MECO46

The 46th International Conference of the Middle European Cooperation in Statistical Physics

11 – 13 MAY 2021

BOOK OF ABSTRACTS

ABOUT THE CONFERENCE

The conference is the 46th in a series of meetings of scientists working in the domain of Statistical Mechanics and Condensed Matter Physics.

The Conferences of the Middle European Cooperation in Statistical Physics (MECO) were initiated in 1974 with the aim of bridging the gap between the communities of scientists from the Eastern and Western blocks of Europe, separated by the iron curtain. Since then, MECO conferences have become the yearly itinerant reference meetings for the community of scientists who are active in the field of Statistical Physics in the broader sense, including modern interdisciplinary applications to biology, finance, information theory, and quantum computation.

Due to the ongoing worldwide pandemic, the MECO46 conference had to be organized as an online conference. The conference was oriented in the direction of applications of statistical mechanics in complex systems. However, contributed talks will be selected from all areas of statistical physics.

Abstract Book edited by: Jevgenijs **Kaupužs**

Cover design: Ramona **Durena**

Riga, 11 May 2021

CONFERENCE PROGRAM

Tuesday, May 11, 2021

time zone "(UTC+03:00) Riga"

TIME	EVENT
10:00 - 10:05	Opening - General Chair **Jevgenijs Kaupužs**
10:05 - 10:20	Welocome to RTU - Vice-Rector for Research **Talis Juhna**, Riga Technical University, Latvia
10:20 - 11:30	**Soft and active matter - Wolfhard Janke**
10:20 - 10:50	➢ Non-equilibrium systems driven by particle rotation - **Andrejs Cebers**, Faculty of physics,mathematics and optometry
10:50 - 11:10	➢ Statistics of percolating clusters in a model of photosynthetic bacteria - **Ferenc IGLOI**, Wigner Research Centre for Physics, Budapest
11:10 - 11:30	➢ Automated discovery of design principles for far-from-equilibrium colloidal self-assembly - **Avishek Das**, Department of Chemistry, University of California, Berkeley
11:30 - 11:50	Coffee break
11:50 - 12:30	**Soft and active matter - Wolfhard Janke**
11:50 - 12:10	➢ Correlation-driven motion. A new mechanism of self-phoresis - **Alvaro Dominguez**, Universidad de Sevilla
12:10 - 12:30	➢ Emergence of an Ising critical regime in the clustering of one-dimensional soft matter revealed through string variables - **Francesco Mambretti**, Universita degli Studi di Padova
12:30 - 14:00	**Posters**
14:00 - 14:40	Lunch
14:40 - 15:50	**Soft and active matter - Ferenc Igloi**
14:40 - 15:00	➢ Thermodynamics of small systems with emergent structures - **Jan Korbel**, Medizinische Universität Wien = Medical University of Vienna
15:00 - 15:20	➢ Superionic liquids in slit nanopores: Bethe-lattice approximation and Monte Carlo simulations - **Maxym Dudka**, Institute for Condensed Matter Physics of NAS of Ukraine, Institute of Theoretical Physics, Faculty of Physics, University of Warsaw
15:20 - 15:50	➢ Size and shape properties of complex macromolecules: universal features - **Viktoria Blavatska**, Institute for Condensed Matter Physics of NAS of Ukraine
15:50 - 16:00	Coffee break
16:00 - 16:40	Cultural program - **Oskars Priede** "Interesting presentation of information is a trainable art of communication"
16:40 - 16:50	Coffee break
16:50 - 19:00	**Non-equilibrium phenomena - Juan P. Garrahan**
16:50 - 17:20	➢ Collective behavior of flickering candle-flames - **Zoltan Neda** - Physics Department, Babes-Bolyai University, Cluj-Napoca
17:20 - 17:40	➢ Reinforcement learning for rare trajectory sampling - **Dominic Rose** - University of Nottingham, UK
17:40 - 18:00	➢ Simultaneous memory effects in the stress and in the dielectric susceptibility of a stretched polymer glass - **Caroline Crauste-Thibierge** - Laboratoire de Physique de l'ENS Lyon
18:00 - 18:20	➢ Widom lines related with the relaxational dynamics for the Ising model - **Songül Özüm** - Hitit University
18:20 - 19:00	➢ Features of nanoscale thermodynamics - **Christopher Jarzynski** - University of Maryland, College Park

CONFERENCE PROGRAM

Wednesday, May 12, 2021

time zone "(UTC+03:00) Riga"

TIME	EVENT
10:00 - 11:50	**Non-equilibrium phenomena - Yurij Holovatch**
10:00 - 10:40	➢ Making rare events typical: from dynamical large deviations to reinforcement learning - **Juan P. Garrahan**, School of Physics and Astronomy, University of Nottingham
10:40 - 11:10	➢ Lindblad-Floquet description of finite-time quantum heat engines - **Dragi Karevski**, Laboratoire de Physique et Chimie Théoriques
11:10 - 11:30	➢ Athermal Uncertainty Relations for Mesoscopic Coherent Light - **Ohad Shpielberg**, University of Haifa
11:30 - 11:50	➢ Depinning transition of charge density waves - **Andrei Fedorenko**, Laboratoire de Physique de l'ENS Lyon
11:50 - 12:10	Coffee break
12:10 - 14:30	**Strongly correlated systems - Wolfhard Janke**
12:10 - 12:40	➢ Quantum criticality driven by magnetic field - **Dariusz Kaczorowski**, Institute of Low Temperature and Structure Research Polish Academy of Sciences
12:40 - 13:10	➢ Emergent Kardar-Parisi-Zhang phase in quadratically driven condensates - **Alessio Chiocchetta**, Institute fo Theoretical Physics, University of Cologne
13:10 - 13:30	➢ Analyticity of critical exponents of the O(N) models from nonperturbative renormalization - **Andrzej Chlebicki**, Institute of Theoretical Physics, Faculty of Physics, University of Warsaw,
13:30 - 13:50	➢ Boundary Critical Behavior of the Three-Dimensional Heisenberg Universality Class - **Francesco Parisen Toldin**, University of Würzburg
13:50 - 14:10	➢ Electron phonon entanglement and the validity of the Luttinger description - **Roósz Gergő**, Wigner RCP Budapest
14:10 - 14:30	➢ Interface in presence of a wall. Results from field theory - **Marianna Sorba**, Istituto Nazionale di Fisica Nucleare, Sezione di Trieste, Scuola Internazionale Superiore di Studi Avanzati / International School for Advanced Studies
14:30 - 15:10	Lunch
15:10 - 16:00	Virtual Excursion **"Latvia. Get to know us!"**
16:00 - 17:30	**Posters**
17:30 - 18:50	**Networks and complex systems - Zoltan Neda**
17:30 - 17:50	➢ A novel quantity for characterizing the dynamics of state-transition networks - **Bulcsú Sándor** - Department of Physics, Babes-Bolyai University [Cluj-Napoca]
17:50 - 18:10	➢ Gintropy: entropic features of the Lorenz curve - **Tamas Biro** - Wigner Research Centre for Physics, Budapest, Complexity Science Hub Vienna
18:10 - 18:30	➢ First-passage process in degree space for networks - **Masayuki Hase** - University of São Paulo - School of Arts, Sciences and Humanities
18:30 - 18:50	➢ Unraveling the role of node metadata in network robustness: the feature-based percolation model - **Oriol Artime** - Bruno Kessler Foundation

CONFERENCE PROGRAM

Thursday, May 13, 2021

time zone "(UTC+03:00) Riga"

TIME	EVENT
10:00 - 11:10	**Networks and complex systems - Ralph Kenna**
10:00 - 10:30	➢ Origin of scaling laws in driven systems - **Stefan Thurner**, Medical University of Vienna, Complexity Science Hub Vienna, Santa Fe Institute
10:30 - 10:50	➢ A message-passing approach to epidemic tracing and mitigation with apps - **Hanlin Sun**, School of Mathematical Sciences, Queen Mary
10:50 - 11:10	➢ The Fate of Articulation Points and Bredges in Percolation - **Reimer Kuehn**, King's College London
11:10 - 11:30	Coffee break
11:30 - 13:00	**Interdisciplinary applications - Tamas Biro**
11:30 - 12:00	➢ Generalised Riemann Hypothesis and the Brownian motion - **Giuseppe Mussardo,** SISSA
12:00 - 12:30	➢ Optimizing returns under extreme-value memory: can you escape the trap of past experience? - **Rosemary Harris** - School of Mathematical Sciences, Queen Mary University of London, UK
12:30 - 12:50	➢ Arbitrage on the energy market as a minority game - **Hildegard Meyer-Ortmanns** - Jacobs University [Bremen]
12:50 - 14:20	**Posters**
14:20 - 14:50	Lunch
14:50 - 15:30	**International Advisory Board Meeting**
15:30 - 16:30	Interdisciplinary applications - Rosemary Harris
15:30 - 16:10	➢ Spontaneous vs. stimulated brain activity: A statistical physics approach - Lucilla de Arcangelis - University of Campania
16:10 - 16:30	➢ Effect of correlated noise on multistable systems with time-delay feedback control - Konstantinos Mamis - Hellenic Naval Academy
16:30 - 16:50	**Quantum many body systems and quantum computation - Rosemary Harris**
16:30 - 16:50	➢ Thermal entanglement of a spin 1 Heisenberg dimer - **Azadeh Ghannadan** - Pavol Jozef Šafárik University
16:50 - 17:10	Coffee break
17:10 - 19:10	**Disordered and frustrated systems - Andrei Fedorenko**
17:10 - 17:30	➢ Relaxation in an ensemble of elongated particles on a line as driven by Brownian diffusion - **Nikolai Lebovka**, Institute of Biocolloidal Chemistry named after F. D. Ovcharenko, NAS of Ukraine, Taras Shevchenko National University - Yuri Tarasevich, Astrakhan State University
17:30 - 17:50	➢ Binary mixtures of particles with soft exclusion: Exact phase diagrams for tree-like lattices - **Dmytro Shapoval**, Institute for Condensed Matter Physics of NAS of Ukraine
17:50 - 18:10	➢ Super-spreader hot-spots, mobility and lock-down effects on the dynamics of SIR epidemic models - **Ódor Géza**, Center for Energy Research, Inst. of Technical Phys. and Materials Science
18:10 - 18:30	➢ Ising and Potts models in a random field: results from (quasi-)exact algorithms - **Martin Weigel**, Chemnitz University of Technology, Coventry University (UK)
18:30 - 18:50	➢ Mixed-order transition in the antiferromagnetic quantum Ising chain in a field - **Péter Lajkó**, Department of Physics, Kuwait University
18:50 - 19:10	➢ Unlocking heterogeneity of node activation in gene regulatory networks - **Giuseppe Torrisi**, King‘s College London
19:10 - 19:30	**Closing**

Keynote talks

Invited talks

Plenary talks

Plenary talks

Poster session 1

Poster session 2

Poster session 3

Features of nanoscale thermodynamics

C. Jarzynski

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In recent decades there has been increasing interest in applying the laws of thermodynamics to systems at very small length scales, such as biomolecules, optically manipulated colloidal particles, single electron devices, and trapped ions. At these scales, new thermodynamic features emerge that are not present, or not relevant, in macroscopic thermodynamics. I will give an overview of theoretical and experimental progress that has been made in understanding these features. I will focus in particular on the second law of thermodynamics, how it applies to nanoscale systems, and what we have learned about non-equilibrium fluctuations, violations of the second law, the thermodynamic arrow of time, nanoscale feedback control, and quantum thermodynamics.

Making rare events typical: from dynamical large deviations to reinforcement learning

Juan P. Garrahan
School of Physics and Astronomy, University of Nottingham, Nottingham, NG7 2RD, UK

I will discuss general ideas for studying atypical dynamics in stochastic systems. Rare events often play a significant role in phenomena occurring across science, but their systematic study is hampered by the fact that they occur with low probability. I will describe the so-called "thermodynamics of trajectories" framework, an ensemble method for quantifying the statistical properties of trajectories of the dynamics, based on the mathematics of large deviations (LDs). I will discuss the use of tensor network methods for computing LD statistics accurately in lattice systems, their use in efficiently sampling rare trajectories, and consider the application of machine reinforcement learning for problems not tractable by LDs. Time permitting I will discuss the extension of this general approach to quantum dissipative systems.

Spontaneous vs. stimulated brain activity: A statistical physics approach

Lucilla de Arcangelis
Department of Engineering
University of Campania "Luigi Vanvitelli"

The understanding of the fundamental relation between brain resting activity and the response to stimuli is a long-standing fascinating question. Recent experiments have shown that the spontaneous brain activity is characterized by avalanches showing absence of characteristic size, result successfully interpreted in the context of criticality. However, in order to support the idea that the brain acts close to a critical point it is crucial to evidence the existence of long-range correlations. The temporal organization of neuronal avalanches in the rat cortex in vitro is characterized by a complex organization, leading to the characteristic brain oscillations and a dynamic balance between excitation and inhibition. The question concerning the relation between spontaneous and evoked activity is addressed by means of the coarse-grained Wilson Cowan model. An approach inspired in non-equilibrium statistical physics allows to derive a fluctuation-dissipation relation, suggesting that measurements of the correlations in spontaneous fluctuations in the brain activity alone could provide a prediction for the system response to a stimulus. Theoretical predictions are in good agreement with MEG data for healthy patients performing visual tasks.

Non-equilibrium systems driven by particle rotation

A.Cebers, R.Livanovics and A.P.Stikuts

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Behavior of non-equilibrium systems with rotating particles (rollers, spinners) attracts interest from the point of view of active systems. Quincke rollers [1] and rotating membrane proteins [2] are just a few examples. An interesting system of this kind is the ensemble of magnetic droplets rotating under the action of a rotating field and forming a structure with hexagonal order [3]. This system is studied experimentally and numerically by modelling the 2D ensemble of rotating particles interacting by hydrodynamic forces. If repulsion is absent the system remains in the disordered state. The process of the ordering is characterized by the hexatic order parameter which increases with time. During this process the number of 5-and 7- fold disclination pairs diminishes as observed in the experiments [3]. The ordered ensembles of the droplets may be classified as rotating crystals. The angular velocity of the rotating crystal is calculated in the continuum approach by coarse graining the spatial distribution of the rotating particles.

The work is supported by M-era-net project FMF No.1.1.1.5 /ERANET/18/04

References

[1] Bricard A., Coussin J.B., Desreumaux N., Dauchot D., and Bartolo D. *Nature*,503 95-98 (2013)

[2] Oppenheimer N.¡ Stein D.B., and Shelley M.J. *Phys.Rev.Lett.*, 123 148101 (2019)

[3] Stikuts A.P., Perzynski R., and Cebers A. *JMMM* 500, 166304 (2020)

Size and shape properties of complex macromolecules: universal features

V. Blavatska

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Prediction of the impact of complex architecture of branched macromolecules on their behaviour in solvents is a problem of continuing interest in polymer physics. In statistical description of polymers, a considerable attention is paid to the universal quantities describing equilibrium size and shape of typical conformation adapted by individual macromolecule in a solvent. In particular, the folding dynamics of macromolecules and hydrodynamics of polymer fluids are strongly dependent on size and shape measures of single macromolecules, which in turn are determined by their topology. We consider a set of complex polymer architectures such as star, rosette and pom-pom polymer, as well as more general polymer networks. By combining both the analytical approach, based on path integration and direct polymer renormalization, and molecular dynamics simulations, the quantitative estimates for the set of universal size and shape characteristics are obtained.

