25th Marian Smoluchowski Symposium on Statistical Physics

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25th Marian Smoluchowski Symposium on Statistical Physics

Sunday 09 September 2012 - Thursday 13 September 2012

Book of abstracts

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Proceedings

As usual, proceedings of the Symposium are going to be published as a special issue of *Acta Physica Polonica B*, a refereed journal recognized by The European Physical Society and Philadelphia Institute of Scientific Information. Everybody is encouraged to contribute, but the invited talks are particularly welcome. However, **all** contributions will go through the regular editorial process, inculding peer review.

Please, visit the publishers' website for instructions to authors. Please, send your contribution to the following address only: **zfs@th.if.uj.edu.pl**. Your contribution should by typeset in LaTeX, figures in Encapsulated PostScript. We are sorry but we will not be able to handle other formats, including MS Word. Please, include a PDF of your contribution with your submission.

The submission deadline is **January 4, 2013**.

Poster Session / 17

Stochastic thermodynamics of small systems: from micro over meso to macro

Mr. ALTANER, Bernhard [1]; Dr. VOLLMER, Jürgen [1]

[1] *Max-Planck-Institute for Dynamics and Self-Organization, Göttingen*

Entropy and entropy production in non-equilibrium systems are key concepts in modern statistical physics. Stochastic thermodynamics and fluctuation theorems readily make use of these notions, though often the interpretation of the mathematical statements can be challenging.

The reason for this is twofold: Firstly, information theory, dynamical systems theory and the theory of Markov processes feature different entropy-like quantities. Secondly, stochastic thermodynamics is considered to describe "small systems" in a "thermodynamic environment" rather than classical (macroscopic) thermodynamic systems.

In our work we connect modern stochastic thermodynamics [1] to results from dynamical systems theory [2]. We give the definition of a small system in a thermodynamic environment and show how entropic quantities from dynamical system and information theory connect to those known from Markov processes. An application coming forth from this enterprise is a method for coarse-graining of finite Markov processes that effectively preserves fluctuations of thermodynamic observables [3].

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Poster Session / 16

Computation of interfacial free energies by non-equilibrium work methods

Dr. BENJAMIN, RONALD [1]; Prof. HORBACH, Juergen [1]

[1] *Heinrich Heine University, Düsseldorf*

Computation of interfacial free energies by thermodynamic integration is computationally expensive and in some cases not possible due to lack of a reversible path connecting the initial and final states. Here, we show that such interfacial free energies can be computed with relatively less computational effort by using the recently derived non-equilibrium fluctuation relations and applying to the Lennard Jones model. Our approach will be mostly useful in cases of complex potentials and in situations where a reversible path could be difficult to achieve.

Thursday Session / 105

Power law behavior in the ion traffic through a lipid bilayer at the melting transition

Dr. GALLAHER, Jill [1]; Prof. BIER, Martin [2]

[1] *Moffitt Cancer Institute*

[2] *East Carolina University*

Power law behavior and 1/f Noise have been observed in currents through ion channels and in the voltage noise across the membrane of live cells. I will show how and why 1/f noise appears in currents through lipid bilayers at the melting transition. It appears to be one of the few cases where the emergence of power laws and 1/f noise can be fully understood. The mechanism appears robust and may share an underlying logic with Zipf's Law and Gambler's Ruin. Possible universalities will be discussed.

Tuesday Session / 71

Overdamped motion in two-dimensional septate channels

Dr. BORROMEO, Marcello [1]

[1] *Universita' di Perugia*

Brownian transport in compartmentalized channels has applications both in natural and artificial devices. While motion 2- and 3 dimensional channels, with walls smoothly depending on the position, can be reduced to a 1-dimensional process, this does not hold for septate channels, that have sharp geometries. The driven motion of overdamped particles in these channels is analysed in several channel types, built with different rectangular cells, measuring mobility and diffusivity.

Poster Session / 24

Recognition of stable distribution with Lévy index alpha close to 2

Dr. BURNECKI, Krzysztof [1]; Dr. WYLOMANSKA, Agnieszka [2]

[1] *Wroclaw University of Technology*

[2] *Hugo Steinhaus Center Institute of Mathematics and Computer Science Wroclaw University of Technology*

We address the problem of recognizing alpha-stable Lévy distribution with Lévy index close to 2 from experimental data. We are interested in the case when the sample size of available data is not large, thus the power law asymptotics of the distribution is not clearly detectable, and the shape of empirical probability density function is close to a Gaussian. We propose a testing procedure combining a simple visual test based on empirical fourth moment with the Anderson-Darling and Jarque-Bera statistical tests and we check the efficiency of the method on simulated data. Furthermore, we apply our method to the analysis of turbulent plasma density and potential fluctuations measured in the stellarator type fusion device and demonstrate that the phenomenon of L-H transition occurring in this device is accompanied by the transition from Lévy to Gaussian fluctuation statistics.

Poster Session / 62

Population ratio between stable states in the presence of a weak temperature gradient

Mr. CAMBONI, Federico [1]; Prof. SOKOLOV, Igor [2]

[1] *Institut für Physik, Humboldt-Universität zu Berlin*

[2] *Institut für Physik, Humboldt Universität zu Berlin*

We let a particle diffusing in a random one-dimensional potential landscape in the presence of a weak temperature gradient and focus our attention on the ratio between the populations of two adjacent steady states. Inspired by a seminal paper published by R. Landauer in 1988, we show the way the temperature inhomogeneity enters the expression of this ratio and, using the same words of Landauer, the way it is affected by "the noise along the whole path connecting the competing states". As an example, we finally consider the simple case in which the model is a pure trap one and potential wells are purely harmonic.

Sunday Session / 82

Facing the coming scientific and social challenges: The role of the NSP division of EPS

CARBONE, Anna [1]

[1] *Politecnico di Torino*

The talk will be addressed to understand the emerging needs of our society and their interlinks to science and technology. A brief history of the role EPS will be given with the main purpose to highlight and compare its areas of excellence. Which actions have been undertaken ? Which ones should be envisaged for the coming decade? The challenges are big and diverse, a concerted cross- disciplinary view seem to be the winning strategy.

Poster Session / 111

Domain structure created by irreversible adsorption of dimers

Dr. BARBASZ, Jakub [1]; Mr. CIESLA, Michal [2]

[1] *Instytut Katalizy i Fizykochemii Powierzchni PAN im. Jerzego Habera oraz Zakład Fizyki Statytycznej FAIS UJ*

[2] *Jagiellonian University*

Structure of monolayers arising during adsorption process is strongly related to properties of adsorbed particles. The most important factor here is its shape. For example, during adsorption of elongated molecules the orientational ordering can appear inside a coverage. Presented work shows that even with no global orientational ordering, layers build of simplest anisotropic molecules like dimers can have orientationally ordered domains. Our investigations focus on dependence between domain size distribution and the environmental parameters like ionic strength, which affects the range of an electrostatic interaction between molecules.

Poster Session / 112

Maximal random packing of spheres in Menger sponge

Dr. BARBASZ, Jakub [1]; Mr. CIESLA, Michal [2]

[1] *Instytut Katalizy i Fizykochemii Powierzchni PAN im. Jerzego Habera oraz Zakład Fizyki Statytycznej FAIS UJ*

[2] *Jagiellonian University*

Maximal random packing of spheres on collectors having fractal dimension d<3 was studied. The packings were generated numerically using RSA (Random Sequantial Adsorption) algorithm. Three dimensional balls were put inside Menger Sponge like fractals. Dimension of the sponge was controlled by the number of subcubes removed in each iteration during fractal creation process. The work focuses mainly on maximal random packing ratio. Additionally, RSA kinetics and density autocorrelations inside packings were measured and compared with theoretical predictions.

Wednesday Session / 106

An RSA of polymers

Mr. CIESLA, Michal [1]

[1] *Jagiellonian University*

Random Sequential Adsorption (RSA) of polymers is systematically studied.
The work focuses on maximal random coverage ratio and adsorption kinetics dependence on polymer size, shape anisotropy and numbers of degrees of freedom. The polymer was modelled as a chain of identical spheres. To precisely control anisotropy and degrees of freedom two different kinds of polymers were used. In the first one monomers were placed along a straight line whereas in the second one particles relative orientations were totally random. Such polymers filled randomly flat homogenous surface. Obtained results were discussed and compared with other numerical experiments and theoretical predictions.

Poster Session / 110

Tracer diffusion inside fibrinogen layers

Mr. CIESLA, Michal [1]; Prof. GUDOWSKA-NOWAK, Ewa [1]

[1] *Jagiellonian University*

We investigate motion of tracer particles in crowded environment by carrying simulations of two-dimensional Gaussian random walk in model fibrinogen monolayers of different orientational ordering. The fibrinogen molecules are significantly anisotropic and therefore they can form structures where orientational ordering, similar to the one observed in nematic liquid crystals, appears. Here, ordered layers are generated numerically by using Random Sequential Adsorption (RSA) algorithm. The work focuses on dependence between level of the orientational order (degree of environmental crowding) inside a layer and non-Fickian character of the diffusion process of spherical tracer particles moving within the domain. In particular, it is shown that in general particles motion is subdiffusive and strongly anisotropic, and it's characteristic features significantly change with the orientational order parameter.

Poster Session / 60

A stochastic reaction-diffusion-taxis model for two picophytoplankton populations

Mr. DENARO, Giovanni [1]; Dr. VALENTI, Davide [1]; Dr. LA COGNATA, Angelo [1]; Prof. SPAGNOLO, Bernardo [2]; Dr. BONANNO, Angelo [3]; Dr. BASILONE, Gualtiero [3]; Dr. MAZZOLA, Salvatore [3]; Dr. ARONICA, Salvatore [3]

[1] *Dipartimento di Fisica, Universita' di Palermo*

[2] *University of Palermo*

[3] *Istituto per l'Ambiente Marino Costiero, CNR, Campobello di Mazara, Trapani*

In this work, the stationary distributions of two populations of picophytoplankton, i.e. picoeukaryotes and Prochlorococcus, are studied. This two groups account on average for 60% of the total chlorophyll a (chl a) and divinil chlorophyll a (divinil chl a) concentration in Mediterranean Sea. The interaction of these populations with the environment occurs through two factors that limit the growth of the aquatic microorganisms: light intensity and nutrient, i.e. phosphorus. The dynamics of the two picophytoplanktonic groups, distributed at different depth along a water column (one-dimensional spatial domain), is analyzed starting from a deterministic reaction-diffusion-taxis model. This consists of a system of three differential equations and an auxiliary equation for light intensity. By numerical methods we calculate the stationary solutions for the spatial distributions of the picophytoplankton biomass along the water column, obtaining the corresponding content of chlorophyll a and divinil chlorophyll a concentration. The results indicate the presence of a maximum of the total concentration of chl a and divinil chl a at a certain depth. Magnitude and localization of this maximum are in a good agreement with experimental findings. In order to consider the effect of the random environmental fluctuations, we modify our equations, by inserting sources of multiplicative white Gaussian noise, then we calculate from the stochastic model the new distributions for the chl a and divinil chl a concentration. The results show that position, shape and magnitude of the peaks agree with the experimental data better than those obtained from the deterministic model.

