1}$. The main goal of these experiments was finding correlation between physicochemical properties and environmental conditions.

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Poster session / 59**Long distance interaction extended model of RSA****Jakub Barbasz¹ ; Kamila Sofinska¹ ; Michal Ciesla² ; Tomasz Witko²**¹ *Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences*² *M. Smoluchowski Institute of Physics, Jagiellonian University, Kraków, Poland***Corresponding Author(s):** michal.ciesla@uj.edu.pl

The phenomenon of interfacial adsorption and adhesion can be encountered at every stage of everyday life, from processes at atomic or cellular level to complex industrial processes taking place on a large scale.

Most commonly used models to describe colloidal particles adsorption are classical RSA and ballistic-deposition model. In this study we presented alternative model to describe adsorption process of "haired" colloidal particles. By combining computational models with advanced optical microscopy methods it is possible to investigate the adsorption process in a wide range of times and directly compare experimental data with mathematical model.

Poster session / 60

Computer augmented microscopy in medicine - cervical cytology

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Computer aided analysis of microscopic images is a rapidly growing field of imaging research. The results of the preliminary assessment of cervical cytology samples made by artificial intelligence systems will be presented. For this purpose, a u-net network of various complexity of architecture has been tested. The obtained results indicate the effectiveness of the solution based on neural networks in the preliminary selection of microscopic images of cervical cytology. The use of the proposed solutions, increases the effectiveness of detecting irregularities without increasing the cost of testing and without additional procedural processes carried out with patients.

Acknowledgements: I acknowledge the support of POIR.01.02.00-00-0038/15-00

Tue noon / 49

Exact results on the kinetics of random sequential adsorption processes

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Random sequential adsorption (RSA) of particles is used in a large variety of contexts to model particle aggregation and jamming. In RSA, a particle's position is selected with uniform probability over the domain and it is then placed sequentially if there is no overlap with any previously placed particles. Particles are not able to move or reorient once being placed. A key feature of these models is the observed algebraic time dependence of the asymptotic jamming coverage. However, the exact value of the scaling exponent is not known apart from the simplest case of the RSA of monodisperse spheres adsorbed on a line (Renyi's seminal 'car parking problem' [1]).

In this talk, I show that exact results on the scaling exponent can be derived for three variants of RSA processes on the line: (i) particles interacting by a finite-range potential; (ii) polydisperse hard spheres; (iii) non-spherical hard particles. These results resolve in particular a long-standing conjecture that the exponent depends solely on the degrees of freedom of a particle [2]. Instead, it is shown that the exponent depends sensitively on both particle shape and the size distribution underlying the polydispersity. Remarkably, for non-spherical particles, the exponent falls into at least two universality classes depending on whether the contact distance has singular features (e.g., for spherocylinder and polyhedra) or not (smooth convex shapes like ellipsoids) [3].

For problems (i,ii) the exact time dependent solution for the interval distribution of the RSA can be found, which reveals that a unique potential/size distribution exists that leads to a maximally dense coverage of the line, which is approached infinitesimally slowly in time [4].

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[3] A. Baule, Physical Review Letters 119, 028003 (2017)

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Poster session / 56

Energy of Quantum Brownian Oscillator

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Models which contain quantum particle coupled to its environment were analysed many times over recent years or even decades. This old and seemingly clichéd system-environment model has been re-considered many, many times by each next generation of physicists. However, it is still difficult to find a transparent presentation of this fundamental issue of the quantum statistical physics. Furthermore by analysing behaviour of quantum Brownian motion one could attempt to find answer for many fundamental questions concerning the very essence of the quantum world, investigate transport phenomena or consider the nature and properties of quantum information. The topic of quantum Brownian motion is fundamental for many fields of physics, for instance in statistical physics, condensed matter and atomic physics. We study the celebrated model of a quantum open system S , i.e. a quantum harmonic oscillator of mass M and eigenfrequency ω_0 . It is in contact with a heat bath B modeled as a collection of independent quantum harmonic oscillators which form thermostat of temperature T being in an equilibrium Gibbs canonical state.

There are plenty of methods for analysing such systems for instance path integrals method, van Kampen method or generalised Langevin equation method. In our considerations we utilise the last listed method and as a starting point in our analysis we took quantum fluctuation-dissipation theorem. We would like to present some of interesting properties exhibited by such systems and exact, analytical results for energy - potential and kinetic - which we have obtained.

Poster session / 43

Errors in Energy Landscapes Measured with Particle Tracking

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Tracking Brownian particles is often employed to map the energy landscape they explore. Such measurements have been exploited to study many biological processes and interactions in soft materials. Yet video tracking is irremediably contaminated by localization errors originating from two imaging artifacts: the “static” errors come from signal noise, and the “dynamic” errors arise from the motion blur due to finite frame-acquisition time. We show that these errors result in systematic and nontrivial biases in the measured energy landscapes. We derive a relationship between the true and the measured potential that elucidates, among other aberrations, the presence of false double-well minima in the apparent potentials reported in recent studies. We further assess several canonical trapping and pair-interaction potentials by using our analytically derived results and Brownian dynamics simulations. In particular, we show that the apparent spring stiffness of harmonic potentials (such as optical traps) is increased by dynamic errors but decreased by static errors. Our formula allows for the development of efficient corrections schemes, and we also present in this work a provisional method for reconstructing true potentials from the measured ones.

Thu noon / 42

Fingering instabilities in tissue invasion: an active fluid model

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We study theoretically a possible physical mechanism for formation of multicellular protrusions in carcinoma at the onset of metastasis. We suggest it might be a consequence of a very simple physical instability resulting from coupling between cell velocity and direction of active traction. It is reminiscent of the classical viscous fingering instability. We use it to show that, for a carcinoma growing in an external environment of comparable viscosity, even weak active traction can lead to the onset of multicellular protrusions, initiating metastasis. We also discuss how further evolution of the fingers would proceed within this model. Due to the simplicity of the mechanism proposed, we think it might be applicable for a wide range of circumstances and might rationalize fingering observed in vivo.

Poster session / 45

Weak initial conditions of RC4 pseudorandom number generator

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Phase space of cryptographic systems, such as RC4 stream cipher is an interesting object, to which statistical physics may be applied. Entropy of a trajectory and of a state space, transient phase, coexisting attractors, 1/f noise and complexity measures are just a few examples of physical ideas, that may be applied to cryptographic systems, which opens the possibility of many new research subjects. The basis for this interdisciplinary research is the fact, that pseudorandom number generators, which form a core of many cryptographic systems, are just strongly mixing deterministic

nonlinear systems in a chaotic state. And the main difference lays in the fact, that basic operations in cryptography, such as XOR operator are in space of integer numbers (as in Bernoulli shift).

In this contribution we expose a weakness of RC4 cipher: that apparently strong cryptographic keys of high entropy can lead to weak initial condition for the pseudorandom number generator. These weak initial conditions lead to poor mixing in the long transient part of a pseudorandom trajectory. This allows to mount a successful attack on this cipher, e.g. using known plaintext attack. We show this by numerical analysis of the space of initial conditions of a simplified version of RC4. We show, that central limit theorem may be applied to this system, and due to this fact many families of weak cryptographic keys may be determined. Basing on these results it is possible to calculate the average weakness of space of all cryptographic keys, which shows an inherent security flaw, built in the structure of priming phase of the RC4 cipher. Current findings confirm that application of nonlinear techniques in cryptology may provide interesting results.