Collective behavior of flickering candle-flames

Zoltan Neda[1] , Attila Gergely[1] , Bulcsú Sándor[1] , Csaba Paizs[2] , Robert Totos[2]

1 : Physics Department, Babes-Bolyai University, Cluj-Napoca (Babes-Bolyai University, Cluj-Napoca)
2 : Dept. of Chemistry, Universitatea Babeș-Bolyai [Cluj-Napoca]

The intimate atmosphere of candlelights fascinated many of us. One might have observed their flickering, but probably did not thought about this as an oscillation phenomenon with an almost perfect periodicity, similar with the periodic beating of pendulum clocks. Using however a high-speed camera we can visualize its periodicity of about 10 flashes per second, a phenomenon that is detected by our eyes as flickering. One can also recall that the flame of a thin candle is usually stable, and flickering appears when bundles of such candles are constructed, unifying their flames. If the candle is thick enough, the flame of a single candle may also become unstable producing hence flickering. The phenomenon becomes even more interesting if we consider multiple oscillating flames, generating fascinating collective oscillation modes. We will present experimental results for the oscillation of a single bundle and the collective behaviour of flames that are nearby. A simple dynamical model is then discussed for understanding both the oscillation of the flames and their collective behavior. Similar phenomena, encountered in the flow of gases are also discussed.

Bibliography:
A. Gergely, B. Sandor, Cs. Paizs, R. Tötös and Z. Néda, *Scientific Reports*, vol. **10**, 21305 (2020)

Lindblad-Floquet description of finite-time quantum heat engines

D. Karevski

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The operation of autonomous finite-time quantum heat engines relies on the existence of a stable limit cycle in which the dynamics becomes periodic. The two main questions that naturally arise are therefore whether such a limit cycle will eventually be reached and, once it has, what the state of the system is within the limit cycle. We show that the application of Floquet's theory to Lindblad dynamics offers clear answers to both questions. By moving to a generalized rotating frame, we show that it is possible to identify a single object, the Floquet Liouvillian, which encompasses all operating properties of the engine.

Quantum criticality driven by magnetic field

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For the past few decades, the unsettling thrust to understand the physics near a quantum phase transition (QPT) has motivated condensed-matter research community to explore more about this precarious point of phase instability. External magnetic field has been recognized as a particularly useful parameter to tune magnetic systems towards QPT. Here, we discuss magnetic field driven classical and quantum criticality in a novel Ce-based compound $CePtIn_4$. The magnetization data revealed the occurrence of long-range antiferromagnetic (AFM) order and two metamagnetic (MM) transitions, while the power law divergence of the differential susceptibility indicated the proximity of QPT. Remarkably, the magnetoresistance measured in the ordered state showed multiple crossover between positive and negative values emphasizing the existence of critical fluctuations. The heat capacity studies revealed a stunning phase diagram that comprises tricritical point separating AFM, MM and paramagnetic phases as well as two quantum critical end points. All these remarkable findings expand the frontier of QPTs, thus offering a playground to further exploit experimental and theoretical understanding of the associated perplexing physics.

Emergent Kardar-Parisi-Zhang phase in quadratically driven condensates

Alessio Chiocchetta
Institute for Theoretical Physics, University of Cologne, Germany

In bosonic gases at thermal equilibrium, an external quadratic drive can induce a Bose-Einstein condensation described by the Ising transition, as a consequence of the explicitly broken U(1) phase rotation symmetry down to Z2. However, in physical realizations such as exciton-polaritons and nonlinear photonic lattices, thermal equilibrium is lost and the state is rather determined by a balance between losses and external drive. A fundamental question is then how nonequilibrium fluctuations affect this transition. Here, we show that in a two-dimensional driven-dissipative Bose system the Ising phase is suppressed and replaced by a nonequilibrium phase featuring Kardar- Parisi-Zhang (KPZ) physics. Its emergence is rooted in a U(1)-symmetry restoration mechanism enabled by the strong fluctuations in reduced dimensionality. Moreover, we show that the presence of the quadratic drive term enhances the visibility of the KPZ scaling, compared to two-dimensional U(1)-symmetric gases, where it has remained so far elusive.

On the origin of scaling laws in driven systems

Stefan Thurner

Sample space reducing (SSR) processes offer a simple analytical way to understand of the origin and ubiquity of power-laws in many path-dependent complex systems. SRR processes show a wide range of applications that range from fragmentation processes, language formation to cascading processes. Here we argue that they also offer a natural generic framework to understand stationary distributions of generic driven non-equilibrium systems that are composed of a driving- and a relaxing process. We show that the statistics of driven non-equilibrium systems can be derived from the nature of the underlying driving process. For constant driving rates exact power-laws emerge, where the exponent is related to the rate. If driving rates become state-dependent, or vary across the life-span of the process, the functional form of the state dependence determines the statistics. Constant driving rates lead to exact power-laws, a linear state dependence function yields exponential or Gamma distributions, a quadratic function yields the normal distribution. Logarithmic and power-law state dependence leads to log-normal and stretched exponential distribution functions, respectively. Also the Weibull, Gompertz and Tsallis-Pareto distributions arise naturally from simple state dependent driving rates.

Generalised Riemann Hypothesis and Brownian motion

Giuseppe Mussardo (SISSA-Trieste, Italy)

Abstract

The seminar presents the main features of the Riemann Hypothesis and discusses its generalisation to an infinite class of complex functions, the so-called Dirichlet L-functions.

The position of the infinite number of zeros of all the Dirichlet L-functions along the axis with real part equal to 1/2 finds a very natural explanation in terms of one of the most basic phenomena in Statistical Physics, alias the Brownian motion. We present the probabilistic arguments which lead to this conclusion and we also discuss a battery of highly non-trivial tests which support with an extremely high confidence the validity of this result.

Optimizing returns under extreme-value memory: can you escape the trap of past experience?

R.J. Harris and E. Mitsokapas

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Snapshots of "best" (or "worst") experience are known to dominate human memory and may thus also have a significant effect on future behaviour. We consider here a model of repeated decision-making where, at every time step, an agent takes one of two choices with probabilities which are functions of the maximum utilities previously experienced. Depending on the utility distributions and the level of noise in the decision process, it is possible for an agent to become "trapped" in one of the choices on the basis of their early experiences. If the utility distributions for the two choices are different, then the agent may even become trapped in the choice which is objectively worse in the sense of expected long-term returns. Using tools from statistical physics and extreme-value theory, we discuss the resulting behaviour for three classes of utility distribution. In particular, we show that for exponential distributions there is an optimal value of noise which maximizes the expected returns in the long run. We also mention some connections to other work on non-Markovian processes.

Statistics of percolating clusters in a model of photosynthetic bacteria

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In photosynthetic organisms, the energy of light during illumination is absorbed by the antenna complexes, which is transmitted by excitons and is either absorbed by the reaction centers (RCs), which have been closed in this way, or emitted by fluorescence. The basic components of the dynamics of light absorption have been integrated into a simple model of exciton migration, which contains two parameters: the exciton hopping probability and the exciton lifetime. During continuous radiation with light the fraction of closed RCs, x, continuously increases and at a critical threshold, x_c, a percolation transition takes place. Performing extensive Monte Carlo simulations we study the properties of the transition in this correlated percolation model. We measure the spanning probability in the vicinity of x_c, as well as the fractal properties of the critical percolating cluster, both in the bulk and at the surface.

1. P. Maróti, I. A. Kovács, M. Kis, J. L. Smart and F. Iglói: *Correlated clusters of closed reaction centers during induction of intact cells of photosynthetic bacteria*, Scientific Reports **10**:14012 (2020)

2. J.-Ch. Anglés d'Auriac and F. Iglói: *Statistics of percolating clusters in a model of photosynthetic bacteria*, preprint arXiv:2101.05517

Automated discovery of design principles for far-from-equilibrium colloidal self-assembly

Avishek Das and David T. Limmer

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Self-assembly is a process where nanoscale building blocks are designed to autonomously come together and form a static or fluxional nanostructure. Predictively directing colloidal self-assembly has seen enormous experimental and theoretical interest due to the independent tunability of size, shape and interactions in colloids and nanoparticles. Design principles thus found are mostly applicable to systems in thermal equilibrium or relaxing to one. This is because equilibrium probability measures are of a Boltzmann form and hence can be modulated by changing the energetic stability of target structures. These approaches cannot predict the transient dynamics of self-assembly and also fail to apply to systems driven by external dissipative forces to a nonequilibrium steady-state. However, far-from-equilibrium assembly environments are the norm in biological systems and also exploited ubiquitously in manufacturing protocols for soft materials. A general framework for predicting design principles in nonequilibrium steady-states is currently lacking.

We demonstrate that nonequilibrium molecular dynamics trajectories conditioned on assembling into a target structure encode a set of optimal interactions and driving forces resulting from a variational principle in the driven trajectory ensemble. We have developed an optimization algorithm to solve this variational problem with explicitly evaluated stochastic gradients in design-space. We have used this algorithm to find general rules for the self-assembly of DNA-labeled colloids in a shear flow, for various target structures and dynamical phases[1]. We discover optimal strategies where a class of transient nonrigid nanoclusters can be made globally stable using dissipative driving. We also find design regimes for amplifying specified probability fluxes and currents in a reaction network of colloidal nanoclusters driven by shear flow. The ability to optimally harness nonequilibrium driving for stabilizing transient structures and to break detailed balance in chosen reaction coordinates can lead to the bottom-up synthesis of new kinds of functional materials.

[1] **A. Das** & D. T. Limmer, *J. Chem. Phys.* **2021**, *154*, 014107.

Correlation–driven motion. A new mechanism of self-phoresis

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The last years have witnessed a growing interest in colloidal particles with a specific surface pattern of catalytic behavior: the particles can thus induce chemical reactions in their environment, a feature dubbed "activity". Specifically, a sufficiently asymmetric pattern ("Janus particles") leads generically to self-propulsion and self-rotation.

The mechanism responsible for this self-propulsion is a matter of recent debate. There seems to be a consensus on the relevance of self-phoresis, that is, the usual diffusiophoretic displacement and rotation of a non-active particle immersed in a chemical solution exhibiting a gradient of solute, except that the gradient is self-induced by the catalytic activity of the particle. This mechanism relies fundamentally on the existence of a differential microscopic interaction between the particles' surface and the molecules of solute or the solvent, respectively — that is, the solute has a tendency to "wet the particle".

We have recently identified a new theoretical mechanism that relies instead on the non-vanishing range of correlations in the fluid solution, usually comparable to the range of the wetting interaction. This mechanism is effective also for neutral particles ("no wetting"), and the model predicts self-propulsion velocities that can reach values comparable to the observed ones. But the mechanism also exhibits certain characteristic features that lead to observable differences as compared to the mechanism based on wetting: most notably, a quadratic dependence of the velocity with the activity, and the absence of self-phoretic rotation. Another important result is the mechanism's irrelevance for the phoresis of non-active particles: therefore, correlation–driven self-phoresis cannot be interpreted as phoresis in an external, albeit self-induced concentration gradient, very much unlike the mechanism based on wetting.

A. Domínguez, M. N. Popescu, C. M. Rohwer, S. Dietrich
Self–Motility of an Active Particle Induced by Correlations in the Surrounding Solution, Phys. Rev. Lett. **125**, 268002 (2020)
DOI: 10.1103/PhysRevLett.125.268002

Emergence of an Ising critical regime in the clustering of one-dimensional soft matter revealed through string variables

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Soft matter systems are renowned for being able to display complex emerging phenomena such as clustering phases, even for some purely repulsive pair potentials models [Likos *et al.*, Phys. Rev. E 63, 031206 (2001)]. Recently, a surprising quantum phase transition has been revealed in a one-dimensional (1D) system composed of bosons interacting via a pairwise soft potential in the continuum [Rossotti *et al.*, Phys. Rev. Lett. 119, 21, 215301 (2017)]. It was shown that the spatial coordinates undergoing two-particle clustering could be mapped into quantum spin variables of a 1D transverse Ising model. In this work ([Mambretti *et al.*, Phys. Rev. E 102, 042134 (2020)]) we investigate the manifestation of an analogous critical phenomenon in 1D classical fluids of soft particles in the continuum. In particular, we explored with stochastic simulation techniques the low–temperature behavior of three different classical models of 1D soft matter, whose inter–particle interactions allow for clustering. The same string variables highlight that, at the commensurate density for the two–particle cluster phase, the peculiar pairing of neighboring soft particles can be nontrivially mapped onto a 1D discrete classical Ising model. We also observe a related phenomenon, namely the presence of an anomalous peak in the low-temperature specific heat, thus indicating the emergence of Schottky phenomenology in a non-magnetic fluid.

Thermodynamics of structure-forming systems

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Structure-forming systems are ubiquitous in nature, ranging from atoms building molecules to self-assembly of colloidal amphibolic particles. The understanding of the underlying thermodynamics of such systems remains an important problem. Here, we derive the entropy for structure-forming systems that differs from Boltzmann-Gibbs entropy by a term that explicitly captures clustered states. For large systems and low concentrations the approach is equivalent to the grand-canonical ensemble; for small systems we find significant deviations. We derive the detailed fluctuation theorem and Crooks' work fluctuation theorem for structure-forming systems. The connection to the theory of particle self-assembly is discussed. We apply the results to several physical systems. We present the phase diagram for patchy particles described by the Kern-Frenkel potential. We show that the Curie-Weiss model with molecule structures exhibits a first-order phase transition.

Reference: J. Korbel, S. D. Lindner, R. Hanel, and S. Thurner, *Nat. Comm.* **12** (2021) 1127.

Superionic liquids in slit nanopores: Bethe-lattice approximation and Monte Carlo simulations

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Superionic liquids are ionic liquids in a superionic state that emerges in narrow conducting pores of supercapacitor electrodes, playing the central role in capacitive energy storage. Here, we report on a theory developed for such superionic liquids confined to ultranarrow slits, admitting a single layer of ions, by mapping this problem onto the well-known Blume-Capel (BC) model. We solve the BC model analytically within the Bethe-lattice approximation [1] and investigate the phase behaviour and pore charging in terms of the key parameters, such as pore ionophilicity, interionic interactions, and applied electrode potential. The phase diagram includes the lines of first- and second-order, direct and re-entrant phase transitions, manifested by singularities in the capacitance-voltage dependence [2]. We reveal that pores that induce ordering of ions at zero voltage can deliver even a few-fold higher stored energies than conventional non-ordering or ionophobic pores. Despite the mean-field character of our analysis, we find a surprisingly good agreement between the theory and Monte Carlo simulations of the same model [3].

