XXIVth Marian Smoluchowski Symposium on Statistical Physics, 17.09-22.09 2011, Zakopane, Poland.

Insights into Stochastic Nonequilibrium

Codirectors:
Christian Van den Broeck (Diepenbeek, Belgium)
Lutz Schimansky Geier (Berlin, Germany)
Ewa Gudowska-Nowak (Kraków, Poland)

The Marian Smoluchowski Symposium on Statistical Physics is a cyclic scientific meeting organized annually in Poland since 1988. The conference takes name after the famous Polish physicist who made huge contributions in the natural science and foundation of statistical physics.

The conference is traditionally organized under the patronage of the Polish Academy of Art and Science, Mark Kac Center for Complex System Research at the Jagiellonian University in Kraków, and the consortium of four other Polish academic institutions, i.e. the Institute of Chemical Physics, Polish Academy of Science (Warszawa), Silesian University of Technology (Gliwice), August Chełkowski Institue of Physics, Silesian University (Katowice) and Wrocław University of Technology.

European Science Foundation which supported the meeting via the program Exploring Physics of Small Devices (EPSD) was also involved in preparation and co-sponsoring of the symposium in the past within the projects PESC/STOCHDYN (2004 and 2006).

The program of the 2011 conference covered:

- General theoretical aspects of statistical physics, new tools and mathematical formalism
- Nonequilibrium phenomena and fluctuation relations
- Classical and quantum diffusive transport
- Thermodynamics of small classical and quantum systems
- Statistical physics of biological selforganization and collective motion

The high quality of invited speakers and active participation of about 60 young researchers and PhD students contributed to the success of the meeting which was very well accepted and appraised by visiting collegues. Most of subjects being recognized as contemporary frontiers of statistical physics have been adequately presented during the Symposium by several collegues pioneering research in the field. A mixture of invited speakers and regular participants from many European countries, in particular those taking parts in the ESF Program Exploring Physics of Small Devices, provided grounds for an exchange of ideas, discussions, strengthening the existing intra-European collaborations and possibly initiating new ones.

One of the strongest qualities of the Symposia is the fact that they have always attracted a good amount of young participants. Therefore, the invited talks are usually split into two, roughly equal, groups: (i) lectures presenting the cutting edge of the modern statistical physics and its diverse applications, and (ii) lectures presenting an overview of a specific subdiscipline, accessible to graduate students, yet going beyond the usual graduate curriculum. The organizers maintained this feature for the event in Zakopane, 2011.

Additionally, the second and third days of the conference had the afternoon „Pre-poster Sessions" which were meant to encourage younger collegues to overview briefly their poster presentations and to give them a chance to advertise their line of reaserch. Judging by our former experience, this form of presentation is highly valued by our students and researchers making their first steps in a scientific carreer.

Proceedings of the Syposium will be published as a peer-reviewed contributions to a special issue of *Acta Physica Polonica B*, a refereed journal recognized by European Physical Society and evaluated by the ISI-Thompson-Reuters organization.

The detailed financial report and program of the meeting are attached to this document.

XXIV th M. Smoluchowski Symposium 17-22.09.2011
Expedinture/Specification

Travel:	3074.00 PLN	711.57 EUR
Accommodation:	60653.20 PLN	14040.09 EUR
Conference hall:	4000.00 PLN	
Accommodation in Zakopane:	55753.20 PLN	
Accommodation in Cracow:	900.00 PLN	
Meals:	30794.40 PLN	7128.33 EUR
Local administrative costs:	1646.96 PLN	381.24 EUR

24th Marian Smoluchowski Symposium on Statistical Physics

Zakopane, Poland, September 17–22, 2011

organized by

Jagiellonian University

Marian Smoluchowski Institute of Physics

European Science Foundation

Mark Kac Complex System Research Center

Polish Academy of Sciences

University of Silesia

Silesian Univerisity of Technology

Wrocław University of Technology

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Symposium Organizing Committee: M. Smoluchowski Institute of Physics, Jagellonian University, ul. Reymonta 4, 30–059 Krak"ow, Poland
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24th Marian Smoluchowski Symposium on Statistical Physics

Zakopane, Poland, September 17–22, 2011

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Pre-poster session

Prior to the poster session, a pre-poster session will be organized. Authors of posters can advertise their posters on a "three by three" basis: not more than three minutes of talking and not more than three slides. We all know that you are grateful for having an opportunity to present your work during this wonderful Symposium, so don't waste your time to thank the Organizers. If you want to have a three-slides computer-based presentation, it must be pre-recorded on a designated computer.

Authors may choose not to advertise their posters and opt out of the pre-poster session, risking a reduced interest in their work.

Proceedings

As usual, proceedings of the Symposium are going to be published as a special issue of *Acta Physica Polonica B*. Everybody is welcome to contribute, but please note that all submissions will go through a full editorial process, including peer review.

Please, send your submissions to the address of the **Organizers**

`zfs@th.if.uj.edu.pl`

Your submission should be in the LaTeX (or plain TeX) format, figures in Encapsulated PostScript. We are sorry but we will **not** be able to handle other formats, including Word. Please, visit the publishers' website `http://th-www.if.uj.edu.pl/acta/` for further instructions for authors.

The submission deadline is **January 4, 2012.**

Saturday, September 17th

Arrival Day

20:00 *Get–together Party*

Sunday, September 18th

8:00	*Breakfast*	
	Chairperson: Igor M. Sokolov	
9:50	Ewa Gudowska-Nowak	Opening address
10:00	**Lutz Schimansky-Geier**	Diffusion of active particles
10:30	**Martin Bier**	Szilard-Machine-Like Features in a Processive Motor Protein
11:00	**Bernardo Spagnolo**	The bistable system: an archetypal model for complex systems
11:30	**Miguel Rubi**	Carbon nanotube-based motor driven by a thermal gradient
12:00	**Alessandro Fiasconaro**	Polymer translocation driven by motors
12:30	*Coffee and Lunch break*	
	Chairperson: Lutz Schimansky-Geier	
15:00	**Fernando Oliveira**	Pattern formation and coexistence domains for a nonlocal population dynamics
15:30	**Jacek Miękisz**	From time-delayed random walks to evolutionary game dynamics and gene expression
16:00	**Michał Kurzyński**	Critical properties of molecular biology networks
16:30	*Coffee break*	
	Chairperson: Lutz Schimansky-Geier	
17:00	**James Gleeson**	Stochastic dynamics on complex networks
17:30	**Davide Valenti**	A stochastic reaction-diffusion-taxis model for picophytoplankton dynamics
	Chairperson: Paweł F. Góra	
18:00	Pre-poster session I	
19:15	*Dinner*	

24th Marian Smoluchowski Symposium on Statistical Physics

Zakopane, Poland, September 17–22, 2011

Monday, September 19th

8:00	*Breakfast*	
	Chairperson: Karina Weron	
9:00	**Christian Van den Broeck**	Three detailed fluctuation theorems
9:30	**Peter Hänggi**	Doing small systems: Concepts, Role of Ensembles, Thermalization and Fluctuation Theorems
10:00	**Andrzej Fuliński**	Anomalous diffusion and weak nonergodicity
10:30	**Werner Ebeling**	Onsagers relaxation-fluctuation theory and new developments
11:00	**Ralf Metzler**	Ageing and ergodicity breaking in anomalous diffusion
11:30	*Coffee break*	
	Chairperson: Bernardo Spagnolo	
12:00	**Alexander Dubkov**	Transient dynamics of Verhulst model with resources fluctuations
12:30	**Igor M. Sokolov**	Harmonic oscillator under Lévy noise: new aspects in the phase space
13:00	**Aleksander Weron**	Ergodicity breaking in the context of anomalous diffusion
13:30	*Lunch break*	
	Chairperson: Werner Ebeling	
15:00	**M. Howard Lee**	Cyclic solutions in chaos, Sharkovskii's theorem and isomorphism
15:30	**Maciej A. Nowak**	Addition and multiplication laws of large random matrices
16:00	**Horacio S. Wio**	Variational Formulation for the KPZ equation and Recent Developments
16:30	**Bertrand Berche**	Gauge field theory approach to spin transport phenomena
17:00	*Coffee break*	
	Chairperson: Paweł F. Góra	
17:30	**Pre-poster session II**	
19:00	*Dinner*	
20:30	Poster Session	

Tuesday, September 20th

8:00	*Breakfast*
	Free time (excursions)
	No lunch is served
19:00	*Concert*
20:00	*Formal dinner*

Wednesday, September 21st

8:00	*Breakfast*	
	Chairperson: Andrzej Fuliński	
9:00	**Jean Pierre Boon**	A microscopic approach to generalized Reaction-Diffusion
9:30	**Francesc Sagués**	Colloidal transport on patterned magnetic films
10:00	**Vladimir Stephanovich**	Random local field method for the description of equilibrium and nonequilibrium properties of disordered solids
10:30	**Steve Dodd**	Charge Transport and Dielectric Properties of Epoxy Resins
11:00	**Robert Hołyst**	Evaporation and condensation in simple liquids
11:30	*Coffee break*	
	Chairperson: Christian Van den Broeck	
12:00	**Christoph Dellago**	Challenges in the simulation of nucleation processes: from transition pathways to reaction coordinates
12:30	**Alex Hansen**	Steady-State Two-Phase Flow in Porous Media: Open Questions
13:00	**Sighart Fischer**	Universal Power-Law Exponents from the Statistics of Quantum Dot Fluorescence Intermittencies derived from Random Matrix Theory
13:30	*Lunch break*	

Wednesday, September **21st** *cont.*

	Chairperson: M. Howard Lee	
15:00	**Jukka Pekola**	Fluctuation relations in driven single-electron transitions: theory and preliminary experiments
15:30	**Jerzy Łuczka**	Distance between states of an open quantum system
16:00	**Jerzy Dajka**	Geometric phase as a determinant of a qubitŃenvironment coupling
16:30	**Piotr Garbaczewski**	(Ab)normal asymptotics of diffusion processes
17:00	*Coffee break*	
	Chairperson: Fernando Oliveira	
17:30	**Łukasz Machura**	Transport control by biharmonic signal in coupled Josephson junctions
18:00	**Jarosław Paturej**	Thermal Breakage and Self-Healing of a Polymer Chain under Tensile Stress
18:30	**Antoni Mituś**	Towards electric field poling of octupolar molecules in nano-scale: statistical mechanics approach
19:15	*Dinner*	
20:30	Poster Session - continuation	

Thursday, September 22nd

Departure Day

8:00	*Breakfast*
9:00	Departure – bus to Krakow

Talks

Gauge field theory approach to spin transport phenomena

Bertrand Berche, Nancy University, France

Abstract: Spin-orbit interaction (SOI) is a very useful tool to manipulate spin degrees of freedom using external gate voltages. This is a major reason why SOIs in various materials, e.g. 2D electron gas, were widely studied in the last decade. From a theoretical point of view, it is also a subject of fascinating interest, since the presence of SOI in the non relativistic Pauli-Schroedinger equation gives a rich U(1) £ SU(2) gauge structure. We investigate some of the consequences (definition of the spin current and spin polarization, conservation equation, spin precession and quantization conditions, spin interferometry, ...) of this structure in simple situations e.g. the case of mesoscopic rings.