Tue morning / 14

Active Lévy matter: Hydrodynamic description and linear stability analysis

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Collective ordered motion can emerge spontaneously in many biological systems, such as bird flocks, insect swarms and tissue under dynamic re-organization. This phenomenon is typically modelled under the active fluid formalism. However, anomalous diffusion, characterizing particles whose position mean-square displacement scales non-linearly in time, is also widespread in biology. For instance, Lévy walks exhibiting super-diffusion can represent an optimal foraging strategy under specific environmental conditions. Surprisingly, the emergence of collective motion in systems displaying such anomalous diffusive behaviour has not yet been discussed. Here, we will investigate a system of active particles performing Lévy flights and endowed with alignment interactions. We will derive the model equation in the hydrodynamic limit and investigate the stability of its ordered and disordered phases. This analysis aims at developing a framework integrating both anomalous diffusive motility and inter-particle interactions, thus paving the way for the definition of more realistic active matter models.

Poster session / 2

Weak Galilean invariance as a selection principle for stochastic coarse-grained diffusive models

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Galilean invariance states that the equations of motion of closed systems do not change under Galilei transformations to different inertial frames. However, real world systems typically violate it, as they are described by coarse-grained models, that integrate complex microscopic interactions indistinguishably as friction and stochastic forces.

This leaves no alternative principle to assess a priori the physical consistency of a given stochastic

model. In this talk, I use the Kac-Zwanzig Hamiltonian model of Brownian motion to clarify how Galilean invariance is broken during the coarse graining procedure to derive stochastic equations and derive a set of rules characterizing systems in different inertial frames, called “weak Galilean invariance”. Several stochastic processes, generating both normal and anomalous diffusion, are shown to be invariant in these terms, except the continuous-time random walk, whose correct invariant description is discussed.

These results are particularly relevant for the modelling of biological systems, as they provide a theoretical principle to select stochastic models of complex dynamics prior to their validation against experimental data.

Poster session / 57

Selected properties of integrated stochastic processes

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Brownian motion (Wiener process) and Ornstein-Uhlenbeck processes are two basic stochastic processes, which are frequently, among others, used in the statistical physics. We consider the full stochastic dynamics, i.e. a situation when a particle is described by the position and velocity. It is assumed that velocity changes according to Wiener or Ornstein-Uhlenbeck processes. Consequently, a particle position is described by an integrated stochastic process. We examine such processes in the free case. Moreover, the problem of first escape from a finite interval for integrated stochastic processes is studied. We show similarities and differences between both processes. These differences arise due to introduction of damping and are especially well visible for a free particle. In the studied range, the problem of first escape seems to be less sensitive to the process describing evolution of the velocity.

Mon afternoon / 5

Two distinguishable impurities in BEC: squeezing and entanglement of two Bose polarons

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We apply the quantum open system formalism to describe the physics of two impurities immersed in a Bose-Einstein condensate. Here, the impurities are considered to be two quantum Brownian particles interacting with a bath of oscillators corresponding to the Bogoliubov modes of the condensate. We characterize the dynamics of the Brownian impurities with Langevin-like quantum stochastic equations carrying an account of memory effects. The Langevin equations are solved to evaluate the covariance matrix. We find that the presence of the bath induces an interaction between the impurities, which leads to entanglement among them. Whether or not the impurities are trapped in an external potential gives rise to different behaviours of such entanglement: (i) In the absence of external potential, we observe sudden death of entanglement, i.e., entanglement disappears at long enough times; (ii) In the presence of external harmonic potential, entanglement survives even at

asymptotic time limit. Our study puts the behaviour of entanglement under scrutiny and captures its response to experimentally tunable parameters.

Besides entanglement, we study the squeezing as well. Interestingly, we find that the mean-square-displacement is super-diffusive, which as we prove, is due to non-Markovianity of the dynamics. Further, a full analysis of squeezing is provided, which explains how experimentally tunable parameters create or destroy squeezing. We emphasize that all of our analysis is rigorously obtained from a realistic physical model; in particular, we avoid manipulating it by introducing artificial Hamiltonians, or by introducing arbitrary spectral densities.

Poster session / 58

Random sequential adsorption of cuboids

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The subject of this study was random sequential adsorption of cuboids of axes length ratio of $a : 1 : b$ for $a \in [0.3, 1.0]$ and $b \in [1.0, 2.0]$ and its aim was to find a shape that provides the highest packing fraction. Obtained results show that the densest packing fraction is 0.402 ± 0.010 , and is reached for axes ratios near cuboids of $0.75 : 1 : 1.30$. Kinetics of packing growth were also studied and it was established that its power-law character is no longer governed by the number of cuboid degrees of freedom. The microstructural properties of obtained packings were studied in terms of density correlation function and propagation of orientational ordering.

Tue noon / 27

Saturated packings of convex anisotropic objects under random sequential adsorption protocol

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The problem of packing hard shapes into limited space has an ancient history and is still of great importance from both utilitarian and fundamental point of view. Random packings are especially important due to their potential application in granular matter and life sciences. There are a number of protocols that allow to generate random packings. One of them is random sequential adsorption. This method is based 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.

When there is no more place for another object, the packing is called saturated. Direct implementation of this algorithm is highly inefficient for almost saturated packings because a very large number

of tries is needed to add next shape. Moreover this method does not stop when packing is saturated already. Here, we present an algorithm to generate two-dimensional, saturated packings built of identical, unoriented, anisotropic convex shapes. The method consists in tracking regions where the next shape can be added. The algorithm was tested on packings built of spherocylinders and ellipses of different width-to-height ratio.

This study was supported by grant no. 2016/23/B/ST3/01145 of the National Science Centre, Poland.

Poster session / 24

Studies on the structure - diffusion relationship for hybrid polymer membranes

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Hybrid alginate membranes filled with various amount of magnetite (Alg/Fe_3O_4) and crosslinked using four different agents, i.e. calcium chloride ($AlgCa$), phosphoric acid ($AlgP$), glutaraldehyde ($AlgGA$) and citric acid ($AlgC$) were applied in pervaporative dehydration of ethanol and were described in paper [1].

In this work, the membranes are characterized by the parameters like: 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. Determination of the above mentioned characteristics base on the image analysis of a sufficiently large cross – sections of the membranes.

Diffusive transport is investigated by simulation of a particle motion in the membrane environment. Diffusion driven by Gaussian random walk and L'evy flights is shown in order to check if the effective diffusion exponent at long time limit is subdiffusive and if it depends on the details of the underlying random process causing diffusion.

Thanks to such research the relationship between chemical composition, structure and morphology, and separation properties of the membranes can be determined.

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Mon noon / 0

Composite Continuous Time Random Walks

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Random walks in composite continuous time have recently been introduced in [1].

Composite time flow is the product of translational time flow and fractional time flow [2]. The continuum limit of composite continuous time random walks gives a diffusion equation where the infinitesimal generator of time flow is the sum of a first order and a fractional time derivative. The latter is specified as a generalized Riemann-Liouville derivative. Generalized and binomial Mittag-Leffler functions are found as the exact results for waiting time density and mean square displacement.