Poster Session / 115

Entropic effects in formation of chromosome territories: towards understanding of radiation-induced gene translocation frequency

DEPERAS-STANDYLO, Joanna [1]; Mr. CIESLA, Michal [2]; Prof. GUDOWSKA-NOWAK, Ewa [2]; Ms. RITTER, Sylvia [3]; Mr. DURANTE, Marco [3]

[1] *M. Kac Complex Systems Research Center and M. Smoluchowski Institute of Physics, Jagiellonian University, Reymonta 4, 30-059 Krakow, Poland*

[2] *Jagiellonian University*

[3] *GSI Helmholtz Centre for Heavy Ion Research, Planckstrasse 1, 64291 Darmstadt, Germany*

A detailed understanding of structural organization of biological target, such as geometry of an inter-phase chromosome, is an essential prerequisite for gaining deeper insight into relationship between radiation track structure and radiation-induced biological damage [1]. In particular, coupling of biophysical models aimed to describe architecture of chromosomes and their positioning in a cell nucleus [2-4] with models of local distribution of ionizations caused by passing projectiles, are expected to result in more accurate estimates of aberration induction caused by radiation.

There is abundant experimental evidence indicating that arrangements of chromosomes in eukaryotic cell nucleus is non random and has been evolutionary conserved in specific cell types. Moreover, the radial position of a given chromosome territory (CT) within the cell nucleus has been shown to correlate with its size and gene density. Usually it is assumed that chromosomal geometry and positioning result from the action of specific forces acting locally, such as hydrogen bonds, electrostatic, Van der Waals or hydrophobic interactions operating between nucleosomes and within their interiors. However, it is both desirable and instructive to learn to what extend organization of inter-phase chromosomes is affected by nonspecific entropic forces.

In this study we report results of a coarse-grained analysis of a chromatin structure modeled by two distinct approaches. In the first method, we adhere to purely statistical analysis of chromatin packing within a chromosome territory. On the basis of the polymer theory, the chromatin fiber of diameter 30nm is approximated by a chain of spheres, each corresponding to about 30 kbp. Random positioning of the center of the domain is repeated for 1000 spherical nuclei. Configuration of the domain is determined by a random packing of a polymer (a string of identical beads) in estimated fraction of space occupied by a chromosome of a given length and mass. The degree of condensation of the chromatin fiber is modeled by changing length of the string: e.g. loosening of the structure is achieved by distributing the chromosome mass into a higher number of smaller beads and tighter configuration corresponds to a lower number of fragments (balls) with a bigger radius. Additionally, for each configuration, a degree of possible overlapping between domains is assumed. This procedure effectively intensifies loosening/tightening of the chromosome structure by changing the radial dimension of the domain while keeping a constant volume of the polymer chain. Such a positioning model is confronted with a minimalistic molecular dynamics model [5] on a similar structure, in which a chain of beads becomes connected by entropic spring energy and subjected to thermal fluctuations.

Comparison of both Monte Carlo models allows to discuss variability of possible configurations as observed in static and dynamic models of chromosome territories along with the effect of compaction and relative arrangements of territorial polymer structures.

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[3] P. Cook and D. Marenduzzo, Journal of Cell Biology 186, 825 (2009).
[4] M. Tark-Dame, R. van Driel, and D. Heermann, Journal of Cell Science 124, 839 (2011).
[5] W. Swope, H. Andersen, P. Berens, and K. Wilson, J. Chem. Phys. 76, 637 (1982).

Poster Session / 52

Brownian motion of nonlinear dynamical systems and the fluctuation-dissipation theorems

Mr. DUBKOV, Alexander [1]; Mr. EFREMOV, Gennady [1]

[1] *Lobachevsky State University*

The consistent statistical approach to derive stochastic equations for nonlinear dynamic subsystem, interacting with Gaussian thermal bath in the presence of external fields, is proposed. Using well-known functional Furutsu-Novikov formula we exclude the thermostat variables and obtain the nonlinear Langevin equations for dynamical system with Gaussian random noises, and their correlation functions are defined on the basis of strong fluctuation-dissipation relations. It should be emphasized that in this approach we do not use the assumptions of Markovianity and small coupling constant which are inherent in the method of kinetic equations. The resulting stochastic equations (containing, in general, in contrast to the Kubo-Mori equations [1, 2], the multiplicative random sources [3]) allow us, in principle, to calculate any statistical characteristics of the subsystem in quasi-equilibrium or far-of-equilibrium states. The devel- oped theory can be easily generalized to quantum systems [4] using the Dirac's quantization rules.

References

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[2] R. Kubo: Rep. Prog. Phys. 29, 255 (1966).
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[4] G. F. Efremov and A. Yu. Smirnov: Sov. Phys. JETP 53, 547 (1981).

Poster Session / 31

Transport equations for modelling membrane vapor separation

Dr. DUDEK, Gabriela [1]; Dr. TURCZYN, Roman [2]; Dr. STRZELEWICZ, Anna [3]; Dr. KRASOWSKA, Monika [1]; Dr. RYBAK, Aleksandra [4]; Prof. GRZYWNA, Zbigniew [1]

[1] *Silesian University of Technology*

[2] *Silesian Universoty of Technology*

[3] *Silesian University of Technology, Faculty of Chemistry*

[4] *Silesian University of Technology, Department of Physical Chemistry and Technology of Polymers*

The problem of a membrane vapor separation in the presence of a magnetic field is considered. Paramagnetism of water and diamagnetic behaviour of ethanol form the basis for vapor separation. A new concept of polymer membranes filled with magnetic nanoparticles i.e. ferroferric oxides (Fe_3O_4) was applied. Membranes with dispersed metal powder were casted in an external magnetic field of a specially designed coil. The simple diffusion equation for water and ethanol behaviour has been discussed. Mass transport coefficients (flux, permeation and selectivity) were evaluated.

Sunday Session / 41

From passive to active Brownian Motion

Prof. EBELING, Werner [1]

[1] *Humboldt University, Institute of Physics*

We review first the way from modelling passive Brownian Motion connected with the names of Smoluchowski, Fokker, Planck, Klein, Kramers, Chapman, Kolmogorov, Döblin and many others to the recent concepts of active dynamics. In the second part we study simple models of active Brownian motion and analyze the role of active friction, energy depots, symmetry-breaking, internal delay and external load, focussing on mechanisms and the efficiency of using free energy. Typical models show a maximum of the efficiency in dependence on the load what agrees with experimental findings.

Refs: P. Romancuk et al.: Eur.Phys.J. ST 202, 1-162 (2012); Chaos Int. J. Nonlin. Sci 21, 047517 (2011); M. Zabicki et al., Acta.Phys.Pol B 41, 1181 (20110), Chem.Phys. (2010); J.Strefler et al. Eur. Phys. J. B 72, 597 (2009);
M. Petit: L'équation de Kolmogoroff , Vie et mort de Wolfgang Doeblin, un génie dans la tourmente nazie. Paris 2005; Die verlorene Gleichung, Eichborn 2005; W. Ebeling, E. Gudowska-Nowak, I.M. Sokolov: On stochastic dynamics in physics – remarks on history and terminology, Acta Phys. Polonica 39, 1003-1018 (2008)

Monday Session / 61

Anomalous thermodynamics at the micro-scale

Prof. CELANI, Antonio [1]; Mr. BO, Stefano [2]; Dr. EICHHORN, Ralf [3]; Prof. AURELL, Erik [4]

[1] *Institut Pasteur and CNRS, Paris*

[2] *Institute for Cancer Research and Treatment, Torino*

[3] *The Nordic Institute for Theoretical Physics*

[4] *KTH - Royal Institute of Technology, Stockholm*

Particle motion at the micro-scale is an incessant tug-of-war between thermal fluctuations and applied forces on one side, and the strong resistance exerted by fluid viscosity on the other. Friction is so strong that completely neglecting inertia – the overdamped approximation – gives an excellent effective description of the actual particle mechanics. In sharp contrast with this result, here we show that the overdamped approximation dramatically fails when thermodynamic quantities such as the entropy production in the environment are considered, in presence of temperature gradients. In the limit of vanishingly small, yet finite inertia, we find that the entropy production is dominated by a contribution that is anomalous, i.e. has no counterpart in the overdamped approximation. This phenomenon, that we call entropic anomaly, is due to a symmetry-breaking that occurs when moving to the small, finite inertia limit.

Monday Session / 85

Stochastic thermodynamics: Engines and demons

Dr. ESPOSITO, Massimiliano [1]

[1] *University of Luxembourg*

I will show how simple Markovian feedbacks, called "Maxwell demon feedbacks", can be incorporated into the formalism of stochastic thermodynamics. I will also show how their efficiency can be analysed similarly as that of standard thermodynamic machines.

Poster Session / 50

Path integral formulation and path probabilities of Continuous Time Random Walks

Dr. EULE, Stephan [1]; Prof. FRIEDRICH, Rudolf [2]

[1] *Max Planck Institute for Dynamics and Self-Organization, Göttingen*

[2] *Institute for Theoretical Physics, WWU Münster*

We present the path integral formulation of a broad class of generalized diffusion processes and employ this formulation to derive exact expressions for the path probability densities and joint probability distributions. After showing how the Continuous Time Random Walk (CTRW) is included in the considered class of processes, we derive a closed expression for the path probability distribution of CTRWs. This solution is given in terms of the waiting time distribution and short time propagator of the corresponding random walk as a solution of a Dyson equation. Furthermore, by applying the corresponding generating functional, we show how response functions can be calculated.

Poster Session / 38

The statistical mechanics of 2s-plats

FERRARI, Franco [1]; Ms. ZHAO, Yani [1]

[1] *University of Szczecin*

We consider the statistical mechanics of a system of 2s-plats. The latter consist in closed curves with a given number s of maxima and minima. 2s-plats play an important role in biochemistry because most, if not all, the topological configurations formed by ring-shaped DNA can be reduced to a 4-plat. We show that the partition function of two polymers linked together to form a 2s-plat is equivalent to that of a system of anyons. Under certain conditions, the two polymers undergo a phase transition, in which the attractive interactions of entropic origin between their monomers become repulsive. At the transition point, the system becomes self-dual and admits configurations minimizing the energy that look like static vortex solutions. The configurations extremizing the energy are computed exactly. The heat capacity of the four-plat is computed numerically.

Thursday Session / 98

Efficient electron transfer via heterogeneous superexchange coupling in photosynthetic bacteria

Prof. FISCHER, Sighart F. [1]; DIETZ, W.; SCHERER, P.O.J.

[1] *Technical University Munich*

The early charge separation after excitation of the special pair in photosynthetic reaction centers is analyzed within a model, which accounts for electronic superexchange coupling via a mediating Chlorophyll monomer with distributed energy locations. The couplings to local vibration are also evaluated. The theory helps to understand the inverted temperature dependence, the non-exponential decay character and the robustness of the process.

Wednesday Session / 114

Brownian motions in systems with variable temperature

Prof. FULIŃSKI, Andrzej [1]

[1] *Jagiellonian University*

It is shown that in systems with time-dependent and/or spatially nonuniform temperature T(t,x) the Brownian motion (BM) is anomalous. A few examples of simple arrangements, easy for experimental realization, are discussed in detail. Most of these processes are isomorphic with weakly non-ergodic diffusion described in literature. New effects: (i) zero-mean oscillations of T(t) accelerate BM (pumping effect), (ii) the combination of temporal and spatial variations of temperature may lead to superballistic BM, (iii) parabolic gradients of T(x) result in an exponential acceleration of BM. One can expect similar effects in inflationary systems with time-dependent metrics.