[1] Gauge symmetry breaking and topological quantization for the Pauli Hamiltonian, Medina E., Lopez A., Berche B., Europhys. Lett. 83 (2008) 47005

[2] Gauge field theory approach to spin transport in a 2D electron gas, Berche B., Bolivar N., Lopez A., Medina E. Cond. Matt. Phys. 12 (2009) 707-716

[3] A perfect spin filtering device through Mach-Zehnder interferometry in a GaAs/AlGaAs electron gas, Lopez A., Medina E., Bolivar N., Berche B. J. Phys.: Condens. Matter 22 (2010) 115303

Szilard-Machine-Like Features in a Processive Motor Protein

Martin Bier, East Carolina University, Greenville, USA

Abstract: The motor protein kinesin literally walks on two legs along the biopolymer microtubule as it hydrolyzes ATP for its fuel supply. The fraction of accidental backsteps that kinesin takes appears to be about seven orders of magnitude larger than what one would expect given the amount of free energy that ATP hydrolysis makes available. This is puzzling as more than a billion years of natural selection should have optimized the motor protein for its speed and efficiency. With an imagined device, Szilard has shown that the dissipation of information can drive motion. A higher backstepping probability creates more randomness in the walk and, consequently, leads to production of more entropy. If the product state of a transition has a higher entropy, then the free energy of that product state is lower. With the free energy that is made available by the production of backstepping entropy, the catalytic cycle of the kinesin can be speeded up. We show quantitatively how the actually measured backstepping rate represents an optimum at which maximal net forward speed is achieved. We, furthermore, show how this thermodynamic mechanism can realistically operate on a biomolecular level. The results suggest that kinesin uses backstepping as a source of energy and that natural selection has manipulated the backstepping rate to optimize kinesin's speed.

Talks (continued)

A microscopic approach to generalized Reaction-Diffusion
Jean Pierre Boon, Université Libre de Bruxelles, Belgium
Abstract: We develop a microscopic theory for reaction-difusion (R-D) processes based on a generalization of Einstein's master equation with a reactive term and we show how the mean field formulation leads to the nonlinear R-D equation with non-classical solutions. For the n-th order annihilation reaction $A + A + A + ... + A \rightarrow 0$, we obtain a nonlinear reaction-diffusion equation for which we discuss scaling and non-scaling formulations. We find steady states with either solutions exhibiting long range power law behavior showing the relative dominance of sub-diffusion over reaction effects in constrained systems, or conversely solutions with finite support of the concentration distribution describing situations where diffusion is slow and extinction is fast. Theoretical results are compared with experimental data for morphogen gradient formation.

Three detailed fluctuation theorems
Christian van den Broeck, Hasselt University, Diepenbeek, Belgium
Abstract: The total entropy production of a trajectory can be split into an adiabatic and a non-adiabatic contribution, deriving respectively from the breaking of detailed balance via nonequilibrium boundary conditions or by external driving. We show that each of them, the total, the adiabatic and the non-adiabatic trajectory entropy, separately satisfies a detailed fluctuation theorem.

[1] M. Esposito and C. Van den Broeck, Phys. Rev. Lett. 104, 090601 (2010)

Geometric phase as a determinant of a qubit-environment coupling
Jerzy Dajka, University of Silesia, Katowice, Poland
Abstract: Geometric phase, a global feature of quantum evolution, reflects various properties of evolving systems. We focus on the relation between the geometric phase of open qubits and the character of their coupling to the environment. We present results for various very different systems: starting from simple but exact dephasing models, via general, but weakly coupled to the environment, systems and ensembles of qubits with an interaction allowing for a mean-field description. We also present how the geometric phase can serve as a potentially useful tool in studies of oscillating neutrinos.

Talks (continued)

Challenges in the simulation of nucleation processes: from transition pathways to reaction coordinates

Christoph Dellago, University of Vienna, Austria

Abstract: Computer simulations of first order phase transitions occurring via nucleation and growth are demanding for several distinct but related reasons. Particularly close to coexistence, the free energy barrier separating the metastable from the stable phase can be high, leading to nucleation times that vastly exceed the time scales accessible to molecular dynamics simulations. Other difficulties arising in the simulation of nucleation processes consist in detecting local structures characteristic for the stable and metastable phases and in identifying the degrees of freedom that capture the essential physics of the transition mechanism. In this talk, I will discuss how these problems can be addressed using transitions path sampling, neural networks, and likelihood optimization, respectively. The freezing of a soft sphere fluid and the pressure induced structural transformation of nanocrystals will be used as illustrative examples.

Charge Transport and Dielectric Properties of Epoxy Resins

Stephen Dodd, University of Leicester, United Kingdom

Abstract: Electrical treeing is an electrical degradation process driven by partial discharge activity in polymeric high voltage insulators as used, for example, as the base resin in impregnated paper transformer bushings. Much work has been directed towards understanding the treeing process, both experimentally and by computer simulation. However, in many such studies, it is common to neglect the electrical properties of the insulation material, even though a small subset of these studies have demonstrated a significant effect of temperature and moisture absorption on the electrical treeing growth behaviour. In this paper, the dielectric properties of epoxy resins are described as a function of temperature and absorbed moisture. Above the glass transition temperature, the dielectric measurements were found to be consistent with a superposition of a number of processes; (1) a bulk DC electrical conductivity, (2) a low frequency dispersion process associated with quasi DC conductivity, (3) an interfacial polarisation that results from inconsistent electrode/sample contact and (4) a frequency independent capacitance. The processes (1), (2) and (3) appeared to scale in the same way with both increasing temperature and increasing moisture content and therefore indicate a common physical origin. The characteristics of the measured quasi DC response were found to be identical in different epoxy compositions when the measurements were conducted at the same temperature above their respective glass transition temperatures and therefore independent of the actual chemical composition of the material.

Talks (continued)

The observed quasi DC response was also similar to that found in many other materials in which proton hopping is expected to occur between cluster centres at frequencies below the critical frequency for the process, whereas at higher frequencies, proton hopping is limited to within the cluster dimensions. It is therefore hypothesised that proton hopping is the dominant charge transport process in epoxy resins and this has supporting evidence from gravimetric and NMR studies of moisture diffusion in epoxy resin in which the moisture was found to exist in two states (1) free (mobile, diffusing) water molecules weakly interacting with the polymer matrix and (2) bonded (trapped) water in which water-water interactions dominate on nucleation of water molecules in regions of free volume within the polymer matrix. The effects of the dielectric properties on the electrical treeing process are briefly discussed.

Transient dynamics of Verhulst model with resources fluctuations

Alexander Dubkov, Lobachevsky State University of Nizhni Novgorod, Russia

Abstract: The stochastic Verhulst equation for the population density with fluctuating resources is considered. Using the exact solution of the equation the conditional probability distribution is calculated for the excitation in the form of Lévy white noise with one-side stable distribution. The analytical results can be obtained for the case of noise with Lévy-Smirnov distribution. The transitions from the initial unimodal distribution of the population density to bimodal and then again to unimodal in asymptotics are discussed. The distribution in the steady state and some first moments are also found.

Onsagers relaxation-fluctuation theory and new developments

Werner Ebeling, Humboldt University, Berlin, Germany

Abstract: On the occasion of the 80th anniversary of Onsagers fundamental paper on irreversible processes we give first a short survey on the old problems and several new solutions for the description of relaxation – fluctuation processes [1]. In the second part we develop the assumption that for many systems the deviations from Gaussian distributions in nonequilibrium systems may be described by convoluted Gauss- Lévy distributions. This means, the central part of the distribution is determined by the Gaussian part, the wings of the distribution maybe of Lévy type, decaying according to a power law. For such systems we develope a generalization of Onsagers theory of linear relaxation processes which includes Gaussian fluctuations and (non-equilibrium) Lévy flights by postulating appropriate Smoluchowski-Fokker-Planck equations in real and in Fourier space. In particular we consider coupled systems of many variables, as a special case the relaxation in the velocity space. This way we reproduce several results obtained earlier.

[1] W. Ebeling, I.M. Sokolov, Statistical thermodynamics and stochastic theory of nonequilibrium systems, World Scientific, Singapore 2005

[2] W. Ebeling, E. Gudowska-Nowak, Including nonequilibrium Lévy fluctuations into Onsagers relaxation – fluctuation theory, Preprint, Jagiellonian University, Krakow, 2010

Talks (continued)

Polymer translocation driven by motors

Alessandro Fiasconaro[1,2] (work done with Juan Jose Mazo[1,2], Fernando Falo[1])
[1] Universidad de Zaragoza, Spain; [2] CSIC-Universidad de Zaragoza, Spain.

Abstract: Transport mechanism of molecules inside cells and/or through cell membranes is getting nowadays more and more attraction. On one hand, because of the increasing abilities to detect and to measure the biological mechanisms at the nanoscale, on the other hand, because of the challenging possibility to construct from scratch structures (with both natural and synthetic materials) able to imitate the biological functioning [1].
Long molecule translocation is usually driven by constant fields in the pore or by chemical potential differences in both sides of the membrane. In other cases the translocation is assisted by an ATP-based molecular motor [2].
Goal of this talk is to present the model of a simple motor with different driving mechanisms: with oscillating, dichotomous, and more realistic ATP activated dichotomous force. In this last case, the model is able to describe the polymer translocation and our results in one dimension agree qualitatively with recent experimental outcomes on DNA packaging of bacteriophages [3].

[1] Mickler M. Schleiff, E., and Hugel T. (2008) Chem. Phys. Chem. 9, 1503-1509
[2] Hänggi P., Marchesoni F., (2009) Rev. Mod. Phys, 81, 683-693
[3] Smith D. E., Tans S. J., Smith S. B., Grimes S., Anderson D. L., and Bustamante C., (2001) Nature 413, 748

Universal Power-Law Exponents from the Statistics of Quantum Dot Fluorescence Intermittencies derived from Random Matrix Theory

Sighart F. Fischer (work done with Wolfgang Dietz), Technical University Munich, Germany

Abstract: The power-law exponent 1.5 observed in the statistics of single quantum dot fluorescence intermittencies is derived from random matrix theory with uncorrelated Gaussian unitary distributions for the excited state energies and the charge transfer matrix elements causing the fluorescence decay. Models predicting larger exponents up to 2 are also presented. The random matrix theory is finally applied to the early charge separation events in Photosynthesis, where a superexchange coupling with distributed intermediate states is considered. It is shown that the effective couplings are strongly peaked in the near resonance regime which helps to understand the robustness of the non- activated transfer rate against changes in the mean of free energy of the intermediate state.

Talks (continued)

How universal is weak ergodicity breaking
Andrzej Fuliński, Jagiellonian University, Kraków, Poland
Abstract: Ergodic behavior of the class of G-processes: $G(t) = \int_{t_m}^{t} du\, K(t,u)\xi(u) - \int_{t_m}^{0} du\, K(0,u)\xi(u)$, $\langle \xi(t) \rangle = 0$, $\langle \xi(t)\xi(s) \rangle = \phi(|t-s|)$ is examined. Ergodic are solely G-extensions of normal diffusion ($K = 1$), and of Mandelbrot-Van Ness fractional diffusion ($K(t,u) = K(t-u)$, $t_m \to -\infty$). Any deviation from these two types results in weak ergodicity breaking which thus is neither exceptional, nor limited to some specific events, but is typical for much wider class of processes. G-processes driven by $\xi(t)$ with non-vanishing correlations are important for description of transport in strongly non-equilibrium systems, and may be responsible for peculiarities of diffusion found in biological, glassy, and nano-scale systems.