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Reinforcement learning for rare trajectory sampling

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Very often when studying non-equilibrium systems one is interested in analysing dynamical behaviour that occurs with very low probability. These so-called rare events play a significant role in phenomena occurring throughout the sciences, ranging from large deviations in time-integrated statistics, to transition paths in chemical processes, up to a macroscopic level in climate models of natural disasters. The rarity of these events makes them inherently hard to observe and understand, necessitating the development of general techniques for their study. Here we develop such an approach by using a deep connection between trajectory sampling and reinforcement learning to develop efficient algorithms for the learning of an efficient sampling dynamics for rare trajectories. This provides access to not only probabilities and statistical information about the rare events studied, but an approximation to the stochastic dynamics by which it is likely to be observed. Applicable to both discrete and continuous time processes with any combination of jumps, drift and diffusion, we demonstrate the approach on a range of problems. These problems include: time-dependent dynamics generating finite-time rare trajectories, such as transition path problems from chemical physics, and time-homogenous dynamics used to study the statistics of time-integrated observables. The approach we take can be further applied to variable time problems such as first passage statistics, and Non-Markovian problems.

Simultaneous memory effects in the stress and in the dielectric susceptibility of a stretched polymer glass

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We report experimental evidence that a polymer stretched at constant strain rate $\dot{\lambda}$ presents complex memory effects after that $\dot{\lambda}$ is set to zero at a specific strain λ_w for a duration t_w, ranging from 100s to 2.2×10^5s. When the strain rate is resumed, both the stress and the dielectric constant relax to the unperturbed state non monotonically. The relaxations depend on the observable, on λ_w and on t_w. Relaxation master curves are obtained by scaling the time and the amplitudes by $\ln(t_w)$. The dielectric evolution also captures the distribution of the relaxation times, so the results impose strong constraints on the relaxation models of polymers under stress and they can be useful for a better understanding of memory effects in other disorder materials.

Widom lines related with the relaxational dynamics for the Ising model

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We have presented a phenomenological description for the relaxation dynamics (RD) of Ising ferromagnets in the presence of external magnetic field (h). We calculate two characteristic times using the rate constants which satify the Onsager reciprocity theorem. The temperature and magnetic field variations of these times were produced. We have shown that the extrema of the curves observed when $h = 0$ determine the loci of correlation length maxima or the Widom lines. Results are compared to those of response functions and thermodynamic curvature and a good agreement is achieved.

Athermal uncertainty relations for mesoscopic coherent light

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Thermodynamic uncertainty relations unveil useful connections between fluctuations in thermal systems and entropy production. This talk extends these ideas to the disparate field of zero temperature quantum mesoscopic physics where fluctuations are due to coherent effects and entropy production is replaced by a cost function defined using a novel disorder reversal operator. A simple expression is obtained for the average cost function, which depends on the dimensionless conductance g and on a geometrical factor $\mathcal{B}$ controlled by boundary conditions. Contrary to thermodynamic machines aimed at minimising fluctuations to increase precision, it is desirable in mesoscopic devices to increase coherent effects. The cost function indicates that increasing coherent effects can be achieved by playing with the geometry and boundary conditions through $\mathcal{B}$ and not only by decreasing the bulk conductance g. The manuscript is available on the arXiv: https://arxiv.org/pdf/2011.07246.pdf

Depinning transition of charge density waves: mapping onto $O(n)$ symmetric ϕ^4 theory with $n = -2$ and loop erased random walks

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Disordered elastic systems such as charge density waves (CDWs) exhibit highly nontrivial glassy like behavior and extremely difficult for studying both analytically and numerically. It is widely believed that to capture the physics of these systems one needs functional renormalization group methods. We show that CDWs can be described by a much simpler model which is the $O(n)$-symmetric ϕ^4 theory taken in the unusual limit of $n = -2$ [1]. This fact, astonishingly overlooked for decades, drastically simplifies studying the depinning transition of periodic elastic systems.

We also prove that both models describe the so called loop-erased random walks [2]. Random walks which are not allowed to self-intersect play an important role in combinatorics, statistical physics and quantum field theory. The two most prominent models are self-avoiding walks and loop-erased random walks. The self-avoiding walks was first introduced in polymer physics to model long polymer chains with self-repulsion due to excluded-volume effects. It was discovered by de Gennes that its scaling behavior in d dimensions is given by the $O(n)$ symmetric ϕ^4 theory in the limit of $n \to 0$. A loop-erased random walk is defined as the trajectory of a random walk in which any loop is erased as soon as it is formed and as we show it can be described by the $O(n)$ symmetric ϕ^4 theory in the limit of $n \to -2$ [3].

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Analyticity of critical exponents of the $O(N)$ models from nonperturbative renormalization

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We employ the functional renormalization group framework at the second order in the derivative expansion to study the $O(N)$ models continuously varying the number of field components N and the spatial dimensionality d. We in particular address the Cardy-Hamber prediction concerning nonanalytical behavior of the critical exponents ν and η across a line in the (d, N) plane, which passes through the point $(2, 2)$. By direct numerical evaluation of $\eta(d, N)$ and $\nu^{-1}(d, N)$ as well as analysis of the functional fixed-point profiles, we find clear indications of this line in the form of a crossover between two regimes in the (d, N) plane, however no evidence of discontinuous or singular first and second derivatives of these functions for $d > 2$. The computed derivatives of $\eta(d, N)$ and $\nu^{-1}(d, N)$ become increasingly large for $d \to 2$ and $N \to 2$ and it is only in this limit that $\eta(d, N)$ and $\nu^{-1}(d, N)$ as obtained by us are evidently nonanalytical. By scanning the dependence of the subleading eigenvalue of the RG transformation on N for $d > 2$ we find no indication of its vanishing as anticipated by the Cardy-Hamber scenario. For dimensionality d approaching 3 there are no signatures of the Cardy-Hamber line even as a crossover and its existence in the form of a nonanalyticity is excluded.

Boundary Critical Behavior of the Three-Dimensional Heisenberg Universality Class

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We study the boundary critical behavior of the three-dimensional Heisenberg universality class, in the presence of a bidimensional surface. By means of high-precision Monte Carlo simulations of an improved lattice model, where leading bulk scaling corrections are suppressed, we prove the existence of a special phase transition, with unusual exponents, and of an extraordinary phase with logarithmically decaying correlations. These findings contrast with naïve arguments on the bulk-surface phase diagram, and allow us to explain some recent puzzling results on the boundary critical behavior of quantum spin models.

Ref: F. Parisen Toldin, Phys. Rev. Lett. **126**, 135701 (2021)

Electron phonon entanglement and the validity of the Luttinger description

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The coupling between electronic and lattice degrees of freedom lies at the core of many important properties of solids. Nevertheless, surprisingly little is known about the entanglement between these degrees of freedom. Here, we calculate the entanglement entropy at zero temperature as well as the mutual information and the logarithmic entanglement negativity at finite temperatures between the electrons and the lattice for a one-dimensional chain. The electrons are described within Luttinger-liquid theory. Our results show that the entanglement entropy diverges when one approaches the limit of stability, the so-called Wentzel-Bardeen singularity. Using combinatoric bound of the entanglement entropy one can establish the range of validity of the Luttinger description. We apply our results to topological insulator nanowire.

Interface in presence of a wall. Results from field theory

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We consider three-dimensional statistical systems at phase coexistence in the half-volume with boundary conditions leading to the presence of an interface. Working slightly below the critical temperature, where universal properties emerge, we show how the problem can be studied analytically from first principles, starting from the degrees of freedom (particle modes) of the bulk field theory. After deriving the passage probability of the interface and the order parameter profile in the regime in which the interface is not bound to the wall, we show how the theory accounts at the fundamental level also for the binding transition and its key parameter.

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A novel quantity for characterizing the dynamics of state-transition networks

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State-transition networks (STN) provide a powerful representation for encoding the dynamics of various complex systems with discrete states. Inspired by the Lyapunov exponents [1], here we introduce a novel network measure for STNs. Together with an adequate sampling of both space and time, continuous-time dynamical systems can also be mapped to STNs. This novel measure is able to reflect the dynamical behavior of the underlying dynamical system, furthermore, unlike the traditional network measures, it may be used to predict upcoming crisis-type bifurcations when changing the control parameters. We explore the measure's properties by a theoretical model and demonstrate its applicability on the STN counterparts of the Henon map and the Lorenz system.

[1] Sándor, B., Schneider, B., Lázár, Z. I., & Ercsey-Ravasz, M., Entropy, 23(1), 2021

Gintropy: entropic features of the Lorenz curve

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The Lorenz curve is known since 1905 in economy, the notion of entropy since 1886 - due to Rudolf Clausius - in thermodynamics. These are distinct concepts. Their mathematical properties, however, show several coincident features. The study of these might help to view the description of income and wealth inequalities in the more general terms of statistical physics.

In this talk we review equivalent formulas for the Gini index describing an overall inequality coded in a probability density function, a PDF. Introducing the gintropy as the deviation of the Lorenz curve from the diagonal in the cumulative wealth – cumulative population possessing it diagram, its several intriguing mathematical properties, like non-negativity, convexity, or the position of its maximum are explored.

Some theoretical examples of having analytically calculable gintropies and Gini indices are presented: genuine communism with a singular PDF describing absolute income equality, a mixed two-class distribution, an eco-window with uniform probability for any income in a fixed interval, and finally the realistic Pareto distribution used to describe capitalism. A particular limit of the latter relates the exponential PDF to a gintropy repeating the Boltzmann–Gibbs entropy formula, while the more general capitalistic case generates a gintropy formula resembling the Tsallis entropy. The eco-window reveals the so called entanglement entropy formula known from quantum physics.

Whether it is more than a formal analogy between mathematical relations is an open question. The corner stone of the test is an analogue of the second law of thermodynamics, identifying a class simple dynamical models of income distributions which are bound to increase the inequality, i.e. the Gini index.

First-passage process in degree space for networks

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From the dynamical point of view, a vertex of a network can gain or lose connection(s) with time, and monitoring this degree variation provides data that aids in the description of the time-evolution of the system. The main aim of the present work is to investigate when a vertex achieves a pre-established degree for the first time. The strategy to tackle this question is to adapt it into a random walk problem (in degree space) and examine the associated first-passage process. The method was illustrated by the dynamical version of the Erdős-Rényi and Watts-Strogatz models, where the vertices are statistically equivalent. Furthermore, their dynamics possess time-translational invariance, which can be explored to access the first-passage time analytically. The dependence of this last quantity - as well as the second moment - with the size of the system, was carefully analyzed.

Unraveling the role of node metadata in network robustness: the feature-based percolation model

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Percolation is an emblematic model used to understand the robustness of interconnected systems, in which the nodes of a network are removed and different topological properties of the resulting structure are analyzed. From a theoretical perspective, this process is usually investigated in relatively simple scenarios, such as the removal of the system's units in random order or sequentially ordered by specific topological descriptors. However, in the vast majority of empirical applications, it is required to dismantle the network following more sophisticated protocols that include non-topological information, such as node metadata.

In this work we propose a novel mathematical framework to fill this gap, and illustrate its applicability with several real networks. The nodes of a network are assigned a set of *features* $\mathbf{F}$, whose nature varies from problem to problem. Therefore we have a multidimensional, correlated joint degree-feature distribution $P(k, \mathbf{F})$ for which we derive several percolation quantities. We focus, theoretically and numerically, on scenarios where nodes are removed according to their importance in the feature space, and finding an excellent match between theory and simulations when the network is intervened following these feature-based protocols.

We apply our framework to degree-feature relations of different nature. We start from ad hoc degree-feature distributions that capture the main characteristics of correlations observed in empirical systems, such as power-law positive and negative degree-feature correlations, moving to features that arise naturally in the process of network growth and ending with the case in which features are coupled to dynamical processes running on top of the network, such as epidemics or biochemical dynamics, among others. Both synthetic and real-world networks of different origin are considered in the analysis. Our results evince how the inclusion of non-topological information in the robustness assessments provides very interesting new phenomenology, offering at the same time insightful lessons to better protect, or dismantle, real systems.

The article has been recently accepted in Nature Communications.

A Message-Passing Approach to Epidemic Tracing and Mitigation with Apps

Ginestra Bianconi, **Hanlin Sun**, Giacomo Rapisardi, Alex Arenas

With the hit of new pandemic threats, scientific frameworks are needed to understand the unfolding of the epidemic. The use of mobile apps that are able to trace contacts is of utmost importance in order to control new infected cases and contain further propagation.

Here we present a theoretical approach [1] that uses both percolation and message--passing techniques to quantify the role of automated contact tracing in mitigating an epidemic wave.

Our approach captures the steady state of the SIR epidemic spreading with contact-tracing and test policies based on the mapping of the process to link percolation. Each individual is assigned a variable indicating the adoption or not of the app. Assuming perfect efficiency of the app, the model is based on the fact that only individuals with the app infected by individuals with the app are not able to spread the disease further if infected (see Figure 1).

Our study goes beyond previous attempts to study the effect of the app by fully capturing the non-linear effects of the dynamics and the phase diagram of the process. Moreover, we show that the adoption of the app by a large fraction of the population increases the value of epidemic threshold, and the best strategy in order to maximally delay the percolation transition is given by targeting the hubs. We use both percolation and message-passing techniques to study the role of contact tracing in mitigating an epidemic wave and we predict analytically the phase diagram of the model in random networks with given degree sequence. The analytical results are compared with extensive Monte Carlo simulations showing good agreement for homogeneous, heterogeneous networks models and for real data.

In conclusion, the proposed theoretical framework is able to assess the expected impact of contact-tracing apps in the course of an epidemic capturing the non-linear effect of the spreading dynamics. These results are important to quantify the level of adoption needed for contact-tracing apps to be effective in mitigating an epidemic.

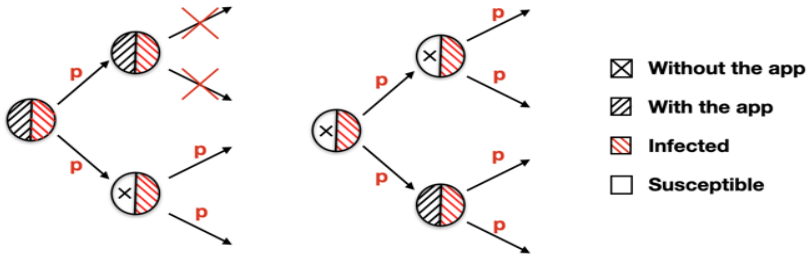

Figure 1: Sketch of the infection pathways that leads to the epidemic spreading in a population in which there are individuals that have adopted the app and individual that have not adopted the app.

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The Fate of Articulation Points and Bredges in Percolation

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We investigate the statistics of articulation points and bredges (bridge-edges) in complex networks in which bonds are randomly removed in a percolation process. Articulation points are *nodes* whose removal would break the network component on which they are located into two or more disconnected components, while bredges are *edges* whose removal would break the network component on which they are located into two components. Because of the heterogeneous nature of complex networks, the probability of a node to be an articulation point, or of an edge to be a bredge will not be homogeneous across the network. We therefore analyze full distributions of articulation point probabilities as well as bredge probabilities, using a message-passing approach to the problem, both for large single instances, and for networks in the configuration model class in the thermodynamic limit. We reveal, and are able to rationalize, a significant amount of structure in the evolution of articulation point and bredge probabilities in response to random bond removal. We argue that our results could be exploited in a variety of applications, including approaches to network dismantling or to vaccination and islanding strategies to prevent the spread of epidemics or of blackouts in process networks. Further details in Phys. Rev. E **103**, 042302 (2021).