For details cf. arXiv:1206.4594.

Poster Session / 20

Regime variance testing - a quantile approach

Mr. GAJDA, Janusz [1]; Mr. SIKORA, Grzegorz [1]; Dr. WYŁOMAŃSKA, Agnieszka [1]

[1] *Hugo Steinhaus Center, Institute of Mathematics and Computer Science, Wroclaw University of Technology, Wroclaw 50-370, Poland*

We examine time series that exhibit behavior related to two or more regimes with different statistical properties. The motivation of our study are two real data sets from plasma physics with an observable two-regimes structure. In this paper we develop a procedure to estimate the critical point of the division in a structural change in a time series. Moreover we propose three tests to recognize such specific behavior. The presented methodology is based on the empirical second moment and its main advantage is the assumption of a lack of distribution. Moreover, the examined statistical properties are expressed in the language of empirical quantiles of the squared data therefore the methodology is an extension of the approach known from the literature. Theoretical results are confirmed by the simulation and analysis of real data of turbulent laboratory plasma.

Tuesday Session / 63

Time-reversal symmetry relation for nonequilibrium flows ruled by the fluctuating Boltzmann equation

Prof. GASPARD, Pierre [1]

[1] *Université Libre de Bruxelles*

A time-reversal symmetry relation is established for out-of-equilibrium dilute or rarefied gases described by the fluctuating Boltzmann equation. The symmetry is proved for the coarse-grained master equation ruling the random jumps in the numbers of particles occupying cells of given position and velocity in the one-particle phase space. Symmetry relations are deduced for the fluctuating particle and energy currents of the gas flowing between reservoirs or thermalizing surfaces at given particle densities or temperatures.

The results are reported in arXiv:1206.0639.

Sunday Session / 103

Electromagnetic waves interaction with various metallic nanomaterials

Prof. GIERSIG, Michael [1]

[1] *Freie University Berlin, Department Physics*

In the last decade the possibility of active interaction of light with the nanosized plasmonic materials has been tremendously growth. The metallic nanoparticles can effectively confine the radiation to nanoscale in the proximity of Plasmon resonance whereby the position of this resonance is controlled by the morphology (size and shape) of the nanostructures. In this lecture we will discussed the physical and chemical preparations methods of various nanostructures and their structural and optical characterization.

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Poster Session / 25

Thermodynamics description of chemical reactions by Isothermal Titration Calorimetry (ITC)

Ms. JANICZEK, Katarzyna [1]; Dr. KRASOWSKA, Monika [2]; Prof. GRZYWNA, Zbigniew [2]

[1] *Politechnika Śląska Gliwice*

[2] *Silesian University of Technology*

Isothermal Titration Calorimetry (ITC) is a technique based on the precise measurement of heat, which is evolved or absorbed during the process. The result is a full description of reaction thermodynamics in a single measurement. By simple calculations, it is possible to obtain such important information as enthalpy change of a reaction (ΔH), binding constant (K), reaction stoichiometry (n), free energy change (ΔG) and entropy change (ΔS).
Low as several micromolar sample concentration and small volume of microcalorimeter (1 μl) are helpful in studying of biological systems. The popularity of ITC can be confirmed by the large number of studies, which can by classified into the following categories:
- protein/peptide- ligand interactions,
- protein/peptide- macromolecule interactions,
- protein/peptide- small molecule interactions,
- small molecule interactions.

ITC can be an important tool for drug design and provides new information about thermodynamics of “new” reactions.

Poster Session / 55

Lifetime of the superconductive state in long Josephson junctions in presence of non-Gaussian noise sources

Mr. GUARCELLO, Claudio [1]; Dr. AUGELLO, Giuseppe [2]; Dr. VALENTI, Davide [3]; Prof. SPAGNOLO, Bernardo [4]

[1] *Dipartimento di Fisica, Group of Interdisciplinary Physics, Università di Palermo and CNISM*

[2] *Dipartimento di Fisica, Group of Interdisciplinary Physics, Università di Palermo and CNISM, sezione di Palermo*

[3] *Dipartimento di Fisica, Universita' di Palermo*

[4] *University of Palermo*

The effects of Lévy noise sources on the transient dynamics of long Josephson junctions (LJJ) are investigated in the presence of both a periodical current signal and a noise source with Gaussian, Cauchy-Lorentz or Levy-Smirnov probability distributions.
In particular, by numerically integrating the Sine-Gordon equation, the mean escape time (MET) from the superconductive metastable state is obtained as a function both of the frequency of the periodical force and amplitude of the noise signal. We find resonant activation (RA) and noise enhanced stability (NES). Significative changes in RA and NES are observed by using Lévy noise sources with different statistics. MET is also studied as a function of the junction length, both for spatially homogeneous and inhomogeneous bias current distributions. In the latter case an enhanced non-monotonic behavior is observed in the presence of Gaussian noise. Conversely, the non-monotonic behavior results to be significatively reduced or completely absent for different statistics of the noise source.

Sunday Session / 118

Smoluchowski Symposia: Why are we here?

Dr. GÓRA, Paweł [1]

[1] *Jagiellonian University*

A popular talk on Marian Smoluchowski, statistical physics, and Marian Smoluchowski Symposia – their past, present and future.

Poster Session / 19

Dynamics and energetics of a molecular zipper under external driving

Mr. HOLUBEC, Viktor [1]; Prof. CHVOSTA, Petr [1]; Prof. MAASS, Philipp [2]; Mr. RYABOV, Artem [3]

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We investigate the dynamics of a single-ended N-state molecular zipper based on a model originally proposed by Kittel. The molecule is driven unidirectionally towards the completely unzipped state with increasing time t, where the driving lowers the energies of states with k unzipped links by an amount proportional to kt. We solve the Pauli rate equation for the state probabilities and the partial differential equations, which yield the probability distributions for the work performed on the zipper and for the heat exchanged with the thermal reservoir. Similarly to the related equilibrium model, two different regimes can be identified at a given temperature with respect to the released molecular degrees of freedom per broken bond. In these two regimes the time evolution of the state probabilities as well as of the work and heat distributions show a qualitatively different behavior.

Poster Session / 58

The effect of depletion layer on diffusion of nanoparticles in solutions of flexible and polydisperse polymers

Dr. OCHAB-MARCINEK, Anna [1]; Dr. WIECZOREK, Stefan A. [2]; Ms. ZIĘBACZ, Natalia [1]; Prof. HOLYST, Robert [3]

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[2] *Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw*

[3] *Institute of Physical Chemistry PAS*

The depletion layer is an exclusion zone that forms around a particle immersed in a solution of non-adsorbing polymer. The effect occurs due to the changes of configurational entropy of polymer chains: Close to the particle surface, the entropy strongly decreases because of chain deformation, so that the centres of masses of polymer chains are excluded from that region. This results in a polymer concentration gradient across the depletion layer boundary.

We introduce a model of diffusion of nanoparticles in solutions of flexible, polydisperse polymers. The model takes into account the effect of depletion layer which leads to nonlinear dependence of the mean square displacement (MSD) on time. Our model may be an alternative choice for the study of those experimental systems where the crossover between subdiffusion and normal diffusion is observed. Its advantage is mathematical simplicity: it allows to easily identify the crossover times and distances, which are here associated with the depletion layer thickness. The soft boundaries of the depletion layer, generated by the flexible and polydisperse polymers, are here approximated by two shells enclosed one in another, which may be interpreted as approximations of polymer density profiles around the probe. We show a very good agreement of the model with dynamic light scattering (DLS) measurements of diffusion of nanoparticles in solutions of polyethylene glycol (PEG).

Poster Session / 44

Biologistics: mobility in cells

Mr. KALWARCZYK, Tomasz [1]; Dr. TABAKA, Marcin [2]; Prof. HOLYST, Robert [1]

[1] *Institute of Physical Chemistry PAS*

[2] *Institute of Physical Chemistry Polish Academy of Sciences*

Poster Session / 45

Taylor dispersion analysis for fast and accurate measurements of diffusion coefficient

Ms. MAJCHER, Aldona [1]; Ms. LEWANDROWSKA, Anna [2]; Prof. HOŁYST, Robert [2]

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Taylor dispersion analysis is a very useful and simple method to accurately determine the diffusion coefficients and ligand-selector equilibrium binding constants. The analysis of macromolecule-ligand binding is an important aspect of many processes in the field of biopharmacy and lets predict the medicinal activity of drugs and fatty acids, hormones, amino acids, cations in human body.
In our experiment we consider dispersion of compound of interest transported by laminar flow in long, thin and coiled capillary. However, during the flow through curved capillary occurs secondary flow, causing local generation of eddies, which changes the effective diffusivity. Nevertheless, basing on dependence of the ratio of the experimental to theoretical dispersion coefficient as a function of Dn2Sc we are able to determine correct value of diffusion coefficient for various substances at high velocity of the flow.

Poster Session / 116

Lehmann effect and rotational viscosity of ferroelectric liquid crystal in Langmuir monolayer

Dr. ŻYWOCIŃSKI, Andrzej [1]; FIAŁKOWSKI, Marcin [1]; NITOŃ, Patrycja [1]; Prof. HOLYST, Robert [2]

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The phenomenon of collective molecular rotation observed in Langmuir monolayers of frroelectric liquid crystalline molecules can be considered as a chemical Lehmann effect because the rotation is driven by a vapor pressure difference, i.e. gradient of chemical potential. The rotating chiral molecules driven by a flux of water molecules can be considered as the smallest possible molecular motors. Continuous precession of the ordering vector at constant angular velocity is a result of balance between the driving torque and the viscous torque related to rotational viscosity, γ_1, of the monolayer. In this work we measured the angular velocity of collective molecular rotation as a function of temperature. The measurements allowed us to calculate the temperature dependence of rotational viscosity and to fit the data to Vogel-Fulcher-Tammann model. We were also able to estimate the torque acting on a single molecule of liquid crystal as comparable to the torque of protein-based biological molecular motors.

Poster Session / 36

Study on the polymerization of Caulobacter crescentus FtsZ by dynamic light scattering

Dr. HOU, Sen [1]

[1] *Department of Soft Condensed Matter, Institute of Physical Chemistry, Polish Academy of Sciences*

We introduce dynamic light scattering spectroscopy (DLS) as a new method to study the polymerization dynamics of FtsZ in solution. Analysis of the DLS data indicates that independent of the concentration of FtsZ monomers, GTP, and GDP, FtsZ polymers are remarkably monodisperse in length. Our measurements of the diffusion coefficient of the polymers show that their length is remarkably stable over time until free GTP is consumed. We estimated the mean size of the FtsZ polymers within this interval of stable length to be between 9 and 18 monomers. The rate of FtsZ polymerization and depolymerization are likely influenced by the concentration of resulting GDP, as the successive addition of GTP to FtsZ increased the rate of polymerization and slowed down depolymerization. Increasing the FtsZ concentration did not change the size of FtsZ polymers; however, it increased the rate of the depolymerization reaction by depleting free GTP. Using transmission electron microscopy we observed that FtsZ forms linear polymers in solutions that rapidly convert to large bundles upon contact with surfaces at time scales as short as several seconds. The best-studied small molecule that binds to FtsZ, PC190723, had no stabilizing effect on C. crescentus FtsZ filaments in vitro, which complements previous studies with Escherichia coli FtsZ and confirms that this class of small molecules binds Gram-negative FtsZ weakly.