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[2] Chem. Phys. 84, 399 (2002)

Thu noon / 41

Flux and storage of energy in non-equilibrium stationary states

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A system kept out of equilibrium in the stationary state by the external source of energy stores an energy in excess over its value at equilibrium. We determine this excess energy, U for two model systems: the ideal gas and the Lennard-Jones liquid. We show that in order to describe non-equilibrium states an external energy source must be explicitly included in the analysis. The final non-equilibrium, stationary state depends not only on the total flux of energy, J_U , but also on the mode of energy transfer into the system. In both systems we study three scenarios of energy transfer: (1) the energy flux per unit volume is constant; (2) the energy flux per unit volume is proportional to the local temperature (3) the energy flux per unit volume is proportional to the local density. Similarly as in equilibrium thermodynamics we introduce internal, adiabatic constraints in the system and find that $U/J_U = \tau$ is minimized in the stationary (unconstrained) state. τ is the characteristic time scale of energy outflow from the system immediately after shut-down of energy flux into the system. Finally we perform MD simulations of 2D Rayleigh-Benard system (RB) of hard discs to check this variational principle for two competing stationary states (conductive and convective). We find that the stable state has smaller value of U/J_U .

Poster session / 38

Formation of modulated structures in random sequential adsorption processes

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Bent-core particles, which are of great importance due to their applications in the liquid crystal industry, gain nowadays more and more interest due to the possibility of formation of novel modulated phases. We investigate the adsorption processes leading to the formation of such structures. We present the role of elastic deformations for the maximum packing in systems composed of particles randomly adsorbed on a surface. We also study the influence of the shape of the particles on the adsorption properties and analyze the packing fraction and its structure.

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Poster session / 37

Ising critical exponents of the frustrated spin-1/2 Heisenberg FM/AF square bilayer in a magnetic field

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The highly frustrated spin-1/2 Heisenberg FM/AF square bilayer in a magnetic field with the ferromagnetic inter-dimer interaction and the antiferromagnetic intra-dimer interaction is explored by the use of localized many-magnon approach, which allows to connect the original purely quantum Heisenberg spin model on a square bilayer with the effective ferromagnetic Ising model on a simple square lattice. Basic magnetic quantities (magnetization, susceptibility, specific heat) are investigated in the proximity of a field-driven phase transition from the singlet-dimer phase towards the fully saturated ferromagnetic phase, which changes from the discontinuous phase transition to the continuous one at a certain critical point. The mapping correspondence between the spin-1/2 Heisenberg FM/AF square bilayer and the ferromagnetic Ising square lattice suggests for this special critical point of the spin-1/2 Heisenberg FM/AF square bilayer critical exponents from the standard two-dimensional Ising universality class.

Poster session / 40

Scattering of the generalized Schrödinger cat state in a harmonic trap. The Wigner function approach.

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An isolated quantum system consisting of a single scattering barrier inside the potential well in the form of double harmonic oscillator is considered. The initial state is assumed to be the Schrödinger cat state [1] which is the superposition of two coherent states but generalized by additional parameter modelling a partial loss of interference which reflects the imperfection of the Schrödinger cat state preparation. The foregoing problem is considered within the phase space description of

quantum mechanics, specifically the Wigner function approach. Time evolution of the considered system is given by the Moyal equation [2]. The major aim of the project is to investigate the dynamical characteristics of such quantum system and how they are affected by the imperfection of initial state preparation.

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Mon evening / 13

When boundary conditions at a thin membrane create nonmarkovian normal diffusion

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In the paper [1] one of the boundary conditions at a thin membrane for normal diffusion has been obtained directly from experimental data. This condition contains the Riemann–Liouville fractional derivative of the 1/2 order and reads $P(0^-, t|x_0, 0) = \left(a + b \frac{\partial^{1/2}}{\partial t^{1/2}}\right) P(0^+, t|x_0, 0)$, the membrane is located at $x = 0$, the fundamental solution to normal diffusion equation $P(x, t|x_0, 0)$ is interpreted as a probability density of finding a diffusing particle at the point x at time t under condition that in the initial moment $t = 0$ the particle was in the initial position x_0 .

The fractional derivative causes that particle’s transition through the membrane can be interpreted as a ‘long memory’ process. The question arises: does the presence of the fractional derivative in a boundary condition cause that the diffusion process in the membrane system is nonmarkovian?

We show that the appearance of an obstacle such as a thin partially permeable membrane can change the nature of normal diffusion which would be considered as a nonmarkovian process.

If the process is markovian, the fundamental solution fulfills the Bachelier-Smoluchowski-Chapman-Kolmogorov (BSCK) equation $P(x, t|x_0, 0) = \int_{-\infty}^{\infty} dx' P(x, t|x', t') P(x', t'|x_0, 0)$.

We conduct the consideration in terms of the Laplace transform $\hat{f}(s) = \int_0^{\infty} e^{-st} f(t) dt$. Boundary conditions at an asymmetric membrane depend on in which part of the system the initial position of the particle is placed.

We assume the boundary conditions at the membrane in terms of the Laplace transform as follows

$$\hat{P}(0^+, s|x_0, 0) = \hat{\Phi}_1(s) \hat{P}(0^-, s|x_0, 0),$$

$$\hat{J}(0^+, s|x_0, 0) = \hat{\Xi}_1(s) \hat{J}(0^-, s|x_0, 0),$$

for $x_0 < 0$ and

$$\hat{P}(0^-, s|x_0, 0) \hat{\Phi}_2(s) \hat{P}(0^+, s|x_0, 0),$$

$$\hat{J}(0^-, s|x_0, 0) = \hat{\Xi}_2(s) \hat{J}(0^+, s|x_0, 0),$$

for $x_0 > 0$, where

$$\hat{J}(x, s|x_0, 0) = -D \partial \hat{P}(x, s|x_0, 0) / \partial x$$

is the Laplace transform of diffusive flux.

The above equations can be considered as general form of boundary conditions at a thin membrane [1].

We will derive the equations that must be fulfilled by the functions $\Xi_{1,2}(s)$ and $\Phi_{1,2}(s)$ so that the function $\hat{P}(x, s|x_0, 0)$ satisfies the BSCK equation.

The functions $\Xi_{1,2}(s)$ and $\Phi_{1,2}(s)$ are measurable experimentally by means of the method presented

in [1]. Thus, it can be checked experimentally if the boundary conditions violate Markov property for the normal diffusion process. The measure of nonmarkovianity is the normalized autocorrelation function [2]. We will also discuss the relation between boundary conditions at the membrane and the measure of nonmarkovianity.

