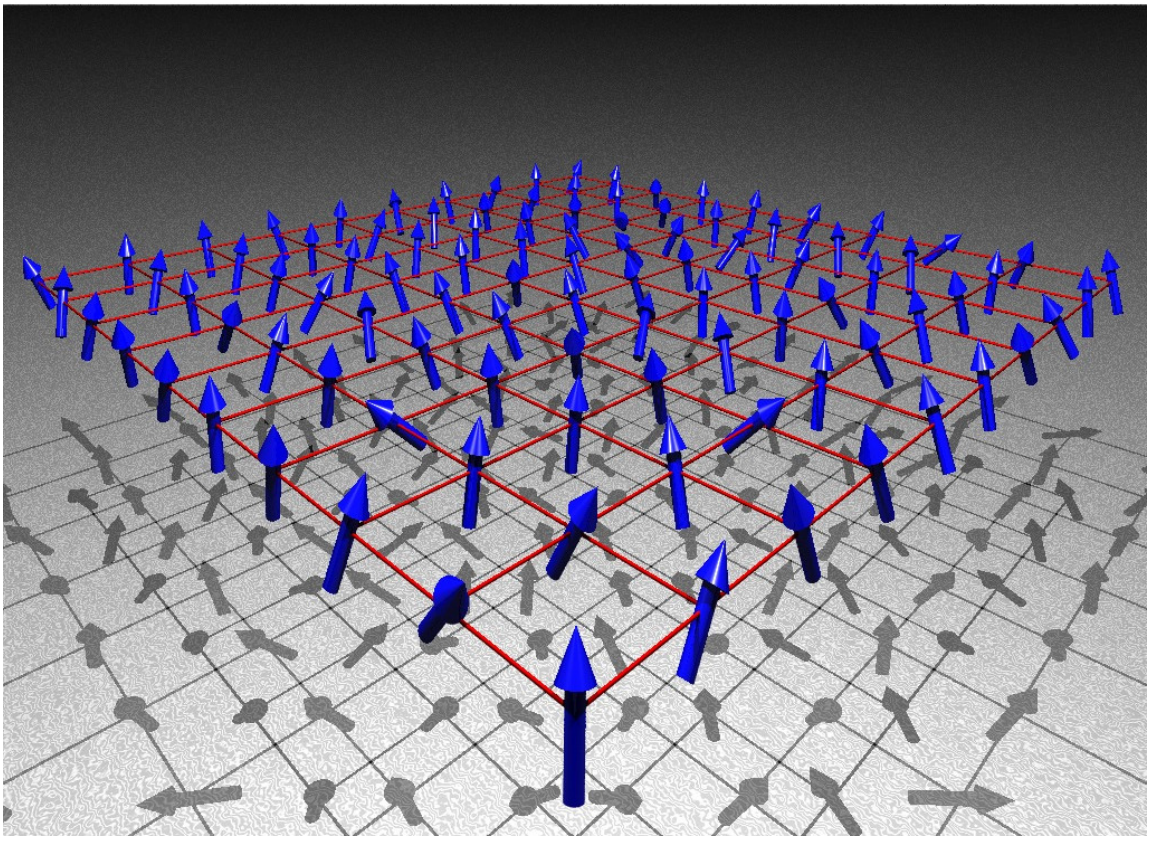
BOOK OF ABSTRACTS

of the

Conference on

Phase Transitions and Critical Phenomena



Coventry, United Kingdom

April 6 – 8, 2016

http://ptcp16.complexity-coventry.org

Preface

Welcome to the 1st conference on "Phase Transitions and Critical Phenomena", April 6–8, 2016 in Coventry, England. Phase transitions in equilibrium and, in particular, in non-equilibrium continue to be an area of great interest in a range of fields, from statistical physics, through lattice field theory, to sociophysics. The present meeting is designed to expose the state of the art in this field as well as to provide a stage for discussions about current challenges and future directions. Additionally, the conference is put together on the occasion of the 60th birthday of Wolfhard Janke, who significantly contributed to this field on a broad range of problems. The topics of this year's conference accordingly cover a broad range from spin systems to macromolecules. In particular, it is focused on spin models and disordered systems, lattice field theory, networks and complex systems, soft matter and biophysics, non-equilibrium processes, and their mathematical aspects. We hope that the chosen format of long, invited lectures and the sessions with contributed posters will create an atmosphere of active scientific discussions and many informal exchanges, celebrating the richness of problems in our field.

We thankfully acknowledge financial support from Springer and the European Physical Journal (EPJ), from Europhysics Letters (EPL) and the IOP with the Journal of Physics A (JPA). Partial travel support is provided by IRSES network "Dynamics of and in Complex Systems" (DIONICOS), funded by the EC's FP7 programme (PIRSES-GA-2013-612707), from the Institute of Mathematics and its Applications (IMA), from Coventry University, and from the Deutsch-Französische Hochschule (DFH-UFA) via the Graduate School Statistical Physics of Complex Systems between Leipzig-Lorraine-Lviv-Coventry ($\mathbb{L}^4$). Moreover, we would like to thank the local staff and all helping hands for their effort.

The organising committee

Michael Bachmann, University of Georgia, Athens (GA) USA
Elmar Bittner, Universität Heidelberg, Germany
Nikolaos Fytas, Coventry University, United Kingdom
Ralph Kenna, Coventry University, United Kingdom
Martin Weigel, Coventry University, United Kingdom
Johannes Zierenberg, Universität Leipzig, Germany

Wednesday, April 6, 2016

08:30 – 09:15		**– Registration and Welcome Coffee –** ☕
09:15 – 09:30		**– Welcome & Opening –**

Session I: (Chair: Elmar Bittner)

09:30 – 10:10	**Joan Adler**	Percolation in education and application in the 21st century
10:10 – 10:50	**Alexander Hartmann**	Large deviations for equilibrium and nonequilibrium processes
10:50 – 11:20		**– Coffee and Tea Break –** ☕

Session II: (Chair: Rudolf Hilfer)

11:20 – 12:00	**Kurt Binder**	Nucleation of colloidal crystals in the bulk and at a substrate
12:00 – 12:40	**Anders Irbäck**	Peptide folding in the presence of protein crowders
12:40 – 14:00		**– Lunch Break –** 🍽
14:00 – 15:30		**– Poster Session I –**