Monday Session / 107

Reversible thermodynamic processes with feedback

Dr. HOROWITZ, Jordan [1]; Prof. RODRIGUEZ PARRONDO, Juan Manuel [1]

[1] *Universidad Complutense de Madrid*

The information acquired during a thermodynamic process with feedback can be converted into useful work. However, the second law of feedback restricts the amount of work that can be obtained from this information. In this talk, I will discuss optimal thermodynamic processes with feedback, where all the information is converted into work. I will demonstrate that such processes are feedback-reversible: they are indistinguishable from their time-reversal, thereby extending the notion of thermodynamic reversibility to feedback processes. Finally, I will build on intuition from analyzing feedback-reversible processes in order to develop a method for designing optimal thermodynamic engines with feedback, using the N-particle Szilard engine as a typical example.

Poster Session / 35

Biologistics: how to optimize regulation of gene expression

Dr. TABAKA, Marcin [1]; Mr. KALWARCZYK, Tomasz [1]; Prof. HOŁYST, Robert [1]

[1] *Institute of Physical Chemistry Polish Academy of Sciences*

Genome regulatory proteins, e.g. transcription factors and RNA polymerases, use non-energy consuming strategies when searching for specific sites on DNA such as operators or promoters. According to the theory of facilitated diffusion proteins speed up the searching by means of one-dimensional diffusion along DNA chain, a process known as sliding. We will show that macromolecular crowding, present in the cytoplasm of Escherichia coli, causes that 1D diffusion constant is 3 orders of magnitude smaller than 3D diffusion making the sliding to be extremely slow and inefficient. Instead transcription factors take advantage of oligomerization and DNA looping. Moreover, in vivo concentrations of nucleoid-associated proteins, which are responsible for structure and compactness of chromosome, match optimal conditions for the searching by transcription factors and RNA polymerases

Monday Session / 40

Fluctuation relations for open systems

Dr. HÄNGGI, Peter [1]

[1] *Universität Augsburg*

Monday Session / 78

Thermodynamics of information processing: A simple, solvable model of Maxwell's Demon

Prof. JARZYNSKI, Chris [1]

[1] *University of Maryland, College Park*

The thermodynamic implications of information processing have received renewed attention, in contexts such as quantum information theory, artificial molecular machines, and microscopic feedback control. I will describe a model system that offers a simple paradigm for exploring the interplay between heat, work and information. This "Maxwell demon" interacts with a thermal reservoir, a stream of bits, and a mass that can be lifted or lowered. Its dynamics are modeled with explicit, thermodynamically consistent equations of motion. The exact solution of these equations is used to construct a nonequilibrium phase diagram, which reveals that the demon can act either as an engine, converting heat to work while writing information to the stream of bits, or as an eraser, using the energy of the falling mass to erase information in the bit stream.

Poster Session / 119

Reaction-diffusion ecological model for coordinating conservation efforts on heterogeneous landscapes

Dr. KLECZKOWSKI, Adam [1]

[1] *University of Stirling*

This poster employs a combination of simulation and percolation theory to study how an agglomeration bonus affects the choice of land management practice and the spatial connectivity of patches of conserved land. Using a reaction-diffusion model of species birth, death and dispersal, we compare three payment regimes: a uniform payment where no reward is applied to connectivity; the standard agglomeration bonus where an additional payment (premium) is made when a neighbouring patch is signed up; and an extended agglomeration bonus, where the premium is only paid for clusters of patches above a threshold.

Poster Session / 15

Exact solutions of time- and space-fractional Legendre-Pearson diffusion equation

Prof. KLIMEK, Malgorzata [1]; Prof. AGRAWAL, Om P. [2]

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[2] *Mechanical Engineering and Energy Processes, Southern Illinois University*

Exact solutions of time- and space-fractional Legendre-Pearson diffusion equation

Poster Session / 32

Boundary conditions at a thin membrane for subdiffusion

KOSZTOŁOWICZ, Tadeusz [1]; Dr. LEWANDOWSKA, Katarzyna [2]

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We consider a subdiffusive system with a thin membrane in which subdiffusion is described by a fractional differential equation. In order to solve this equation we need two boundary conditions at the membrane. One of them is quite obvious and demands a continuity of a flux at the membrane. The second boundary condition is not determined in an unambiguous way. The most used boundary conditions assume that the flux is proportional to the concentration difference between membrane surfaces or that the ratio of the concentration at the membrane surfaces is constant. However, there are observed situations in which the permeability of the membrane changes over time due to blocking the membrane channel by subdiffusive particles. In our contribution we present a new boundary condition taking into account the effect mentioned above.This boundary condition will be derived within the Continous Time Random Walk formalism and the queueing theory.

Poster Session / 28

Fractal analysis of the fracture profiles

Dr. KRASOWSKA, Monika [1]; Dr. STRZELEWICZ, Anna [2]; Dr. DUDEK, Gabriela [1]; Dr. RYBAK, Aleksandra [3]; Dr. BARSZCZEWSKA-RYBAREK, Izabela [1]; Dr. TURCZYN, Roman [1]; Prof. GRZYWNA, Zbigniew [1]

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[2] *Silesian University of Technology, Faculty of Chemistry*

[3] *Silesian University of Technology, Department of Physical Chemistry and Technology of Polymers*

The concept of fractal was used to analysis of the fracture surfaces of three different polymeric materials. The fracture profile was characterized by the modified fractal dimension. The profile lines were subjected to the analysis, in which the length of each fracture profile was measured with steps of varying length (the step in each following operation was reduced by half). The modified fractal dimension is considered as a diagnostic tool for structure-morphology analysis of fracture path and roughness parameter. A quantitative description of fracture surface is an important link in the investigation of the mechanisms of materials' decohesion and crack resistance.

Poster Session / 47

Monte Carlo studies of the ferromagnetic p-spin models on scale-free hypernetworks

Dr. KRAWIECKI, Andrzej [1]

[1] *Faculty of Physics, Warsaw University of Technology*

Results of Monte Carlo simulations of p-spin Ising models on scale-free hypernetworks are presented. The hypernetworks are obtained using the preferrential attachment algorithm, the spins are located in the nodes and the hyperedges connecting p nodes correspond to non-zero ferromagnetic interactions involving p spins. Such models show high degeneracy of the ground state: apart from the ferromagnetic state, depending on the parameters of the preferrential attachment algorithm leading to different topologies of the obtained hypernetworks, there are several or even infinitely many disordered (glassy) states with the same energy. For various network topologies quantities such as the specific heat or magnetic susceptibility show maxima as functions of the temperature, which suggests the occurrence of the glassy and/or ferromagnetic phase transition in the models under study. The transition seems to be a second-order one, in contrast with similar transition in the p-spin ferromagnetic Ising model on 3d regular lattice, where there is a first-order glassy transition.

Poster Session / 59

Dissipated work and fluctuation relations in non-equilibrium single-electron transitions

Mr. KUTVONEN, Aki [1]; Prof. PEKOLA, Jukka [2]

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[2] *Aalto University*

We discuss a simple but experimentally realistic model system, a single-electron box (SEB), where common fluctuation relations can be tested for driven transitions. When the electronic system on the SEB island is driven out of equilibrium by the control parameter (gate voltage) non-isothermally, we obtain deviations from the work fluctuation theorem.

Sunday Session / 66

Marian Smoluchowski on sources of randomness in physics and deterministic chaos

Prof. KUŚ, Marek [1]

[1] *Center for Theoretical Physics PAS*

Development of statistical physics at the turn of the 19th century brought about conceptual problems of justifying probabilistic methods on the ground of other physical theories. The conspicuous determinism of mechanics and electrodynamics demanded reconciliation with merely statistical predictions offered by the newly offered approach. Various attempts to justify statistical physics on the basis of deterministic laws of classical mechanics resulted in such fundamental achievements like e.g. ergodic theory of dynamical systems and a vast research area of what is nowadays called “the deterministic chaos theory”.

Smoluchowski contributed to the topic in two papers. In Über den Begriff des Zufalls und den Ursprung der Wahrscheinlichkeitsgesetze in der Physik published in 17. volume of Naturwissenschaften which appeared in 1918 after his death and in an earlier contribution Remarks on the notion of chance in physical phenomena published in Polish in 1916 he discussed a notion we now call “the sensitivity to initial condition” – a fundamental concept for the deterministic chaos theory. I will discuss the novelty of Smoluchowski’s approach from a broader perspective aiming at explanations to which extend the classical mechanics is really deterministic.

Tuesday Session / 90

Define chaos in 1d from first principles

Prof. LEE, M Howard [1]

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Chaotic behavior is a manifestation of some underlying basic property. By Sharkovskii's theorem of chaos applied on multi-cycles of the logistic map, we find that chaos is defined by a finite spectral measure in the space of the fixed points. This definition of chaos satisfies Birkhoff's ergodicity condition indicating why a chaotic trajectory can also be ergodic. By finding the same spectral property in an infinite harmonic chain, we have concluded that there is chaos in the local variables of the chain and that chaos can occur without nonlinearity if there are infinitely many degrees of freedom.

Poster Session / 33

Subdiffusion in a three part system with a mixture of particles having different subdiffusion coefficients

Dr. LEWANDOWSKA, Katarzyna [1]; KOSZTOŁOWICZ, Tadeusz [2]

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[2] *Institute of Physics, Jan Kochanowski University, ul. Świętokrzyska 15, 25-406 Kielce, Poland*

We consider a model which describe subdiffusion in a three part system. The middle part contains a mixture of particles having different subdiffusion coefficients D_α whereas the external parts contain a pure solvent at the initial moment. The external parts have a different subdiffusion parameter α to the one of the middle part. Assuming that subdiffusion is described by a fractional differential equation we will find concentration profiles of the particles in all parts of the system and a time evolution of a substance released from the middle part. In our consideration different distributions of the subdiffusion coefficients in the middle part will be taken into account. We will also discuss possible applications of the model in describing real biological processes.

Wednesday Session / 26

Synchronization of globally coupled two-state stochastic oscillators

Prof. LINDENBERG, Katja [1]; Prof. ESCAFF, Daniel [2]; Prof. HARBOLA, Upendra [3]

[1] *University of California San Diego*

[2] *Universidad de Los Andes*

[3] *Indian Institute of Science*

We present a model of identical coupled two-state stochastic units each of which in isolation is governed by a fixed refractory period. The nonlinear coupling between units directly affects the refractory period, which now depends on the global state of the system and can therefore itself become time dependent. At weak coupling the array settles into a quiescent stationary state. Increasing coupling strength leads to a saddle node bifurcation, beyond which the quiescent state coexists with a stable limit cycle of nonlinear coherent oscillations. We explicitly determine the critical coupling constant for this transition.