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Mon evening / 23

Stereological-fractal analysis as a tool for a precise description of the morphology of hybrid alginate membranes

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A precise description of the morphology of a material is necessary in order to establish structural and functional relationships [1]. Tools (methods) for morphological analysis should be quantitative techniques, which would yield objective and reproducible values for any morphological structure and enable statistically defined comparisons. The combination of the stereological analysis and fractal analysis provides the researchers with such a tool. This work investigated hybrid alginate membranes filled with various amount of magnetite (Fe_3O_4) and crosslinked using four different agents, i.e. calcium chloride (*AlgCa*), phosphoric acid (*AlgP*), glutaraldehyde (*AlgGA*) and citric acid (*AlgC*). Alginate membranes can be used to dehydrate ethanol in the process of pervaporation [2–3]. The morphology of the studied membranes was characterized on the basis of the image analysis of the membrane's cross-section obtained from a scanning electron microscope Phenom Pro-X. The quantitative analysis of the structure and morphology of the above-named materials included the stereological analysis and the fractal analysis. The stereological analysis was based on shape descriptors (elongation factor f_1 , surface factor f_2 , irregularity parameter f_3) and bulkiness f [2, 4]. Generalized fractal dimension [5] and lacunarity [6] constitute the basis of fractal analysis. In relation to the membranes subjected to the tests, it was possible to identify the correlation between transport properties (pervaporation separation index (*PSI*)) and morphological parameters. The use of a comprehensive analysis made it possible to determine the morphology of the membrane with the best separation properties. The membranes of the highest self-similarity were also characterized by the highest separation properties.

Acknowledgments

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Tue evening / 30

Spin-glass-like transition in the Ising models with locally competing temperatures.

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The possibility of the occurrence of the spin-glass-like and ferromagnetic transitions in nonequilibrium systems based on the Ising model with spin-flip rates combining two Glauber rates at different temperatures is discussed. The models comprise the Sherrington-Kirkpatrick model and the Ising model on random graphs with edges corresponding, with certain probability, to positive and negative exchange integrals. Only in rare cases such nonequilibrium systems with non-zero heat flux can be mapped onto equilibrium ones at certain effective temperature. Nevertheless, Monte Carlo simulations show that transitions to the ferromagnetic and spin-glass-like phases occur in all cases under study as the probability of contact with each thermal bath is varied, and the phase diagrams resemble qualitatively those for the corresponding equilibrium models obtained with varying temperature. Theoretical calculations based on the mean-field approximation and the TAP equations predict correctly the location of the phase border between the paramagnetic and ferromagnetic phases, while in the case of the border between the paramagnetic and spin-glass-like phases only qualitative agreement between theoretical and numerical results is achieved. The obtained results can be interesting for modelling the opinion formation by means of the well-known majority-vote and related models.

Tue noon / 47

Random Sequential Adsorption of Platonic and Archimedean Solids

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Packings of objects attracted people's interest for many centuries. For example, during colonial era packings of spheres were studied to find the most optimal way to transport cannonballs. Today, densest packings are utilized in a variety of areas starting from condensed matter physics where they can model crystalline structures, and ending with telecommunication where they indicate how to optimize transfer rates. Besides densest random packing, a lot of attention is focused on random packings as they can model granular matter and biological objects. One of the easiest protocols used to obtain such packings, is random sequential adsorption (RSA): particles of random position and orientation are added to the packing one after the other if they do not overlap with any of previously placed objects. This study focuses on RSA packings build of identical Platonic and Archimedean solids. Besides finding a mean packing fraction, they are analyzed in terms of kinetics of packing growth as well as propagation of translational and orientational order. Moreover, an effective intersection test for those objects is provided.

Poster session / 12

How to recognize if any absorption occurs in a subdiffusive medium

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Various kinds of diffusion in membrane systems commonly occur in biology (see, for example, \cite{h} and references cited in \cite{k1}). The example of diffusion in a composite system is diffusion of drugs through biofilms in which subdiffusion can be present \cite{awdk}. We consider subdiffusion in a system which consists of two different media separated by a thin membrane. In one of the media particles' absorption can occur. Such systems can be studied experimentally but, due to technical reasons, it is not always possible to measure concentration profiles in the medium in which absorption can be present. For example, when we study the process experimentally by means of the laser interferometric method \cite{awdk} and one of the media in which absorption can occur is opaque. We show the method which allows one to recognize whether absorption is present in such a medium knowing concentration profiles of diffusing substance in the other medium \cite{klk}. This method is based on a simple random walk with absorption model in a membrane system. Within this model we firstly consider particles' transport in a system with both discrete time and space variable. Next, we move to continuous variables. Similar models have been used in modelling diffusion in a membrane system \cite{k1,k2,k3}, to derivation of parabolic \cite{kl} and hiperbolic \cite{k4} subdiffusion–reaction equation, in modelling subdiffusion–absorption process in a membrane system \cite{kl1} and in the description of subdiffusion–absorption process in a composite medium \cite{k5}. Furthermore, the presented method also allows one to determine subdiffusion parameter in the medium which cannot be studied experimentally, for the system without absorption.

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Thu / 53

Active noisy oscillators - analytical approaches, stochastic phase description, and coupling effects

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Many systems in physics and biology display somewhat irregular (noisy) but clearly oscillatory behavior. Most of these systems are kept outside of thermodynamic equilibrium (they are active) and can be well described in a stochastic framework.

In the talk I review a number of new developments from the theoretical side: how we can test whether the oscillator's dynamics is Markovian (using a non-equilibrium fluctuation-dissipation theorem), how we can define a phase for a stochastic oscillator (there are two proposals of a phase definition), how we can calculate correlation statistics like the power spectrum for a specific oscillator, and what can happen to the correlation statistics if we couple active noisy oscillators with each other.

Poster session / 19

Brownian Asymmetric Simple Exclusion Process

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We present a model of a Brownian asymmetric simple exclusion process (BASEP) with underdamped Brownian Dynamics, which is an extension on the well-known asymmetric simple exclusion process (ASEP) defined on a discrete lattice. In the BASEP, particles of size σ with hardcore interaction are driven by a constant drag force through a one-dimensional cosine potential with period λ . The amplitude of the cosine potential is much larger than $k_B T$, leading to an effective hopping motion of particles between potential wells. Under periodic boundary conditions, the system reaches a non-equilibrium steady-state (NESS) with a constant particle current. In general, the character of these NESS is strikingly different from the one in the ASEP. Compared to the particle current in a system of non-interacting particles, we observe an enhancement for small σ/λ ratios, caused by a barrier reduction effect arising from multi-occupation of potential wells. Larger ratios lead to a suppression of the current because of strong blocking effects. Surprisingly, an exchange-symmetry effect leads to a current-density relation identical to that of non-interacting particles for the commensurate length $\sigma = \lambda$. A current-density relation similar to the ASEP is obtained only for a limited parameter regime. The rich behavior of the current-density relation is reflected in non-equilibrium phase-diagrams for open-systems, which can exhibit up to five phases. The topology of these phase diagrams changes with varying σ/λ ratio. We furthermore discuss transition times and splitting probabilities for a tagged particle in the BASEP. These quantities exhibit a remarkable asymmetry, which we relate to the collective particle motion in the NESS.

Mon afternoon / 44

Quantum law for partition of kinetic energy

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One of the fundamental laws of classical statistical physics is the energy equipartition theorem which states that for each degree of freedom the average kinetic energy equals $E_k = k_B T/2$, where k_B

is the Boltzmann constant and T is temperature of the system. Despite the fact that quantum mechanics has already been developed for more than 100 years still there is no quantum counterpart of this theorem. We attempt to fill this far-reaching gap and formulate the **quantum law for equipartition of energy** in the appealing form $E_k = \langle \mathcal{E}_k \rangle$, where \mathcal{E}_k is thermal kinetic energy per one degree of freedom of the thermostat consisting of harmonic oscillators and $\langle \dots \rangle$ denotes averaging over frequencies ω of those thermostat oscillators which contribute to E_k according to the probability distribution $\mathbb{P}(\omega)$.