(Ab)normal asymptotics of diffusion processes
Piotr Garbaczewski, Opole University, Poland
Abstract: We show that, under suitable confinement conditions, the ordinary Fokker8211;Planck equation may generate non-Gaussian heavy-tailed probability density functions (pdfs) (like, for example, Cauchy or more general Lévy stable distributions) in its long-time asymptotics. In fact, all heavy-tailed pdfs known in the literature can be obtained this way.

Stochastic dynamics on complex networks
James Gleeson, University of Limerick, Ireland
Abstract: How much detail is needed about the structure of a large-scale network in order to predict the evolution of a dynamical system running on the nodes of the network? Can statistical characteristics, such as the degree distribution, contain sufficient information to give accurate predictions for dynamics on real-world networks? This talk will review some statistical physics approaches to these questions, including heterogeneous mean-field theories and improvements thereon. The focus will be on binary-state dynamics (such as the susceptible- infected-susceptible model of disease spread, and systemic risk models for banking networks) for which a hierarchy of approximation techniques will be described.

Talks (continued)

Doing small systems: Concepts, Role of Ensembles, Thermalization and Fluctuation Theorems

Peter Hänggi, University of Augsburg, Germany

Abstract: This talk is aimed at highlighting issues that relate of doing thermodynamics and statistical physics of finite size systems. This theme gained considerable importance in view of fascinating advances in nanotechnology and system biology. While the fathers of thermodynamics developed the famous Laws having in mind macroscopic systems these grand concepts need to be inspected anew in view of the fact that the fluctuations grow with decreasing size to a level where they even may play the dominant role. The symposium touches upon several timely issues in designing, measuring and operating systems at the submicron scale, both IN and also FAR AWAY from thermal equilibrium. With this introduction I discuss subtleties related to thermodynamics of small systems, such as (i) the role of finite size for quantities such as (in some cases negative-valued) heat capacitance [1], (ii) the role of entropy and temperature in these small systems, or (iii) the issue of thermalization [2]. Moreover, a key role in doing statistical physics of submicron systems relates to (iv) the choice of the ensemble description and the inter-relationships between the sizable fluctuations of measures like work, heat heat flow and thermodynamic equilibrium quantifiers such as free energy changes or changes of entropy [3].

[1] P. Hänggi and G. L. Ingold, Quantum Brownian motion and the third law of thermodynamics, Acta Physica Polonica B 37, 1537–1550 (2006); P. Hänggi, et al., Finite quantum dissipation: the challenge of obtaining specific heat, New J. Phys. 10, 115008 (2008); see also in:G. Ingold, et al., Phys. Rev. E 79, 061105 (2009) .

[2] A. V. Ponomarev, S. Denisov, and P. Hänggi Thermal equilibration between two quantum systems Phys. Rev. Lett. 106, 010405 (2011).

[3] M. Campisi, P. Hänggi, and P. Talkner Quantum fluctuation relations: Foundations and applications Rev. Mod. Phys. 83, 771–791 (2011).

Steady-State Two-Phase Flow in Porous Media: Open Questions

Alex Hansen, Norwegian University of Science and Technology, Trondheim, Norway

Abstract: Whereas instabilities during injection of a fluid into a porous medium already saturated with another fluid immiscible with respect to the first, have been extensively studied, the simultaneous flow of two immisicble fluids under steady-state conditions have been received surprisingly little attention. We will in this talk present a number of open questions - and some attempts at answering them. Among the questions we pose is what happens to the interface between two immiscible fluids flowing in parallel; why does the effective permeability scale with the average pressure gradient with a non-trivial exponent.

Talks (continued)

Evaporation and condensation in simple liquids
Robert Hołyst, Institute of Physical Chemistry PAS, Warsaw, Poland
Abstract: The evaporation of simple liquids has been studied since the seminal paper written by J.C.Maxwell. One important issue related to mechanical equilibrium was overlooked in previous studies. The mechanical equilibrium establishes very fast even at high evaporation rates and even during evaporation into vacuum. This strong constraint on the dynamics of evaporation governs the mass flux. In the particular case of evaporation into vacuum the mass flux of evaporating molecules follows from their momentum flux, which excatly matches the pressure inside the liquid. This observation has allowed us to correct the Hertz-Knudsen formula. We also tested new equation for the evaporation flux in computer simulations of Lennard-Jones fluid reaching perfect agreement between theory and simulations. Independent simulations on other molecules performed in Sandia Laboratories also confirmed our theory. In a different system of liquid evaporating into its own vapor the mechanical equilibrium in the system governs the spatial distribution of temperature (between hot walls and cold liquid inside a system). In turn the temperature distribution governs the energy flux arriving at the surface of the liquid and thus the mass flux via the enthlapy of evaporation). One of the reasons for the slow progress in the theoretical study of evaporation is the lack of good experiments. If time allows I will also present some results on the collapse of vapor bubbles in simple liquids and its relation to sonoluminescence.

Critical properties of molecular biology networks
Michał Kurzyński, Adam Mickiewicz University, Poznań, Poland
Abstract: Since the formulation by Bak and Sneppen a cellular automaton model of the punctuated equilibria, the biological evolution is more and more often considered as a self-organized criticality phenomenon. Soon it appeared that the protein interaction and metabolic networks of the systems biology have a scale-free structure like the model evolving networks of Barabasi and Albert. Contrary to the latter, however, the protein interaction and metabolic networks display the small-world property only in large length-scales, having in smaller scales an evidently self-similar (fractal) organization. There are premises that also the conformational transition networks in native proteins are scale-free but whether they have a small-world or a self-similar organization remains a still open question. The Barabasi-Albert trees are considered as a possible theoretical model of these networks, having certainly a small-world property but displaying a power-low distribution density of the first-return times, characteristic for fractals with an effective dimension one. The model appeared successful in explaining a possible higher than one output-input ratio in biological molecular machines.

Talks (continued)

Cyclic solutions in chaos, Sharkovskii's theorem and isomorphism
M. Howard Lee, University of Georgia, Athens, USA
Abstract: At the fully developed chaos in the logistic map it is possible to solve analytically the 3-cycle problem. There are found two 3-cycles, each with a simple structure. By Sharkovskii's theorem, we can assert that there are all other multi-cycles of the same structure given by a set of all rational numbers in the interval of (0,1). We shall show that the resultant invariant density of cycles is isomorphic to the frequency density of a harmonic oscillator chain at the thermodynamic limit. This isomorphism shows the same underpinnings for ergodicity in two entirely unrelated systems.

Distance between states of an open quantum system
Jerzy Łuczka, University of Silesia, Katowice, Poland
Abstract: Intriguing features of the distance between two arbitrary states of an open quantum system are identified that are induced by initial system-environment correlations. As an example, we analyze a qubit dephasingly coupled to a bosonic environment. Within tailored parameter regimes, initial correlations are shown to substantially increase a distance between two qubit states evolving to long-time limit states according to exact non-Markovian dynamics. It exemplifies the breakdown of the distance contractivity of the reduced dynamics.

Current-flux characteristics in mesoscopic nonsuperconducting rings
Łukasz Machura, University of Silesia, Katowice, Poland
Abstract: The world of mesoscopic objects is one of the most intriguing domains of science and one that in many respects remains terra incognita. The mesoscopic world is characterized by small length scales and low temperatures. At sub-Kelvin temperatures, the length scales are of the order of micrometers. A prominent example of such a mesoscopic system is a normal (i.e. nonsuperconducting) metal ring threaded by a magnetic ux. Such a ring can support 'persistent current' and occurs when electrons maintain their phase coherence around the ring. It is purely a quantum mechanical phenomenon and, in fact, a manifestation of the famous Aharonov–Bohm effect. Persistent currents were predicted by Hund in 1938 and until the early 1990s their detection has been considered an experimental challenge. In 2009 paper by *Bluhm et al. (Phys. Rev. Lett. 102 136802)* the results of experiments on 33 individually scanned gold rings were presented for the first time. We propose four different mechanisms responsible for the paramagnetic or diamagnetic persistent currents in normal metal rings and determine the circumstances for changes of the current from paramagnetic to diamagnetic and vice versa.

Talks (continued)

Ageing and ergodicity breaking in anomalous diffusion

Ralf Metzler, Technical University of Munich, Germany

Abstract: In 1905 Einstein formulated the laws of diffusion, and in 1908 Perrin published his Nobel-prize winning studies determining Avogadro's number from diffusion measurements. With similar, more refined techniques the diffusion behaviour in complex systems such as the motion of tracer particles in living biological cells is nowadays measured with high precision. Often the diffusion turns out to deviate from Einstein's laws. This talk will discuss the basic mechanisms leading to such anomalous diffusion as well as point out its consequences. In particular the unconventional behaviour of non-ergodic, ageing systems will be discussed within the framework of continuous time random walks. Indeed, non-ergodic diffusion in the cytoplasm of living cells as well as in membranes has recently been demonstrated experimentally.

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Towards electric field poling of octupolar molecules in nano-scale: statistical mechanics approach

Antoni C. Mituś[1] (work done with Grzegorz Pawlik[1] and Joseph Zyss[2])
[1] University of Technology, Wrocław, Poland; [2] Ecole Normale Superieure de Cachan, France

Abstract: Conditions towards effective electric field poling in two dimension of octupolar molecules are being addressed, based on a lattice model studied using the complementary approaches of analytical methods in statistical mechanics and Monte Carlo simulations [1]. The poling field is imparted by a system of cylindrical electrodes. A topologically rich structure of local and global inhomogeneous octupolar order is present in the system. The poling criteria are show to vary strongly throughout the cell. In particular, octupoling in the center of the cell requires temperatures as low as 10-4 K. It is argued that a weak global octupolar order can be reached at Helium temperatures, thanks to advances in optical techniques and nanotechnologies.

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Talks (continued)

From time-delayed random walks to evolutionary game dynamics and gene expression

Jacek Miękisz, Warsaw University, Poland

Abstract: It is well known that time delays may cause cyclic behavior in dynamical systems. Here we would like to point out that the presence of oscillations may depend on particular causes of a time delay. One of the first examples of stochastic dynamics with time delay is a time-delayed random walk [1].We discuss here its stationary behavior in the limit of zero noise [2]. We review two specific examples of evolutionary games - replicator dynamics with time delay [3,4] In a social-type model, where individuals react to the information concerning the state of the population at some earlier time, the population oscillates around an unstable stationary point. On the other hand, in a biological-type model, where some changes already take place in the population at an earlier time, oscillations are not present for any time delay. We propose a new methodology to deal with time delays in biological systems and apply it to simple models of gene expression with delayed degradation [5,6]. We show that delayed degradation in gene expression does not cause oscillations as it was recently argued [7]. It follows from our rigorous analysis that one should look for different mechanisms than just delayed protein degradation to explain causes of oscillations observed in certain biological experiments. We develop a systematic analytical treatment of stochastic models of time delays. Specifically we take into account that some reactions, for example degradation, are consuming, that is once molecules start to degrade, they cannot be part in other degradation processes.