Session III: (Chair: Nikolaos Fytas)

15:30 – 16:10	**Walter Selke**	Classical and quantum anisotropic Heisenberg antiferromagnets
16:10 – 16:50	**Subir Das**	Kinetics of Vapor-Solid Phase Transition
16:50 – 17:30		**– Coffee and Tea Break –** ☕

Session IV: (Chair: Michael Bachmann)

17:30 – 18:10	**Malte Henkel**	Ageing and dynamical symmetries in the kinetics of interface growth
18:10 – 18:50	**Christian Holm**	Influence of the permittivity gradient on static and dynamic properties of charged macromolecules

Thursday, April 7, 2016

08:45 – 09:30		**– Wake-up Coffee and Tea –** ☕

Session V: (Chair: Martin Weigel)

09:30 – 10:10	**Wolfgang Paul**	Stochastic approximation Monte Carlo applied to polymer phase transitions
10:10 – 10:50	**Peter Grassberger**	To protect your own network and to destroy your opponent's: The importance of being explosive
10:50 – 11:20		**– Coffee and Tea Break –** ☕

Session VI: (Chair: Fred Hucht)

11:20 – 12:00	**David Landau**	Pushing the limits of Monte Carlo simulations for the 3d Ising model
12:00 – 12:40	**Christian Borgs**	Graph convergence and estimation
12:45 – 13:00		**– Conference Photo –**
13:00 – 14:00		**– Lunch Break –** 🍽
15:00		**– Excursion to Kenilworth –**
19:00		**– Dinner at The Queen & Castle –** 🍽

Friday, April 8, 2016

08:45 – 09:30		**– Wake-up Coffee and Tea –** ☕

Session VII: (Chair: Ralph Kenna)

09:30 – 10:10	**Tilman Sauer**	A look back at the Ehrenfest classification
10:10 – 10:50	**Lev Shchur**	Exploring first order phase transition with population annealing algorithm
10:50 – 11:20		**– Coffee and Tea Break –** ☕

Session VIII: (Chair: Johannes Zierenberg)

11:20 – 12:00	**Bartlomiej Waclaw**	Computer models of bacterial colonies
12:00 – 12:40	**Bernd Berg**	Brief history of the use of generalized ensembles in Markov chain Monte Carlo simulations
12:40 – 14:00		**– Lunch Break –** 🍽
14:00 – 15:30		**– Poster Session II –**

Session IX: (Chair: Thomas Prellberg)

15:30 – 16:10	**Zdzislaw Burda**	Adding and multiplying invariant random matrices
16:10 – 16:50	**Hsiao-Ping Hsu**	Static and dynamic properties of polymer melts: equilibrium and non-equilibrium molecular dynamics studies
16:50 – 17:30		**– Coffee and Tea Break –** ☕

Session X: (Chair: Wolfhard Janke)

17:30 – 18:10	**Christophe Chatelain**	Old, recent and new results concerning the perturbed Potts model
18:10 – 18:50	**Des Johnston**	Degeneracy and first order phase transitions

T1 – Percolation in education and application in the 21st century

Joan Adler
Technion, Israel Institute of Technology, Haifa, Israel
phr76ja@tx.technion.ac.il

Percolation, "so simple you could teach it to your wife" (Chuck Newman, last century) is an ideal system to introduce young students to phase transitions. Two recent projects in the Computational Physics group at the Technion make this easy. One is a set of analog models to be mounted on our walls and enable visitors to switch between samples to see which mixtures of glass and metal objects have a percolating current. The second is a website enabling the creation of stereo samples of two and three dimensional clusters, (suited for viewing with Oculus rift) on desktops, tablets and smartphones. Although there have been many physical applications for regular percolation in the past, for Bootstrap Percolation, where only sites with sufficient occupied neighbours remain active, there have not been a surfeit for condensed matter physics. We have found that the creation of diamond membranes for quantum computers can be modeled with a bootstrap process of graphitization in diamond, enabling prediction of optimal processing procedures.

T2 – Large deviations for equilibrium and nonequilibrium processes

Alexander Hartmann
Institute for Physics, University of Oldenburg, Germany
a.hartmann@uni-oldenburg.de

Large deviations and rare events play an ever increasing role in science, economy and society. Often this concerns non-equilibrium processes, where large deviations play a crucial role for example for the estimation of impacts of storms, the calculation of probabilities of stock-market crashes or the sampling of transition paths for protein simulations. Here, we study rare events in the context of numerical simulations. We develop a very general black-box method, based on sampling vectors of random numbers within an artificial finite-temperature (Boltzmann) ensemble to access rare events and large deviation for almost arbitrary equilibrium and non-equilibrium processes. In this way, we obtain probabilities as small as 10^{-500} and smaller, hence rare events and large-deviation properties can be easily obtained. As pedagogical example, the distribution of the components of random graphs are obtained. Furthermore, applications from different fields are displayed, e.g., Fractional Brownian motion (fBm) characterized by the Hurst exponent H: Distribution of end-points of non-absorbed walks for different values of H; Distribution of work performed for a critical ($T = 2.269$) two-dimensional Ising system of size $L \times L = 128 \times 128$ upon rapidly changing the external magnetic field (related to the free energy difference via the Jarzynski theorem); Distribution of perimeters and area of convex hulls of two-dimensional single and multiple random walks; Distribution of scores of biological sequence alignments for local pairwise and multiple sequence alignments.

T3 – Nucleation of colloidal crystals in the bulk and at a substrate

Kurt Binder
Institut für Physik, Johannes Gutenberg Universität Mainz, Germany
kurt.binder@uni-mainz.de

For the nucleation of crystals from fluid phases, an important question concerns the role of a possible anisotropy of the interfacial tension. This problem is studied by analyzing the properties of a crystal nucleus surrounded by fluid in a finite box in thermal equilibrium. Using a model for weakly attractive colloidal particles, it is shown that the surface excess free energy of the nucleus can be determined accurately over a wide range of nucleus sizes, and the resulting nucleation barriers are completely independent from the size of the total volume of the system. [1,2]

[1] A. Statt, P. Virnau, K. Binder, Phys. Rev. Lett. 114 (2015) 026101.

[2] A. Statt, P. Virnau, K. Binder, Mol. Phys. 113 (2015) 2556.