It is valid for an arbitrary strength of the system-thermostat coupling.

We derive it for two paradigmatic and exactly solvable models of quantum open systems: a free Brownian particle and a harmonic oscillator. We formulate conditions for validity of the relation $E_k = \langle \mathcal{E}_k \rangle$ for other quantum systems.

Mon noon / 17

Information and regularity of Brownian particle dynamics

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The common definition of entropy is that it represents some quantifier of disorder. In classical physics, the entropy of a physical system is proportional to the quantity of energy no longer available to do physical work. In dynamical systems analysis it usually refers to the rate at which signal loses or gains information. In information theory it directly measures the information in a signal. The information can be seen as a number of possible states a system can take [1,2].

In this talk the description of the dynamics of the Brownian particle moving in the periodic potential [3] from the point of view of the information theory [2] will be address. We will discuss the role of the external forces as a source of disorder and regularities for the global dynamics and examine key time scales at which a maximum insight into the stochastic dynamics can be expected. The results of Shannon, Spectral and approximate entropies will be presented and compared.

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Thu noon / 39

The divergence of collective dissipation length in SCN-induced glass-like transition

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Spatially Correlated Noise (SCN) emerges in various physical systems, e.g. plasma dynamics, ensembles of active particles and in the self-assembly phenomena. SCN-driven dynamics resembles also the dynamic heterogeneity, i.e. the coexistence of domains with highly correlated mobility, which emerge in the glass transition. In this talk the multi-particle collective dynamics of particles driven by SCN will be discussed. Thermodynamic consistency requires that SCN must be accompanied by the collective dissipation, i.e. the matrix of friction coefficients that depend on the inter-particle

distances. Recently, this matrix has been shown to encode the glass-like transition, i.e. the rise in the viscosity of disordered system by a few orders of magnitudes upon reaching a certain critical packing. This effect will be discussed from the perspective of divergence in collective dissipation length. The open problem in the glass transition physics is the existence of a length-scale that diverges at the transition point. Collective dissipation length can be proposed as a novel approach to this problem. The results for hard spheres and soft particles will be compared.

Poster session / 62

Energetics of the undamped stochastic oscillators

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We present results for undamped stochastic oscillators driven by additive noise. For various noise types we study analytically and numerically energetic properties of stochastic systems. In general, action of an additive noise results in pumping of energy into the system through an interesting interplay between kinetic and potential energies which are sensitive to the shape of the potential well and noise type.

We show that in the long time limit, the total energy grows in time with characteristic exponents depending on the type of noise.

Tue morning / 29

Anomalous diffusion, ergodicity, ageing, and non-gaussianity

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A surging amount of experimental and simulations studies reveals persistent anomalous diffusion in the membranes and volume of living biological cells as well as other complex fluids [1]. This anomalous diffusion is observed for micron-sized objects down to labelled single molecules such as green fluorescent proteins [2].

In this talk I will present results from large scale computer simulations and stochastic analysis of the motion of lipids and embedded proteins in lipid bilayer model membranes [3], indicating that increased disorder leads to longer and longer lasting anomalous diffusion. In particular, the motion of lipids and proteins can become non-Gaussian [3]. In the membranes of living cells anomalous diffusion of embedded protein channels can last over several hundreds of seconds [4].

Anomalous diffusion inside the volume of cells will be discussed, as well. In particular, the emergence of non-Gaussian diffusion patterns for both Fickian and non-Fickian diffusion will be addressed within the framework of diffusing diffusivities [5].

The observed stochastic dynamics may be ergodic or not, depending on the exact physical mechanisms governing the motion of the test particle. The talk will discuss how non-ergodic behaviour needs to be taken into account when interpreting data from stochastic systems. In addition effects of ageing will be explained [6].

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Thu / 18

Scale-dependent anomalous diffusion in spatially disordered environments

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Recent advances in single particle tracking techniques have led to a growing interest in the theoretical study of the motion of microscopic particles in biological environments. It is of key importance for the field of biology to characterize the diffusion of such particles. Many experimental observations have been linked to already existing frameworks such as the continuous time random walks, Lévy walks, ... However, as we show in our work, if one faces a system with spatial disorder, the scale at which we are able to track the particles is a key factor for the characterization of its motion.

We exemplify this issue with a simple system, which allows us to create an anomalous diffusion process by means of the interaction of the particles and its environments. We consider a compartmentalized space, where each compartment is characterized by a size L and a transmittance of the boundaries T . We show that the motion of a Brownian particle moving in such environment, in the case in which we are able to follow its position at each time step - the microscopic scale - can be mapped to a CTRW.

In the other hand, we consider that we are only able to track the particle once it has exited a compartment - the macroscopic scale. This is often the case in biological systems. Then, the motion of the particle can be modeled as a Lévy walk, in which the step size has a length L (which in 2D is related to the area) and the time step is the time the particle takes to exit the compartment. This time is related to the size and the transmittance of such compartment.

To give a concrete example, we take power law distribution of the probability distribution functions of the sizes L and transmittances T . In our work, we show how the diffusion evaluated at the micro- and macroscopic scales, even coming from the same underlying process, show completely different behaviors. Moreover, these two are related as the variance in the position of the microscopic scale is the square root of the variance of the macroscopic scale. The previous proofs the importance of characterizing the different scales of a spatially disordered system before studying the diffusion process taking place on it.

Tue evening / 33

Interplay of Katsura-Nagaosa-Balatsky mechanism and zigzag geometry of lattice bonds: exactly solvable model of the $S = 1/2$ XY magnetoelectric.

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We consider exactly solvable model of the $S = 1/2$ XY one-dimensional magnetoelectric with zigzag geometry of the exchange interaction bonds between the spins. The system is supposed to exhibit the magnetoelectric effect due to Katsura-Nagaosa-Balatsky (KNB) mechanism, connecting the local bond polarization with the spin-current flowing through it. Mapping the quantum spin chain onto the spinless fermion system we presented the exact description of the zero-temperature as well as thermodynamic properties of the model. The main goal is the analysis of the interplay between the zigzag geometry of the bond and the KNB mechanism. We analyze the ground-state phase diagram of the model, zero and finite temperature magnetoelectric effect, obtain the magnetization and polarization curves versus magnetic and electric fields, as well as the parameters of anisotropic dielectric and magnetoelectric response. It is also shown that the electric field may enhance the magnetocaloric effect in the model. Some of our results are universal and can be extrapolated to the quantum spin chains with isotropic Heisenberg interaction between the spins. For instance, when the magnetic field is collinear with the bonds of the zigzag chain the direction of the polarization does not depend on the magnitudes of the magnetic and electric fields.

Mon evening / 7

Emergence of Kardar-Parisi-Zhang dynamics from the etching model: A nonphenomenological description.