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Talks (continued)

Addition and multiplication laws of large random matrices

Maciej A. Nowak, Jagiellonian University, Kraków, Poland

Abstract: Random matrices play an increasingly important role in mathematics, physics, multivariate statistics and interdisciplinary research. Among various formulations of random matrices one particular formalism is flourishing — free random variables calculus (hereafter FRV). FRV formalism can be viewed as a striking analogue of classical probability calculus, where the role of random variables is played by random operators, represented by large (infinite) matrices drawn from some probability distribution. The large size of the matrices is by no means a restriction: first, contemporary data incude samples of several orders of magnitude, with dimensionality ranging from thousands (physics), through milions (telecommunication, internet) up to bilions (genetics); second, the formalism becomes exact precisely in the limit when the size of the random matrix tends to infinity. The cornerstones of this success are the so-called R and S transforms. The R transform allows one to infer the spectral properties of the sum of random operators, provided the individual spectral measures are known for each of them and they are independent in the noncommutative sense a.k.a. free. The S transform plays a similar role for the multiplication of free random operators. These constructions allow for fast decomposition of several problems for complicated random operators into simple ingredients. In this talk we present these transformations as analogues to conventional Fourier and Mellin transforms for sums and products of random variables in classical probability theory. After short summary of the known results we will present new results by the author on addition and multiplication laws of random operators which are non-hermitian, i.e. they eigenvalues are complex. Such case is by no means academic – important applications cover dissipative phenomena, directed percolations in random media, analysis of various kinds of so-called lagged correlations and several other examples from various branches of physics. Explicit illustrations will be provided, and new potential domains of applications will be proposed.

Thermal Breakage and Self-Healing of a Polymer Chain under Tensile Stress

Jarosław Paturej[1,2] (work done with V.G. Rostiashvili[1], A. Ghosh[1], J. Paturej[1,2], A. Milchev [1,3], T.A. Vilgis[1])
[1]Max-Planck-Institut für Polymerforschung, Mainz, Germany; [2]University of Szczecin, Poland; [3]Bulgarian Academy of Science, Sofia, Bulgaria

Abstract: We consider the thermal breakage of a tethered polymer chain of discrete segments coupled by Morse potentials under constant external force. The chain dynamics at the onset of fracture is studied analytically by Kramers-Langer multidimensional theory and by extensive Molecular Dynamics simulations in $1D$- and $3D$-space. Comparison with simulation data in one- and three dimensions demonstrates that the Kramers-Langer theory provides good qualitative description of the process of bond-scission as caused by a *collective* unstable mode. We derive distributions of the probability for scission over the successive bonds along the chain which reveal the influence of chain ends on rupture in good agreement with theory.

Talks (continued)

The breakage time distribution of an individual bond is found to follow an exponential law as predicted by theory. We have also shown that the mean life time of the chain becomes progressively independent of the number of bonds as the pulling force grows. Special attention is focused on the recombination (self-healing) of broken bonds. Theoretically derived expressions for the recombination time and distance distributions comply with MD observations and indicate that the energy barrier position crossing is not a good criterion for true rupture. It is shown that the fraction of self-healing bonds increases with rising temperature and friction.

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Fluctuation relations in driven single-electron transitions: theory and preliminary experiments

Jukka Pekola, Helsinki University of Technology, Finland

Abstract: I discuss the distribution of generated heat in a driven single-electron box (SEB) [1]. In this system one can test fluctuation relations (FRs) conveniently by performing a large number of accurately controlled gate sweeps. We find interesting limitations in applying the most common FRs when the box gets overheated or is otherwise driven into non-equilibrium. A variation of a SEB, a single-electron trap, is a candidate of realizing Maxwell's demon [2]. At the end I present preliminary experimental results on the distribution of generated heat.

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Carbon nanotube-based motor driven by a thermal gradient

Miguel Rubi, University of Barcelona, Spain

Abstract: We present a model able to reproduce experimental observations and computer simulation results of the movement of two coaxial carbon nanotubes induced by a thermal gradient. The model is formulated in terms of a Langevin equation which includes the friction force, the van der Waals forces between both nanotubes, that depend on their chiralities, and the inhomogeneous temperature distribution which give rise to an inhomogeneous phonon distribution. The random force term is assumed to be related to the fluctuations of the heat current along the inner nanotube and therefore its intensity is proportional to the heat conductivity. The model reproduces the rich variety of possible dynamic behaviors and proves the conjecture that the driving force is the phononic current induced by the thermal gradient. Applications to other nano-electromechanical devices are also analyzed.

Talks (continued)

Colloidal transport on patterned magnetic films

Francesc Sagués, University of Barcelona, Spain

Abstract: A review of our recent work on transport of paramagnetic micron-size particles on patterned magnetic films will be sketched. The basic principle of the ratcheted motion under an oscillating external magnetic field will be first introduced. Related dynamic modes such as localized, anomalously diffusive, ballistic, etc. will be also mentioned [1]. In particular, a more detailed attention will be paid to an scenario where single particle enhanced diffusion [2] combines with a collective behavior of driven colloidal chains that is reproduced with the Rouse- like model of polymer physics [3]. I will finish by addressing a different situation that refers to autonomous chemically-driven motion of ellipsoidal-like colloidal particles in simple water dispersions in absence of both the patterned support and the external field [4].

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Harmonic oscillator under Lévy noise: new aspects in the phase space

Igor M. Sokolov (work done with B. Dybiec and W. Ebeling), Humboldt University, Berlin, Germany

Abstract: A harmonic oscillator under influence of the noise is a basic model of various physical phenomena. Under Gaussian white noise the position x and velocity v of the oscillator are independent random variables which are distributed according to the bivariate Gaussian distribution with elliptic level lines. The distribution of phase is homogeneous. None of these properties hold in the general Lévy case. Thus, the level lines of the joint probability density are not elliptic. The distribution of the phase is inhomogeneous and highly nontrivial. The coordinate and the velocity of the oscillator are strongly dependent. This dependence of these variables can be quantified by introducing the corresponding parameter ("width excess"), similar in spirit to but different from the codifference of the variables. The correlation of velocity and position have large influence on e.g. level-crossing properties of the x(t)-process.

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Talks (continued)

The bistable system: an archetypal model for complex systems

Bernardo Spagnolo[1] (work done with P. Caldara[1] , A. La Cognata[1], D. Valenti[1] , A. Fiasconaro[2,3]),
[1] University of Palermo, Italy; [2] Centro Universitario de la Defensa de Zaragoza, Spain; [3] Departamento de Fisica de la Materia Condensada and ICMA, Zaragoza, Spain

Abstract: Bistable systems often play the role of archetypal models to understand the dynamical behavior of complex systems. Examples range from microphysics to macrophysics, biology, chemistry and also econophysics. Moreover the statistical mechanics is essential to study the physical properties of complex systems and to investigate stochastic systems in which the microscopic degrees of freedom behave collectively over large scales. We investigate the nonlinear relaxation in a bistable system in classical and quantum systems. (i) As a first classical system, the role of the multiplicative and additive noise in the mean life time of the metastable state of an asymmetric bistable system is investigated. This model is useful to describe the dynamical behavior of an out of equilibrium Ising spin system. Nonmonotonic behavior of the average lifetime as a function of both additive and multiplicative noise source intensities is found. (ii) The role of a non-Gaussian Lévy noise on the nonlinear dynamics of: a) a particle moving in a metastable system, b) an ecosystem composed by two competing species interacting with the surrounding environment, and c) a short overdamped Josephson junction is investigated. a) By using the backward fractional Fokker–Planck equation we investigate the barrier crossing event and the nonlinear relaxation time for a metastable system; b) In the ecosystem, the role of two non-Gaussian noise sources in the exclusion and coexistence regimes is analyzed. Quasiperiodic oscillations and stochastic resonance phenomenon in the dynamics of the competing species are found; c) In the short overdamped Josephson, the mean escape time of the junction is investigated considering Gaussian, Cauchy-Lorentz and Lévy-Smirnov probability distributions of the noise signals. In these conditions we find resonant activation and the first evidence of noise enhanced stability in a metastable system in the presence of Lévy noise. For Cauchy-Lorentz noise source, trapping phenomena and power law dependence on the noise intensity are observed. (iii) Finally the dynamics of a quantum particle subject to an asymmetric bistable potential and interacting with a thermal reservoir is investigated. We obtain the time evolution of the population distributions in the position eigenstates of the particle, for different values of the coupling strength with the thermal bath. The calculation is carried out by using the Feynman-Vernon functional under the discrete variable representation.

Talks (continued)

Random local field method for the description of equilibrium and nonequilibrium properties of disordered solids

Vladimir Stephanovich, Opole University, Poland

Abstract: We suggest an approach to describe the equilibrium (like static magnetization, electric or magnetic susceptibility, specific heat etc) and nonequilibrium (like frequency dependent susceptibilities) physical properties of disordered dielectric and/or magnetic systems. These systems are characterized by randomly positioned and oriented spins (dipoles) situated in a host crystal lattice. The spins or dipoles, being randomly positioned and oriented in a host lattice, create the random magnetic or electric fields in it. The distribution function of these random fields, defined as an average (over spatial and orientational fluctuations) of Dirac delta contributions of each spin (dipole), enables us to obtain the self-consistent equations for order parameters. The exact form of distribution function (which is not Gaussian) and character of order parameters (it can be average magnetization (polarization) $\langle S \rangle$, equilibrium spin-glass order parameter $\langle S^2 \rangle$ and/or general quantities like $\langle S^n \rangle$, $\langle \ldots \rangle$ mean double average over spatial and orientational disorder) depend on specific form of microscopic interaction between spins or dipoles in a host. The solution of equations for order parameters permits to obtain the equilibrium thermodynamic characteristics of the systems under consideration. In some cases the equations for order parameters permit to derive the continuous free energy functional of a substance, substituting initial "disordered" Hamiltonian. Such free energy functional permit to investigate both equilibrium and non- equilibrium properties of a system using well-known methods like Landau-Khalatnikov equations for ferroelectrics. Our theory delivers pretty good description of experiments in disordered ferroelectrics, multiferroics, magnets and diluted magnetic semiconductors.

Pattern formation and coexistence domains for a nonlocal population dynamics

Fernando A. Oliveira[1,4] (work done with Jefferson A.R. da Cunha[3,4], Andre L.A. Penna[2,4])
[1]Universidade de Brasilia, Brazil; [2]FGA-Universidade de Brasilia, Brazil; [3]Universidade Federal de Goias, Goiania, Brazil; [4]International Center for Condensed Matter Physics, Brasilia DF, Brazil

Abstract: The violation of the Ergodic Hypothesis have been discussed in recent investigations about diffusion[1,2,3]. We give here a practical character to this concept, i.e. we make that the basic concept within pattern formation in bacterial growth and diffusion. The violation of ergodicity may leed to the lack of a detailed balance relation wich may require a specific analysis of each case [3]. In this communication we propose a most general equation[4] to study pattern formation for one-species population and their limit domains in systems of length L.