Arbitrage on the energy market as a minority game

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As a consequence of the energy transition, the energy market is reorganized towards more decentralized structures. Retailers on local markets try to optimize their own profit while possibly losing track of the physical grid stability. Occasionally it is observed that the reserve energy is almost completely exhausted due to strong fluctuations in renewable energy, so that drastic changes in the price for reserve energy are very likely abused by arbitrageurs. We map this situation to a minority game. We determine the average arbitrage over the number of players and over a certain period of time with a focus on its fluctuations, as large fluctuations in arbitrage may destabilize the grid. The fluctuations depend non-monotonously on a parameter that is the ratio of P, a measure for the complexity of available information, and the number N of arbitrageurs. This dependence results from an underlying phase transition that has its counterpart in spin glasses where it corresponds to replica symmetry breaking. Depending on the choice of parameters, the fluctuations may grow even proportional to N. When other external fluctuations are included to represent uncertainties of different sources, their combination with a nonlinear price function may actually reduce the arbitrage and effectively stabilize the grid. We also analyze the impact of risk aversion of arbitrageurs. Based on our results we propose economic and statutory measures to reduce the amount of arbitrage below a tolerable low threshold. Our results complement those obtained from an economic perspective, as we deal with collective effects, manifest in the signatures of an underlying phase transition, and with the interplay of nonlinear price functions with stochastic fluctuations. This understanding supports decisions, for example, regarding an optimal choice of the market size in terms of the number of retailers.

T. Ritmeester and H. Meyer-Ortmanns, Physica A 573, 125927 1-19 (2021).

Effect of correlated noise on multistable systems with time-delay feedback control

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Dynamical systems modeling real-life applications are excited by environmental noises that are correlated, and thus cannot be assumed as white. The noise-induced transitions that these systems exhibit, due to bistabilities in their potential, can be mitigated by considering linear time-delay feedback control. After a general result determining the effects of control in multidimensional systems under colored noise, we focus on scalar stochastic differential equations (SDEs) excited by additive or multiplicative Ornstein-Uhlenbeck noise. For small time delay, the control of these SDEs results in the introduction of an effective potential, and the intensification of both the noise intensity and correlation time by factors $(1-a\tau)^{-1/2}$ and $(1-a\tau)^{-1}$ respectively, with τ being the time delay and a the control gain. By determining the stationary solution of a novel nonlinear Fokker-Planck equation, we are able to approximate SDE's stationary response distribution. This response distribution approximation is fairly accurate, eliminating thus the need for Monte Carlo simulations. Furthermore, we are able to accurately predict, as well as to suppress via the control term, the peak drift phenomenon, and the appearance of inflated tails in the controlled stationary distributions. To the best of our knowledge, these phenomena have not been systematically examined before.

Thermal Entanglement of Dinuclear Nickel Complexes as the Case Study of a Spin-1 Heisenberg Dimer with an Uniaxial Single-Ion Anisotropy in a Magnetic Field

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The bipartite entanglement in pure and mixed states of a quantum spin-1 Heisenberg dimer with an exchange and uniaxial single-ion anisotropy is qualified through a negativity in a presence of the external magnetic field. In the case of easy-axis single-ion anisotropy a kink is observed in the temperature dependence of the negativity due to a sudden death of one contribution to the negativity at a given temperature. Zero-temperature density plot of the negativity is in full agreement with the ground-state phase diagram. The experimental values of the exchange constant and the single-ion anisotropy parameter previously reported for the homodinuclear nickel compound $[Ni_2(Medpt)_2(\mu-ox)(H_2O)_2](ClO_4)_2.2H_2O$ which serves as a good representative of the antiferromagnetic spin-1 Heisenberg dimer, have allowed us to estimate a strength of the bipartite entanglement as well as threshold temperature above which entanglement vanishes. It is shown that the negativity is most persistent against rising temperature at the magnetic field, for which an energy gap between a ground state and a first excited state is highest.

Relaxation in an ensemble of elongated particles on a line as driven by Brownian diffusion

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Relaxation in an ensembles containing identical elongated particles (discorectangles) on a line was studied by using kinetic Monte Carlo simulations. The initial state was produced by using a random sequential adsorption (RSA) model ("Paris car parking problem"). In RSA model the overlapping of particles is strictly forbidden, i.e., excluded volume interaction between particles is assumed. The partially oriented systems with the preassigned order parameter within the range $S \in [-1; 1]$ were considered. Particularly, for $S = 1$ all particles are oriented along the line, and for $S = -1$ they oriented perpendicularly to the line. The aspect ratio (length-to-width ratio) for the particles was varied within the range $\epsilon \in [1; 20]$. During the relaxation (some kind of aging), the particles underwent translational and rotational Brownian motions. Distribution functions of the shortest distance and angle between near-neighbor particles were calculated. The relaxation behaviors of the order parameter, packing density and percolation connectivity were analyzed.

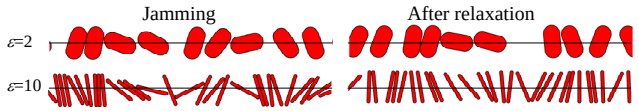

Figure 1: Examples of RSA packings in jamming state and after relaxation for the preassigned order parameter $S = 0$ (random orientation).

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Binary mixtures of particles with soft exclusion: Exact phase diagrams for tree-like lattices

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We study equilibrium properties of binary lattice gases comprising A and B particles, which undergo continuous exchanges with their respective reservoirs, maintained at chemical potentials $\mu_A = \mu_B = \mu$. The particles interact via on-site hard-core exclusion and also between the nearest-neighbours: there are a soft repulsion for AB pairs and interactions of strength J for AA and BB pairs. For tree-like Bethe and Husimi lattices we determine the full phase diagram of such a ternary mixture of particles and voids. We show that for J being above a lattice-dependent threshold value, the critical behaviour is similar: the system undergoes a transition at $\mu = \mu_c$ from a phase with equal mean densities of species into a phase with a spontaneously broken symmetry, in which the mean densities are no longer equal. Depending on the value of J, this transition can be either continuous or of the first order. For sufficiently big negative J, the behaviour on two lattices becomes markedly different: while for the Bethe lattice there exists a continuous transition into a phase with an alternating order, and a continuous re-entrant transition into a disordered phase, such a phase does not exist on the Husimi tree due to strong frustration effects.

Our work generalizes a previous exact analysis of the behaviour in disordered one-dimensional systems [D. Shapoval, M. Dudka, O. Bénichou, and G. Oshanin, *Phys. Rev. E* **102**, 032121 (2020)].

Super-spreader hot-spots, mobility and lock-down effects on the dynamics of SIR epidemic models

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Power-law (PL) time dependent infection growth has been reported in many COVID-19 statistics. In simple SIR models the number of infections grows at the outbreak as $I(t) \propto t^{d-1}$ on d-dimensional Euclidean lattices in the endemic phase or follow a slower universal PL at the critical point, until finite sizes cause immunity and a crossover to an exponential decay. Heterogeneity may alter the dynamics of spreading models, spatially inhomogeneous infection rates can cause slower decays, posing a threat of a long recovery from a pandemic. COVID-19 statistics have also provided epidemic size distributions with PL tails in several countries. Here I investigate SIR like models on hierarchical modular networks, embedded in 2d lattices with the addition of long-range links. I show that if the topological dimension of the network is finite, average degree dependent PL growth of prevalence emerges. Supercritically the same exponents as of regular graphs occurs, but the topological disorder alters the critical behavior. This is also true for the epidemic size distributions. Mobility of individuals does not affect the form of the scaling behavior, except for the $d = 2$ lattice, but increases the magnitude of the epidemic. The addition of a super-spreader hot-spot also does not change the growth exponent and the exponential decay in the heard immunity regime.

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Ising and Potts models in a random field: results from (quasi-)exact algorithms

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The non-trivial critical behavior of the random-field Ising model is governed by a zero-temperature fixed point. As a consequence, ground-state calculations provide an alternative avenue for studying critical behavior, in particular since algorithms borrowed from computer science allow for the exact calculation of ground states for large systems. While extensive work in recent years has covered the behavior of this system in three, four, and even five dimensions, less attention has been paid to the two-dimensional model which, however, is no less fascinating (and experimentally much more relevant than 4D and 5D). We solve a long-standing puzzle by presenting compelling numerical evidence for the scaling behavior of the correlation length ξ, showing that it scales like $\xi \sim \exp[A/h^2]$ with the strength h of the random field. For the related problem of *Potts* spins in a field, no exact algorithms are available, and very little is known for this system. As it is shown here, it is possible to arrive at accurate predictions for such systems based on techniques used in computer vision if combined with suitable extrapolation methods. For the $q = 3$ random-field Potts model in three dimensions, extensive simulations based on these approaches show a continuous transition of a type that is distinct from the Ising system, thus allowing us to uncover a new universality class of systems subject to quenched randomness.

Mixed-order transition in the antiferromagnetic quantum Ising chain in a field

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The antiferromagnetic quantum Ising chain has a quantum critical point which belongs to the universality class of the transverse Ising model (TIM). When a longitudinal field (h) is switched on, the phase transition is preserved, which turns to first-order for $h/\Gamma \to \infty$, Γ being the strength of the transverse field. Here we will re-examine the critical properties along the phase transition line. During a quantum block renormalization group calculation, the TIM fixed point for $h/\Gamma > 0$ is found to be unstable. Using DMRG techniques, we calculated the entanglement entropy and the spin-spin correlation function, both of which signaled a divergent correlation length at the transition point with the TIM exponents. At the same time, the bulk correlation function has a jump and the end-to-end correlation function has a discontinuous derivative at the transition point. Consequently for finite h/Γ the transition is of mixed-order.

Unlocking heterogeneity of node activation in gene regulatory networks

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The regulation of gene expression is at the core of all biological processes inside a cell. Differential gene expression in cell types can be interpreted as the result of collective properties of the entire genome. We study gene expression through the tools of network and disordered systems theory (using dynamical message passing). We investigate networks of effective gene-to-gene interactions, which mutually determine whether a gene is active or not. We propose simple update rules to characterise the time evolution in presence of noise and external signals. To solve the dynamics in noisy conditions, we develop a method that dramatically reduces the computational complexity of the dynamical message passing algorithm from exponential to quadratic in the degree for a fully asymmetric network. We use the power of the algorithm to unlock the noise dependent heterogeneity of stationary node activation patterns in such systems.

First-passage bias of learning in stochastic environments

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Physics of active matter is a natural sandbox for control algorithms. The group of control methods known as reinforcement learning presents a promising way to control active particles. Many of the relevant environments are governed by stochastic dynamics. Hence, the impact of stochasticity on learning needs to be investigated.

We use Q-learning with table Q-function to find the fastest path to a target. As an environment we consider 1D and 2D gridworlds having regions with different levels of noise. The noise is modelled as a fixed number of random actions, added to every action of an agent. In such systems without noise it is well known that RL converges to optimal paths readily.

Contrary to that scenario in our systems we observe stable bias in policy selection, connected with noise level. On realistic timescales, the bias leads to selection of suboptimal strategies, increasing presence of agents in regions with high noise.

In addition to Q-learning we have tested Double Q-learning, Expected SARSA and SARSA algorithms that produce qualitatively similar results.

Aging in the Two-Dimensional Long-Range Ising Model with Power-Law Interactions

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The current understanding of aging phenomena is mainly confined to systems with short-ranged interactions. Little is known about the aging of long-ranged systems. Here we present first results of Monte Carlo simulations for the aging in the phase-ordering kinetics of the $d = 2$ dimensional Ising model with power-law long-range interactions $\propto r^{-d+\sigma}$. The dynamical scaling of the two-time spin-spin autocorrelator is shown to be well described by simple aging for all interaction ranges studied. The autocorrelation exponents are consistent with $\lambda = 1.25$ in the effectively short-range regime with $\sigma > 1$, while for stronger long-range interactions with $\sigma < 1$ the data are consistent with $\lambda = d/2 = 1$. For very long-ranged interactions, strong finite-size effects are observed. We discuss whether such finite-size effects could be misinterpreted phenomenologically as sub-aging.

[1] H. Christiansen, S. Majumder, M. Henkel, and W. Janke, *Aging in the Long-Range Ising Model*, Phys. Rev. Lett. **125**, 180601-1–7 (2020).

Analytical estimation of the percolation threshold for mixed site-bonds problems by the renormalization group method

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Many properties of composite materials such as electrical conduction, dielectric response and oth. are closely related to the geometrical arrangement of the constitutive phases. Percolation theory, whose objective is to characterize the connectivity properties in random geometries and to explore them with respect to physical processes, thus provides a natural frame for the theoretical description of random composites.

In recent years, great progress has been made in the field of numerical methods of percolation theory; however, analytical descriptions for many important cases still remain open. In particular, mixed problems, in which both nodes and bonds can be removed from the lattice, are resource-demanding for numerical experiments and require at least rough methods of analytical estimates.

We propose applying the generalized renormalization group method to obtain the position of the percolation threshold for a mixed problem. The work considers mixed percolation problems on square and cubic lattices. Polynomial mappings were constructed for the relationship between the probability p_{n+1} of a renormalized cell conductance at $n+1$ iteration and p_n at the n-th iteration. The percolation threshold was calculated as the position of the real-space fixed points of the mentioned polynomial mapping. The estimates were verified using a numerical method based on the construction of regular graphs of the corresponding lattices for different probabilities of filling with conducting nodes and connections. In the figure, the dots indicate the results of the numerical calculation of the position of the percolation threshold, and the solid lines - analytical estimates by the proposed method.

Approach to consensus in models of continuous-opinion dynamics: A study inspired by the physics of granular gases

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A model for continuous-opinion dynamics is proposed and studied by taking advantage of its similarities with a mono-dimensional granular gas. Agents interact as in the Deffuant model, with a parameter α controlling the persuasibility of the individuals. The interaction coincides with the collision rule of two grains moving on a line, provided opinions and velocities are identified, with α being the so-called coefficient of normal restitution. Starting from the master equation of the probability density of all opinions, general conditions are given for the system to reach consensus. The case when the interaction frequency is proportional to the β-power of the relative opinions is studied in more detail. It is shown that the mean-field approximation to the master equation leads to the Boltzmann kinetic equation for the opinion distribution. In this case, the system always approaches consensus, which can be seen as the approach to zero of the opinion temperature, a measure of the width of the opinion distribution. Moreover, the long-time behaviour of the system is characterized by a scaling solution to the Boltzmann equation in which all time dependence occurs through the temperature. The case $\beta = 0$ is related to the Deffuant model and is analytically soluble. The scaling distribution is unimodal and independent of α. For $\beta > 0$ the distribution of opinions is unimodal below a critical value of $|\alpha|$, being multimodal with two maxima above it. This means that agents may approach consensus while being polarized. Near the critical points and for $|\alpha| \geq 0.4$, the distribution of opinions is well approximated by the sum of two Gaussian distributions. Monte Carlo simulations are in agreement with the theoretical results.