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In a recent work [1] a method to derive analytically the roughness evolution was exposed. The method allows to obtain analytically the growths exponents of a surface of $1 + 1$ dimensions whose dynamics is ruled by cellular automata. The method was successfully applied to the etching model[2,3]

and the dynamical exponents were obtained. Those exponents are exact and they are the same as those exhibited by the KPZ model[4] for this dimension. Here we revisit the dynamics of corrosion of an interface and we define a distribution of height difference $P(h_i - h_j)$, between a site i and its first neighbour j . We present a simple proof that in the continuous limit the etching mechanism leads us to the Kardar-Parisi-Zhang (KPZ) equation in a $d + 1$ dimensional space. We show that the parameter λ associated with the nonlinear term of the KPZ equation is not phenomenological, rather it stems from $P(h_i - h_j)$. The Galilean invariance is recovered independent of d , and we illustrate this via very precise numerical simulations. Moreover, we strengthen the argument that there is no upper critical limit for the KPZ equation [6].

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Thu / 11

Short-time molecular motion in simple liquids reflected in temporal, ensemble and wavelet variance MSD for self-diffusion

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The conventional object of interest for studies related to random motions or relatively large walkers in a complex medium having traps and obstacles, e.g. biological soft matter that is motivated by a clear separation of scales between their dynamics. On the other hand, molecular motion in simple liquids, where the walker and its surrounding are composed of identical particles may exhibit a demonstrable non-Gaussianity as it has been found in the classic Rahman's work on molecular dynamics (MD) simulations of liquid argon. Although the typical time range of this phenomenon is sufficiently shorter than for the self-diffusion coefficient considered thermodynamically, this feature may be closely connected with the behaviour of the macroscopic isochoric heat capacity and the fluctuation theory-based prediction of the liquid density under elevated pressure.

Thus, this work explores MD-based trajectories of molecular motions analysing time, wavelet variance, and ensemble averaged mean-square displacements (MSD). This approach allows for an explicit separation of the characteristic spatiotemporal time scales corresponding to the direct localized intermolecular interactions leading to a sufficiently different ensemble- and single trajectory-based pictures, and the normal ergodic Brownian motion for time scales available for experimental detection. At the same time, there will be discussed, how the characteristics of a microscopic compound process formed by localised fluctuational oscillations and stochastic jumping displacements can be accessed from the macroscopic thermodynamic quantities. The work has a financial support from the project No. 2016/23/B/ST8/02968 by the National Science Centre (Poland).

Poster session / 10

Power fluctuations close to the Carnot efficiency

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We show that work and power fluctuations in quasi-static periodically driven heat engines (PHEs) operating with the Carnot efficiency at nonzero output power are finite and can even vanish. This result contradicts the corresponding findings for steady state HEs (SSHEs), where the Carnot efficiency at nonzero power with finite fluctuations cannot be reached quasi-statically. Moreover, the Fano factor for work done by the SSHEs operating at the Carnot efficiency necessarily diverges, while it is constant for the PHEs. In the studied regime, the PHEs thus can be mapped onto the SSHEs on the level of mean values only. We exemplify our findings for the PHEs using an exactly solvable and experimentally relevant model of an overdamped Brownian HE. In this model, the finite-time quasi-static Carnot cycle can be realized due to the possibility to control the relaxation time of the system. Our results can be used to engineer efficient, powerful and reliable HEs.

Mon noon / 9

Non-equilibrium Steady States of the Brownian Asymmetric Simple Exclusion Process

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We discuss non-equilibrium steady states of a system of Brownian hard spheres diffusing in a one-dimensional cosine potential, where a small static bias is driving the particles in one direction. The amplitude of the cosine potential in this Brownian asymmetric simple exclusion process (BASEP) is assumed to be large compared to the thermal energy, leading to a hopping motion of the particles between potential wells. Thus, one may expect that the non-equilibrium steady states of the BASEP are similar to those of its lattice counterpart, the asymmetric simple exclusion process (ASEP). Contrary to this expectation, the BASEP exhibits a much richer behavior due to the additional length scale in the problem brought by the particle diameter. Compared to the case of non-interacting particles, we find both current enhancement caused by multi-occupation of potential wells for small particle diameters and current suppression caused by a blocking effect for large diameters. The phase diagram of the BASEP with open boundaries depends on the particle diameter and can contain five phases. The ASEP-like behavior is observed only in a limited range of parameters. We furthermore discuss transition times and splitting probabilities for a tagged particle in the BASEP. These quantities exhibit a remarkable asymmetry, which we relate to the collective particle motion.

Mon morning / 52

Celestial mechanics of fruit flies or a theory for mushroomers

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The topic of global search in complex environments have been often investigated. But a search can also be local in the sense that it is centered at a given home position. In the latter case, the searcher does not only look for a new target but is also required to regularly return to the home position. Such behavior is typical for many insects and achieves technical importance for self-navigating robotic systems. We propose a stochastic nonlinear model for local search which does not distinguish between the two aims. The dynamics bases on an active particle moving with constant speed. It performs a pursuit and escape behavior of the heading from the position vector realizing thereby optimal exploration of space and the return to the home. We discuss the mechanics of the searcher and inspect the role of noise. Such randomness is present in the decision making rule of selecting the new heading direction. We consider Levy noises with different degree of discontinuity and report about steady spatial densities for the searchers. Also we report about an optimal noise intensity that a searcher finds a target at nearby places. For this noise value the required time for finding the target becomes minimal which appears to be the consequence of different relaxation processes in the spatial and the angular dynamics. Further extensions of the model are discussed during the lecture.

J. Nötel, V.L.S. Freitas, E. E.N. Macau, and L. Schimansky-Geier, “A class of stochastic models for local search”, *Phys. Rev. E* accepted for publication.

J. Nötel, V.L.S. Freitas, E. E.N. Macau, and L. Schimansky-Geier, “Search and return model for stochastic path integrators”, *CHAOS*, accepted for publication.

Tue morning / 1

Robust Active Force Detection with the Overdamped Langevin Equation

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The Overdamped Langevin equation describes the inertialess motion of a particle under deterministic drift and thermal noise. The deterministic drift is the result of the combined action of active forces and the diffusivity gradient (the “spurious” force). For biological applications, it is important to distinguish between the two components, because the former indicates specific interactions, while the latter is due to a heterogeneous environment, in which these interactions take place. The spurious force is always proportional to the diffusivity gradient, but the proportionality coefficient is only known for equilibrium systems. This leads to a range of possible spurious force values in out-of-equilibrium systems and leads to ambiguity in the interpretation of the observed drift. This ambiguity is known as the Itô-Stratonovich dilemma.

In this work, we do not try to resolve the dilemma, but analyze the information that can be extracted about the active forces in an *a priori* unknown out-of-equilibrium system. To this end, we propose a Bayesian method that marginalizes over all possible values of the spurious force and allows robust identification of active forces in both equilibrium and out-of-equilibrium setups. Under certain assumptions, the main result can be obtained in an analytical form. The method has a significantly decreased false positive rate of active force detection as compared to conventional approaches. We illustrate the practical value of the method by integrating it into an open-source software project and applying it to both numerical trajectories and experimental single-biomolecule tracks recorded on the cell membrane.