T4 – Peptide folding in the presence of protein crowders

Anders Irbäck
Department of Theoretical Physics, Lund University, Sweden
anders@thep.lu.se

In the crowded interior of a cell, macromolecules may occupy 30% of the volume. So far, computational studies of the effects of crowding on properties such as protein stability have mainly focused on purely steric effects, using simple spherical crowder particles. In this talk, I present an atomic-level Monte Carlo study of the folding thermodynamics of two structurally dissimilar peptides in the presence of protein crowders. The simulated systems consist of one test peptide and eight copies of either BPTI or GB1, which are two thermally highly stable proteins. In the simulations, the interaction with the crowders tends to distort the folding of one of the peptides, while having a stabilizing effect on the other. The observed effects are contrasted with those seen in reference simulations with purely steric crowders.

T5 – Classical and quantum anisotropic Heisenberg antiferromagnets

Walter Selke
Institut für Theoretische Physik, RWTH Aachen, Germany
selke@physik.rwth-aachen.de

XXZ antiferromagnetic Heisenberg models, with and without single-ion anisotropy term, in a magnetic field are studied for spin values 1/2 and 1 as well as in the classical limit for one-, two- and three-dimensional lattices, using, mainly, Monte Carlo and density matrix renormalization group techniques. The model displays interesting structures, such as spin-flop and biconical ("supersolid") phases as well as various multicritical phenomena, like critical end-points, bi- and tetracritical points.

T6 – Kinetics of Vapor-Solid Phase Transition

Subir Das
Theoretical Sciences Unit, JNCASR, Bangalore, India
das@jncasr.ac.in

In this talk I will present results on the kinetics of vapor-solid phase transition (the solid phase possessing only quasi-long-range order) from molecular dynamics simulations of a single component Lennard-Jones system in space dimension $d = 2$. Having been quenched from high temperature to inside the vapor-solid coexistence region, the system evolves towards the new equilibrium via formation and growth of fractal domains of the solid phase in the vapor background. For very low overall density, these fractal objects exhibit ballistic motion and grows via coalescence mechanism, the average mass obeying a power-law with time. The exponent of the power-law is approximately 1.15 which we understand via appropriate theoretical argument.

T7 – Ageing and dynamical symmetries in the kinetics of interface growth

Malte Henkel
Laboratoire de Physique des Materiaux, Université de Lorraine, Nancy, France
malte.henkel@univ-lorraine.fr

The long-time behaviour and the physical ageing in the kinetics of interface growth provides paradigmatic examples for dynamical scaling and furnishes case studies for searches of possible extensions. Results from numerical simulations and exactly solvable models will be presented and the validity of dynamical scaling will be discussed in detail. The extension of simple dynamical scaling to local scale-invariance requires to introduce new concepts not seen in equilibirum critical phenomena. These are related to more general representations of the conformal algebra than the one usually studied at equilibrium phase transitions.

T8 – Influence of the permittivity gradient on static and dynamic properties of charged macromolecules

Christian Holm
Institute for Computational Physics, Universität Stuttgart, Germany
holm@icp.uni-stuttgart.de

Dissolved ions can alter the local permittivity of water, nevertheless most theories and simulations ignore this fact. We present a novel algorithm for treating spatial and temporal variations in the permittivity, and show several examples where this leads to large qualitative and quantitative differences. A dynamic example is the equivalent conductivity of a salt-free polyelectrolyte solution. Our new approach quantitatively reproduces experimental results unlike simulations with a constant permittivity that even qualitatively fail to describe the data. We can relate this success to a change in the ion distribution close to the polymer due to the built-up of a permittivity gradient.

T9 – Stochastic approximation Monte Carlo applied to polymer phase transitions

Wolfgang Paul
Institut für Physik, Martin-Luther Universität Halle, Germany
wolfgang.paul@physik.uni-halle.de

We will explain Stochastic Approximation Monte Carlo (SAMC) in its relation to the Wang-Landau Monte Carlo version of flat histogram simulations. These methods, as well as the multi-canonical Monte Carlo method, determine the density of states of a model system and from this its complete thermodynamics. Morphological observables are obtainable from standard Markov chain Monte Carlo simulations having this density of states providing the invariant probability distribution. We will show applications to two polymer physics problems. The first one concerns the collapse transition of a single homo-polymer chain in a regime of control parameters where this transition reproduces the thermodynamics of two-state folding proteins. We elucidate the reason for this and discuss the "folding" path of these chains. The second example concerns the ordering transition of a melt of short, semi-flexible polymer chains. We show that these undergo a first-order crystallization transition into a rotator-like phase, known from alkane chains. We also discuss the droplet evaporation-condensation transitions found in the coexistence regime of the crystalline and molten phases.

T10 – To protect your own network and to destroy your opponent's: The importance of being explosive

Peter Grassberger
Forschungszentrum Jülich, Germany
p.grassberger@fz-juelich.de

We present a new strategy to immunize networks against SIR attacks, and to destroy networks by targeted attacks. It is based on the Achlioptas et al. concept of explosive percolation. More precisely, we propose an "inverse targeting" approach as in C.M. Schneider et al., EPL 98, 46002 (2012), but with improved scoring and with vastly improved speed. As a result, the algorithm seems superior to all previous ones both with respect to efficiency (speed) and with respect to effectiveness (number of immunized/attacked sites).

T11 – Pushing the limits of Monte Carlo simulations for the 3d Ising model

David Landau
Center for Simulational Physics, The University of Georgia, Athens (GA), USA
dlandau@physast.uga.edu

The critical behavior of the 3d Ising model has defied analytic solution for almost a century. Numerical results from heroic series expansions provided very precise values for the critical temperature and critical exponents, but Monte Carlo and Monte Carlo renormalization group studies soon became competitive. In 1991, the use of vector supercomputing, histogram reweighting, and the simultaneous analysis of multiple thermodynamic quantities permitted Monte Carlo simulations to set a new standard. These were surpassed by later simulations, including a seminal contribution by Weigel and Janke who recognized the importance of the systematic inclusion of cross-correlations in the analysis of different thermodynamic quantities derived from the same data stream. Using very high resolution Monte Carlo simulations employing Wolff cluster flipping for simple cubic lattices as large as $L = 1024$ and analyzing the data with cross correlations included, we have now determined the critical temperature and critical exponents with much greater precision than previously possible. We will compare our current estimates (simulations are still ongoing) $J/k_bT_c = K_c = 0.221\,654\,655(33)$, $\nu = 0.62986(27)$ with those of earlier simulations as well as those from the latest high precision predictions made using modern theoretical approaches.