Balanced and fragmented phases in societies with homophily and social balance

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We try to understand the recent increase of social fragmentation with a simple model where we use spins to represent G-dimensional vectors of binary opinions of individuals and use a positive (negative) link weight to represent friendship (enmity), respectively. We take into account the joint effects of (1) homophily—the tendency of people with similar opinions to establish positive relations, and (2) social balance—the tendency to establish balanced triadic relations. These two mechanisms are incorporated in a localized Hamiltonian that minimizes social stress through the co-evolution of opinions of individuals and their social networks. Specifically, starting from a random assignment of opinions for each of N agents, an initial social network is constructed from the similarities between pairs of connected agents. The dynamics is iterated in four steps until the system reaches a steady state: i) we randomly select an agent, i, and within its social neighbourhood a fraction of Q triads is randomly chosen among all possible $N_\Delta^{(i)}$ triads of node i. The social stress H of i is calculated; ii) one of i's opinions is flipped and the weights of all links which are part of the Q selected triads are reevaluated. Now we re-calculate the stress of i, H'; iii) The update is accepted, if either the stress is reduced, i.e. $H' < H$, or in case it increases, with probability $e^{-H'+H}$, otherwise the opinions and network remain unchanged. We show how the likelihood of social fragmentation increases as individuals care more about social balance. We identify the critical size of the social neighbourhood, Q_c, above which society must fragment into communities that are internally cohesive and hostile towards other groups.

Changeover phenomenon in randomly colored Potts model

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A hybrid q-state Potts model where a random fraction p of the spins assume q_0 states and a random fraction $1-p$ of the spins assume $q > q_0$ states is introduced. It is known that when the system is homogeneous, with a spin number q_0 or q, it undergoes a second or a first order transition, respectively. Heuristic arguments together with simulations of two-dimensional systems show that there is a fraction p^* such that a first order transition is exhibited for $p < p^*$. The presence of p^* is also indicated for the mean field hybrid model. An exact expression for the second order critical line in concentration-temperature parameter space of that model is obtained.

Conformational Entropy Estimation of a Non-Markovian Random Walk by Autoregressive Generative Modeling

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We propose a new flexible method of calculating conformational entropy of lattice polymer and random walk models and apply it to reconstruct phase diagram of a novel model of non-Markovian discrete random walk on a three-dimensional lattice, which we call volume and surface reinforced random walk. The idea of the model is that each step of the walk depends on the entire previous trajectory: we differentiate between probabilities of (i) steps directed to already visited points of the lattice (volume reinforcement), (ii) steps along the surface of the previously visited volume (surface reinforcement), and (iii) all others steps. This model is a generalization of volume reinforced walks previously studied in the literature, in a certain range of parameter values, its trajectories demonstrate the presence of hierarchical folded structures resembling the three-dimensional structure of DNA in chromosomes.

The method approximates the full-dimensional probability density function over all possible conformations by deep autoregressive generative model resembling the PixelCNN. The joint distribution $p(x|\theta)$ of a trajectory x conditioned on a vector θ of macroscopic parameters is expanded as $p(x|\theta) = \prod_{i=1}^{len(x)} p(x_i|x_{<i}, \theta)$, where conditional distributions are modelled by a deep neural network. We present the adaptive masking mechanism which takes into account sequential nature of the trajectory generation process and allows to define sparse three-dimensional generalization of conditional PixelCNN capable of computing all conditional distributions in a single forward pass. The network then is trained on the ensemble of trajectories generated for different macroscopic parameters using maximum likelihood estimation. Given a trained network we compute conformational entropy by averaging negative log-likelihood over ensemble of trajectories generated at fixed values of macroscopic parameters $S(\theta) = -\mathbb{E}_x \log p(x|\theta)$.

Controlled crack patterns in thin brittle layers

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Shrinkage induced cracking of thin material layers attached to a rigid substrate is abundant in nature giving rise to the formation spectacular polygonal crack patterns. Examples can be mentioned on a wide range of length scales from dried out lake beds through permafrost regions, to the columnar joints formed in cooling volcanic lava. Under laboratory conditions the simplest realization of such crack patterns can be achieved by desiccating thin layers of dense colloidal suspensions in a container, which typically leads to isotropic polygonal crack patterns.

Anisotropic crack patterns emerging in desiccating layers of pastes on a substrate can be exploited for controlled cracking with potential applications in microelectronic manufacturing. Recently, a promising method of the generation of controlled crack patterns has been suggested by applying mechanical excitation to dense calcium carbonate and magnesium carbonate hydroxide pastes before desiccation sets in. As a result of excitation the main cracks emerged perpendicularly the applied vibration.

Due to its potential technological applications, we investigated how the competition of the initially imposed anisotropy and the structural disorder of the thin layer affects the formation of the structure of the crack pattern. We studied the process of shrinkage induced cracking by means of realistic discrete element simulations where anisotropy is captured by the directional dependence of the local cohesive strength. We demonstrate that the strength of anisotropy has a decisive effect on the emerging crack pattern. In particular, cracking is found to evolve through three distinct phases of formation of long cracks aligned with a direction of initial mechanical excitation, secondary cracking in the perpendicular direction, and after the formation of a connected crack network binary fragmentation sets. The anisotropic crack patterns gives rise to fragments with an elongated shape which gradually gets reduced by binary fragmentation. Nonetheless the statistics of fragment masses exhibits a high degree of robustness which can be described by log-normal distribution.

Controlling Particle Currents with Evaporation and Resetting from an Interval

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We investigate the Brownian diffusion of particles in one spatial dimension and in the presence of finite regions within which particles can either evaporate or be reset to a given location. For open boundary conditions, we highlight the appearance of a Brownian yet non-Gaussian diffusion: at long times, the particle distribution is non-Gaussian but its variance grows linearly in time. Moreover, we show that the effective diffusion coefficient of the particles in such systems is bounded from below by $(1 - 2/\pi)$ times their bare diffusion coefficient. For periodic boundary conditions, i.e., for diffusion on a ring with resetting, we demonstrate a "gauge invariance" of the spatial particle distribution for different choices of the resetting probability currents, in both stationary and non-stationary regimes. Finally, we apply our findings to a stochastic biophysical model for the motion of RNA polymerases during transcriptional pauses, deriving analytically the distribution of the length of cleaved RNA transcripts and the efficiency of RNA cleavage in backtrack recovery.

Crackling avalanches due to short range interaction in the limit of high disorder

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Under a slowly increasing mechanical load the fracture of heterogeneous materials proceeds in bursts which generate acoustic noise, and hence, can be recorded by acoustic emission techniques. The time series of such crackling events provide a deep insight into the dynamics of fracturing and can be exploited to forecast the imminent catastrophic collapse of the system. Recently, we have shown in a fiber bundle model (FBM) of long range load sharing that the record statistics of crackling events can be exploited to increase the precision of failure forecast methods, since it clearly signals the onset of acceleration towards global failure.

Here we consider the limiting case of short range load sharing and study the evolution of the sequence of crackling events using record statistics. We generate fracture processes using a fiber bundle model where fibers are organized on a square lattice and load is redistributed over the intact nearest neighbors of broken fibers. As the external load increases, the fracture process is driven by the competition of the evolving stress field and of the disordered strength of fibers. Computer simulations showed that for low strength disorder the stress concentration dominates the fracture process making the overall response of the system highly brittle, i.e. the system evolves through breaking avalanches, however, no acceleration of the process, hence, no signal of the imminent failure can be detected. At a sufficiently high degree of disorder, global failure is preceded by an acceleration regime which gets broader as the amount of disorder increases. However, the analysis of record statistics revealed that this acceleration is rather short, making forecasting practically impossible when the load sharing is short ranged.

Critical Behaviour of Magnetic Polymers in Two and Three Dimensions

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We explore the critical behaviour of the a magnetic polymer in solution modelled by a self-avoiding walk on the square (2d) or cubic (3d) lattice where each monomer (site visited by the walk) carries an Ising spin which interacts with nearest-neighbour spins on the lattice. This model was first studied in three dimensions by Garel, Orland and Orlandini, European Physical Journal B, **12**, 261 (1999) using mean-field theory and multi-Markov chain Monte-Carlo methods. We revisit the 3d case and explore for the first time the 2d case using flatPERM to estimate the coefficients of the finite-length partition functions, coupled with finite-size scaling methods, to look at the critical behaviour particularly in zero field, but also as the external field, h. is varied.

For $h = 0$ in three dimensions we confirm the presence of a first-order collapse transition, as predicted by Garel *et al.*, whilst in two dimensions we find a non-trivial second-order collapse transition with a magnetic field exponent $\beta = 1/8$ as for the usual two-dimensional Ising model, but a critical length exponent $\nu \approx 0.585$.

In 3d it is expected that the first-order behaviour persists up to a finite field value before the behaviour becomes the usual second-order transition for an interacting self-avoiding walk. The location of the multicritical point separating these two behaviours will be discussed. In two dimensions $h = 0$ is a special point, and the usual collapse transition is observed for all $|h| > 0$.

Critical scaling in the random-field Potts model

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Unlike the random-field Ising model, an exact ground-state algorithm for the *random-field Potts model* (RFPM) with more than two states does not exist. Using a computationally efficient *graph-cut method*, however, we solve the ground state problem approximately in polynomial time. Combining this technique with a sophisticated extrapolation method, we can guarantee results that are representative of the exact ground-state behavior up to reasonably large system sizes. A comprehensive study is carried out to predict the critical behavior for the case of the 3-state model in three dimensions from such approximate ground-state calculations. In particular, we determined the magnetization, Binder cumulant, specific heat, as well as the connected and disconnected susceptibilities for many random initial conditions and extrapolated them to the limit of quasi-exact solutions. These results are used to (precisely) locate the critical point and to calculate (accurately) the critical exponents that characterize the singular behavior near the phase transition.

Cross-correlations in the Brownian motion of colloidal nanoparticles

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The two-body cross-correlation for the diffusive motion of colloidal nano-spheres is experimentally investigated. Polystyrene nano-spheres were used in a very low concentration suspension in order to minimize the three- or more body collective effects. Beside the generally used longitudinal and transverse component correlations we investigate also the Pearson correlation in the magnitude of the displacements. In agreement with previous studies we find that the longitudinal and transverse component correlations decay as a function of the inter-particle distance following a power-law trend with an exponent around -2. The Pearson correlation in the magnitude of the displacements decay also as a power-law with an exponent around -1.

Crystal growth rates in supercooled atomic liquid mixtures

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Crystallization is a fundamental process in materials science, providing the primary route for the realization of a wide range of novel materials and probing glass-forming ability [Tang *et al.*, Nature Mater., 12, 507 (2013)]. At the microscopic level, crystallization is described by the classical crystal nucleation and growth theories [Jackson, *Kinetic Processes* (2004)]. The observation of apparently different crystal growth regimes in many binary liquid mixtures greatly challenges our understanding of crystallization, being the classical models of crystal growth unable to fully describe the available data [Orava and Greer, J. Chem. Phys., 140, 214504 (2014)]. In this work ([Schottelius, Mambretti *et al.*, 19, 512-516 (2020)]), we study by experiments, theory, and computer simulations the crystallization of supercooled mixtures of argon and krypton. X-ray scattering experiments performed at DESY (http://www.desy.de/) synchrotron source in Hamburg, Germany, used to probe the crystallization process of supercooled liquid Ar-Kr microjets, are supported by Molecular Dynamics simulations of seeded crystal growth of several mixtures studied at different krypton concentration. We leveraged Local Bond Order Parameters [Lechner and Dellago, J. Chem. Phys., 129, 114707 (2008)] to analyze the configurations, and also to calculate crystal growth rates as a function of mixing ratio. Our work shows that crystal growth rates in these systems can be reconciled with existing crystal growth models, only by explicitly accounting for the non-ideality of the mixtures, as we demonstrated through thermodynamic calculations. These results highlight the importance of thermodynamic aspects in describing the crystal growth kinetics, providing a major step towards a more sophisticated theory of crystal growth.

Defects Superdiffusion and Unbinding in a 2D Active XY Model

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Active matter constitutes a novel and rapidly growing field gathering interests and contributions from very diverse communities. Among the variety of cooperative behaviors displayed by active systems, particular attention is being paid to topological defects. These play a salient role already in equilibrium systems, as they drive topological phase transitions –the so-called Berezinskii-Kosterlitz-Thouless (BKT) transition– in a variety of contexts. In active matter, they behave in a different and richer fashion : many recent theoretical and experimental works have shown that defects can self-propel in the presence of activity, driving complex collective dynamics. However, despite a great deal of recent research efforts, a full characterization of their dynamics is still lacking.

To address these questions, we consider a non-equilibrium extension of the two-dimensional (2D) XY model, equivalent to the noisy Kuramoto model of synchronization with short-range coupling, where rotors sitting on a square lattice are self-driven by random intrinsic frequencies.

We show that self-spinning induces a new behavior compared to the standard 2D XY model and provides a generic route to pattern formation and super-diffusion of topological defects. We show that activity results in the emergence of a finite characteristic length, controlled by the forcing intensity. Upon self-driving, vortices generically *unbind*, breaking the BKT picture and display *superdiffusion* $\langle r^2(t)\rangle \sim t^{3/2}$ — following simple Gaussian statistics. Our simple framework reproduces the findings of very recent experimental studies, opening new directions of research to understand general features of topological defects in active systems.

Development of a Low Variance Entropy Estimator and its Application to a Stock Network to Quantify the Covid-19 Shock Response of Financial Markets

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Shannons information entropy is a vital quantity to characterize discrete data samples. It lays the foundation for higher-order measures integral to non-linear systems analysis such as mutual information and transfer entropy. Though generalizations for (quasi) continuous distributions exist, these depend on the possibly unknown underlying probability density and lack desirable attributes such as non-negativity and coordinate invariance. Resultingly, it is common practice to use discrete information entropy, even for continuous data. This approach introduces partition-hyperparameters to the model that substantially influence results. Therefore, we conduct a systematic analysis of different binning techniques concerning entropy calculation with Monte-Carlo methods. We then develop a modified entropy estimator by positively associating the number of data contained in a bin and its width with its probability, normalize by the number of frequency classes and make the bias consistent through an entropy maximizing binning algorithm. This approach outperforms other binning techniques in terms of the relative variance. It further enables comparability of entropy of multiple samples if their respective characteristics force different binning. Subsequently, we apply our entropy-maximizing estimator to construct a directed temporal network of a subset of S&P 500 titles. Here, the transfer entropy between two stocks defines the edge weight. We find substantial evidence for higher information transfer in times of high economic policy uncertainty. This relationship shows to be particularly tight on the onset of the current COVID-19 pandemic.