Poster session / 34**Many body localization of bosons in optical lattices.****Author(s):** Piotr Sierant¹**Co-author(s):** Jakub Zakrzewski¹¹ Jagiellonian University in Kraków**Corresponding Author(s):** sierant.piotr@gmail.com

This contribution is based mainly on [1]. Many-body localization for a system of bosons trapped in a one dimensional lattice is discussed.

Two models that may be realized for cold atoms in optical lattices are considered.

The first one is Bose–Hubbard model with a random on–site potential

$$H = -J \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) + \sum_i \mu_i \hat{n}_i$$

where a_i^\dagger and a_i are operators creating and annihilating boson at site

i of the lattice, J and U are respectively tunneling amplitude and interaction strength

and μ_i is a random on–site potential distributed uniformly in interval $[-W, W]$.

The random on–site potential model is compared with random interactions model [2-3]

$$H = -J \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \frac{1}{2} \sum_i U_i \hat{n}_i (\hat{n}_i - 1)$$

where $U_i \in [0, U]$ is random interaction strength.

While the origin and character of the disorder in both systems is different they show interesting similar properties. In particular, many-body localization appears for a sufficiently large disorder strengths W and U as verified by a time evolution of initial density wave states as well as using statistical

properties of energy levels for small system sizes. Starting with different initial states, we observe that the localization properties are energy-dependent which reveals an inverted many-body localization edge in both systems – that finding is also verified by statistical analysis of energy spectrum – see Fig.~1.

Moreover, we consider computationally challenging regime of transition between many body localized and extended phases where we observe a characteristic algebraic decay of density correlations which may be attributed to subdiffusion (and Griffiths-like regions) in the studied systems. Ergodicity breaking in the disordered Bose-Hubbard models is compared with the slowing-down of the time evolution of the clean system at large interactions.

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Many-body localization of bosons in optical lattices,
New J. Phys. **20** 043032 (2018)

[2] Piotr Sierant, Dominique Delande, and Jakub Zakrzewski,
Many-body localization due to random interactions,
Phys. Rev. A **95**, 021601 (2017)

[3] Piotr Sierant, Dominique Delande, Jakub Zakrzewski,
Many-body localization for randomly interacting bosons,
Acta Physica Polonica A **132**, 1707 (2017)

Mon afternoon / 50**Weighted models for level statistics across the many–body localization transition****Author(s):** Piotr Sierant¹

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We study level statistics across the many-body localization transition. An analysis of the gap ratio statistics from the perspective of inter- and intra-sample randomness allows us to pin point differences between transitions in random and quasi-random disorder, showing effects due to Griffiths rare events for the former case. Defining a mean gap ratio for a single realization of disorder we show that it has a broad, system specific distribution across the whole transition. That explains the necessity of introducing weighted random matrix ensembles that correctly grasp the sample-to-sample variation of system properties including the rare events. We consider two such approaches. One is a weighted short-range plasma model, the other a weighted power-law random banded matrix model. Treating the single sample gap ratio distribution as input, the considered weighted models yield a very good agreement both for spacing distribution including its exponential tail and the number variance up to tens of level spacings. We show explicitly that our weighted models describe the level statistics across the whole ergodic to many-body localized transition much more faithfully than earlier predictions. We also demonstrate that our model describes level statistics in variety of spin, bosonic and fermionic systems. The remaining deviations for long-range spectral correlations are discussed and attributed mainly to the intricacies of level unfolding.

[1] P. Sierant and J. Zakrzewski, *Intermediate spectral statistics in the many-body localization transition*, arXiv:1807.06983

[2] P. Sierant and J. Zakrzewski, *Weighted models for level statistics across the many-body localization transition*, arXiv:1808.02795

Poster session / 48

Negative mobility for controlled mass-based particle separation

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Dynamics of the systems at the sub-micro level can reveal astounding effects and may often mislead our intuition. However, since fluctuations play a key role at this scale, unexpected physical phenomena that contradict our everyday experience should not be a surprise. In this study we consider one of the anomalous transport effects, namely the directed transport of the particles in the opposite direction to an external static force applied to the system. Such a behaviour, referred to as negative mobility, was predicted theoretically in 2007 in a system consisting of inertial Brownian particle moving in a one-dimensional periodic symmetric potential [1]. A year later it was confirmed experimentally in the experiment involving determination of current-voltage characteristics of the microwaved-driven Josephson junction [2]. In 2010 negative mobility has been observed for sub-micro colloidal particles [3] and in 2016 for intracellular organelles [4].

In terms of the Brownian motion the following problem is considered: is it possible to use negative mobility in order to mechanically separate a mixture of various particles in a controlled manner? A number of experiments involving negative mobility already report on successful separation of two types of particles with different sizes in a microfluidic devices [3, 4]. However, no investigation on

how to isolate particles with desired parameters has been found. We performed a number of numerical simulations in order to reveal conditions that guarantee controlled particles isolation by the means of difference in their mobility. In the mechanism proposed here the distinction between particles is based on their absolute mass, i.e. parameter of the model reflecting the correlation between particle mass, applied potential and friction forces present in the system.

[1] L Machura, M Kostur, P Talkner, J Luczka, and P Hanggi. Absolute negative mobility induced by thermal equilibrium fluctuations. *Physical Review Letters*, 98(4):040601, 2007

[2] J Nagel, D Speer, T Gaber, A Sterck, R Eichhorn, Peter Reimann, K Ilin, M Siegel, D Koelle, and R Kleiner. Observation of negative absolute resistance in a Josephson junction. *Physical Review Letters*, 100(21):217001, 2008

[3] Ralf Eichhorn, Jan Regtmeier, Dario Anselmetti, and Peter Reimann. Negative mobility and sorting of colloidal particles. *Soft Matter*, 6(9):1858–1862, 2010.

[4] Jinghui Luo, Katherine A Muratore, Edgar A Arriaga, and Alexandra Ros. Deterministic absolute negative mobility for micro- and submicrometer particles induced in a microfluidic device. *Analytical Chemistry*, 88(11):5920–5927, 2016

Mon morning / 46

Random search with resetting: A unified renewal approach

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We provide a unified renewal approach to the problem of random search for several targets under resetting. This framework does not rely on specific properties of the search process and resetting procedure, allows for simpler derivation of known results, and leads to new ones. Concentrating on minimizing the mean hitting time, we show that resetting at a constant pace is the best possible option if resetting helps at all, and derive the equation for the optimal resetting pace. No resetting may be a better strategy if without resetting the probability of not finding a target decays with time to zero exponentially or faster. We also calculate splitting probabilities between the targets, and define the limits in which these can be manipulated by changing the resetting procedure. We moreover show that the number of moments of the hitting time distribution under resetting is not less than the sum of the numbers of moments of the resetting time distribution and the hitting time distribution without resetting.