Poster Session / 109

"Cargo-mooring" as the general principle for molecular motors

Mr. LISOWSKI, Bartosz [1]; Mr. ZABICKI, Michal [2]

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[2] *Jagiellonian University*

Routinely navigating through ever–changing and unsteady envi- ronment, utilizing chemical energy, molecular motors transport the cell's crucial components, such as neurotransmitters and organelles. A widely accepted assumption is that they do so by generating force and pulling the cargo, while literally walking along the polymeric tracts, e.g. microtubules. However, using experimental data one may calcu- late that the energy needed for this pulling would take the most part of around 22 kT available for each step, even without any external forces opposing the motion. In such a case there would be no energy left for all conformational change of protein and for chemical tran- sitions. Moreover, the cost of pulling increases in viscoelastic media — the motor would consume more energy pulling cargo inside living cell than in the experimental test tube filled with buffer solution. We propose different mechanism that explains how motor proteins utilize chemical energy. In our model the energy is used for ratcheting the free diffusion of a cargo. Motor no longer pulls, but only holds the bead or a vesicle, allowing for Brownian motion in a range limited by the elasticity of motor–cargo–track system. The consequence of such mechanism is the dependency of motion not only on the motor, but also on the cargo (especially it's size) and on the environment (i.e. it's viscosity, crowding and temperature). However, current experimen- tal works rarely provide this type of information for in vivo studies. We suggest that even small differences between assays can impact the outcome. Our results agree with those obtained in the wet laborato- ries and provide novel insight in the mechanism of molecular motor's functioning.

Poster Session / 34

External noise effects in silicon MOS inversion layer

Mrs. PERSANO ADORNO, Dominique [1]; Mrs. LODATO, Maria Antonietta [1]; Mr. SPEZIA, Stefano [1]; Mr. PIZZOLATO, Nicola [1]; Prof. SPAGNOLO, Bernardo [2]

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[2] *University of Palermo*

In the present work we investigate the effect on the intrinsic noise caused by the addition of an external correlated noise source in a quasi-two-dimensional electron gas (2DEG) in a Silicon MOS inversion layer, driven by a high-frequency periodic electric field in cyclostationary conditions [1]. The electron dynamics is simulated by a Monte Carlo procedure which keeps into account non-polar optical phonon and acoustic phonon [2]. In particular, in our modeling of the quasi-2DEG gas, (i) the potential profile perpendicular to the MOS structure is assumed in the triangular potential approximation, (ii) only the lowest three energy subbands are taken into account and (iii) non-degenerate conditions are simulated [3].
With the aim to study the effect on the electron transport of the added fluctuations, we calculate the changes in the spectral density of the velocity fluctuations, at different values of field strength, lattice temperature, noise amplitude, noise correlation time and width of the well. Our findings show that, under specific conditions, the presence of a fluctuating component added to an oscillating electric field can significantly affect the total noise power. Our study reveals that, critically depending on the external noise correlation time, the dynamical response of the quasi-2DEG driven by a periodic electric field receives a benefit by the constructive interplay between the fluctuating field and the intrinsic noise of the system [4].

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Poster Session / 51

Geometric properties of 2D CTRWs

Mr. LUKOVIC, Mirko [1]; Dr. EULE, Stephan [1]; Prof. GEISEL, Theo [1]

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We investigate geometric properties of 2D continuous time random walks (CTRWs). In particular, we determine analytical expressions for the time-evolution of the average perimeter and area of convex hulls of CTRWs, which are of relevance to ecology-related problems such as animal foraging. In addition, we support these results with numerical simulations.

Poster Session / 37

Current control in a set of Josephson junctions

Dr. MACHURA, Lukasz [1]; Prof. ŁUCZKA, Jerzy [2]; Mr. SPIECHOWICZ, Jakub [3]

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Transport phenomena in periodic structures by harvesting the unbiased external time-periodic stimuli and thermal equilibrium fluctuations have been one of the hottest topic in nowadays science. Examples range from biology and biophysics explaining directed motion of biological motors or particle transport in ion channels, through the new separation techniques to meso-- and nano--physics covering newest and up-to-date experiments with optical lattices, persistent currents in quantum rings and Josephson junctions, to mention only a few.

The physics of the latter has been studied for almost five decades now [1]. Devices with Josephson junctions constitute a paradigm of nonlinear systems exhibiting many interesting phenomena in classical and quantum regimes. Yet new and interesting phenomena arise as researchers are able to use an advantage of powerful computer simulations followed by real experiments on junctions proving theoretically predicted findings [2],[3],[4]. Although many papers deepen the general knowledge on the dynamics of such systems studying currents, fluctuations or the dynamical regimes of underlying chaos, the knowledge of the interacting junctions were addressed only recently [5].

The schematic set of dimensionless equations of motion for n interacting identical Josephson junctions under the influence of the thermal noise and external forces read $\dot{\varphi}i = -\sin\varphi i + Fi(t) + I(\{\varphi\},\{F\}) + \xi i(t)$, where F denotes the set of all individual forces applied to all junctions except the force Fi(t) which is applied to i-th junction. This forces represents all possible external sources of energy and can be time periodic, constant, impulses or even random. φ stands for phase differences on all other junctions except the i-th one. Symbolically I indicates the interactions between all connected junctions. Usually we can control the coupling by tuning the external resistance in the circuit. Terms ξi represent the δ-correlated Gaussian white noises of zero mean and should be interpreted as the typical equilibrium Jonhson-Nyquist noise terms. For a certain realisation of two coupled junction dynamics please read [5].

We will focus on the dynamical properties of the certain realisation the system, namely two junctions driven separately by the unbiased, simple periodic forces $ai \cos(\omega it + \theta i)$. A single junction forced with this kind of signal will not produce net average current. But what about the coupled junctions? We will like to show the possibility of steering a certain junction by driving the other one. Additionally we aim to identify the regimes of locked and operational states and present the structure of actively working junctions. The simple classification of the performance of junctions producing the current of the same or opposite signs or locked-active regions for the same values of all system parameters will be demonstrated.

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Poster Session / 56

Dynamics of a quantum particle interacting with a thermal bath and subject to an oscillating asymmetric bistable potential

Mr. MAGAZZÙ, Luca [1]

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Exploiting the approach of the Feynman-Vernon functional within the framework of the discrete variable representation (DVR), we consider a quantum particle described by the Caldeira-Leggett model. The particle, “moving” in an asymmetric bistable potential subject to a periodical driving, interacts with a thermal bath of harmonic oscillators. In this conditions we study the dynamics of the particle by analyzing the time evolution of the populations in the DVR. Specifically we focalize on the position eigenstate located in the shallower well, i.e. metastable state, finding a nonmonotonic behaviour of the corresponding population as a function of the frequency. Moreover, for different values of the coupling strength with the thermal bath, we obtain the equilibrium energy of the particle as a function both of the amplitude and frequency of the periodical driving.

Wednesday Session / 74

Ergodicity and mixing of anomalous diffusion processes

Dr. MAGDZIARZ, Marcin [1]

[1] *Wroclaw University of Technology*

We study ergodic properties of some classes of anomalous diffusion processes. Using the recently developed measure of dependence called the Levy autocorrelation, we derive a generalization of the classical Khinchin theorem. This result allows us to determine ergodic properties of the class of Levy flights. Moreover, taking advantage of the so-called dynamical functional we show how to verify ergodicity/ergodicity breaking in experimental data. Some examples are presented.

Poster Session / 113

Polymer unfolding induced by spatially correlated noise

Mr. MAJKA, Maciej [1]

[1] *Uniwersytet Jagielloński, Instytut Fizyki Astronomii i Informatyki Stosowanej*

In contrast to the time-correlated noise, which is extensively researched on in the context of sub-diffusion and synchronization effects, little work has been done to understand its spatial counterpart and its consequences. Therefore, we have analyzed the behavior of 2D polymer-like chain under the influence of spatially correlated Gaussian noise.

By means of Langevin equations, we have simulated a bead-spring chain, where the nearest neighbors interact via the harmonic potential and every node interacts globally by Lennard-Jones potential, which provides excluded volume. We have also introduced a harmonic interaction between beads i and i+2 which resulted in a saw-like conformation of the chain. This system has been forced by the spatially correlated Gaussian noise, which amplitude and the correlation length have been varied.

Our investigation into the system revealed several effects, namely: beads motion synchronization, increased time-correlation of the nearest neighbors distance and angles between modules, and, most notably, chain unfolding due to the rise in the correlation length.

Poster Session / 39

Network representation of cardiac interbeat intervals for monitoring restitution of autonomic control for heart transplant patients.

Dr. ŻARCZYNSKA-BUCHOWIECKA, Marta [1]; Prof. GRUCHAŁA, Marcin [1]; Prof. RYNKIEWICZ, Andrzej [2]; Dr. GRAFF, Beata [1]; Prof. MAKOWIEC, Danuta [3]; Prof. KRYSZEWSKI, Stanislaw [3]; Dr. WDOWCZYK-SZULC, Joanna [1]

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[2] *Gdanks Medical University*

[3] *Gdansk University*

It is generally believed that time intervals between subsequent heart contractions (so-called RR-intervals) carry the information about the cardiac control system mainly driven by autonomic nervous system. However, heart transplantation (HTX) interrupts the possibility of autonomic control over the heart beating. Therefore, heart rate variability (HRV) in patients after HTX is low, regardless of the time elapsed since surgery. It is controversial whether the cardiac reinnervation occurs after HTX nevertheless it is expected that progressive reinnervation sets in and it is a good prognosis for survival. We believe that changes that occur in the heart rhythm may provide signals of recovery of the cardiac control. Moreover, these signals should be connected with the increasing influence of the sympathetic nervous system. Therefore we hope that observing these changes, with the help of carefully selected tools, we can describe the process of cardiac reinnervation.

The considerable success of the network theory in various fields of research motivated us to explore these ideas in the analysis of HRV. Here we use the networks of transitions applied to study RR-intervals in patients after HTX. We will also raise the question whether these transitions build a monotonic sequence of accelerations or decelerations. We are of opinion that sequences of monotonic accelerations or decelerations may indicate response of the cardiac system to some special needs of the organism what offers a chance for additional insights into the emergence of the heart regulatory control.

It appears that the network of transitions provides yet another way to assess the heart rhythm. Since RR-series leads to transition networks of the characteristic shape, then one can classify typical properties of these networks, and then construct a measure of heart rhythm changes. The network representation, first of all, offers a total assessment of increments between the consecutive RR-intervals. However, additionally, it gives the eye-catching picture of RR-intervals as a map from which one can read at what RR-interval and how frequently the particular increase> Such presentation is particularly attractive for the clinical application.

Poster Session / 18

Impact of inertia on biased Brownian transport in confined geometries

Mr. MARTENS, Steffen [1]; Prof. SCHIMANSKY-GEIER, Lutz [2]; Prof. SOKOLOV, Igor [2]

[1] *Humboldt-University Berlin, Department of Physics, Newtonstr. 15, 12489 Berlin*

[2] *Humboldt-University Berlin, Department of Physics*

The impact of inertia on biased Brownian motion of point-size particles in a two-dimensional channel with sinusoidally varying width is investigated. We demonstrate that inertial effects cannot be neglected as long as the width of the channel bottlenecks is smaller than the characteristic length along particle's velocity becomes uncorrelated. If the time scales of the problem separate, the adiabatic elimination of the transverse degrees of freedom leads to an effective description for the motion along the channel given by the potential of mean force. We show that the result for the latter is absolutely general for arbitrary friction coefficient and that the validity of such reduced description is intimately connected with equipartition. Numerical simulations show that in the presence of external bias the equipartition may break down leading to non-monotonic dependence of mobility on the external dc force and to a giant enhancement of the effective diffusivity.