Discontinuous quantum and classical magnetic response of the pentakis dodecahedron

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The pentakis dodecahedron, the dual of the truncated icosahedron, consists of 60 edge-sharing triangles. It has 20 six-fold and 12 five-fold coordinated vertices, with the former forming a dodecahedron, and each of the latter connected to the vertices of one of the 12 pentagons of the dodecahedron. When spins mounted on the vertices of the pentakis dodecahedron interact according to the nearest-neighbor antiferromagnetic Heisenberg model, the two different vertex types necessitate the introduction of two exchange constants. As the relative strength of the two constants is varied the molecule interpolates between the dodecahedron and a molecule consisting only of quadrangles. The competition between the two exchange constants, frustration, and an external magnetic field results in a multitude of ground-state magnetization and susceptibility discontinuities. At the classical level the maximum is ten magnetization and one susceptibility discontinuities when the 12 five-fold vertices interact with the dodecahedron spins with approximately one-half the strength of their interaction. When the two interactions are approximately equal in strength the number of discontinuities is also maximized, with three of the magnetization and eight of the susceptibility. At the full quantum limit, where the magnitude of the spins equals $\frac{1}{2}$, there can be up to three ground-state magnetization jumps that have the z-component of the total spin changing by $\Delta S^z = 2$, even though quantum fluctuations rarely allow discontinuities of the magnetization. The full quantum case also supports a $\Delta S^z = 3$ discontinuity. Frustration also results in nonmagnetic states inside the singlet-triplet gap. These results make the pentakis dodecahedron the molecule with the most discontinuous magnetic response from the quantum to the classical level.

DNA thermal denaturation by polymer field theory approach

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We discuss possible mechanisms that may impact the order of the transition between denaturated and bounded DNA states and lead to changes in the scaling laws that govern conformational properties of DNA strands. To this end, we re-consider the Poland-Scheraga model and apply a polymer field theory to calculate entropic exponents associated with the denaturated loop distribution. For the $d = 2$ case the latter are deduced from mapping the polymer model onto a two- dimensional random lattice, i.e. in the presence of quantum gravity. For the $d = 3$ case we get the corresponding (diverging) ε^4 expansions evaluating them by restoring their convergence via the resummation technique.

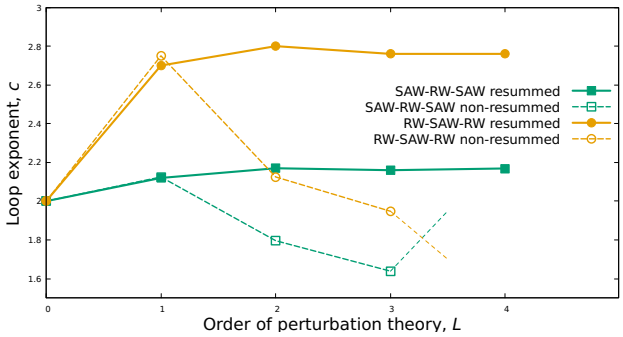

Fig.1. *Loop closure exponent c for DNA of heterogeneous compositions modeled as sequences of random and self-avoiding walks in different orders of $\varepsilon = 4 - d$ expansion at space dimension $d = 3$. Solid and dashed lines show resummed (convergent) and non-resummed (divergent) values, correspondingly. Value $c = 2$ discriminates between the first (at $c \geq 2$ and the second (at $1 \leq c < 2$) order transition.*

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Effect of Vicsek-like Activity on the Dynamics of a Flexible Polymer

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The dynamics of many biological filaments can be understood within the framework of active polymer models. We construct a flexible bead-spring model with attractive Lennard-Jones interactions in which the activity among the beads is introduced via a Vicsek-like alignment rule. Due to the additional activity, the beads will try to align their velocities towards a particular direction with time. Following a quench from the high-temperature coil phase to a low-temperature state, we study its kinetics via molecular dynamics (MD) simulations using Langevin thermostat. For the passive polymer, we confirm the earlier observation from Monte Carlo studies that the low-temperature equilibrium state is a compact globule. Our results for active beads reveal that the typical final steady state is also of globular form. The nonequilibrium pathway, however, changes due to the effect of activity. In this work, we focus on the nonequilibrium coarsening kinetics and the associated scaling laws for the collapse time and growth of clusters. Interestingly we observe nonmonotonic behavior in coarsening with the variation of the strength of activity. In the final steady state, we study the motion of the polymer globule which changes from super-diffusive to ballistic behavior with increasing activity compared to a diffusive motion for the passive case.

Effects of inhomogeneous bulk magnetization of magnetic particles on the magnetic energy of a magneto-sensitive elastomer

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Magneto-sensitive elastomers are composite materials with magnetic and elastic subsystems. Magnetic particles, which comprise magnetic subsystem, strongly influence mechanical and rheological properties of the elastomer. Usual approach is to treat the interparticle interactions as the point-like dipole-dipole ones. However, when the interparticle distances are comparable with their size, the effects of inhomogeneous bulk magnetization become increasingly important. As a result, in the case of the systems with a tendency to form column-like clusters or with high concentration of the particles the point-like dipole-dipole approximation may not be accurate enough.

In the current paper we develop the self-consistent dipole (SCD) energy model, which allows description of the effects of inhomogeneous bulk magnetization for two particles. For example, it predicts attraction for wider amount of mutual configurations than the point-like dipole-dipole one, thus, enhances the ability of the particles to form column-like clusters. Than, we compare it to several others, notably the expression of energy of two magnetizable spheres, which was obtained elsewhere via numerical solution of the Laplace equation (LE). We also show that formalism of the microsphere, obtained earlier, do not suffer from altering the potential energy. To do so, we calculate the shape factor of the macroscopic spheroidal sample using the LE particle interactions. This shape factor expression is in a full agreement with the continuum mechanics result and with the one obtained earlier for point-like dipole interactions.

Entanglement measure of frustrated Heisenberg octahedral chain within the localized-magnon approach

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Localized-magnon theory is a powerful tool for rigorous determination of the ground state and detailed study of the thermodynamic properties of a special class of frustrated quantum Heisenberg antiferromagnets under certain conditions (strong magnetic fields and low temperatures) [1-2]. In the present study we verify another application of localized-magnon concept for calculation of bipartite entanglement [3-4] between the nearest-neighbor and next-nearest-neighbor spin pairs of frustrated spin-1/2 Heisenberg octahedral chain [5] in a presence of the external magnetic field. It was shown that localized-magnon theory can be straightforwardly adapted in order to calculate concurrence, which measures a strength of the pairwise entanglement. For verification of localized-magnons predictions we have performed a full ED of the finite-size spin-1/2 Heisenberg octahedral chain with 4 unit cells (20 spins). The obtained results confirm a new possibility of application the localized-magnon concept for simple calculation of concurrence for the frustrated Heisenberg antiferromagnets.

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Explicit formulas for the probability of percolation on finite graphs

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For the site percolation on a square lattice, percolation thresholds have been were calculated with an accuracy of 10-12 [1]. Moreover, the proposed methods also allow finding explicit analytical formulas for the percolation probability. We analyze the various ways to enhance these methods. Some possible ways are as follows:

- Finding explicit formulas for the probability of percolation on finite arbitrary graphs, in particular, on a torus;
- Use of topological dynamic programming methods;
- Finding heuristic algorithms for finding the optimal turn in monotone win-lose random turn games on graphs (for example, a Random-Turn Hex game);
- Use of heuristic methods.

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Extracting partition function zeros from Fukui-Todo simulations

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The Fukui-Todo algorithm is an efficient Monte Carlo tool for sampling states of a spin system near a phase transition. Accuracy of the qualitative and quantitative conclusions about the phase transition depends much on how the Monte Carlo data are subsequently analyzed. An elegant solution here is a numerical study of the structure of the partition function zeros. However, because the Fukui-Todo algorithm bypasses sample-by-sample energy computation, zeros cannot easily be harnessed through the energy distribution. Here this obstacle is overcome by a novel reweighting technique and zero-detection protocol. The efficacy of the approach is demonstrated in a square lattice Potts model for the number of states $q = 2, 3$ in the second order transition regime and $q = 6$ in a first order regime.

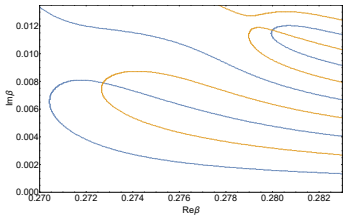

Figure 1: Lines of zeros of the real part (blue) and imaginary part (orange) of the partition function. Intersections of these contours show location of Fisher zeros for 2D Ising model on a 48×48 square lattice.

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Finding the Theta temperature of a polymer with long-range interactions

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Recently we adapted a Monte Carlo method for generating self-avoiding walks on lattice geometries which employs a binary-tree data-structure for polymers with continuous degrees of freedom. Data suggests that the time per Monte Carlo move scales logarithmically with polymer length. Here, we generalize the method to Lennard-Jones polymers with untruncated monomer-monomer interaction. To this end we propose a variant of the Metropolis algorithm which in combination with the tree data-structure preserves logarithmic scaling. We determine the Theta-temperature for Lennard-Jones polymers using two different approaches and present the results for chains with up to 16384 repeat units.

A new method of solution of the Wetterich equation and its applications

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A new truncation scheme is proposed [1] to solve the Wetterich exact renormalization group equation [2,3]

$$\frac{\partial}{\partial k}\Gamma_k[\phi] = \frac{1}{2}\mathrm{Tr}\left\{\left[\Gamma_k^{(2)}[\phi] + R_k\right]^{-1}\frac{\partial}{\partial k}R_k\right\}$$

for the the effective average action $\Gamma_k[\phi]$, depending on the averaged order parameter ϕ in presence of external sources and the running infrared cut-off scale k, induced by the cut-off function R_k in the wave-vector space. It allows us to calculate the two–point correlation function depending on the wave-vector magnitude q and the cut-off scale k. The natural domain of validity of the derivative expansion appears to be limited to small values of q/k. To the contrary, the new approximation scheme has the advantage to be valid for any q/k, therefore, it can be auspicious in many current and potential applications of the celebrated Wetterich equation and similar models. In distinction from the derivative expansion, derivatives are not truncated at a finite order in the new scheme. It is shown that the derivative expansion up to the ∂^2 order is just the small-q approximation of our new equations at the first order of truncation. The RG flow equations at this order are derived and approximately solved as an example. Furthermore, a new method of functional truncations is tested for such a solution.

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Geometrical Aspects of the Multicritical Phase Diagrams for the Blume-Emery-Griffiths Model

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A Ruppeiner metric is defined on a 2D phase space of dipolar (m) and quadrupolar (q) order parameters for the spin-1 mean-field Blume-Emery-Griffiths model. Then, an expression for the Ricci scalar (R) is derived and temperature/crystal field variations of R are presented using four different phase diagram topologies introduced by Hoston and Berker (1991). Its behaviour near the continuous/discontinuous phase transition temperatures as well as the multicritical points is investigated. Besides the study of R along the phase equilibria we have located the $R = 0$ boundry lines in the multicrital phase diagrams.

Gravity driven fragmentation of a cohesive granular column

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Natural catastrophes like landslides are typically initiated on steep hillsides by heavy raining when water penetrates the pores and reduces the cohesion of soils [1]. To understand the emergence of landslides and debris flows we investigated the collapse of a granular column under the action of gravity by means of discrete element simulations. Cohesion is introduced by connecting the particles with non-linear spring elements. The constitutive law of springs captures the elastic behavior of particle contacts at small deformations, the plasticity beyond a yield threshold, and the gradual softening and final breaking at large separation distances. A very important feature of the interaction is that particle contacts can be healed, i.e. if two particles approach each other within a capture distance, a new cohesive contact is established between them.

Our calculations revealed that at high cohesion the granular column sinks in but keeps its integrity. When the cohesion is week, the process of collapse cannot stop: the system breaks up into a large number of fragments. The two phases of high and low cohesion represent the landslide and the debris flow states respectively. We demonstrate that the transition occurs at a critical cohesion showing analogies to continuous phase transitions. The fragment mass distribution in the debris flow phase has a power law behaviour with an exponent which falls close to the corresponding value of brittle fragmentation in two dimensions [2].

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Hematite cube chains in static magnetic fields

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Hematite from a physical viewpoint is a weak ferromagnetic material. This means that it has three orders of magnitude smaller permanent magnetization than magnetite. Therefore, hematite colloids allow us to explore a different physical particle interaction parameter range compared to ordinary ferromagnetic particle colloids. In this case the steric forces compete with the magnetic forces and thermal fluctuations play an important role.

In the presence of a weak static external magnetic field (B <0.1 mT) the particles of hematite with cubic shape tend to align and form straight chains along the direction of the applied magnetic field. An increase in the strength of the applied field causes an additional rearrangement of the chains. Chains reorganize in the kinked structures. Here we explain why such kinked structures are formed. In order to explain this we examine the most energetically favorable configurations of hematite cube chains and observe what changes if thermal fluctuations are taken into account. We calculate distributions for angle between the orientation of a chain and the direction of the external magnetic field. The obtained results are also compared with experiments. The work was funded by PostDocLatvia grant No. 1.1.1.2/VIAA/3/19/562 and M.era-net project FMF No.1.1.1.5/ERANET/18/04.

Heterogeneous excitable systems exhibit Griffiths phases below hybrid phase transitions

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In $d > 2$ dimensional, homogeneous threshold models discontinuous transition occur, but the mean-field solution provides $1/t$ power-law activity decay and other power-laws, thus it is called mixed-order or hybrid type. It has recently been shown that the introduction of quenched disorder rounds the discontinuity and second order phase transition and Griffiths phases appear. Here we provide numerical evidence, that even in case of high graph dimensional hierarchical modular networks a Griffiths phase in the $K = 2$ threshold model is present below the hybrid phase transition. This is due to the fragmentation of the activity propagation by modules, which are connected via single links. This provides a widespread mechanism in case of threshold type of heterogeneous systems, modeling the brain or epidemics for the occurrence of dynamical criticality in extended Griffiths phase parameter spaces. We investigate this in synthetic modular networks with and without inhibitory links as well as in the presence of refractory states.

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Hidden Markov Models: A Breakdown of Random Matrix Universality and The Brain Criticality Hypothesis

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Complex systems typically display a broad spectrum of relaxation timescales, a phenomenon often linked to criticality. However, in discrete Markovian systems, generic large transition matrices are governed by random matrix theory, which predicts the absence of long timescales unless fine-tuned. Here we show a simple scenario for the emergence of long time-scales in discrete Markovian systems, by varying the dynamic range of matrix elements. We show that as the dynamic range increases, a phase transition occurs whereby the random matrix theory result is avoided, and long relaxation times ensue, in the entire 'ordered' phase. We furthermore show that this phase transition is accompanied by scale-free behaviour. The findings are then used to test the brain criticality hypothesis using fMRI data and show that brains lie in a critical region identified by this phase transition.

How does homophily shape the dynamics of an evolving network?

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We consider a dynamic network of individuals that may hold one of two different opinions in a two-party society. As a dynamical model, agents can endlessly create and delete links to satisfy a preferred degree, and the network is shaped by *homophily*, a form of social interaction. Characterized by the parameter $J \in [-1, 1]$, the latter plays a role similar to Ising spins: agents create links to others of the same opinion with probability $(1 + J)/2$, and delete them with probability $(1 - J)/2$. Using Monte Carlo simulations and mean field theory, we focus on the network structure in the steady state. We study the effects of J on degree distributions and the fraction of cross-party links, ρ, and on the degree distribution. While the extreme cases of homophily or heterophily ($J = \pm 1$) are easily understood to result in complete polarization ($\rho = 0$) or anti-polarization ($\rho = 1$), intermediate values of J lead to interesting behavior of the network, especially when the communities are of different sizes. In addition, we introduce a novel measure of polarization which displays distinct advantages over a commonly used quantity - the average edge homogeneity.