T12 – Graph convergence and estimation

Christian Borgs
Microsoft Research New England, Cambridge (MA), USA
borgs@microsoft.com

When studying large graphs, two of the fundamental questions one might want to answer are the following: (1) when should we consider two large graphs similar, and (2) what is a good class of stochastic models to describe large graphs, and how can one "learn" the generating model from an observed, large graph. In this talk, I will outline the theory of graph convergence and non-parametric graph model estimation that was developed in the past decade, at least in part motivated by the above two questions, highlighting in particular the relationship to what we call the thermodynamic limit in statistical physics.

T13 – A look back at the Ehrenfest classification

Tilman Sauer
Institut für Mathematik, Johannes Gutenberg Universität Mainz, Germany
tsauer@uni-mainz.de

A broad historical account of the introduction and evolution of the notion of phase transitions of higher order was given by Gregg Jäger in 1998. I will review that account and focus in on Paul Ehrenfest's initial classification of 1933. The classification was proposed in Ehrenfest's last publication before his tragic death. Although problematic from today's understanding, it proved to be very influential by its introduction of the concept of an order of a phase transition.

T14 – Exploring first order phase transition with population annealing algorithm

Lev Shchur
Landau Institute for Theoretical Physics, Chernogolovka, Moscow region, Russia
shchur@itp.ac.ru

We use theory of correction to scaling for the first order phase transition developed by Wolfhard Janke (CS-WJ) in the numerical analysis of data computed using extended version of population-annealing algorithm. We add warming procedure to the cooling procedure of population-annealing algorithm that allows us to obtain hysteresis in the behavior of observables computed along the cooling and warming curves. We found corrections to scaling follows to CS-WJ theory, and give estimations of the observables for the 2D Potts model for a number of values of number of states.

T15 – Computer models of bacterial colonies

Bartlomiej Waclaw
School of Physics and Astronomy, University of Edinburgh, United Kingdom
bwaclaw@staffmail.ed.ac.uk

Bacteria are ubiquitous in nature and play an important role in medicine and industry. Bacteria often grow in colonies - large aggregates in which cells behave as colloidal particles interacting mechanically with one another. However, an important difference between bacterial conglomerates and passive colloids is that bacteria grow and replicate. This leads to many interesting non-equilibrium phenomena. In my talk I will discuss how bacterial colonies can be simulated on a computer, what these simulations predict about the non-equilibrium behaviour of real bacterial colonies, how this can be experimentally verified, and what it implies for the biology of bacteria.

T16 – Brief history of the use of generalized ensembles in Markov chain Monte Carlo simulations

Bernd Berg
Department of Physics, Florida State University, Tallahassee (FL), USA
berg@hep.fsu.edu

The most efficient weights for Markov chain Monte Carlo calculations of physical observables are not necessarily those of the canonical ensembles. Generalized ensembles, which do not exist in nature but can be simulated on computers, lead often to a much faster convergence. In recent years they have in particular been used for simulations of first order phase transitions and of systems in which conflicting constraints lead to bottlenecks in a rugged free energy landscape. Starting of with the Metropolis algorithm and Hasting's extension, I give in my talk a mainly chronological overview of frequently used methods, including umbrella sampling, multicanonical algorithms, replica exchange simulations, expanded ensembles and Wang-Landau sampling. Illustrations are given, which range from simple spin models and lattice gauge theories to complex free energy barriers in biologically relevant molecules.

T17 – Adding and multiplying invariant random matrices

Zdzislaw Burda
AGH University of Science and Technology, Kraków, Poland
zdzislaw.burda@uj.edu.pl

We sketch the idea behind the free probability calculus and discuss how to use it to calculate eigenvalue densities of sums and products of random matrices. We give a couple of examples to illustrate the idea.

T18 – Static and dynamic properties of polymer melts: equilibrium and non-equilibrium molecular dynamics studies

Hsiao-Ping Hsu
Max-Planck-Institut für Polymerforschung, Mainz, Germany
hsu@mpip-mainz.mpg.de

We present a detailed study of the static and dynamic behavior of semiflexible polymer chains in a melt starting from the previously obtained fully equilibrated high molecular weight polymer melts by a hierarchical strategy [1,2]. For semiflexible chains in a melt, we see that results of the mean square internal distance, the probability distributions of the end-to-end distance, and the chain structure factor are all described by the theoretical predictions for ideal chains to some extent. We examine the motion of monomers in polymer melts by molecular dynamics (MD) simulations using the *ESPResSo++* package [3]. The scaling predictions of the mean square displacement of inner monomers, center of mass, and the relative behavior between them based on the Rouse model, and the reptation theory are verified, and the related characteristic relaxation time scales are determined. We also check the topological structures of polymer chains through the primitive path analysis (PPA) [4], and give the evidence that the entanglement length determined through PPA in the standard expression of the plateau modules is consistent with the value obtained from stresses using the Green-Kubo relation [5]. Finally, the non-linear viscoelastic properties of deformed polymer melts after a step uniaxial elongation and the conformational changes of chains during the relaxation process are investigated through a non-equilibrium MD study.

[1] G. Zhang, L. A. Moreira, T. Stuehn, K. Ch. Daoulas, and K. Kremer, ACS Macro Lett. 3, 198 (2014).

[2] G. Zhang, K. Ch. Daoulas, and K. kremer, Macromol. Chem. Phys. 214, 214 (2013), Macromolecules, 43, 1592 (2010).

[3] *ESPresSo++*: J. D. Halverson, T. Brandes, O. Lenz, A. Arnold, S. Bevc, V. Starchenko, K. Kremer, T. Stuehn, and D. Reith, Comput. Phys. Commun. 184, 1129 (2013).

[4] R. Everaers, S. K. Sukumaran, G. S. Grest, C. Svaneborg, A. Sivasubramanian, and K. Kremer, Science 303, 823 (2004).

[5] H.-P. Hsu, and K. Kremer, preprint (2016).