Poster Session / 21

Stochastic representation of modified double-order time-fractional diffusion equation

Mr. ORZEŁ, Sebastian [1]; Prof. MYDLARCZYK, Wojciech [2]

[1] *Hugo Steinhaus Center, Wrocław University of Technology*

[2] *Wrocław University of Technology*

We find a stochastic representation for process whose probability density function evolves according to double-order time-fractional Fokker-Planck equation of Riemann-Liouville type (in modified form). We prove that subdiffusive process can be constructed by using subordination technique. The explicit form of subordinator will be given in terms of Levy exponent and Levy measure.

Monday Session / 87

Information engines

Prof. RODRIGUEZ PARRONDO, Juan Manuel [1]

[1] *Universidad Complutense de Madrid*

Wednesday Session / 95

Distribution of dissipated energy in electron tunneling

Prof. PEKOLA, Jukka [1]

[1] *Aalto University*

We present experimental results on tests of Jarzynski and Crooks fluctuation relations in driven electron tunneling [1]. In the most recent experiments [2] we have demonstrated the validity of integral fluctuation relation under full non-equilibrium experimental conditions.

We propose a calorimetric experiment to investigate the distribution of dissipation and fluctuation relations in a two-level quantum system coupled to dissipative environment [3,4].

[1] O.-P. Saira, Y. Yoon, T. Tanttu, M. Möttönen, D. V. Averin, and J. P. Pekola, arXiv:1206.7049.
[2] J. V. Koski et al., in preparation (2012).
[3] P. Solinas, D. V. Averin, and J. P. Pekola, arXiv:1206.5699.
[4] J. P. Pekola et al., in preparation (2012).

Monday Session / 108

Recent progress in free energy recovery from irreversible pulling experiments

Prof. RITORT, Felix [1]

[1] *Universitat de Barcelona*

Fluctuation theorems establish relations governing energy exchange processes in systems in contact with thermal sources, providing new methodologies to obtain equilibrium information from non-equilibrium experiments [1,2]. In this talk I will show several new applications to free energy recovery of DNA and RNA structures in single molecule experiments using an extended version of Crooks fluctuation relation [3,4]. New applications extend to free energy recovery of kinetic molecular structures such as intermediate states, misfolded states and protein/peptide nucleic acid binding. Finally I will also show how fluctuation relations applied to unzipping experiments [5,6] are useful to recover base pairing free energies in RNA, essential to improve free energy prediction of RNA secondary structures.

Tuesday Session / 88

Fluctuations, symmetries and energy sorting in driven systems

Prof. RUBI, Miguel [1]

[1] *University of Barcelona*

Poster Session / 30

Influence of various parameters on structure and morphology of magnetic membranes

Dr. RYBAK, Aleksandra [1]; Dr. KRASOWSKA, Monika [2]; Dr. DUDEK, Gabriela [2]; Dr. STRZELEWICZ, Anna [3]; Prof. GRZYWNA, Zbigniew [2]

[1] *Silesian University of Technology, Department of Physical Chemistry and Technology of Polymers*

[2] *Silesian University of Technology*

[3] *Silesian University of Technology, Faculty of Chemistry*

Membrane technology for separating gas mixtures (including air separation) is undergoing intensive development [1]. The main property of membranes used for the separation of different mixtures is the preferential transport of one of their component. The research is directed therefore not only toward exploring new membrane materials, but also to understanding the nature and details of transport and separation phenomena. The classic theories of transport do not apply in systems where other processes accompany diffusion or when molecules of penetrant react on each other or on molecules of surrounding as well as when there is an external force present. In our research we have proposed magnetic membranes (polymer membranes filled with magnetic neodymium powder and magnetized) [2, 3]. They could be considered as the disordered system because of penetrant-scale gaps whose size and position are changing randomly. One of the main tools for characterizing and studying disordered systems is the concept of fractals. Fractal models may be used both, in the study of static as well as dynamic properties of disordered structures [4, 5]. Fractal theory as the alternative and more suitable tool for analysis of natural phenomena, allows to characterise the objects in terms of their self-similar (scale-invariant) properties (i.e. parts of the object are similar to the whole after rescaling) [6, 7]. 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 [8]. In this paper, we try to investigate the influence of various parameters on structure and morphology of membranes and their transport and separation properties.

[1] Y. Yampolskii, B. Freeman, I. Pinnau, Materials Science of Membranes for Gas and Vapor Separation, New York: John Wiley and Sons; 2006
[2] A. Rybak, Z. J. Grzywna, W. Kaszuwara, On the air enrichment by polymer magnetic membranes, J. Membr. Sci. 336 (2009) 79-85.
[3] B. Freeman, Y. Yampolskii, Membrane Gas Separation, Z.J. Grzywna, A. Rybak, A. Strzelewicz, Air enrichment by polymeric magnetic membranes, John Wiley and Sons, (2010) 159.
[4] A. Bunde, S. Havlin, Fractals and disordered systems, Springer, 1991
[5] B.B Mandelbrot The Fractal Geometry of Nature, W. H. Freeman and Co., 1982.
[6] M. Krasowska, Z. J. Grzywna, M. E. Mycielska, M. B. A. Djamgoz, Fractal analysis and ionic dependence of endocytic membrane activity of human breast cancer cells, Eur. Biophys. J. 38 (2009) 1115-1125.
[7] T. Miyata, T. Takagi, J. Higuchi, T. Uragami, Two types of fractal dimensions for phase separation in multicomponent polymer membranes, J. Polym. Sci. Part B: Polym. Phys. 37, (1999) 1545-1550.
[8] D. Avnir (ed.). The Fractal Approach to Heterogeneous Chemistry – Surfaces, Colloids, Polymers, John Wiley and Sons; 1989

Poster Session / 48

Competing of Sznajd and voter dynamics in the Watts-Strogatz network

Mr. RYBAK, Marcin [1]; Prof. KUŁAKOWSKI, Krzysztof [2]

[1] *AGH University of Science and Technology Faculty of Physics and Applied Computer Science*

[2] *AGH*

We investigate the Watts-Strogatz network with the clustering coefficient C dependent on the rewiring probability. The network is an area of two opposite contact processes, where nodes can be in two states, S or D. One of the processes is governed by the Sznajd dynamics: if there are two connected nodes in D-state – all their neighbors become D with probability 1. For the opposite process it is sufficient to have only one neighbor in state S; this transition occurs with given probability p. The concentration of S-nodes changes abruptly at given value of the probability p. The results are presented in the form of phase diagrams.

Thursday Session / 73

Synchonization of stochastic oscillators

Prof. SCHIMANSKY-GEIER, Lutz [1]

[1] *Instiute of Physics, Humboldt-University at Berlin, Germany*

Monday Session / 70

Momentum transfer in nonequilibrium steady states

Prof. SEKIMOTO, Ken [1]

[1] *Paris7 & ESPCI*

When a Brownian object interacts with noninteracting gas particles under nonequilibrium conditions, energy dissipation associated with Brownian motion causes an additional force on the object as a ‘‘momentum transfer deficit.’’ This principle is demonstrated first by a new nonequilibrium steady state model and then applied to several known models such as an adiabatic piston for which a simple explanation has been lacking.
This work has been done in collaboration with Antoine Fruleux (ESPCI, Paris) Ryoichi Kawai (Alabama Univ. Alabama).

[Refs. PRL 108, 160601 (2012) , arXiv:1204.6536v1]

Poster Session / 43

Statistical modelling of subdiffusive dynamics in the cytoplasm of living cells: A FARIMA approach

Dr. BURNECKI, Krzysztof [1]; Mr. SIKORA, Grzegorz [2]; WERON, Aleksander [1]; Dr. MUSZKIETA, Monika [1]

[1] *Wroclaw University of Technology*

[2] *Politechnika Wrocławska*

Golding and Cox (Phys. Rev. Lett., 96 (2006) 098102) tracked the motion of individual fluorescently labelled mRNA molecules inside live E. coli cells. They found that in the set of 23 trajectories from 3 different experiments, the automatically recognized motion is subdiffusive and published an intriguing microscopy video. Here, we extract the corresponding time series from this video by image segmentation method and present its detailed statistical analysis. We find that this trajectory was not included in the data set already studied and has different statistical properties. It is best fitted by a fractional autoregressive integrated moving average (FARIMA) process with the normal-inverse Gaussian (NIG) noise and the negative memory. In contrast to earlier studies, this shows that the fractional Brownian motion is not the best model for the dynamics documented in this video.

Wednesday Session / 94

Models and tests for anomalous diffusion in crowded environments

Prof. SOKOLOV, Igor [1]

[1] *Instiute of Physics, Humboldt-University at Berlin, Germany*

Many experiments on the motion of particles in crowded environments (artificial or biological, e.g. in cell interior) hint towards anomalous diffusion, mostly subdiffusion. The nature of this subdiffusion can be quite diverse, and therefore needs for description within theoretical models based on different physical assumptions. Recent development in single particle tracking techniques urge for understanding what information about the physical (or biological) system can be extracted from particle trajectories, and how this information can be extracted, i.e. how different model assumptions about the nature of the subdiffusive process can be falsified within statistical tests. The difference between time-inhomogeneous, non-ergodic models (trap model, continuous-time random walks) and ergodic ones (fractional Brownian motion and motion under geometric restrictions, e.g. in percolation) is deeply rooted in the thermodynamics of the corresponding processes. The distinction of these classes is therefore relatively simple and can be done either by running a test for ergodicity (e.g. the test based on comparing the moving time average with the ensemble average) or a one for time homogeneity (e.g. the p-variance test). The distinction within the ergodic class is tricky. This one can be based on specific tests of homogeneity of filling of the space by the corresponding trajectory and will be discussed in some detail based on analytical and numerical examples.

Poster Session / 64

Statistical equivalence of constant bias and compound poissonian driving in the anomalous transport regime

Mr. SPIECHOWICZ, Jakub [1]; Dr. MACHURA, Lukasz [2]; Prof. ŁUCZKA, Jerzy [3]

[1] *University of Silesia, Department of Theoretical Physics*

[2] *University of Silesia*

[3] *Univesrity of Silesia*

We study the dynamics of inertial Brownian particles which move in one-dimensional, symmetric periodic potentials and driven by both a time periodic and a constant biasing force or a compound poisson process. It is known [1] that in the first case for certain parameter regimes, thermal equilibrium fluctuations induce the phenomenon of absolute negative mobility (ANM), i.e. particle moves backwards against a small constant force. We replace the bias with the compound poisson process and examine its influence on the average velocity of an inertial Brownian particle for various distributions of the heights of the δ-pulses. A general observation is statistical equivalence of constant bias and compound poissonian driving in this particular parameter regime. The experimental verification of this finding is a setup consisting of a resistively and capacitively shunted Josephson junction device.