Influence of the thickness on optical properties of cadmium sulfide thin films

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Cadmium sulfide thin films with different thickness were deposited on quartz substrates by the method of high-frequency magnetron sputtering using a VUP-5M vacuum station (Selmi, Ukraine). Commercial target of 99.99 % purity was used for deposition. The target–substrate distance was equal to 60 mm. The start and end of the sputtering process were controlled by means of a movable shutter.

The phase analysis and crystal structure refinement was examined with X-ray diffraction data (XRD) obtained on DRON-2.0M diffractometer at room temperature with the Kα radiation (λ= 1.936087 $\mathring{A}$) of Fe. The spectral dependence of optical transmittance and reflection of the obtained samples were measured in the visible and near infrared regions (300-1500 nm) at room temperature using the spectrometer Shimadzu UV-3600.

The optical constants and the band gap of the films under study have been determined. Optical properties (refractive index $n(\lambda)$, absorption coefficient $\alpha(\lambda)$, extinction coefficient $k(\lambda)$, dielectric functions $\varepsilon(\lambda)$ and optical conductivity $\sigma(\lambda)$) of thin films and thickness d can be determined from the transmission and reflection spectrum. The increase of the bandgap width was revealed by comparing obtained value ultra-thin films with the known results for single crystal. The dispersion of the refractive index was explained using a single oscillator model. Single oscillator energy and dispersion energy are obtained from fitting. Optical parameters of the films were determined using the Cauchy, Sellmeier and Wemple models.

Ising universality in the two-dimensional Blume-Capel model with quenched random crystal field

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Using high-precision Monte Carlo simulations based on a parallel version of the Wang-Landau algorithm and finite-size scaling techniques, we study the effect of quenched disorder in the crystal-field coupling of the Blume-Capel model on a square lattice. We mainly focus on the part of the phase diagram where the pure model undergoes a continuous transition, known to fall into the universality class of a pure Ising ferromagnet. A dedicated scaling analysis reveals concrete evidence in favor of the strong universality hypothesis with the presence of additional logarithmic corrections in the scaling of the specific heat. Our results are in agreement with an early real-space renormalization-group study of the model as well as a very recent numerical work where quenched randomness was introduced in the energy exchange coupling. Finally, by properly fine tuning the control parameters of the randomness distribution we also qualitatively investigate the part of the phase diagram where the pure model undergoes a first-order phase transition. For this region, preliminary evidence indicate a smoothing of the transition to second-order with the presence of strong scaling corrections.

Knots are Generic Stable Phases in Semiflexible Polymers

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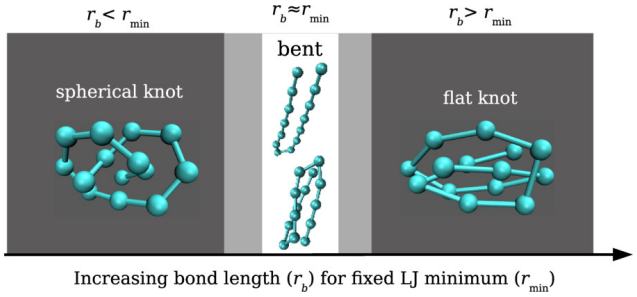
While investigations of knots in polymers have lured scientists for decades, the existence of phases characterized by a stable knot of specific type has attracted attention only recently. In this work, we treat two popular models that encompass the complete spectrum of real polymers (flexible to stiff) via extensive replica exchange Monte Carlo simulations, and show that the existence of stable knots in the phase diagram depends only on the ratio $r_b/r_{\min}$, where r_b is the equilibrium bond length and $r_{\min}$ is the distance for the strongest nonbonded contacts in an attractive Lennard-Jones (LJ) potential. Our results provide evidence that irrespective of the specific model, bead-stick or bead-spring, if the ratio $r_b/r_{\min}$ is outside a small window around unity then one always encounters for semiflexible polymers stable knotted phases at low temperatures.



Lagrangian discripton of dissipative oscillator

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The damped harmonic oscillator is the most elementary classical mechanical system that shows dissipative behavior. Describing such a process in Langrangian formalism can be problematic due to mathematical difficulties. As it is a statistical process, either the environment must be included in the model, or a trick must be used to receive the proper equations of motion.

Introducing a potential, in a more general sense than what it means in electrodynamics, it is possible to obtain a Lagrangian, and also the solution for the potential function, including initial conditions. Generally, potentials contain non-physical solutions, but these can be eliminated naturally by choosing initial conditions cleverly.

It seems that this method proves to be effective in solving classical transport processes. On the other hand, the possibility of dealing with such systems in Lagrangian formalism suggests the idea of quantization. Hopefully, the discussed method may also be used for modern problems, such as loss of information or restoring the coherence of a system.

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Modeling Earthquake statistics by a Burridge-Knopoff-type spring-block chain

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Due to their disastrous socio-economic impacts studying earthquakes is indisputably important. Our long-term aim is to predict large magnitude earthquakes, both by finding precursor events or using statistical methods. Due to our present information revolution, nowadays we are able to access uniformly structured, large online earthquake databases. Carefully collected and categorized data are perfect instruments for the statistical investigation of earthquakes. In previous empirical studies interesting universalities were found. It was shown that the distribution of the released energies, for different tectonic zones, are well described by a Tsallis-Pareto (Lomax II) distribution. An other universality is related to the recurrence times: the distribution of the interval times between earthquakes over a given cut magnitude (CM) for a tectonic region collapse on a universal curve and can be fitted with a Gamma distribution. In the present work, we intended to explain these empirical results, by a simple one dimensional spring- block model, known as the Burridge-Knopoff model. Previous studies already concluded that this model reproduces successfully the Tsallis-Pareto distribution for the released energies. We prove here, that with properly adjusted parameters, the exponent of this scale-free distribution becomes close to the one found in experimental data. Furthermore, we prove that the model is able to reproduce also the Gamma distribution for the recurrence times. These results give further confidence for the use of spring-block models in approaching universalities found in earthquake statistics.

Monte Carlo simulation of particle dynamics in bi-dispersed colloidal droplets

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Colloidal droplets are used in a variety of applications. Some of them require the presence of particles of different sizes. These include methods of medical diagnostics, the creation of photonic crystals, the formation of supraparticles, and the production of membranes for biotechnology.

Some experiments have previously shown the possibility of particle separation by their size near the contact line. We have developed a mathematical model that describes this process. Bi-dispersed colloidal droplets during their evaporation on the hydrophilic substrate with a small contact angle were taken in our consideration. In such a system, a monolayer of particles is formed near the periphery of the drop. This pattern form is associated with the effect of coffee rings. The model takes into account the transport by the flow caused by the evaporation of the liquid and the diffusion of particles.

We carried out a Monte Carlo simulation for several particle concentrations. The results of the calculations correspond to experimental observations when smaller particles accumulate closer to the contact line than relatively large particles.

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Nanorod-based transparent electrodes as random resistor networks

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Computer simulation of the physical properties of nanomaterials is an urgent task for improving nanotechnology. Electrically conductive and at the same time transparent in the visible range of electromagnetic radiation films are widely used in touch screens, photovoltaic devices, displays based on organic light-emitting diodes, etc. Transparent electrodes based on nanowires, nanorods, and nanorings are considered as a promising alternative to titanium oxide electrodes. The report will review our recent works devoted to modeling the electrical conductivity of two-dimensional random systems of nanorods.

We mimic nanorod-based transparent electrodes as random resistor networks produced by the homogeneous, isotropic, and random deposition of conductive zero-width sticks onto an insulating substrate. The number density (the number of objects per unit area of the surface) of these sticks is supposed to exceed the percolation threshold, i.e., the system under consideration is a conductor. To identify any current-carrying part (the backbone) of the percolation cluster, we have proposed and implemented a modification of the well-known wall follower algorithm —one type of maze solving algorithm. The advantage of the modified algorithm is its identification of the whole backbone without visiting all the edges. The algorithm has been applied to backbone identification in networks with different number densities of conducting sticks. We have found that (i) for number densities of sticks above the percolation threshold, the strength of the percolation cluster quickly approaches unity as the number density of the sticks increases; (ii) simultaneously, the percolation cluster becomes identical to its backbone plus simplest dead ends, i.e., edges that are incident to vertices of degree 1. This behavior is consistent with some analytical evaluations.

Failure avalanches on complex networks

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The fracture of heterogeneous materials under a slowly increasing external load proceeds in avalanches of local failure events, where the cracking of a material region can trigger additional cracking events due to the subsequent redistribution of mechanical load over the intact elements. The range of interaction, i.e. load sharing after failure events and the degree of disorder of the strength of individual elements of the system play a crutial role in the evolution of failure avalanches. Two limiting cases of load sharing has been extensively studied, i.e. the equal load sharing where no stress fluctuations can arises, and the localized load sharing which results in strong stress concentration around failed regions. Based on a fiber bundle model, here we investigate how the topology of the connections of material elements affects the time evolution of failure cascades and the statistics of their characteristic quantities. In the model, initially fibers are placed on a square lattice which is then rewired according to the Watts-Strogatz method. Fibers have a random strength which is sampled from an exponential distribution. Tuning the rewiring probability from 0 to 1, we generate fracture processes by slowly increasing the external load to break a single fiber and record the triggered avalanche of failures as the load is redistributed along the connections of fibers. We show that the temporal profile of avalanches has a right handed asymetry, i.e. avalanches slowly accelerate and stop suddenly. The asymmetry of the average profiles proved to depend on the network topology: increasing the rewiring probability reduces the asymmetry, however, even in the case of the perfectly random network the avalanche profile is not symmetric. The distribution of avalanche sizes and durations have power law functional form where the exponents are increasing from the rewiring probability. We show that the dynamics and statistics of cascading failures on random graphs are different from the characteristics of equal load sharing systems.

On the equilibrium states of thermodynamic systems in a small vicinity of the equilibrium values of parameters

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The dynamic behavior of thermodynamic systems described by a single order parameter and several control parameters is studied in a small neighborhood of ordinary and bifurcation equilibrium values of the system parameters. Using the general methods of investigating the branching (bifurcations) of solutions for nonlinear equations, we performed an exhaustive analysis of the order parameter dependences on the control parameters in a small vicinity of the equilibrium values of parameters, including the stability analysis of the equilibrium states, and the asymptotic behavior of the order parameter dependences on the control parameters (bifurcation diagrams). One shall adopt the most convenient general form of the applied methods, because both the order and control parameters are singnificantly different for distinct physical systems, and the analysis of equilibrium states relevant, in particular, to the crystal-nucleation phenomena in supercooled liquids as well as protein crystallization by using these general results is presented in the recently published paper (A.A. Barsuk, F. Paladi, Physica A 527 (2019) 121303-20). The novelty value of the research results refers indeed to the complete list of canonical forms and bifurcation diagrams, as well as the sensitivity analyses of the ordinary and bifurcation equilibrium values of the order parameter as a function of control parameters, and the estimation of the phase transition time. We also consider important from both theoretical and practical point of view represented in a general form results relating to the analysis of the sensitivity of parameters describing the equilibrium states of dynamical (thermodynamic) systems for both ordinary and bifurcation values of parameters. These results are an important generalization of the well-known form of the equation of state in differential form, which is referred to as the "cyclic identity" in thermodynamics (A.A. Barsuk, F. Paladi, J. Stat. Phys. 171 (2018) 361), that is, one can rewrite the partials in terms of other partials using the cyclic and reciprocity relationships.

Operator expansions, layer susceptibility and correlation functions in boundary CFT

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We show that in boundary conformal field theories, there exists a one-to-one correspondence between the boundary operator expansion of the two-point correlation function and a power series expansion of the layer susceptibility. This general property allows the direct identification of the boundary spectrum and expansion coefficients from the layer susceptibility and opens a new way for efficient calculations of two-point correlators in BCFTs. To show how it works we derive an explicit expression for the correlation function $\langle \phi_i \phi^i \rangle$ of the $O(N)$ model at the extraordinary transition in $4-\varepsilon$ dimensional semi-infinite space to order $O(\varepsilon)$. The bulk operator product expansion of the two-point function gives access to the spectrum of the bulk CFT. In our example, we obtain the averaged anomalous dimensions of scalar composite operators of the $O(N)$ model to order $O(\varepsilon^2)$. These agree with the known results both in ε and large-N expansions.

Parallel structure factors of lateral and transverse phase separations in bilayer biomembranes: Effects of the presence of an interacting wall

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Abstract

The adsorption of biomolecules such as lipids or proteins on a solid substrate has numerous significant applications in different fields such as drug delivery, pharmaceutics, and tissue engineering. In such situations, the phase transitions in the lipid membrane are influenced by the presence of an interacting wall. We consider, in this context, a bilayer biomembrane made up of two amphiphiles A and B. Under a variation of a suitable parameter, such as temperature or difference of lengths of hydrophobic chains, these systems undergo a phase separation from a homogeneous liquid phase to two distinct liquid phases. Two physical situations can be distinguished: (i) The amphiphiles A and B prefer to jump from a monolayer to the other (transverse or flip-flop transition), (ii) the mixture phase separates on each monolayer, and there is no jump from one sheet towards the second one (lateral transition). The physical system, here, is modeled by a two-order parameter field theory. The mixture is considered to be in a semi-infinite *three-dimensional* space limited by an interacting $2D$ −wall. The adsorption on the wall of one or both amphiphile species is assumed to be strong. We investigate, in this work, the influence of this adsorbing surface on the parallel structure factors $S(z,z')$ of the lipid mixture. These structure factors are exactly calculated in all cases: below T_c, above T_c, and at $T = T_c$, as well as their associated local compressibilities $S(z)$. Scaling laws, for these latter, are also derived.

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Phase behavior of a cell model with Curie-Weiss interaction

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An accurate calculation of the equation of state of a one-component cell model with Curie-Weiss potential is made. It is found that this model has a sequence of first order phase transitions at temperatures below the critical one. We analyzed the mechanism of these transitions based on the behavior of the chemical potential as a function of density. Isotherms, phase diagrams, and coexistence curves of the system are obtained and investigated, as well as the coordinates of a critical point and the order parameter behavior in the first three phase transitions of the cascade are determined.

Phase transitions in low-velocity impact phenomena

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We investigate the impact induced breaking of heterogeneous materials in the range of low impact velocities far below the fragmentation threshold. Particle breakage is widely used by the industry in comminution processes of ores and minerals, where particles collide both with each other and with hard components of the process equipment. Over the past decades, a detailed knowledge has been accumulated in physics, and engineering on single impact breakage phenomena, however, a comprehensive understanding of low velocity impact sequences responsible for the the gradual mass reduction and rounding of solid particles is still lacking. Here we present a theoretical study of the phase structure of impact induced attrition processes. Based on realistic discrete element simulations of sequences of particle-wall collisions, we show that depending on the impact velocity, three distinct phases of breakage emerge: at sufficiently low velocities repeated impacts result in abrasion of the body and lead to a finite asymptotic residual mass, however, above a threshold velocity a complete destruction is achieved within a finite number of repetitions. Instantaneous fragmentation occurs above a second critical velocity where cracks span the entire body and the sample rapidly falls apart into a large number of small pieces. The transitions between the abrasion, cleavage, and fragmentation phases occur at well-defined critical velocities analogous to continuous phase transitions. Our computer simulations revealed that the evolution of the mass and shape of the solid is governed by scaling laws in terms of the impact velocity. Most notably, in the cleavage phase the sample lifetime decreases as a power law of the impact velocity analogous to the Basquin law of sub-critical fracture. In the abrasion phase the shape evolution of the sample is described by a universal scaling form with a power law dependence on the impact velocity. The precise phase structure and scaling laws of impact induced attrition are important to understand the evolution of landforms, and can be exploited in the design of comminution technologies.