T19 – Old, recent and new results concerning the perturbed Potts model

Christophe Chatelain
Laboratoire de Physique des Materiaux, Université de Lorraine, Nancy, France
christophe.chatelain@univ-lorraine.fr

The occasion of a collaboration with Wolfhard was given to me with the study of the influence of randomness on the critical behavior of the 3D 4-state Potts model. The strong first-order phase transition of the pure model is smoothed and, for sufficiently strong disorder, it becomes continuous with a new universality class. In 2D, the new random fixed point was shown, both numerically and analytically, to depend on the number of states q of the Potts model. In contrast, the critical behavior of the Potts model with layered disorder is q-independent and is governed by Fisher infinite-randomness fixed point. Recently, we have shown by Monte Carlo simulations that a disorder with long-range correlations may also lead to a q-independent critical behavior. Finally, we will discuss again the old problem of the influence of aperiodic perturbations for which, earlier Monte Carlo simulations predicted a q-dependent critical exponents, even though the system is strongly correlated in one direction of the lattice.

T20 – Degeneracy and first order phase transitions

Des Johnston
Department of Mathematics, Heriot-Watt University, Edinburgh, United Kingdom
des@ma.hw.ac.uk

I review some recent work with Wolfhard and a graduate Student Marco Müller on the effect of degeneracy on the scaling behaviour at first order phase transitions. The 3d plaquette Ising model provides a useful test case.

P1 – Monte Carlo Studies of the Dipolar Random Field Ising Model

Arunkumar Bupathy
Indian Institute of Technology Delhi, New Delhi, India
arunbupathy@gmail.com

We present our ongoing work on the dipolar random field Ising model (RFIM+D) on a body centered cubic (bcc) lattice using Monte Carlo (MC) simulations. We choose the bcc lattice as it is realized by many experimental systems (eg., dilute antiferromagnets such as $Co_xZn_{1-x}F_2$, dilute ferromagnet $LiHo_{1-x}Y_xF_4$, etc.). Dipolar interactions are long-ranged and can be ferromagnetic or antiferromagnetic depending on the relative positions of the spins. Therefore, the free energy landscape is complex with many deep local minima. This makes it an analytically and computationally difficult problem to study. As a result, the understanding of phases and phase transitions in these systems is still incomplete. In a recent paper, we studied the RFIM on cubic lattices using Graph Cut technique which gives exact ground states (GS). In this work, we study typical morphologies of the RFIM+D on a bcc lattice for different values of dipolar interaction strength D and random field (rf) strength Δ. We use the Ewald summation technique to compute the dipolar energies and parallel tempering MC for efficient sampling. Our preliminary simulations show that at $\Delta = 0$, the GS is ferromagnetic in agreement with predictions. For $\Delta > 0$, the typical morphologies show elongated column-like domains, suggesting an intermediate columnar phase prior to the paramagnetic phase. We believe that our study could provide useful insights on dipolar systems.

P2 – MuCa vs WL: A comparison

Elmar Bittner
Institut für Theoretische Physik, Universität Heidelberg, Germany
e.bittner@thphys.uni-heidelberg.de

We perform a competitive analysis to study the relative performance of the two best-known generalized-ensemble algorithms: the multicanonical Monte Carlo and the Wang-Landau method. To keep things as simple and clear as possible, we take the exactly solvable two-dimensional Ising model as test case and we show also some results for the three-dimensional Ising model.

P3 – Topological-sector fluctuations and ergodicity breaking at the Berezinskii-Kosterlitz-Thouless transition

Michael Faulkner
University of Bristol, United Kingdom
michael.faulkner@bristol.ac.uk

The Berezinskii-Kosterlitz-Thouless (BKT) phase transition drives the unbinding of local topological defects in many two-dimensional systems. In the two-dimensional Coulomb gas, it corresponds to an insulator-conductor transition driven by charge deconfinement. We investigate the global topological properties of this transition, both analytically and by numerical simulation, using a lattice-field description of the two-dimensional Coulomb gas on the torus. The BKT transition is shown to be an ergodicity breaking between the topological sectors of the electric field, which implies a definition of topological order in terms of broken ergodicity. The breakdown of local topological order at the BKT transition leads to the excitation of global topological defects in the electric field, corresponding to different topological sectors. The quantized nature of these classical excitations, and their strict suppression by ergodicity breaking in the low-temperature phase, afford striking global signatures of topological-sector fluctuations at the BKT transition.

P4 – Role of Fourier Modes in Finite-Size Scaling above the Upper Critical Dimension

Emilio J. Flores-Sola
Coventry University, United Kingdom
Laboratoire de Physique des Materiaux, Université de Lorraine, Nancy, France
floresse@uni.coventry.ac.uk

Renormalization-group theory has stood, for over 40 years, as one of the pillars of modern physics. As such, there should be no remaining doubt regarding its validity. However, finite-size scaling, which derives from it, has long been poorly understood above the upper critical dimension d_c in models with free boundary conditions. In addition to its fundamental significance for scaling theories, the issue is important at a practical level because finite-size, statistical-physics systems with free boundaries and above d_c are experimentally relevant for long-range interactions. Here, we address the roles played by Fourier modes for such systems and show that the current phenomenological picture is not supported for all thermodynamic observables with either free or periodic boundaries. In particular, the expectation that dangerous irrelevant variables cause Gaussian-fixed-point scaling indices to be replaced by Landau mean-field exponents for all Fourier modes is incorrect. Instead, the Gaussian-fixed-point exponents have a direct physical manifestation for some modes above the upper critical dimension.

P5 – Parallel multicanonical simulations on GPUs

Jonathan Gross
Institut für Theoretische Physik, Universität Leipzig, Germany
gross@itp.uni-leipzig.de

In this study we present an adaptation of the parallel multicanonical sampling technique on general purpose graphics processing units (GPGPUs) using CUDA. As a benchmark system we apply our implementation to the two-dimensional Ising model and provide the complete and documented source code. It turns out that our GPU implementation yields a significant speedup compared to the identical MPI version running on multiple CPUs. This allows for major time and energy savings.