Talks (continued)

To accomplish this we include non-locality in the growth and competition terms where the integral kernels are now depend on characteristic length parameters α and β. Therefore, we derived a parameter space (α, β) where it is possible to analyze a coexistence curve $\alpha^* = \alpha^*(\beta)$ which delimits domains for the existence (or not) of pattern formation in population dynamics systems. We show that this curve has an analogy with coexistence curve in classical thermodynamics and critical phenomena physics. We have successfully compared this model with experimental data for diffusion of *Escherichia coli* populations.

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A stochastic reaction-diffusion-taxis model for picophytoplankton dynamics
Davide Valenti, University of Palermo, Italy
Abstract: The dynamics of picophytoplankton communities in marine environment is studied by a stochastic reaction- diffusion-taxis model, analyzing the time evolution of the biomass concentration along a water column. The model is based on two stochastic differential equations, where the random fluctuations of the environmental variables are considered by inserting two multiplicative noise terms. Specifically, the model describes the dynamics of diffusion of picophytoplankton biomass and nutrient concentrations. In the proposed model the marine environment is characterized by poorly mixed waters and picophytoplankton is subject to intraspecific competition for light and nutrients. By numerically solving the system equations, we obtain the spatio-temporal dynamics of phytoplankton biomass, nutrients and light along the water column at different depths. The results indicate that the distributions of the picophytoplankton biomass concentration along the water column are characterized by a peak. The comparison with experimental data show that height and localization of these peaks are in a good agreement with experimental maxima obtained from data collected in a real marine ecosystem. Finally, we consider the effect of seasonal variations of temperature by studying the picophytoplankton dynamics in the presence of a periodical driving force. The model proposed represents an improvement of previous deterministic models for phytoplankton dynamics and is able to reproduce the spatio-temporal distributions of picophytoplankton concentration observed in real marine ecosystems.

Talks (continued)

Ergodicity breaking in the context of anomalous diffusion

Aleksander Weron, Wrocław University of Technology, Poland

Abstract: L.Boltzmann in his papers on the kinetic theory of gases introduced a special hypothesis according to which leaving a system in free evolution and waiting for a sufficient long time, the system will pass through all the states consistent with its general conditions, namely with given value of the total energy,[1]. This hypothesis was later called the Boltzmann ergodic hypothesis. With J.W.Gibbs's work and the subsequent arrangement by P. and T. Ehrenfest, this hypothesis acquired a central position in statistical mechanics. At the begining of the 1930s, a complete new and original approach was attempted by G.D.Birkhoff, B.Koopmann and J.von Neumann. They proposed the idea of proving the equality of phase average with inifinite time average without using the Boltzmann hypothesis[2]. A.I.Khinchin in 1949 proposed a new approach to the ergodic problem and maintains that furnishing an approximate method for evaluating phase avaerages is part of the solution to the ergodic problem. The celebrated Khinchin theorem [3] shows that the measure of phase points for which the infinite time average of whatever function differs from the phase average more than a number small as we please, tends to zero. In other words Khinchin links the ergodicity of a physical system with the irreversibility of the corresponding autorelation function. However, the Kchinchin theorem cannot be successfully applied to processes with infinite second moment, in particular to the relevant class of Lévy flights,[4]. In this talk we show how to solve this challenging problem in full generality and clarify the role of ergodicity and ergodicity breaking in the context of anomalous diffusion processes,[5]. Also we demonstrate how to detect ergodicity breaking from experimental data.

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Diffusion of active particles

Lutz Schimansky-Geier, Humboldt-University, Berlin, Germany

Abstract: We introduce equations of motion of particles which convert energy into motion by negative friction. We discuss different random forces which act possibly on the particles and describe then by stochastic differential equations as well as by corresponding probability densities and its kinetics. The case that the particle have a preferred turning angle in their motion is modeled by a Lorentz-like force. Motion with preferred turning angle reduces drastically the diffusion coefficient of the organisms compared to the free situation. It leads to am enhanced consumption of food of these organisms compared to the case of the consumption of freely diffusing particles. We also discuss the motion of cluster of particles in dependence on the intensity of present fluctuating forces.

Talks (continued)

Variational Formulation for the KPZ equation and Recent Developments

Horacio S. Wio[1] (work done with J.A. Revelli[2], C. Escudero[3], R.R. Deza[4])
[1] University of Cantabria, Santander, Spain; [2] University of Cordoba, Argentina; [3]Autonomous University of Madrid, Spain, [4]National University of Mar Del Plata, Argentina

Abstract: It is well known that in the literature associated to growth processes there is a reiterated claim indicating that "the KPZ equation is in fact a genuine kinetic equation describing a nonequilibrium process...that cannot be derived from an effective free energy;..". In opposition to such a statement, here we present a variational formulation for the Kardar- Parisi-Zhang (KPZ) equation leading to a nonequilibrium potential (a kind of thermodynamic- like potential in a far from equilibrium situation) for the KPZ as well as a general form for such thermodynamic-like potential of generalized KPZ and other related kinetic equations [1]. Its knowledge allows us to prove some global shift invariance properties previously conjectured by other authors, and also discuss a few results about the form of the stationary probability distribution function for arbitrary dimensions. In addition, we can extract some strong constraints for the choice of real-space discrete representation schemes , by means of the exploitation of the known fact that the KPZ equation results from a diffusion equation (with multiplicative noise) through a Hopf–Cole transformation. It implies a tight relation between the discrete forms for the diffusive and the nonlinear terms, i.e. they cannot be independent. Whereas the nearest-neighbor discrete representation passes the resulting consistency tests, several known examples in the literature do not. We propose a consistent and highly accurate scheme, and emphasize the importance of the Lyapunov functional as a natural starting point for a real-space discrete representation. As an extremely relevant byproduct, in the light of these findings, the mainstream opinion on the relevance of Galilean invariance in determining the KPZ scaling properties, as well as the fluctuation–dissipation theorem (peculiar of 1D) is challenged [2,3,4]. The results of thorough numerical analysis strongly indicates, in good agreement with some recent theoretical arguments, that the Galilean invariance does not seems to play the relevant role usually assumed in the literature for determining the KPZ universality class. Finally, we discuss further exploitation of the variational approach as well as a new perspective from a path integral point of view that can shed some light over the KPZ dynamics.

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Posters

1.

Rupture dynamics of macromolecules

Jarosław Paturej[1,2] [1]Max-Planck-Institut für Polymerforschung, Mainz, Germany; [2]University of Szczecin, Poland;

Abstract:
In this contribution scission kinetics of polymer molecules induced by constant tensile stress as well as by increase in temperature will be presented.

2.

Some extensions of Lévy walk via coupled continuous time random walk framework

Marcin Magdziarz, Władysław Szczotka, Piotr Żebrowski
Wrocław University of Technology, Poland

Abstract:
Lévy walk is a coupled continuous time random walk in which the length of each jump is equal to the waiting time for this jump to occur. By application of recent results from theory of coupled continuous time random walks we obtain the Langevin form of the stochastic process being a weak limit of sequence of properly scaled Lévy walks. Next we introduce extensions of Lévy walk in which jump sizes are some functions of waiting times. We prove that under proper scalings such processes are weakly convergent and we find Langevin forms of limiting processes. We also investigate asymptotic of mean square displacements for proposed extensions showing that choice of different functions leads to various types of anomalous diffusion.

3.

A novel microfluidic technique of droplets generation

Krzysztof Churski
Institute of Physical Chemistry, PAN, Poland

Abstract:
The most of techniques of microfluidic generation of 'droplets on demand' bases on control of flow of discontinuous phase. The disadvantage of this approach is a hydrodynamic limit for the largest possible to generate droplet - if the 'tongue' of the aqueous phase is too long, it is broken by the continuous phase. Limitation of the range of volumes which we can generate with the use of a standard procedure of droplet on demand systems is a significant problem. It disables formation of droplets with strongly varying concentrations of individual substances. Here we present a solution of this problem. We control the flow of both phases – continuous and discontinuous with the use of external electromagnetic valves. This allow creation of droplets of arbitrarily large volume range, limited only by the geometry of a chip. Moreover, the characteristic of valves is independent of the material of a chip (polycarbonate, polydimethylsiloxane)

Posters (continued)

4.

Microdevices for generation of gradient of chemistry in droplets

Paweł Jankowski , Dominika Ogończyk , Adam Samborski, Judyta Węgrzyn, Piotr Garstecki
Institute of Physical Chemistry, PAN, Poland

Abstract:
We demonstrate fabrication of a microfluidic chip that transforms two miscible and continuous input streams (colorful and colorless water solutions) into a series of streams of droplets suspended in the third, non-miscible fluid (2The process of fabrication of the used microdevice includes milling microchennels with milling machine in polycarbonate (PC) plates and bonding them based on a controlled exposition of the machined material to vapours of solvents and subsequent compression at an elevated temperature below the temperature of glass transition. The last step in preparation of a chip is a modification of the surface of the microchannels. That modification changes the surface properties making them more hydrophilic or hydrophobic, respectively. Our adequately prepared microfluidic chip presents a model demonstration of parallel formation of droplets (in 8 parallel T-junction droplet generators), and, at the same time, utilizes the linear character of flow at low and moderate Reynolds numbers to generate gradients of the concentration of any chemistry in the streams of droplets. Microfluidic devices have been used for many various purposes. The microchip like ours, which enables parallel observation of the influence of different concentrations, could be usefull in experiments involving procedures of optimisation of environment of reaction or conditions necessary to grow living cells.

5.

Numerical investigations of stochastic models for fractional-power-law dielectric relaxation patterns

Agnieszka Jurlewicz, Justyna Trzmiel
Wrocław University of Technology, Poland

Abstract:
We present the results of numerical investigations of stochastic models for fractional-power-law relaxation responses. By means of Monte Carlo methods we analyze the asymptotic behavior of the effective relaxation rate reflecting the internal dynamics of the considered dielectric complex system. Moreover, we discuss the rate of convergence to illustrate the effective-relaxation-rate approximation by its limiting distribution.

6.

Variational approach to tracking cells in microscopic images

Monika Muszkieta
Wrocław University of Technology, Poland

Abstract:
Segmentation and tracking of objects from dynamic microscopy data is of great interest for biomedical applications. In the talk, we will present an variational approach to the problem of cell tracking from the 2D + time sequence of fluorescence microscopy images.

Posters (continued)

7.

Speed of droplets in square microchannels

Sławomir Jakieła, Piotr Korczyk, Sylwia Makulska, Piotr Garstecki
Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland

Abstract: Miniaturization of microfluidic systems is the basis for finding applications in many interesting areas such as biotechnology or biochemistry. Design of automated microchips for reactions inside the droplet requires an understanding of physical phenomena of the transport in microchannels, which is not yet fully known. This transport depends on many parameters, including velocity and viscosity of both phases, as well as surface tension between them. These relations are very sensitive, what brings about difficulty in developing a unified description. Performed experiments are the first fully automated and such a scrupulous attempt to analyze the droplet translation in microfluidic square channels. Obtained results contradict the prevailing assumption, that the droplet speed in the channel is related to its dimensions. Obtained results of measurements show, that not only the length of droplets, but also the differences in viscosities between both phases, have a significant influence on the speed of droplets. This dependence is both quantitative and qualitative. Performed experiments allow to predict the behavior of droplets which is important from a practical point of view in various applications especially when the droplet liquid is less viscous than the continuous liquid.