Ref:
[1] Machura L, Kostur M, Talkner P, Łuczka J and Hänggi P 2007, Phys. Rev. Lett. (98) 040601

Poster Session / 29

Anomalous diffusion on fractal structure of magnetic membranes

Dr. STRZELEWICZ, Anna [1]; Dr. KRASOWSKA, Monika [2]; Dr. DUDEK, Gabriela [2]; Dr. RYBAK, Aleksandra [3]; Dr. TURCZYN, Roman [2]; Prof. GRZYWNA, Zbigniew [2]; Dr. CIEŚLA, Michał [4]

[1] *Silesian University of Technology, Faculty of Chemistry*

[2] *Silesian University of Technology*

[3] *Silesian University of Technology, Department of Physical Chemistry and Technology of Polymers*

[4] *Jagiellonian University*

The anomalous diffusion on fractal structure of polymer membrane with dispersed magnetic powder is discussed. Magnetic 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). Random walk dimensions dw were also evaluated. The diffusion equation to describe diffusion processes in the aforementioned membranes was proposed.

Wednesday Session / 77

Quantum fluctuation theorems for different initial states

Prof. TALKNER, Peter [1]

[1] *Institut fuer Physik, Universitaet Augsburg, Germany*

The fluctuation theorems of Jarzynski and Crooks impose restrictions on the statistics of work performed by an external force acting on a system. Originally, these relations were proven in the framework of classical statistical mechanics when the system initially stays in a canonical state.
In this talk we discuss the generalization to quantum fluctuation relations and to the different forms which they take, depending on whether the considered system initially is prepared in a micro-canonical, canonical, or grand-canonical state.

Poster Session / 54

From molecules to patchy colloids: Network fluids and bigels

Prof. TELO DA GAMA, Margarida [1]

[1] *Universidade de Lisboa*

Patchy colloids are characterized by anisotropic short-range interactions and self-assemble into a variety of equiibrium and non-equilibrium structures. We consider binary mixtures of patchy colloidal particles with three sites of two types, one of which promotes bonding of particles of the same species while the other promotes bonding of different species. We find up to four percolated structures at low temperatures and densities: two gels where only one species percolates, a mixed gel where particles of both species percolate but neither species percolates separately, and a bicontinuous gel where particles of both species percolate separately forming two interconnected networks. Appropriate mixtures exhibit one or more connectivity transitions between the mixed and bicontinuous gels, as the temperature and/or the composition changes.

Poster Session / 27

Scaling limits of multidimensional Levy walks

Mr. TEUERLE, Marek [1]; Dr. MAGDZIARZ, Marcin [1]; Mr. ZEBROWSKI, Piotr [2]

[1] *Wroclaw University of Technology*

[2] *Wroclaw University*

We present the scaling limit of multidimensional Levy walk and we describe the detailed structure of the limiting process. It occurs that the scaling limit is a multidimensional subordinated Levy-stable motion with the parent process and subordinator being strongly dependent processes. The corresponding Langevin picture of scaling limit is derived. We also introduce an useful method of simulating Levy walks, which approximates the limiting process. Our approach can be used when one works with real-life data described by the limiting process. Namely, by estimating the spectral measure from the data we are able to recover a full description of L´evy walk approximating the limiting process. We also give examples of analytical representations of spectral measure, which cover large class of possible application in the modeling of real-life phenomena.

Monday Session / 79

Maxwell's Demon and information thermodynamics

Prof. UEDA, Masahito [1]

[1] *Department of Physics, University of Tokyo*

The three fundamental inequalities concerning information thermodynamics are discussed. They place the fundamental bounds on the work that can be extracted from the heat engine and the minimum energy costs for measurement and erasure of information. We also discuss a Jarzynski-like equality in the presence of feedback control, and its experimental verification.

Poster Session / 57

Stochastic model for a biological complex system: analysis of the bacterial growth in food products

Dr. VALENTI, Davide [1]; Prof. SPAGNOLO, Bernardo [2]; Prof. GIUFFRIDA, Alessandro [3]; Prof. ZIINO, Graziella [3]; Prof. PANEBIANCO, Antonio [3]

[1] *Dipartimento di Fisica, Universita' di Palermo*

[2] *University of Palermo*

[3] *Dipartimento di Sanita' Pubblica Veterinaria, Universita' di Messina*

The Physics of Complex Systems has recently taken a more and more important role in the description of natural systems because of the interactions, both deterministic and noisy, between such systems and the environment. In particular the noise plays a relevant role in biological systems, whose dynamics is strongly influenced by environmental variables subject to random fluctuations. In this work a stochastic model is exploited to reproduce the growth of bacteria in food of animal origin. Specifically the dynamics of a bacterial species, Listeria monocytogenes, is analyzed in the presence of lactic acid bacteria (LAB) during the period of the fermentation of meat products. The model, based on a generalization of the Lotka-Volterra equations in the presence of noise sources, takes into account the random fluctuations of physical and chemical variables such as temperature, pH and activity water, which are treated as stochastic variables. The presence in the model of appropriate levels of noise allows to obtain theoretical results in a good agreement with experimental data.

Wednesday Session / 65

On the efficiency of (small) machines

Prof. VAN DEN BROECK, Christian [1]

[1] *Hasselt University*

I evaluate the efficiency of machines, discussing both the case of thermal machines (heat to work conversion) and iso-thermal machines (work to work conversion). Universal features of efficiency at maximum power are revealed.

Refs.
C. Van den Broeck, Phys. Rev. Lett. 95, 190602, 1-3 (2005).
C. Van den Broeck, Adv. Chem. Phys. 135, 189-201 (2007).
M. Esposito, K. Lindenberg, and C. Van den Broeck, EPL 85, 60010, 1-5 (2009).
M. Esposito, K. Lindenberg, and C. Van den Broeck, Phys. Rev. Lett. 102, 130602 (2009).
M. Esposito, R. Kawai, K. Lindenberg, and C. Van den Broeck, Phys. Rev. E81, 041106 (2010).
M. Esposito, R. Kawai, K. Lindenberg, and C. Van den Broeck, Phys. Rev. Lett. 105, 150603 (2010).
C. Van den Broeck, N. Kumar and K. Lindenberg, "Efficiency of isothermal molecular machines at maximum power", to appear Phys. Rev. Lett. (2012).

Tuesday Session / 42

On anomalous diffusion and the out of equilibrium response function in one-dimensional models

Prof. VULPIANI, Angelo [1]

[1] *Dipartimento di Fisica, Università degli Studi di Roma "Sapienza"*

We study how the Einstein relation between spontaneous fluctuations and the response to an external perturbation holds in the absence of currents, for the comb model and the elastic single-file, which are examples of systems with subdiffusive transport properties. The relevance of non-equilibrium conditions is investigated: when a stationary current (in the form of a drift or an energy flux) is present, the Einstein relation breaks down, as is known to happen in systems with standard diffusion. In the case of the comb model, a general relation, which has appeared in the recent literature, between the response function and an unperturbed suitable correlation function, allows us to explain the observed results. This suggests that a relevant ingredient in breaking the Einstein formula, for stationary regimes, is not the anomalous diffusion but the presence of currents driving the system out of equilibrium.

Poster Session / 53

From CTRW models to some fractional evolution equations

WEBER, Piotr [1]; Mr. PEPŁOWSKI, Piotr [1]

[1] *Uniwersytet Mikołaja Kopernika*

The aim of this paper is to associate a stochastic model, describing with some accuracy, probability density obtained in the computer simulations of certain dynamical systems. We build a few models of stochastic processes within the framework of the continuous time random walks (CTRW). For each of these models two concurrent processes are considered: normal diffusion and Levy flights leading to different forms of anomalous diffusion. For each of the considered models we derive fractional differential equations with the solution given in the integral form.

Poster Session / 14

Anomalous diffusion. An identification algorithm for telomere motion data

Prof. WERON, Aleksander [1]; Dr. JANCZURA, Joanna [1]; Dr. BURNECKI, Krzysztof [1]

[1] *Wroclaw University of Technology*

We present a systematic statistical analysis of the recently measured individual trajectories of fluorescently labeled telomeres in the nucleus of living human cells. The experiments were performed in U2OS cancer cell line. We propose a new algorithm for identification of the telomere motion. By expanding the previously published data set we are able to explore the dynamics in six time orders, a task not possible earlier. As a result we establish a rigorous mathematical characterization of the stochastic process and identify the basic mathematical mechanisms behind the telomere motion. We find that the increments of the motion are: stationary, Gaussian, ergodic and even more chaotic - mixing. Moreover, the obtained memory parameter estimates, as well as, the ensemble average MSD reveal subdiffusive behavior at all time spans. All these findings suggest a fractional Brownian motion for the telomere trajectories which is confirmed by a generalized p-variation test. In addition, these results shed new light on other studies of telomere motion and the Alternative Telomere Lengthening mechanism. We hope, that identification of these mechanisms will allow to develop a proper physical and biological model for telomere subdynamics. This array of tests can be easily implemented to other data sets to enable quick and accurate analysis of their statistical characteristics.

Poster Session / 9

Noise induced phase transitions and coupled Brownian motors: non standard hysteretic cycles

Prof. WIO, Horacio S. [1]

[1] *Instituto de Fisica de Cantabria*

Recent work [1,2,3] have shown the possibility, through a noise induced symmetry breaking leading to a nonequilibrium phase transition, of obtaining a set of coupled Brownian motors. It was also shown [4] that in some parameter region such a system could show negative mobility (that is motion opposed to the applied force) and anomalous hysteretic behavior (clockwise in opposition to the usual counter-clockwise). Using an explicit mean-field approximation and colored multiplicative noises, it was found a contraction of the ordered phase (and re-entrance as a function of the coupling) on one hand, and a shift from anomalous to normal hysteretic behavior on the other [5]. This behavior was obtained in systems presenting a noise induced phase transition that originates from a short time instability. Here we discuss a similar system, but where the noise induced phase transition is originated in an entropic mechanism [6]. Some preliminary studies that exploits such a mechanism indicate the possibility of obtaining no standard hysteretic cycles: anti-clockwise but showing a staircase-like structure. Depending on the parameter region, the hysteresis diagram could have one or more blocks, that can be explored as a whole or step by step, opening the possibility of exploiting it as a noise-controlled multipurpose logic gate.

[1] Sagués et al, Rev. Mod. Phys. 79, 829 (2007)
[2] van den Broeck et al, Phys. Rev. E 55, 4084 (1997)
[3] Mangioni et al, Phys. Rev. E 61, 223 (2000)]
[4] Reimann et al, Europhys.Lett. 45, 545 (1999)
[5] Mangioni et al, Phys. Rev. E 66, 051106 (2002)
[6] Carrillo et al, Phys. Rev. E 67, 04611 (2003)

Poster Session / 22

Stochastic modeling of indoor air quality data

Dr. WYLOMANSKA, Agnieszka [1]; JANCZURA, Joanna [2]; Dr. MACIEJEWSKA, Monika [3]; Dr. SZCZUREK, Andrzej [3]

[1] *Hugo Steinhaus Center Institute of Mathematics and Computer Science Wroclaw University of Technology*

[2] *Wroclaw University of Technology*

[3] *Institute of Air Conditioning and District Heating, Wroclaw University of Technology*

Finding a proper model for a description of experimentally recorded data dynamics is an important issue in modeling of physical processes. In this paper we apply a range of statistical tests, in order to verify main statistical properties such as stationarity, stochastic dynamics and distributional features of experimental data related to indoor air quality. Such procedures can be very helpful in confirming or rejecting a hypothesized anomalous diffusion model as a proper one for analyzed dataset.