Poster session / 35

Spin frustration of a mixed spin-1/2 and spin-3/2 Ising model on a decorated square lattice driven by a magnetoelastic coupling

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The mixed spin-1/2 and spin-3/2 Ising model on a decorated planar lattice accounting for lattice vibrations of decorating atoms is treated by making use of the canonical coordinate transformation, the decoration-iteration transformation, and the harmonic approximation. It is shown that the magnetoelastic coupling gives rise to an effective single-ion anisotropy and three-site four-spin interaction, which are responsible for the anomalous spin frustration of the decorating spins in virtue of a competition with the equilibrium nearest-neighbor exchange interaction between the nodal and decorating spins. The ground-state and finite-temperature phase diagrams are constructed for the particular case of the mixed spin-1/2 and spin-3/2 Ising model on a decorated square lattice for which thermal dependencies of the spontaneous magnetization and specific heat are also examined in detail. It is evidenced that a sufficiently strong magnetoelastic coupling leads to a peculiar coexistence of the antiferromagnetic long-range order of the nodal spins with the disorder of the decorating spins within the frustrated antiferromagnetic phase. The investigated model displays a variety of temperature dependencies of the total specific heat, which may involve in its magnetic part one logarithmic divergence from the Ising universality class apart from one or two additional round maxima superimposed on a standard thermal dependence of the lattice part of the specific heat.

Tue afternoon / 54

Deterministic Loewner equation and unstable growth processes

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The Loewner equation in its stochastic incarnation has proved to be an insightful method in studying scaling limits of critical two-dimensional lattice models in statistical mechanics. However, a deterministic counterpart of this equation is also a valuable tool, particularly well-suited for the description of diffusion-controlled growth problems, such as electrodeposition, dielectric breakdown or viscous fingering [1-3]. In this communication, we use this formalism to describe the growth of finger-like protrusions driven by the gradient of a harmonic field. Following Carleson and Makarov [1] we assume that the growth takes place only at the tips of long-and-thin fingers. However, in contrast to [1], we allow the fingers to split, which is crucial to obtain the patterns corresponding to those observed in nature. We discuss different splitting criteria and study the dynamics of the model in variety of geometries. In particular, we demonstrate that tip-splitting instability of the growing fingers can lead to the stable, regular movement of the envelope of the growing structure [4]. Finally, we show how this formalism can be applied to the evolution of the river networks [5-7] and demonstrate that it correctly predicts the branching angle between the streams to be 72 degrees.

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Poster session / 25

Multifractal characteristics of BK channels' activity in human glioblastoma cells

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BK channels are voltage-gated potassium channels that exhibit large single-channel conductance. They are involved in a number of important physiological processes including the pathogenesis of several diseases. In this work, we analyze the multifractal properties of glioblastoma BK channels activity in different experimental conditions. The sequences of ion currents and dwell times of BK channels' states are analyzed under the influence of such factors like the mechanical strain of the cell membrane at its hyper- and depolarization. In addition, the different stages of membrane fatigue obtained by the repeated membrane stimulation (by suction) are taken into consideration. Among the several methods used for the investigation of the ion channels dynamics here, the advantage lies within the techniques which take into account its nonlinear character. This approach offers a better insight into a complex nature of the biosystem and is closely related to the real phenomena associated with its ability to adapt to the ever-changing environment. For a comprehensive evaluation of analyzed time series, the Multifractal Detrended Fluctuation Analysis was applied. Through this method, the long-range memory effect measured by the Hurst exponent was examined at different scaling regimes.

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Poster session / 21

Cardiovascular dynamics models for hypertension patients based on symbolized signals of heart rate and arterial blood pressure

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Hypertension - a long-term elevation of blood pressure - is a major risk factor for cardiovascular disease like coronary artery disease, stroke and kidney failure. The dynamic relationships in cardiovascular system are altered in hypertensive patients but there is a lack of methods providing qualitative and quantitative assessment of these changes. Therefore, the aim of the study is to compare the dynamics of the cardiovascular system of healthy and hypertensive people using symbolization by three-event-patterns, and then to reproduce the properties of physiological series in simulations. The study was based on symbolized signals of heart rate and arterial pressure recorded in 25 healthy people and 38 hypertension patients, resting in the comfortable supine position. Two types of pattern symbolization were used for the subsequent three signal values. The first one focuses on variations of signal values and the second type emphasizes monotonic trends of a signal. For each signal representation, a transition matrix, describing probability to observe pair of patterns subsequently in a time series, was constructed. Transition matrices offer a Markov chain approach to the signal dynamics.

It has occurred that there are only irrelevant differences between transition matrices arising from signals of the healthy group and of hypertensive patients. One could claim that both dynamics are driven by the same Markov rules, though dynamics are performed with specific to the group: healthy or hypertensive. Based on the Markov rates the artificial signals were produced. Their complexity were compared to the original signals by Shannon entropy. The Shannon entropy indicates at almost flat distribution of patterns in artificial signals for both symbolizations ($SE(\text{MAP}, \text{dyn})=1.59 \pm 0.03$, $SE(\text{MAP}, \text{det})=1.33 \pm 0.06$) what is significantly different from entropy of physiological signals ($SE(\text{MAP}, \text{dyn})=1.24 \pm 0.13$, $SE(\text{MAP}, \text{det})=1.02 \pm 0.11$). Hence the Markovian approach is not efficient in revealing complexity of vascular dynamics. There is not such evident difference when signals of RR-intervals are considered (artificial signals: $SE(\text{RR}, \text{dyn})=1.50 \pm 0.03$, $SE(\text{RR}, \text{det})=1.27 \pm 0.05$, physiological signals: $SE(\text{RR}, \text{dyn})=1.34 \pm 0.23$, $SE(\text{RR}, \text{det})=1.08 \pm 0.19$).

Tue evening / 51

Duality in Percolation

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In this talk we discuss the importance of duality in two-dimensional percolation, from the determination of thresholds exactly (the star-triangle transformation, the triangle-triangle transformation, the isoradial construction) to the question of the behavior of the number of clusters at the critical point, in which duality and the Euler graph formula play important roles. (Work here with Christian Scullard, Youjin Deng and Stephan Mertens). A connection is also made to numerical methods and recent incredibly precise work done by Jesper Jacobsen and Chris Scullard, which takes advantage of duality considerations. Other applications of duality include crossing problems, which are also closely connected with conformal invariance. Applications of percolation to models of cancer growth, epidemic spreading, and general phase transitions will also be discussed.

Tue afternoon / 4

Nurturing Nature for Nanotechnology

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It has long been a dream to design molecular devices and machines. We are not, though, very good at it, but Nature is. From the complex machinery of the ribosome to the integration of information, sensing, and actuation in cells, biological systems conduct the most exquisite nanofabrication and molecular operation that we know of. Our best methods so far for creating nanoscale objects mimic and exploit biological systems – top-down lithographic techniques notwithstanding. DNA nanotechnology, in particular, makes information – the sequence of bases – into structures by taking advantage of the specificity of Watson-Crick pairing. An appropriate chosen sequence of DNA, or sequences of many pieces of DNA, will self-assemble into different shapes and patterns, and can even generate structures that move and respond to different stimuli. This assembly process, though, is not fool proof; it does not always give us what we want. To do as biology does (whether chemical, e.g., ribosomal, or structural), we better develop the tools to measure, model, and understand biomolecular assembly. I will present theoretical principles of biomolecular nanostructure design, as well as experimental results to test these principles in the context of DNA origami. In other words, I will discuss how we can better nurture Nature to give us novel structures and devices, from sensors to machines to drug delivery systems.