8.

On the interaction between sodium channels and internal calcium distribution in galvanotaxis

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Abstract: We discuss the galvanotaxis of human breast cancer cells. The research reveals the role of voltage gated sodium channels in the disturbances of calcium distribution which can lead to an asymmetry in the cytoskeleton development on two ends of the cell, initiating cellular movement.

9.

The perturbation method to solve subdiffusion-reaction equations

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Abstract: Subdiffusion-reaction equations are nonlinear differential equations with the Caputo fractional derivative. As far as we know, the exact solutions of these equations remain unknown. In order to find the approximate solutions to the- se equations the quasistatic approximation method and scaling method were mainly used. In our paper we will present an application of the perturbation method to solve subdiffusion-reaction equations and new explicit solutions with corrections of the first and the second order.

Posters (continued)

10.

The nonextensive entropy approach versus the fractional model to describe subdiffusion

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Abstract: In this contribution we will study the similarities and differences between different models describing subdiffusion. We will consider two sets of subdiffu- sive models having different physical origins. The first set contains the models derived from nonextensive entropy and the second contains the fractional model which utilizes a differential equation with fractional derivative. We will find the accordance conditions between models from both sets using first passage time (FPT) distributions, which can be calculated from Green's functions. These Green functions are solutions to the nonlinear differential equations obtained from Sharma-Mittal's, Tsallis's and Gauss's nonextensive entropies for the first set of models, and the linear differential equation with a fractional time deriva- tive for the fractional model. All these Green functions give us exactly the same standard relation $< (\Delta x)^2 >= D_\alpha t^\alpha$ which defines subdiffusion ($0 < \alpha < 1$), but generally FPT's are not equivalent to one another. We will show here that both the FPT distribution and Green's functions for the fractional model are very similar to the Sharma-Mittal model only if in the latter case the parameters characterizing this model depend on α, and satisfy the specific equation. We will also discuss the interpretation of subdiffusion models based on nonextensive entropies and the possibilities of experimental measurement of the subdiffusion model parameters.

11.

Transport control by biharmonic signal in coupled noisy Josephson junctions

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Abstract:
The typical periodic stimulus applied to any mechanical system contains not only fraction with tuned frequency but also higher harmonics with different strengths. We study the system of two coupled noisy Josephson junctions propelled by biharmonic ac current. The influence of the shape of the external signal applied to active junction only on the transport across the passive one is presented.

Posters (continued)

12.

Random search strategies driven by the Lévy walk with bivariate Lévy-stable jumps

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Abstract: The random search strategy driven by the Lévy walk appears to be a useful tool in modelling the movement patterns of foraging animals. In this work we investigate the search strategy driven by the Lévy walk with bivariate Lévy-stable jumps, which is an alternative to well-known random search strategy driven by the Lévy walk with jumps described by Pareto distribution. We compare, via the Monte Carlo simulations, the efficiency of the search strategy for different parameters of bivariate Lévy-stable jump. The optimality of the searching strategy is examined for destructive and non-destructive character of target sites. Moreover, we investigate whether this strategy is advantageous in searching for fractally-distributed targets.

13.

The rigid spheres model as a stochastic discontinuous process

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Abstract: We implement a stochastic microscopic description of the unidimensional model of a gas compounded by rigid spheres submitted to elastic collisions as a further treatment of the theoretical model known as Rayleigh Piston. First, we show how it is possible to express the velocity probability transition of the Brownian particle as a purely stochastic discontinuous process. We perform molecular dynamics simulations to obtain the corresponding Kramers-Moyal coefficients in order to assess the accuracy of this description in the case of our unidimensional model. In the following, we show what are the general prescriptions to construct transition probabilities as stochastic discontinuous processes and apply it in the improvement of the results already obtained in the case of the Rayleigh Piston.

14.

Fractional differential equation for probability density function generated by dynamical system with mixed phase space

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Abstract: We discuss continuous time random walks (CTRW) as a model of momentum diffusion in the modified standard map (MSM). The presence of accelerating modes in the MSM results in spatiotemporal coupling which is described by Lévy walks. In the absence of accelerating modes one observes in the MSM the Gaussian diffusion, therefore we consider both processes - Lévy Walks and standard diffusion and treat them as competing ones. We derive and solve the fractional differential equation for evolution of probability density function. We provide also comparison of the analytical solution with results obtained from numerical simulations of the MSM.

Posters (continued)

15.

Comparative studies of reversible aggregation of X-, T-, and anchor-shaped bolaamphiphiles in monolayers at the air/water interface

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Abstract: We present the results for new compounds from the group of specific surfactants known as bolaamphiphiles. The partially fluorinated bolaamphiphiles exhibit an unusual reversibility of Langmuir isotherms even though compressed at maximum rate of compression up to a total collapse of the film1. Aggregation in Langmuir films is usually meant as a disorderly grouping of the molecules into the chaotic three dimensional aggregates and is considered as unwanted phenomenon causing irreversible changes. The key property of these compounds is partial fluorination of the lateral chains linked to the rigid cores of the molecules. The molecules of different shape (X-, T-, and anchor shaped) are studied. The most interesting feature of the compounds is that depending on shape and degree of fluorination they are able to resist aggregation remaining as a monolayer until relatively high surface pressures (T-shaped molecules), or create bilayers (X-shaped molecules) and trilayers (anchor-shaped molecules).

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16.

Anomalous diffusion models: different types of subordinator distributions

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Abstract: Subordinated processes play an important role in modeling anomalous diffusion-type behavior. In such models the observed constant time periods are described by the subordinators distribution. Therefore on the basis of time series it is possible to conclude on the main properties of the subordinator, like asymptotic behavior of moments, tail characteristics or its distribution. In this paper we analyze the anomalous diffusion models with different types of subordinator's distribution. We present similarities and differences between the analyzed processes and point at their main properties. Moreover we discuss the estimation scheme for parameters of the considered distributions and validate the presented procedure.

Posters (continued)

17.

A stochastic reaction-diffusion-taxis model for picophytoplankton dynamics

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Abstract: The dynamics of picophytoplankton communities in marine environment is studied by a stochastic reaction-diffusion-taxis model, analyzing the time evolution of the biomass concentration along a water column. The model is based on two stochastic differential equations, where the random fluctuations of the environmental variables are considered by inserting two multiplicative noise terms. Specifically, the model describes the dynamics of diffusion of picophytoplankton biomass and nutrient concentrations. In the proposed model the marine environment is characterized by poorly mixed waters and picophytoplankton is subject to intraspecific competition for light and nutrients. By numerically solving the system equations, we obtain the spatio-temporal dynamics of phytoplankton biomass, nutrients and light along the water column at different depths. The results indicate that the distributions of the picophytoplankton biomass concentration along the water column are characterized by a peak. The comparison with experimental data show that height and localization of these peaks are in a good agreement with experimental maxima obtained from data collected in a real marine ecosystem. Finally, we consider the effect of seasonal variations of temperature by studying the picophytoplankton dynamics in the presence of a periodical driving force. The model proposed represents an improvement of previous deterministic models for phytoplankton dynamics and is able to reproduce the spatial distributions of picophytoplankton concentration observed in real marine ecosystems.

18.

Optimization in the resizing procedure for compression purposes

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Abstract: We address the problem of resizing an image as an alternative to the frequency filtering, found for example in the JPEG standards. It is obvious that reduction of the image size reduces the frequency content of the image but the traditional interpolation techniques used in this procedure are concerned with obtaining a high quality resized image rather than obtaining a good compression, with a reasonable PSNR coefficient. In this research we address the problem of downsizing an image in such a way that the resizing back to the original dimensions retains a high contrast of the original image.

Posters (continued)

19.

Induction of bimodal gene expression in open-loop regulatory systems

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Abstract: We will show theoretically that bimodal gene expression can be generated even for the simplest gene regulatory system without deterministic bistability, cooperativity of transcription factor binding and feedback loops [1]. The system is a two-step gene cascade that consists of the regulatory gene producing transcription factors and the target gene. The bimodality is caused by a unimodal distribution of transcription factors having a nonlinear effect on the promoter activity of the target gene. We will present a method of prediction of the bimodality that does not require solving of the master equation and it is only based on a simple geometric construction. This construction involves the parameters of regulatory gene bursting and the dose-response function of the target gene. By means of the method, we will show that the gene expression may switch between unimodal and bimodal as the concentration of inducers/corepressors is varied.

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20.

The Stokes-Sutherland-Einstein equation for scale dependent diffusion of nano-particles in complex liquids

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Abstract: We determine nano-particles diffusion in polymer (polyethylene glycol) solutions as a function of the ratio of the particle size, R, to the radius of gyration, Rg of the polymer. The Stokes - Sutherland - Einstein (SSE) formula with the viscosity of the polymer solution accurately predict particle diffusion coefficient for R>Rg. For R comparable to Rg we report a scale dependent diffusion due to the non-uniform viscosity arising from the layer depleted from polymer coils (depletion layer) around the particles. Inside the depletion layer viscosity is orders of magnitude smaller than the viscosity of polymer solution. We determine diffusion coefficients at large and short spatial scale and the size of the depletion layer as a function of polymer concentration.

Posters (continued)

21.

Structure and morphology analysis of magnetic membranes used in the air separation

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Abstract: Structure and morphology of dense polymer membranes with dispersed magnetic powder (magnetic membranes) for air separation were investigated. Study of transport processes in the air separation using polymeric membranes with magnetic powder was performed experimentally [1, 2]. Based on experimental data we have observed that enrichment of air in oxygen rises with the increase of magnetic powder amount (magnetic induction) and decrease of its granulation. We have used fractal analysis for qualitative and quantitative description of structure and morphology of membranes with dispersed magnetic particles based on the generalized fractal dimension and f(alpha) formalism [3]. We have found that structure of magnetic powder in membranes are fractals with fractal dimension df = 1,44-1,87. These fractals have stochastic characteristics (multifractal spectrum has light asymmetry and the value of DD=0,27-0,41). Such fractals have smaller complexity, larger homogeneity and self-similarity, which grows with increase of amount of magnetic powder and decrease of powder granulation.

Acknowledgements: The authors would like to thank The Ministry of Science and Higher Education for providing financial support under the project N N508 409137

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Posters (continued)

22.

Diffusion on fractal structure of polymeric membrane with magnetic powder

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Abstract: The problem of a membrane air separation in the presence of a magnetic field is considered by our team from several years [1, 2]. We observed that external field i.e. magnetic field, amount and granulation of added magnetic neodymium powder remarkably influence the oxygen content in permeate. In this paper we focus our attention on understanding the anomalous diffusion on fractal structure of polymer membrane with dispersed magnetic powder. Such membrane is a medium with penetrant-scale gaps whose size and position are changing randomly, and it exhibits distinctive fractal characteristics and can be described by using the fractal geometry (fractal dimension df, generalized fractal dimension Dq). We will simulate structures with the same value of fractal parameters as for real membranes and random walk dimensions will be evaluated. The diffusion equation with a spatial dependent diffusion coefficient of self-similar type to describe diffusion processes in the aforementioned membranes will be proposed.