P6 – Scaling functions for vesicle models

Nina Haug
Queen Mary University of London, United Kingdom
n.a.haug@qmul.ac.uk

We consider a class of two-dimensional directed polygon models, weighted with respect to their perimeter and area. They can be used to model cell membranes, in which case the area generating variable is interpreted as an osmotic pressure. The phase diagrams of the different models share similar features, including a tricritical point around which the generating function is expected to show a scaling behaviour with the scaling function being given by the logarithmic derivative of the Airy function. In order to prove this rigorously for a given model, we apply a set of techniques, including the method of steepest descents, generalized to the case of several coalescing saddle points.

P7 – Time Automorphisms on C*-Algebras

Rudolf Hilfer
Universität Stuttgart, Germany
hilfer@icp.uni-stuttgart.de

The existence of time automorphisms on commutative and noncommutative C*-algebras for interacting many-body systems is investigated in this presentation. A mathematical framework is given to discuss local stationarity in time and the global existence of fractional and nonfractional time automorphisms. The results challenge the concept of time flow as a translation along the orbits and support a more general concept of time flow as a convolution along orbits. Implications for the distinction of reversible and irreversible dynamics are discussed. The generalized concept of time as a convolution reduces to the traditional concept of time translation in a special limit.

P8 – Many-body critical Casimir interactions in colloidal suspensions

Fred Hucht
University of Duisburg-Essen, Germany
fred@thp.uni-due.de

We study the fluctuation-induced Casimir interactions in colloidal suspensions, especially between colloids immersed in a binary liquid close to its critical demixing point. To simulate these systems, we present a highly efficient cluster Monte Carlo algorithm based on geometric symmetries of the Hamiltonian. Utilizing the principle of universality, the medium is represented by an Ising system while the colloids are areas of spins with fixed orientation. Our results for the Casimir interaction potential between two particles at the critical point in two dimensions perfectly agree with the exact predictions. However, we find that in finite systems the behavior strongly depends on whether the Z_2 symmetry of the system is broken by the particles. We present Monte Carlo results for the three-body Casimir interaction potential and take a close look onto the case of one particle in the vicinity of two adjacent particles, which can be calculated from the two-particle interaction by a conformal mapping. These results emphasize the failure of the common decomposition approach for many-particle critical Casimir interactions. [1]

[1] H. Hobrecht and A. Hucht, Phys. Rev. E 92, 042315 (2015)

P9 – Spin glasses with variable frustration

Ravinder Kumar
Institut für Theoretische Physik, Universität Leipzig, Germany
Coventry University, United Kingdom
kumarr31@uni.coventry.ac.uk

Together with randomness, frustration is believed to be a crucial prerequisite for the occurrence of glassy behavior in spin systems. The degree of frustration is normally the result of a chosen distribution of exchange couplings in combination with the structure of the lattice under consideration. Here, however, we discuss a process for tuning the frustration content of the Edwards-Anderson model on arbitrary lattices. With the help of extensive parallel-tempering Monte Carlo simulations we study such systems on the square lattice and compare the outcomes to the predictions of a recent study employing the Migdal-Kadanoff real-space renormalization procedure.

P10 – Ising-like systems without temperature

Krzysztof Malarz
AGH University of Science and Technology, Kraków, Poland
malarz@agh.edu.pl

For Ising model [1,2] the spin s_i flip rate w_n depends on the state of the spin and on the state of its nearest-neighbors, where n is the number of spins also being in the state s_i. For example, for a square lattice and the Metropolis scheme these flips rates are $w_0 = w_1 = 1$, $w_2 = \frac{1}{2}$, $w_3 = \exp(-4J/T)$ and $w_4 = w_3^2$, where J and T stand for the exchange integral and temperature, respectively. Here we show that an arbitrary choice of the set of flip probabilities $w_0(x) \geq w_1(x) \geq \cdots \geq w_{z-1}(x) \geq w_z(x)$ does not destroy the phase transition for both square ($z = 4$, Ref. [3]) and triangular ($z = 6$, Ref. [4]) lattice, where z in the number of nearest-neighbours and x is a model control parameter. In particular we show that assuming $w_0(x) = w_1(x) = 1$, $w_2 = x$, $w_3 = x/2$, $w_4 = x/4$ (for square lattice) or $w_0 = 1$, $w_1 = 3x$, $w_2 = 2x$, $w_3 = x$, $w_4 = x/2$, $w_5 = x/4$ and $w_6 = x/6$ (for triangular lattice) leads to magnetization $m(x)$, the Binder's fourth-order cumulant $U_4(x)$ and susceptibility $\chi(x)$ dependencies qualitatively similar to the shapes $m(T)$, $U_4(T)$ and $\chi(T)$ obtained when the Metropolis algorithm is applied. The only exception is the critical point x_C position, which does not correspond to well known T_C for square and triangular lattices. Also an introduction of a fraction $f \in [0, 1]$ of long-range interactions does not change this picture [4], which however influence further the critical point $x_C(f)$. These results indicate that the idea of the order-disorder transition is not limited to thermally induced phenomena. A short discussion of an social equivalent of temperature can be found in Ref. [5].

[1] W. Lenz, Z. Phys. 21, 613 (1920)

[2] E. Ising, Z. Phys. 31, 253 (1925)

[3] K. Malarz, R. Korf, K. Kułakowski, Int. J. Mod. Phys. C 22, 719 (2011)

[4] K. Malarz, M. J. Krawczyk, K. Kułakowski, Acta Phys. Pol. B Proc. Suppl. 7, 371 (2014)

[5] K. Kułakowski, arXiv:0807.0711v2

P11 – On the metal-insulator transition of disordered materials: May its character be determined by how one looks at it?