Poster Session / 49

Thermal properties of knotted polymer rings

Ms. ZHAO, Yani [1]; FERRARI, Franco [1]

[1] *University of Szczecin*

The problem of the statistical mechanics of polymer rings is relevant in biochemistry, because in mitocondria, bacteria and viruses often DNA strands form rings which occur in topologically nontrivial configurations. Nontrivial polymer knots may also be synthetized in the laboratory. In this contribution the results of recent calculations of the heat capacity of a polymer knot will be presented. The calculations are performed numerically using the Wang-Landau algorithm. The excluded volume forces acting on the monomers are taken into account by counting the so-called number of contacts, see for example P.N.

Refs: Vorontsov-Belyaminov et Al., J. Phys. A 37 (2004), 1573 and A. Swetnam et Al. PRE 85 (2012), 031804.

Poster Session / 23

Self-similarity index estimation based on p-variations

Mr. ŚLĘZAK, Jakub [1]; Dr. MAGDZIARZ, Marcin [2]; Ms. WÓJCIK, Justyna [1]

[1] *Wrocław University of Technology*

[2] *Wroclaw University of Technology*

The recently introduced p-variation method appeared to be a useful tool in distinguishing between different types of anomalous diffusion. Based on this method, we introduce a new estimator of a self-similarity index of the fractional Brownian motion. We compare the proposed estimator with other widely used in statistics. Efficiency of the estimator is checked for different values of the self-similarity indices and lengths of simulated and experimental data. As a conclusion we point out advantages and limitations of this technique.

Thursday Session / 117

Quantum entanglement - a statistical approach

Prof. ŻYCZKOWSKI, Karol [1]

[1] *Uniwersytet Jagielloński*

We study statistical properties of an ensemble of quantum states describing composite systems. Such states arise as a result of action of a generic Hamiltonian on an arbitrary product state. Reviewing geometric properties of higher dimensional spheres we show that such states are generically entangled and present estimations for the average entanglement entropy. The latter quantity characterizes, to what extent a given bi-partite pure state is entangled, or alternatively, to what extent the corresponding monopartite reduced state is mixed.

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Applications of self-avoiding walk concept as a type of Smoluchowski dynamics' realization under a suitably chosen external driving field

Prof. GADOMSKI, ADAM [1]; Mr. BEŁDOWSKI, Piotr; Ms. KRUSZEWSKA, Natalia; Mr. PAWLAK, Zenon

[1] *INSTITUTE OF MATHS & PHYSICS, UNIVERSITY OF TECHNOLOGY & LIFE SCIENCES IN BYDGOSZCZ*

Self-avoiding random walk/polygon (SARW/P) concept involves stochastic dynamics driven by some decisive external fields. The decision-making belongs to a choice of external potential, driving the system of interest, since in general, the Smoluchowski dynamics are governed by the chemical potential, being a sum of the physical potential, and a thermal-energy assisted logarithmic concentration term. Moreover, the dynamics express a space-dimensionality dependence too, see R. Zallen, The physics of amorphous bodies, Wiley, NY, 1983.

The applications of SARW/P concept can last over the fields as distant as superconductivity and superlubrication, wherein in the former both electron (super)passage and structure of the nanotube (or, superconducting ceramic sample), in a contact with external, mechanical-stress yielding surroundings, become intriguingly interdependent; cf. M. Gitterman, J. Stat. Phys. 146, 239 (2012); N. Kruszewska, A. Gadomski, Physica A389, (3053) 2010.

As for the latter, the protons' passages through meandric amphiphilic structures of the membranes under adequate alterations upon external/lateral dynamic excitation, appear to be the case for useful comprehension; cf. W.K. Auge II Nano Energy 1, 309 (2012).

Both of the main instances addressed involve a structure-property paradigm, see A. Gadomski, BioSystems 94, 215 (2008), to be tackled within the framework of Smoluchowski dynamics, possibly when based upon proposed-for-testing scaling laws. This way, transport process (coupled to the structure) is meant to be dealt with in terms of nonequilibrium thermodynamics at meso- and nanoscopic levels of matter organization, see A. Gadomski, Z. Pawlak, A. Oloyede, Tribol. Lett. 30, 83 (2008).

25th Marian Smoluchowski Symposium on Statistical Physics

Kraków, Poland, September 9-13, 2012

Program

Sunday, 9 September 2012

10:00 Conference Opening and Awarding of the Henryk Niewodniczański Prize (45')

Sunday Session (10:45 ->12:15)

Session in memoriam of Marian Smoluchowski, prepared by the Institute of Physics, Jagiellonian University

Chairperson: Ewa Gudowska-Nowak (Jagiellonian University)

10:45 **Smoluchowski Symposia: Why are we here?** (45') — Paweł Góra (Jagiellonian University)

11:30 **From passive to active Brownian Motion** (45') — Werner Ebeling (Humboldt University, Institute of Physics)

12:15 Coffee Break (30')

Sunday Session (12:45 ->15:00)

Session in memoriam of Marian Smoluchowski, prepared by the Institute of Physics, Jagiellonian University

Chairperson: Margarida Telo da Gama (Universidade de Lisboa)

12:45 **Facing the coming scientific and social challenges: The role of the NSP division of EPS** (45') — Anna Carbone (Politecnico di Torino)

13:30 **Marian Smoluchowski on sources of randomness in physics and deterministic chaos** (45') — Marek Kuś (Center for Theoretical Physics PAS)

14:15 **Electromagnetic waves interaction with various metallic nanomaterials** (45') — Michael Giersig (Freie University Berlin, Department Physics)

15:00 Lunch

19:00 Get Together Party (4h0')

Monday, 10 September 2012

Monday Session (09:00 ->11:15)

Chairperson: Christian Van den Broeck (Hasselt University)

09:00 **Thermodynamics of information processing: A simple, solvable model of Maxwell's Demon** (50') — Chris Jarzynski (University of Maryland, College Park)

09:50 **Maxwell's Demon and information thermodynamics** (50') — Masahito Ueda (Department of Physics, University of Tokyo)

10:40 **Reversible thermodynamic processes with feedback** (35') — Jordan Horowitz (Universidad Complutense de Madrid)

11:15 Coffee Break (20')

Monday Session (11:35 ->13:00)

Chairperson: Lutz Schimansky-Geier (Instiute of Physics, Humboldt-University at Berlin, Germany)

11:35 **Stochastic thermodynamics: Engines and demons** (50') — Massimiliano Esposito (University of Luxembourg)

12:25 **Anomalous thermodynamics at the micro-scale** (35') — Ralf Eichhorn (The Nordic Institute for Theoretical Physics)

13:00 Lunch (2h0')

Monday Session (15:00 ->16:40)

Chairperson: Igor Sokolov

15:00 **Recent progress in free energy recovery from irreversible pulling experiments** (50') — Felix Ritort (Universitat de Barcelona)

15:50 **Information engines** (50') — Juan M.R. Parrondo (Universidad Complutense de Madrid)

16:40 Coffee Break (20')

Monday Session (17:00 ->18:40)

Chairperson: Igor Sokolov

17:00 **Momentum transfer in nonequilibrium steady states** (50') — Ken Sekimoto (Paris7 & ESPCI)

17:50 **Fluctuation relations for open systems** (50') — Peter Hänggi (Universität Augsburg)

Tuesday, 11 September 2012

Tuesday Session (09:00 ->11:15)

Chairperson: Peter Hänggi (UNIV AUGSBURG)

09:00 **Fluctuations, symmetries and energy sorting in driven systems** (50') — Jose Miguel Rubi (University of Barcelona)

09:50 **On anomalous diffusion and the out of equilibrium response function in one-dimensional models** (50') — Angelo Vulpiani (Dipartimento di Fisica, Università degli Studi di Roma "Sapienza")

10:40 **Overdamped motion in two-dimensional septate channels** (35') — Marcello Borromeo (Universita' di Perugia)

11:15 Coffee Break (30')

Tuesday Session (11:45 ->13:25)

Chairperson: Peter Talkner (Institut fuer Physik, Universitaet Augsburg, Germany)

Location: Collegium Novum (Main Aula)

11:45 **Time-reversal symmetry relation for nonequilibrium flows ruled by the fluctuating Boltzmann equation** (50') — Pierre Gaspard (Université Libre de Bruxelles)

12:35 **Define chaos in 1d from first principles** (50') — M Howard Lee (University of Georgia)

13:25 Lunch (2h5')

14:45 City Tour (3h15')

19:00 Concert and Banquet (3h0')

Wednesday, 12 September 2012

Wednesday Session (09:00 ->12:05)

Chairperson: Karina Weron (Institute of Physics, Wrocław University of Technology)

09:00 **On the efficiency of (small) machines** (50') — Christian Van den Broeck (Hasselt University)

09:50 **Quantum fluctuation theorems for different initial states** (50') — Peter Talkner (Institut fuer Physik, Universitaet Augsburg, Germany)

10:40 **Brownian motions in systems with variable temperature** (35') — Andrzej Fuliński (Jagiellonian University)

11:15 Coffee Break (30')

Wednesday Session (11:45 ->13:10)

Chairperson: Juan Parrondo

Location: Collegium Novum (Main Aula)

11:45 **Distribution of dissipated energy in electron tunneling** (50') — Jukka Pekola (Aalto University)

12:35 **Ergodicity and mixing of anomalous diffusion processes** (35') — Marcin Magdziarz (Wroclaw University of Technology)

13:10 Lunch (2h20')

Wednesday Session (15:30 ->17:10)

Chairperson: Jose Miguel Rubi

Location: Collegium Novum (Main Aula)

15:30 **Models and tests for anomalous diffusion in crowded environments** (50') — Igor Sokolov (Instiute of Physics, Humboldt-University at Berlin, Germany)

16:20 **Synchronization of globally coupled two-state stochastic oscillators** (50') — Katja Lindenberg (University of California San Diego)

Poster Session (18:00 ->21:00)

PRE-POSTER SESSION and POSTERS' PRESENTATION

session and catering

Chairperson: Zbigniew Grzywna (Silesian University of Technology), Paweł Góra

Location: Institute of Physics

Thursday, 13 September 2012

Thursday Session (09:30 ->11:10)

Chairperson: Jerzy Łuczka (Univesrity of Silesia)

09:30 **Quantum entanglement - a statistical approach** (50') — Karol Życzkowski (Uniwersytet Jagielloński)

10:20 **Power law behavior in the ion traffic through a lipid bilayer at the melting transition** (50') — Martin Bier (East Carolina University)

11:10 Coffee Break (30')

Thursday Session (11:40 ->13:05)

Chairperson: Robert Holyst (Institute of Physical Chemistry PAS)

11:40 **Efficient electron transfer via heterogeneous superexchange coupling in photosynthetic bacteria** (35') Sighart F. Fischer (Technical University Munich)

12:15 **Synchonization of stochastic oscillators** (50') Lutz Schimansky-Geier (Instiute of Physics, Humboldt-University at Berlin, Germany)

13:05 Lunch (2h5')