Acknowledgements: The authors would like to thank The Silesian University of Technology for providing financial support under the project BK-M 228/RCh-4/2011 and The Ministry of Science and Higher Education for providing financial support under the project N N508 409137

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23.

Fuzzy analysis of the cancer's risk factor

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Abstract: Using fuzzy set theory, we have created a system which allows predicting type of cancer on the basis of the largest risk factors for particular patient. We have taken into account lung, colon, breast, colorectal, stomach, cervical and prostate cancer. In our analysis we have used the Mamdani model which is implemented in the Fuzzy Logic Toolbox in Matlab. As inputs to our system we have taken genetic, biological (race, age, sex) and behavioral (overweight, alcohol consumption, tabacco smoke) risk factors. The output was "the kind of cancer". This study suggests that fuzzy logic can be an effective tool in dealing with this kind of medical problem.

Posters (continued)

24.

Percolation phenomena in polymeric membranes with magnetic particles

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Abstract: Transport properties in disordered systems are often described using percolation theory. In many fields polymeric membranes with additional particles to gas separation are used. These materials are of great interest because of mixed components with different properties. Mixing the various components can help to overcome the respective drawbacks like low selectivity or low permeability of separating chemical species [1]. In our work, we consider the influence of structural properties of a polymer membrane with magnetic powder on the gas transport through this object [2-3]. This process can be considered as percolation process [4]. The percolation paths in scanning microscope image of polymeric membrane with magnetic powder are observed. The physicochemical structure of polymer affects the percolation threshold and the percolation concentration. Membranes with various amount and granulation of magnetic powder have different topological structures and may lead to different behaviours of the penetrant.
Acknowledgements: The authors would like to thank The Ministry of Science and Higher Education for providing financial support under the project N N508 409137.

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Posters (continued)

25.

Enhanced Escape Times of Interacting Brownian Particles

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Abstract: We investigate a diffusive motion of interacting Brownian particles in quasi-one-dimensional micropores. The small diameter of the pore imposes the non-crossing condition for the trajectories of the individual particles. In particular, we consider a semi-infinite 1D geometry with an imperfectly absorbing boundary and the hard-core inter-particle interaction. Due to the absorbing boundary the number of particles in the pore gradually decreases. We present an exact analytical solution of the problem. Our procedure merely requires the knowledge of the corresponding one-particle problem. At the initial time we assume a general N-particle probability density. First, we calculate the simultaneous probability density of having at a definite time still a definite number $N - k$ of surviving particles at definite coordinates (i.e., k particles have already left the pore). Focusing on an arbitrary tagged particle, the marginal probability density of its coordinate simply follows by spatial integrations of many-particle densities. Secondly, we present a complete probabilistic description of the emerging escape process. The distribution functions for the escape times of the individual particles and the corresponding mean lifetimes have been calculated. Generally speaking, although the original inter-particle interaction possesses a point-like character, it induces entropic repulsive forces which, e.g., push the leftmost (rightmost) particle towards (opposite) the absorbing boundary thereby accelerating (decelerating) its escape. More importantly, as compared to the reference problem for the non-interacting particles, the interaction changes the dynamical exponents which characterize the long-time asymptotic dynamics.

26.

Learning invariant color features with Sparse Topographic Restricted Boltzmann Machines

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Abstract: Our objective is to learn invariant color features directly from data via unsupervised learning. We introduce a method to regularize restricted Boltzmann machines during training to obtain features that are sparse and topographically organized. Upon analysis, the features learned are Gabor-like and demonstrate a coding of orientation, spatial position, frequency and color that vary smoothly with the topography of the feature map. There is also differentiation between monochrome and color filters, with some exhibiting color-opponent properties. We also found that the learned representation is more invariant to affine image transformations and changes in illumination color.

Posters (continued)

27.

Effect of a fluctuating electric field on electron spin dephasing in III-V semiconductors

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Abstract: In the present work we investigate electron spin relaxation in low-doped n-type GaAs semiconductor bulks driven by a static electric field. The electron dynamics is simulated by a Monte Carlo procedure which keeps into account all the possible scattering phenomena of the hot electrons in the medium and includes the evolution of spin polarization [1-2]. Spin relaxation lengths are computed through the D'yakonov-Perel process [3], which is the only relevant relaxation mechanism in zinc-blende semiconductors [4-5]. Since semiconductor based devices are always imbedded into a noisy environment that can strongly affect their performance, the decay of initial spin polarization of conduction electrons is calculated in the presence of a fluctuating component added to the static driving electric field. The starting point for our analysis is the computation of changes in the depolarization length caused by the addition of an external correlated noise source, at different values of field strength, lattice temperature, doping density, noise amplitude, noise correlation time, etc. Our findings show that, only for values of noise correlation time comparable to the dephasing time, relaxation lengths decrease with the increasing of noise intensity. Moreover, for each value of the noise amplitude, a nonmonotonic behavior of spin depolarization length with the noise correlation time is found. The presence of a minimum is well explained by studying the effective mean electric field experienced by the electrons ensemble within the relaxation time. Furthermore, our study reveals that the system receives a benefit in terms of weakening of the length reduction by the inclusion of the electron-electron scattering mechanism. This effect will be also discussed.

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Posters (continued)

28.

Modeling of the fractional dynamics based on experimental studies of the ammonium dihydrogen phosphate $NH_4H_2PO_4$: porous glass composites

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Abstract: The fingerprint of the fractional dynamics is seen in the non-Debye relaxation behaviour of the investigated system. A deviation from the classical Debye pattern is represented by the low- and high-frequency power-law dependency of the complex dielectric permittivity $\varepsilon(\omega) = \varepsilon'(\omega) - i\varepsilon''(\omega)$ in frequency:

$$\begin{aligned} \varepsilon''(\omega) &\propto (\frac{\omega}{\omega_p})^m, \quad \omega = \omega_p \\ \varepsilon''(\omega) &\propto (\frac{\omega}{\omega_p})^{n-1}, \quad \omega \neq \omega_p \end{aligned} \tag{1}$$

where ω_p denotes the loss peak frequency and the power-law exponents m and n fall in the range of (0, 1). The above relaxation behavior, characteristic for dipolar complex systems, was observed by us in ammonium dihydrogen phosphate NH4H2PO4 (ADP) ferroelectric crystals placed into porous silica glass matrix. The power-law exponents, obtained for this nanocomposite, satisfy relation m<1-n. This property is characteristic for the so called 'less typical' relaxation data which, unfortunately, cannot be interpreted by means of the well-known Havriliak-Negami function, yielding the opposite inequality m 1-n [1]. In order to explain the origins of such a relaxation response of ADP nanocrystals we propose a correlated-cluster relaxation model leading to a new relaxation pattern recently derived by Stanislavsky and Weron [2]

$$\phi^*_{JWS} = 1 - \frac{1}{\left[1 + \left(\frac{i\omega}{\omega_p}\right)^{-\alpha}\right]^\gamma}, 0 < \alpha, \gamma < 1 \tag{2}$$

Formula (2) is the explicit frequency-domain representation of the generalized Mittag-Leffler relaxation response derived for the first time in the continuous time random walk framework by Jurlewicz and Weron [3]. We show that the JWS function (2) is able to reproduce relaxation patterns obtained for the studied ADP nanocomposite. The proposed model, taking into account the local randomness resulting from the microscopic anisotropy of this material, allows one to investigate mutual correlations between the NH4+-HPO-4 dipoles formed in the system and brings into light the scale invariant spatio-temporal properties of the studied nanocomposite. We believe that this study will not only broaden the knowledge on the properties of this important, from the practical point of view, class of ferroelectric materials but also provide useful tools to find the microscopic origins of the two-power-law dielectric relaxation responses for which m<1-n.

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Posters (continued)

29.

Studies of the low-frequency dispersion in bioglass composite materials. Continuous time random walk model

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Abstract: Recent advances in material engineering resulted in manufacturing of biocompatible materials which can be used as a bone implants. Such an application is possible due to the fact that these materials posses an ability to bond chemically to bone through a biologically active layer of bonelike apatite. In order to understand the mechanisms of bioactivity it is of a great importance to investigate the surface charge dynamics of such composite materials. We analyze the dielectric properties of the gel-derived CaO-SiO2-P2O5 glasses coatings on corundum porous material which can be used as a bone implant core. The effect of a physiological solution on the surface properties of bioglasses and composites slightly differing in their chemical compositions were examined by impedance spectroscopy. It was found that the investigated samples of the bioglass composites exhibit the fractional power-law behavior

$$\chi'(\omega) \sim \chi''(\omega) \sim (\frac{i\omega}{\omega_c})^{n_1-1}, \quad \omega < \omega_c$$
$$\chi'(\omega) \sim \chi''(\omega) \sim (\frac{i\omega}{\omega_c})^{n_2-1}, \quad \omega > \omega_c$$

with the power-law exponents $0 < n_1 < 0.5$ and $0 < n_2 < 1$. Such a response with characteristic overlap at a crossover frequency ω_c is known as a low frequency dispersion (LFD). The obtained results indicate that a certain type of ion hopping transport mechanism may take place at the bioglass – submicrocrystalline corundum grains interface. A continuous time random walk approach is applied to analyze this phenomenon. Within the proposed model the complex internal dynamics of the investigated composites is considered. The properties of trapping times and the hopping charge step length underlying the experimentally observed LFD-type of response are specified. It is shown that the observed relaxation response can be attributed to the self-similar character of the transport mechanism.

Posters (continued)

30.

The simultaneous adsorption two types of latex particles. Comparison of theory with experiment.

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Abstract: Irreversible deposition process of a mixture of latex particles (142 and 551nm) was studied experimentally and theoretically. Particles properties were measured in an environment characterized by various parameters (ionic strength 0.15M – 10-4 M and pH 3-10). Experimentally it was found that pH has no impact on hydrodynamic particle radius. Theoretical results were derived from RSA (random step adsorption) algorithm. To model intermolecular forces hard-sphere and screened electrostatic potentials were used. The maximal surface coverage was calculated for different bulk particles concentration ratio between 10:1 and 1:10. The surface structure dependence on coverage and also on large to small particles ratio were also investigated. It was interesting to find changes of small particles surface concentration versus time of adsorption experiment.

31.

Ordering in a fibrinogen layers.

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Abstract: Ordered protein layers are active field of biomedical research, because usually they have interesting physicochemical properties like permeability, stiffness and pours structure. In presented work we focused on layers build of fibrinogen molecules characterized by strong shape anisotropy. Using RSA (Random Sequential Adsorption) we simulated adsorption process where orientation of adsorbate was given by a non-uniform probability distribution. Thus obtained covering layers were characterized by different global orientational ordering. This allowed finding dependence between main properties of layers, like maximal random coverage ratio, and an order parameter. For better description and deeper understanding of obtained structures the autocorrelation function and distribution of uncovered space were designated. Additionally we calculated the ASF (Available Free Surface) function, which is essential in finding adsorption kinetics.