Arnulf Moebius
Institute for Theoretical Solid State Physics, IFW Dresden, Germany
a.moebius@ifw-dresden.de

In a recent experiment, Siegrist et al. studied the metal-insulator transition (MIT) of phase-change materials [1]. They conclude that these substances exhibit a finite minimum metallic conductivity. The striking contrast to reports on other disordered substances motivates the present in-depth study of the influence of the MIT criterion used on the character of the MIT obtained [2]. First, we discuss inherent biases of various approaches to locating the MIT. Second, reanalyzing $GeSb_2Te_4$ data from [1], we show that this solid strongly resembles other disordered materials: These data may also be interpreted in terms of a continuous MIT. Checking the justification of these fits, however, uncovers data inconsistencies preventing an unambiguous interpretation. Third, comparing with previous experiments on crystalline Si:As, Si:P, Si:B, Ge:Ga, CdSe:In, disordered Gd, and nano-granular Pt-C, we show that such an inconclusive behavior occurs frequently. The logarithmic temperature derivative of the conductivity highlights serious inconsistencies in original data evaluations in terms of a continuous MIT: In part, they are common to all such studies and seem to be generic, in part, they vary from experiment to experiment. Fourth, for four qualitatively different empirical models of the temperature and control parameter dependence of the conductivity, we present the respective flow diagrams of this logarithmic derivative. In consequence, the likely generic inconsistencies seem to indicate discontinuous MITs, in contradiction to the original interpretations. For these reasons, the question for the character of the MIT of these materials has to be considered as still open. The primary challenge now lies in improving the measurement precision and accuracy rather than in extending the temperature range.

[1] T. Siegrist et al., Nature Materials 10 (2011) 202.

[2] A. Moebius, arxiv.org/abs/1308.1538.

P12 – Planar ("fuki-nuke") ordering and finite-size effects for a model with four-spin interactions

Marco Müller
Institut für Theoretische Physik, Universität Leipzig, Germany
mueller@itp.uni-leipzig.de

We analyse a model with local four spin interaction of Ising spins, which appears as a special, plaquette-only case of the so-called gonihedric Ising model, a discrete variant when describing interacting surfaces. In three dimensions, it shows a strong first-order phase transition from a disordered high-temperature phase to a phase with exponentially degenerate low-temperature states and this degeneracy gives rise to a nonstandard finite-size scaling of the transition temperature. Our multicanonical simulations that confirmed this unusual finite-size scaling in the first place also provide a way of measuring planar order parameters. These come from considering an exactly solvable anisotropic limit of the model and can distinguish the low- and high-temperature phases in both the anisotropic and isotropic cases. In two dimensions, the model may serve as a pedagogical example on calculating how different finite-size corrections appear from different boundary conditions.

P13 – Winding angle distributions for two-dimensional collapsing polymers

Arturo Narros Gonzalez
Queen Mary University of London, United Kingdom
a.n.gonzalez@qmul.ac.uk

We provide numerical support for a long-standing prediction of universal scaling of winding angle distributions. Simulations of interacting self-avoiding walks show that the winding angle distribution for N-step walks is compatible with the theoretical prediction of a Gaussian with a variance growing asymptotically as $C\log(N)$, with $C = 2$ in the swollen phase (previously verified), and $C = 24/7$ at the θ-point. At low temperatures weaker evidence demonstrates compatibility with the same scaling and a value of $C = 4$ in the collapsed phase, also as theoretically predicted [1]. We will also show winding angle distribution and variance simulation results for self-avoiding trails (ISAT) model in swollen and collapse phase, and at critical point. Such results in collapse phase are seen for the first time in such model, where there is not theoretical predictions. Simulations were performed with a modified version of flatPERM algorithm [2], allowing to obtain the microcanonical partition function as a function of chain size, energy and winding. The quality of the data shows the expected corrections due to finite size, never seen so clearly before in both models [3].

[1] B. Duplantier and H. Saleur, Phys. Rev. Lett. 60, 2343 (1988).

[2] T. Prellberg and J. Krawczyk, Phys. Rev. Lett. 92, 120602 (2004).

[3] A. Narros, A. L. Owczarek, and T. Prellberg. Journal of Physics: Conference Series, 686(1), Oct 2016.

P14 – A dynamic transition in the relaxation time of a condensing zero-range process

Thomas Rafferty
University of Warwick, United Kingdom
t.rafferty@warwick.ac.uk

The relaxation time of a Markov process controls the asymptotic rate of convergence towards its stationary distribution, which is also a key estimate in calculating hydrodynamic limits. We consider zero-range processes that exhibit condensation due to site defects (slow exit rates), where above a critical density a non-zero fraction of the particles accumulate on the defect sites. We compute the relaxation time for dynamics on the complete graph, which we show to exhibit a dynamic transition in the system size as the density crosses the critical density. A key step in this calculation is to compare the zero-range process with a birth-death chain generated via a decomposition of the state space. A method previously used to calculate relaxation times for non-condensing zero-range processes and the Ising model with Kawasaki dynamics. This is joint work with Paul Chleboun and Stefan Grosskinsky.

P15 – Linear and ring polymer chains in confined geometries

Zoryana Usatenko
Institute of Physics, Cracow University of Technology, Poland
zusatenko@pk.edu.pl

The investigation of a dilute solution of linear and phantom ring polymer chains confined in a slit geometry of two parallel repulsive walls, two inert walls and for the mixed case of one inert and other one repulsive wall was performed. Taking into account the well known correspondence between the field theoretical ϕ^4 $O(n)$-vector model in the limit $n \to 0$ and the behavior of long-flexible polymer chains in a good solvent the investigations of dilute solution of long-flexible linear and ring polymer chains with excluded volume interactions (EVI) confined in a slit geometry of two parallel walls were performed in the framework of the massive field theory approach at fixed space dimensions $d = 3$ up to one-loop order. For all the above mentioned cases the correspondent depletion interaction potentials, depletion forces and the forces which exert linear and ring polymer chains on the walls were calculated, respectively. Besides, taking into account the Derjaguin approximation the depletion interaction potentials between big colloidal particle and a wall and between two big colloidal particles were calculated for all the above mentioned cases of dilute solution of linear and ring polymer chains. The obtained results are in good qualitative agreement with previous theoretical investigations and with the results of Monte Carlo simulations.