Phase-ordering kinetics and persistence of the two-dimensional long-range Ising model at zero temperature

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We investigate the phase-ordering kinetics of the $d = 2$ dimensional long-range Ising model with power-law decaying interactions $\propto 1/r^{d+\sigma}$. Recently, we have numerically confirmed that the characteristic length $\ell(t)$ after a quench to $0 < T < T_c$ grows like a power law $\ell(t) \sim t^{\alpha}$ in accordance with a long-standing prediction by Bray and Rutenberg, i.e., with $\alpha = 1/2$ for $\sigma > 1$ and $\alpha = 1/(1+\sigma)$ for $\sigma < 1$ [1]. This means, for quenches to finite T the growth is σ *dependent*. We now perform a quench to $T = 0$ [2], for which we observe that the growth exponent $\alpha \approx 3/4$ is *independent* of σ and different from $\alpha = 1/2$ as one would expect for the nearest-neighbor model. Additionally, we investigate the persistence of the local order parameter and provide estimates for the persistence exponent θ and the fractal dimension d_f of the persistent lattice. In the limit of large σ only the fractal dimension d_f of the nearest-neighbor Ising model is recovered, while θ differs significantly. This we understand from the unexpected value for α and a conjectured relation between these exponents, which we confirm numerically for the long-range model.

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Proposals for Hybrid Monte Carlo Simulations of Macromolecules

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Even nowadays, when simulations focus mostly to study biomacromolecules using Molecular Dynamics, Monte Carlo based methods still play a very important role. Using MD we are usually able to reach equlibrium and then sample a few microseconds of the macromolecule's life, but the number of independent samples is usually relativelly poor. Monte Carlo methods are usually much more efficient in walking through the phase space and therefore we would like to take the advantage of using it.

We can use various proposals for the Monte Carlo moves of macromolecular chains, like pivot move or time evolution using molecular dynamics. The latter approach is known as Hamiltonian Monte Carlo.

In this work we introduce new proposals for off-lattice Monte Carlo. We use various geometrical moves similar to pivot move and proposals based on Andersen thermostat. We also compare these Monte Carlo proposals from the point of view of computational efficiency as well as their efficiency in obtaining independent samples of the phase space of linear polyelectrolyte chain.

Possibility of a continuous phase transition in random-anisotropy magnets with a generic random axis distribution

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The structural disorder is inevitably present in many magnetic systems which undergo a phase transition. Of particular interest is its impact near the critical points, where even weak disorder can drastically modify the scaling behavior. In this work we analyze the critical properties of magnetic systems with continuous symmetry where the coupling of the order parameter to disorder is bilinear. Their critical behavior is usually described by the random-anisotropy model (RAM) which was first introduced to describe magnetic properties of amorphous alloys of rare-earth compounds with aspherical electron distributions and transition metals. Using two different field-theoretical renormalization group approaches we analyze how the critical properties depend on the local anisotropy axis distribution. We analyze the corresponding renormalization group flows with the help of the Padé-Borel resummation technique. We show that there is no stable fixed point accessible from physical inital conditions whose existence was argued in a recent study. This may indicate the absence of a long-range ordered phase in the presence of random-anisotropy disorder with a generic trimodal random-axis distribution [1].

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Random surface roughening with quenched disorder and turbulent environment

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The random surface roughening under the influence of quenched disorder and chaotic (turbulent) motion of the environment is studied by the means of the field-theoretic renormalization group on the base of Kardar-Parisi-Zhang nonlinear equation. The disorder is modelled by a time-independent, short-correlated random noise, while the motion of the environment is described by the Kazantsev- Kraichnan "rapid-change ensemble".

The absence of Galilean symmetry leads to a new qualitative effect: the advection term, being irrelevant by itself in regards to critical exponents, gives rise to a new effect: "digging" of the underlying substrate by unexpectedly emerging term, quadratic in the velocity field.

The scaling exponents of the resulting asymptotic regime are calculated to the leading order. Other possible infrared asymptotic regimes are also studied.

Pressure effect on the ferroelectric ordering in the framework of the Blume–Emery–Griffiths model

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We propose a modified deformable version of the Blume–Emery–Griffiths (dBEG) model taking into account a microscopic mechanism of the applied external pressure influence on thermodynamics and phase transitions in crystals with a multi-well (specifically, three-well) local lattice potential. Our approach is based on the idea that the crystal deformation leads to the change of internal field and displacements of atoms surrounding the structure elements (ionic groups); configurations of the latter are determined by the mentioned above local potential. Our modification of the model supplementarily considers the shift of local energy levels (due to restructuring of local anharmonic potentials formed by the electron subsystem) under the influence of deformation caused by a uniform pressure or tension. Such an approach allows to describe the deformational effects accompanying the phase transitions to the state with a dipole ordering (the ferroelectric phase).

The $Sn_2P_2S_6$ crystal is considered as an example. Experimental measurements reveal that the temperature of the phase transition to the ferroelectric phase decreases under the influence of the hydrostatic pressure resulting in a subsequent suppression of the ferroelectric ordering. The *ab initio* calculations indicate rearrangement of the local anharmonic potential under pressure. We demonstrate in this case that the interaction of energy states of the mentioned structure elements (e.g., groups P_2S_6 for the $Sn_2P_2S_6$ crystal) with the lattice deformation, taken into account in the framework of the proposed dBEG model, allows us to explain the observed suppression of the ferroelectric ordering under the pressure as well as predict a peak-like behaviour of the compressibility in the vicinity of the phase transition which also coincides with the observed one. In the regime of a clamped crystal our approach suggests a separation into differently strained fragments of the paraelectric and ferroelectric phases.

Potts model with invisible states: critical behaviour on a scale-free network

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Different models are proposed to understand the phase transitions in (magnetic) systems through the prism of competition between the energy and the entropy. One of such models is a Potts model with invisible states [1]. This model introduces r invisible states such that if spin lies in one of them, it does not interact with the rest of the system.

We consider such a model on an annealed scale-free network where the probability of a randomly chosen vertex having a degree k is governed by the power-law $P(k) \sim k^{-\lambda}$.We confirm the previously obtained results and conclusions [2-3], namely that the number of invisible states can change the universality class of models on graphs. In particular, on a complete graph or even on a scale-free network [3], when the degree distribution decay exponent plays an important role. Here, after numerical analysis of the free energy of the Potts model with invisible states on a scale-free network, we conclude that q, r, λ play a role of global parameters that influence the critical behaviour of the system [4]. The phase diagram in q, r, λ space can be separated into two main regions. In the region $1 < q \leq 2$, $3 \leq \lambda \cup q > 2$, $3 \leq \lambda \leq \lambda_c(q)$ we found two marginal values of r dependent on λ and q. They divide the phase diagram into three domains with different critical behaviour. For $q > 2, \lambda > \lambda_c(q)$ only first order phase transition is observer regardless of values of r.

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Simple models for complex polymers: hyperbranched polymers

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Many physical properties of polymer solutions strongly depend on the topology of the macromolecules. We study the size characteristics of a number of complex polymers by the means of Edwards model. All the chains are considered to be Gaussian thus allowing us to receive an exact expressions for gyration radius and hydrodynamic radius of the considered topologies. This model allows for an approximate description of the solution's properties in the vicinity of the θ-point. Here we concentrate on polymers with multiple branching points that form periodic structures as well as some simple polymer networks.

Synchronization in locally coupled one dimensional oscillator systems

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Synchronization in one-dimensional oscillator systems are studied both experimentally and by computer simulations. The oscillators have a spread in their natural frequencies and are arranged in a ring-like topology, interacting only with their nearest neighbors. According to the well-known Mermin-Wagner theorem in the thermodynamic limit the system should not be able to synchronize. Our aim here is to investigate how the synchronization order parameter vanishes as the system size is increased.

First we considered electronically coupled mechanical metronomes, where a magnetic braking force acts at each period of the oscillation cycle, when the limb of the metronomes reached the maximum amplitude at one side. Each metronome had a reference signal sent by it's previous neighbor. If the metronome's period was shorter than it's reference, the limb's motion was delayed by the implemented magnetic braking. Multiple measurements were done with closed 1D loops containing from 2 up to 9 metronomes.

On the computational side we first considered locally coupled Kuramoto oscillators in a closed circle. Extended numerical simulations were considered to show the dependence of the synchronization order parameter as a function of the system size and other model parameters (coupling strength and the variance of the oscillators natural frequencies). The second computational model is based on a realistic mechanical model of the metronomes with an interaction mechanism closely resembling the experimentally implemented one. We solved numerically the involved evolution equations and determined the same synchronization order parameters as the ones in the experiments.

Experiments and computational models yield similar results for the monotonic decaying trend of the synchronization order parameters as a function of the system size. We learned that the simple locally coupled Kuramoto model is already able to describe qualitatively the behavior of realistic oscillator systems like the ones formed by interacting metronomes.

The effect of interfacial morphology on the magnetic and magnetocaloric properties of ferromagnetic nanoparticles with core-shell geometry: A Monte Carlo study

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We present Monte Carlo simulation results for the magnetic and magnetocaloric properties exhibited by a magnetic nanoparticle composed of a ferromagnetic core which is surrounded by a ferromagnetic shell. The model is defined by an atomistic interaction Hamiltonian including the exchange couplings and a Zeeman term. Different shapes for the core and shell parts have been modelled by introducing the interparticle distance between the sites $A : (x_1, y_1, z_1)$ and $B : (x_2, y_2, z_2)$ in terms of the Minkowski distance

$$D_p(A, B) = (|x_1 - x_2|^p + |y_1 - y_2|^p + |z_1 - z_2|^p)^{1/p}, \qquad (1)$$

where $p = p_c, p_s$ denotes the metric order for the core and shell parts, respectively. Our results show that the magnetic and magnetocaloric properties are highly sensitive to the interface structure of the particle. Specifically, as a result of a competition mechanism between the core and shell magnetizations, the isothermal magnetic entropy change as a function of temperature may exhibit a double-peak behavior for a suitable selection of exchange coupling parameters.

The energetic performance of a critical thermal systems

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Heat transfer is very important for good design and reliable operation of a system. Reliability and system performance are highly dependent on the operating temperature, in particular, in electronic equipment. Several cooling methods have been proposed in order to improve the heat transfer. These techniques include two: which consists in grafting blades offering a greater contact surface with the environment; and which consists of using nanofluids comprising. The latter is currently present the best solution. This work could beused as the basis of 2D dimension numerical of heat transport models, which can be helpful to develop newer numerical technical models the coupled fluid flow and heat transfer of two tandem equal isothermal to find an optimal geometry for good cooling.

This work represents the results of extensive numerical simulations of 2D nanofluid flow around of heated bloc cylinder with different incidence angle and aspect ratio. The continuity and momentum equations have been numerically solved. Two types of nanofluids consisting of two type of nanoparticles with base fluids of water and ethylene glycol mixture were selected to evaluate their effect on the flow over a bloc cylinder, also their superiority over conventional fluids.The thermo-physical parameters of nanofluid have been estimated using the theory of one fluid phase, a contemporary correlations of thermal conductivity and viscosity of nanofluids have been used in this paper, which are functions of particle volumetric concentration as well as temperature.

Key words: Nanofluid, Fluid flow, Heat transfer

The Role of Resampling in Population Annealing

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Population Annealing (PA) is a population-based algorithm that can be used for equilibrium simulation of thermodynamic systems with a rough free energy landscape. It is known to be more efficient in doing so than standard Markov chain Monte Carlo alone. The algorithm has a number of parameters that can be fine-tuned to improve performance. While there is some theoretical and numerical work regarding most of these parameters, there appears to be a gap in the literature concerning the role of resampling in PA, which this work attempts to bridge.

The $d = 2$ Ising model is used as a benchmarking system for this study. At first various resampling methods are implemented and numerically compared using a GPU PA implementation. In a second part the exact solution of the Ising model is utilized to create an artificial PA setting with effectively infinite Monte Carlo updates at each temperature as well as an infinite population. This allows one to look at resampling in isolation from other parameters.

We identify when resampling choices affect the simulation outcome and obtain some results that are model-independent. Further, we name two resampling methods that appear preferable over the widely used multinomial resampling.

Universal shape properties of mesoscopic polymer stars and their aggregates

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We analyse macromolecular shape by the dissipative particle dynamics simulations. In the **case study A** we discuss homo- and hetero-stars immersed in a solvent of variable quality [1]. Asphericity and related properties are examined at various arms compositions as the functions of solvent quality. For the homo-star, the asphericity maximum is found close to the θ-point condition explained by the interplay between the enthalpic and entropic contributions to the free energy. In the **case study B** we consider the changes in shape-related universal ratios for a homo-star and for its individual arms with the increase of the number of arms f. The results for the universal ratios show very good agreement with the available data from the Monte Carlo and molecular dynamics simulations [2], whereas some of the ratios are calculated for the first time. In the **case study C** we extend our analysis to the simplest representative of the class of multiply branched polymer macromolecules, known as a pom-pom structure [3]. Whereas rheological behaviour of melts of pom-pom molecules are intensively studied so far, we turn our attention towards conformational properties of such polymers in a regime of dilute solution. In the **case study D** we looked at the aggregation of the amphiphilic stars in a solvent. Four architectures are examined: the miktoarm star, two different diblock stars and a set of four disjoint linear diblock copolymers. We observed four different shapes of aggregats: spherical, rod-like and disc-like micelles and a spherical vesicle. The change from a spherical to aspherical micelle shape is monotonous, whereas that from an aspherical micelle into a spherical vesicle is found to be discontinuous.

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Zero-Temperature Coarsening in the Two-Dimensional Long-Range Ising Model

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We investigate the nonequilibrium dynamics following a quench to zero temperature of the non-conserved Ising model with power-law decaying long-range interactions $\propto 1/r^{d+\sigma}$ in $d = 2$ spatial dimensions. The zero-temperature coarsening is always of special interest among nonequilibrium processes, because often peculiar behavior is observed. We provide estimates of the nonequilibrium exponents, viz., the growth exponent α, the persistence exponent θ, and the fractal dimension d_f. It is found that the growth exponent $\alpha \approx 3/4$ is independent of σ and different from $\alpha = 1/2$ as expected for nearest-neighbor models. In the large σ regime of the tunable interactions only the fractal dimension d_f of the nearest-neighbor Ising model is recovered, while the other exponents differ significantly. For the persistence exponent θ this is a direct consequence of the different growth exponents α as can be understood from the relation $d-d_f = \theta/\alpha$; they just differ by the ratio of the growth exponents $\approx 3/2$. This relation has been proposed for annihilation processes and later numerically tested for the $d = 2$ nearest-neighbor Ising model. We confirm this relation for all σ studied, reinforcing its general validity.


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