Posters (continued)

32.
Adsorption on fractal collectors.
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Abstract: Coverage ratio is a basic characteristic of layers, produced in adsorption process. Measured values of a random maximal coverage for one-, two- and three-dimensional collectors can suggest a possibility of some scaling behaviour. To test this hypothesis we performed numerical study of irreversible adsorption of spherical molecules over collectors characterized by fractional dimension. Results presented here were obtained by utilising RSA (Random Sequential Adsorption) algorithm with Sierpinski Triangle, Sierpinski Carpet, General Cantor Set and similar fractals as a collector for adsorption process.

33.
Kinetic equation for the self-correlation function in external non-conservative field
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Abstract: It is considered an auxiliary distribution function $f(k, v_1, t)$ for a dilute gas subject to an external non-conservative potential in frame of classical statistical mechanics. Integration of $f(k, v_1, t)$ with respect to v_1 yields the intermediate scattered function $I_s(k, t)$ being a Fourier transform of the van Hove function $G_s(r, t)$. A kinetic equation for $f(k, v_1, t)$ is derived by the technique of projection operators applied to the appropriate Liouville equation. Equation the right-hand side of which has a time-convolution form, describes the Brownian motion of a marked particle scattered by anonymous non-localized particles of the gas. The limiting cases of k->o and gas of hard spheres are discussed.

34.
Competing contact processes on the Erdos-Renyi network with tunable clusterization
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Abstract: We investigate the random Erdos-Renyi network with tunable clustering coefficient <C>. The network is an area of the two opposite contact processes, where nodes can be in two states, S or D. A node in state S becomes D with probability 1, if at least two its mutually linked neighbours are in state D. A node in state D becomes S with a given probability p if at least one its neighbour is in state S. At $p = p_{crit}$, the system is in a stationary state. The competition between the processes is described by a phase diagram, p_{crit} against <C>. In particular, p_{crit} is positive when <C> is larger than its critical value.

Posters (continued)

35.

A probabilistic model of anomalous multiplicity fluctuations in high-energy hadron-nucleus collisions

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Abstract: High-energy hadrons collisions observed in particular in the Large Hadron Collider are attended by production of greate numbers of secondary particles. The peculiarity of this process is in high level of relative fluctuations in multyplicity, power-type increasing of the mean multiplicity with the total energy and the so-called leading-effect: about a half of the total energy is taking away with only one of the produced particles. Because of the evident inconsistency of these features with a classical statistical scheme, they are intetrpreted as a consequence of dynamical processes. The present report shows that all these property can be revealed in frame of a very simple kinematic model assuming that the virtual particle produced by collision are mutually independent and becomes real particles in case their total energy coincide with the collision energy. A keystone of the model is the energy spectrum of virtual particles. If it possesses a finite second moment, we observe a classical picture: the mean multiplicity inreases linearly with the total energy E, fluctuations rapidly fall and the leading is absent. However, if the spectrum has a power-type heavy tail, that is belongs to the domain of attraction of Lévy-stable laws, we meet all above-mentioned pecularities observed in experiments. As follows from this result, the kinematic constrains together with the Lévy-stable statistics can mimic dynamical effects, and this should be taken into account when analyzing new experimental results.

36.

Complex network models of intramolecular dynamics of biological molecular machines

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Abstract: The central task of biological molecular machines is the free energy transduction in a system of coupled biochemical reactions. The significant role in these processes plays the internal dynamics of conformational transitions within the native protein domains. To this end the models of random walks on the complex networks joining a set of conformational sub-states is to be proposed. The application of Monte Carlo simulations allows to estimate a few thermodynamic quantities which explicitly characterize the action of the machine: the degree of coupling of the fre energy-donating and the free energy-accepting reactions, the flux-force dependence for the two coupled reactions and the efficiency of the machine.

Posters (continued)

37.

Analysis of polymer fragmentation in extensional flow: simulation and theory

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Abstract: In this work we present an analysis of fragmentation of dilute polymer solutions in extensional flow. In order to gain an insight into the process of polymer fragmentation we shall perform Langevin dynamics simulations of a chain with N beads of mass M in a center-symmetrical extensional flow. The simulation model attempts to incorporate just enough details to observe fragmentation without impeding the efficiency of the simulation. As a result, we ignore the internal dynamics of the beads and treat them as particles of mass M. The theoretical analysis was made by the effective potential of breaking. The intra chain interaction is given by a 12:6 Lennard-Jones potential and the interaction with the fluid by a viscous force proportional to the relative velocity VF between the chain and the extensional flow. The effective potential for a polymer in an extensional flow allows the study of the fragmentation process as a generalized thermal activation process over a barrier. The simulation shows that the time variation of breaking with the temperature is an Arrhenius process with activation energy Es. The activation energy Eb determined from the effective potential approaches from Es only at low temperatures: Eb>9kbT (N = 100, VF = 0.02 and g=0.25. wo is the friction constant and wo is the maximum phonon frequency). The dispersion of breaks with temperature s also shows a good agreement between theory and simulation. For small values of Eb argument is excellent. New theoretical [4,5] results stimulates more research in this field.

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Posters (continued)

38.

Analytical results for long time behavior in anomalous diffusion

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Abstract: We investigate through a Generalized Langevin formalism the phenomenon of anomalous diffusion for asymptotic times. To confirm our analytical re- sult, we have also developed a computational algorithm to calculate some quantities like correlation function, diffusion coefficient and mean square dis- placement, necessary to identify the type of diffusion mechanism [1]. The results are then compared through the introduction of a time scaling factor, and very good agreement is observed, between both methods for intermedi- ate and long times. The result is general and may be applied to many types of diffusion regimes. This analytical result is important to discuss some im- portant aspects of physics, such as the violation of the Ergodic Hypothesis discussed in recent investigations about diffusion[2,3,4].

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39.

Three-dimensional simulations of nucleus architecture

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Abstract: Motivation: many experimental studies suggest correlation between topological proximity of chromosomes located inside cell nucleus and frequency of interchromosomal translocations observed after ionizing radiation. Additionaly, relations between genomic regions, gene activity and relaxation of local chromatin structure are elaborated. Purpose: to model chromosomal rearrangement in human lymphocyte nuclei by performing computer MC simulations incorporating two different packing modes have been analyzed. Based on information of radial distance between the nucleus center and mass center of a chromatin domains and chromosome territories with respect to DNA content of each chromosome are investigated.

Posters (continued)

40.

Understanding disease control: influence of epidemiological and economic factors

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Abstract:
The goal of our work is to find optimal control strategy of epidemics. We have considered an extended SIR model including pre- and symptomatic cases for a disease spreading on a regular network. The effective treatment strategies for a disease control are expected to minimize the total cost of an epidemic. However, in designing efficient control strategies, we have to consider both – epidemiology and economics. The most optimal control is determined by the relative costs of treatment and infection, as well as by the initial distribution of infectious cases and kinetics of its spread and transformation. We have shown that even if the knowledge of a pathogen is limited, or its origin is unknown, one is still able to make a valuable prediction about the evolution of the epidemics, based on the economic analysis only. Although economics determines control strategies, the range of applicability of chosen scenarios depends strongly on epidemiological factors such as infectiousness, detectability, recovery, removal and map of contacts in population. Some of those factors such as e.g. contagion or mortality are specific for a particular disease and hard to control. On the other hand, we can have an influence on some parameters affecting kinetics of the epidemics spread. For example, the quicker the symptoms occur or the higher is the recovery level, the smaller control radius can be applied. Additionally, we have analyzed the relationship between an efficient control and the size of an infected neighbourhood.
Our studies allow to devise the most influential epidemiological parameters for such a control.

41.

The polymer chain dynamics driven by the spatially correlated noise.

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Abstract: In our work we have examined the influence of the purely spatially correlated noise on a 2D polymer-like chain modeled with harmonic bonds and angular interactions and a global Lennard-Jones potential. Simulations show that as the noise correlation length is increased, the synchronization of beads motion occurs and correlations between conformation transitions are affected.

Posters (continued)

42.

Dynamics of Maximal Entropy Random Walk: Solvable Cases

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Abstract: We consider the Maximal Entropy Random Walk (MERW) on graphs (Burda, et al. 2009), which maximises entropy globally (which means all paths of a given length and endpoints are equally probable) in contrast to the Generic Random Walk (GRW), which maximises entropy locally (moves to neighbouring nodes are chosen with equal probabilities). Any impurities on a graph affect MERW non-locally, in contrast to GRW. The most spectacular difference is the localisation phenomenon, which arises in the case of weakly diluted lattices, where a particle performing MERW eventually gets trapped in the largest nearly spherical region which is free of impurities (Burda, et al. 2010). We obtain the stationary state probability distribution (given by the eigenvector to the largest eigenvalue of the graph's adjacency matrix) for the case of Cayley tree (Bethe lattice) with arbitrary number of generations, branching parameter and degree of the root. While the probability distribution for GRW concentrates in the last but one generation of the tree, the stationary state for MERW has high occupation probability near the root. We also show that the second largest eigenvalue of the adjacency matrix does not suffice to describe relaxation process of the probability distribution to the stationary state. We also consider relaxation dynamics on defected ladder graphs. In the case of GRW, we observe the usual scaling relation between the relaxation time and the system size with the exponent of two. In the case of MERW, however, where the stationary distribution is localised in the regions free of defects, we find that for a given size of the ladder the relaxation time grows exponentially with the gap size (i.e. a number of consecutive rungs taken out of the ladder).

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43.

Modeling Energetics of Kinesins with Different Approaches

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Abstract: Motor proteins, sometimes referred to as mechanoenzymes, are a group of proteins that maintain a large part of intracellular motion. Being enzymes, they undergo chemical reactions leading to energy conversion and changes of their conformation. Being mechano, they use the chemical energy to perform mechanical work, leading to the phenomena of motion. We present three complementary approaches to modeling kinesin's step-by-step walk along its microtubular tract (MT). We show how by combining those techniques one may gain deeper understanding of mechanoenzymes' behavior in crowded intracellular environment in presence or absence of an external force (e.g. load force).

Posters (continued)

44.

Biaxial phase in nematic liquids under influence of external fields

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Abstract: By means of Monte Carlo lattice simulations and generalized Landau expansion we study the effects of interaction with an external field (magnetic or electric) on the biaxial nematic phase in a minimal-coupling model of interacting quadrupoles [1-3]. The field is coupled to the quadrupolar tensor in the second order. Phase diagrams in the space of temperature and field magnitude are found for different biaxiality parameters, including the self-dual Landau point of the zero-field model. Cases of both positive and negative molecular anisotropy are studied. The familiar phase transition sequence: I→NU→NB is altered. In the case of positive anisotropy, the high-temperature I→NU transition ends at a critical point. In the case of negative anisotropy a tricritical point for the NU→NB transition is found. The resulting phase transition sequences are presented on phase diagrams in the experimentally relevant range of parameters.

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XXIV Marian Smoluchowski Symposium on Statistical Physics Zakopane, Poland September 17–22, 2011

Insights into Stochastic Nonequilibrium

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