Joan Adler phr76ja@tx.technion.ac.il	Technion, Israel Institute of Technology, Haifa, Israel
Michael Bachmann bachmann@smsyslab.org	Center for Simulational Physics, The University of Georgia, USA
Bernd Berg berg@hep.fsu.edu	Department of Physics, Florida State University, Tallahassee (FL), USA
Kurt Binder kurt.binder@uni-mainz.de	Institut für Physik, Johannes Gutenberg Universität Mainz, Germany
Elmar Bittner bittner@thphys.uni-heidelberg.de	Institut für Theoretische Physik, Universität Heidelberg, Germany
Christian Borgs borgs@microsoft.com	Microsoft Research New England, Cambridge (MA), USA
Arunkumar Bupathy arunbupathy@gmail.com	Indian Institute of Technology Delhi, New Delhi, India
Zdzislaw Burda zdzislaw.burda@uj.edu.pl	AGH University of Science and Technology, Kraków, Poland
Christophe Chatelain christophe.chatelain@univ-lorraine.fr	Laboratoire de Physique des Materiaux, Université de Lorraine, Nancy, France
Subir Das das@jncasr.ac.in	Theoretical Sciences Unit, JNCASR, Bangalore, India
Robin de Regt ab2589@coventry.ac.uk	Coventry University, United Kingdom
Charo del Genio C.I.del-Genio@warwick.ac.uk	University of Warwick, United Kingdom
Michael Faulkner michael.faulkner@bristol.ac.uk	University of Bristol, United Kingdom
Christian von Ferber c.vonferber@coventry.ac.uk	Coventry University, United Kingdom
Emilio J. Flores-Sola floresse@uni.coventry.ac.uk	Coventry University, United Kingdom Laboratoire de Physique des Materiaux, Université de Lorraine, Nancy, France
Nikolaos Fytas ab5298@coventry.ac.uk	Coventry University, United Kingdom
Peter Grassberger p.grassberger@fz-juelich.de	Forschungszentrum Jülich, Germany
Jonathan Gross gross@itp.uni-leipzig.de	Institut für Theoretische Physik, Universität Leipzig, Germany

Alexander Hartmann a.hartmann@uni-oldenburg.de	Institute for Physics, University of Oldenburg, Germany
Nina Haug n.a.haug@qmul.ac.uk	Queen Mary University of London, United Kingdom
Malte Henkel malte.henkel@univ-lorraine.fr	Laboratoire de Physique des Materiaux, Université de Lorraine, Nancy, France
Rudolf Hilfer hilfer@icp.uni-stuttgart.de	Universität Stuttgart, Germany
Christian Holm holm@icp.uni-stuttgart.de	Institute for Computational Physics, Universität Stuttgart, Germany
Hsiao-Ping Hsu hsu@mpip-mainz.mpg.de	Max-Planck-Institut für Polymerforschung, Mainz, Germany
Fred Hucht fred@thp.uni-due.de	University of Duisburg-Essen, Germany
Anders Irbäck anders@thep.lu.se	Department of Theoretical Physics, Lund University, Sweden
Wolfhard Janke wolfhard.janke@itp.uni-leipzig.de	Institut für Theoretische Physik, Universität Leipzig, Germany
Des Johnston des@ma.hw.ac.uk	Department of Mathematics, Heriot-Watt University, Edinburgh, United Kingdom
Ralph Kenna r.kenna@coventry.ac.uk	Coventry University, United Kingdom
Ravinder Kumar kumarr31@uni.coventry.ac.uk	Institut für Theoretische Physik, Universität Leipzig, Germany Coventry University, United Kingdom
David Landau dlandau@physast.uga.edu	Center for Simulational Physics, The University of Georgia, Athens (GA), USA
Krzysztof Malarz malarz@agh.edu.pl	AGH University of Science and Technology, Kraków, Poland
Arnulf Moebius a.moebius@ifw-dresden.de	Institute for Theoretical Solid State Physics, IFW Dresden, Germany
Marco Müller mueller@itp.uni-leipzig.de	Institut für Theoretische Physik, Universität Leipzig, Germany
Arturo Narros Gonzalez a.n.gonzalez@qmul.ac.uk	Queen Mary University of London, United Kingdom
Joel Nicholls joel.nicholls@warwick.ac.uk	University of Warwick, United Kingdom

Wolfgang Paul wolfgang.paul@physik.uni-halle.de	Institut für Physik, Martin-Luther Universität Halle, Germany
Andrea Pizzoferrato ap@andreapizzoferrato.com	University of Warwick, United Kingdom
Thomas Prellberg t.prellberg@qmul.ac.uk	Queen Mary University of London, United Kingdom
Thomas Rafferty t.rafferty@warwick.ac.uk	University of Warwick, United Kingdom
Sutapa Roy sutapa@is.mpg.de	Max-Planck Institute for Intelligent Systems, Stuttgart, Germany
Tilman Sauer tsauer@uni-mainz.de	Institut für Mathematik, Johannes Gutenberg Universität Mainz, Germany
Walter Selke selke@physik.rwth-aachen.de	Institut für Theoretische Physik, RWTH Aachen, Germany
Lev Shchur shchur@itp.ac.ru	Landau Institute for Theoretical Physics, Chernogolovka, Moscow region, Russia
Maggie Simmons angela.gage@iop.org	IOP Publishing, United Kingdom
Zoryana Usatenko zusatenko@pk.edu.pl	Institute of Physics, Cracow University of Technology, Poland
Bartlomiej Waclaw bwaclaw@staffmail.ed.ac.uk	School of Physics and Astronomy, University of Edinburgh, United Kingdom
Martin Weigel Martin.Weigel@coventry.ac.uk	Coventry University, United Kingdom
Taras Yavorskyi ab3785@coventry.ac.uk	Coventry University, United Kingdom
Johannes Zierenberg johannes.zierenberg@itp.uni-leipzig.de	Institut für Theoretische Physik, Universität Leipzig, Germany

CALL FOR PAPERS

for a

Topical Issue of EPJST on

Phase Transitions and Critical Phenomena

We are preparing the publication of an issue of the European Physical Journal – Special Topics (EPJST) summarising the research discussed at the conference and further recent developments in the field of phase transitions and critical phenomena. EPJ – Special Topics is devoted to the rapid and timely publication of complete topical issues in all fields pertaining to the pure and applied physical sciences. All contributions undergo regular peer review according to EPJ's standards.

Contributions fall in one of three categories:

(a) 10-15 pages minireview on a subtopic

(b) 15+ pages tutorial review on a subtopic

(c) up to 10 pages original paper, i.e. with mostly new material

If you would like to contribute an article, please send a (tentative) title, short abstract and article category (a), (b) or (c) to `ptcp16@complexity-coventry.org` or any of the organisers no later than **April 30, 2016**.

Michael Bachmann
Elmar Bittner
Nikolaos Fytas
Ralph Kenna
Martin Weigel
Johannes Zierenberg