November 24, 2009

ABSTRACTS

of contributions to the

10th International NTZ-Workshop on

New Developments in Computational Physics

CompPhys09

Institut für Theoretische Physik, Universität Leipzig, Germany

26 – 29 November 2009

http://www.physik.uni-leipzig.de/~janke/CompPhys09

Supported by Centre for Theoretical Sciences (NTZ) of Universität Leipzig, Deutsch-Französische Hochschule (DFH-UFA), Alexander von Humboldt Foundation, DFG Research Group 877, Research Academy Leipzig (RAL), Priority Research Area PbF2 (Mathematical Sciences), and Graduate School "BuildMoNa".

Preface

This year we celebrate a double jubilee – the 10th Workshop of this series and the 600th anniversary of the University of Leipzig a few days later on 02 December 2009, the "Dies Academicus"!

Also the 10th NTZ-Workshop *CompPhys09* on *New Developments in Computational Physics* covers again a broad spectrum of different fields ranging from general aspects of computational and statistical physics over applications in condensed and soft matter physics, including biological applications, to lattice gauge theories of high-energy physics. And as in all previous years, the idea of the Workshop is to provide a forum for an informal exchange of ideas and to meet in a relaxed atmosphere in Leipzig around Christmas time.

The Workshop takes place from 26 – 29 November 2009 in the Theory Lecture Hall ("Theorie Hörsaal") and the "Aula" of the Experimental Physics building. We are very grateful to all colleagues who helped moving their regular lecture courses to another place or date.

Finally, we and the Centre for Theoretical Sciences (NTZ) gratefully acknowledge financial support of the Workshop from Deutsch-Französische Hochschule (DFH-UFA), Alexander von Humboldt Foundation, DFG Research Group 877, Research Academy Leipzig (RAL), Priority Research Area PbF2 (Mathematical Sciences), and Graduate School "BuildMoNa".

Leipzig, November 2009
Wolfhard Janke

Abstracts

Properties of exact ground states of the random-field Ising magnet around the upper critical dimension

Björn Ahrens
Institut für Physik, Universität Oldenburg, Germany
bjoern.ahrens@uni-oldenburg.de

We consider the random-field Ising magnet (RFIM) in dimensions from $d = 3$ to $d = 7$. The RFIM is a disordered system. It consists of ferromagnetically coupled Ising spins with an additional quenched local magnetic field. Here the field is distributed according to a Gaussian with zero mean and a tuneable standard deviation.
To obtain the ground state for a single realisation of the disorder we map the random field to a graph with suitible chosen edge capacities [Picard and Ratliff, Networks 5 (1975) 357]. For these graphs we calculate the maximum flow using a fast max-flow/min-cut algorithm, recently developed in algorithmic graph theory. Therein the minimum cut corresponds to a ground-state configuration of the system.
We measure the energy per spin, the magnetisation and the susceptibility by applying a small extern field. Using finite-size scaling we can calculate the specific-heat exponent α, the order parameter exponent β, the susceptibility exponent γ and the correlation length exponent ν. The results for $d = 6$ and $d = 7$ are compared with the mean-field exponents of the RFIM, since $d_u = 6$ is the upper critical dimension from which on the mean-field exponents are expected to hold.
Our special interest lies in the scaling of the exponents as function of the dimension. Therefore we use earlier results [Hartmann and Young, Phys. Rev. B 64 (2001) 214419; Hartmann, Phys. Rev. B 65 (2002) 174427] and calculate ground states up to sizes of $8^7 \approx 2 \cdot 10^6$ spins.

Thermodynamics of tubelike flexible polymers (P)

Michael Bachmann[1]
(with Thomas Vogel[1]**, Thomas Neuhaus**[2]**, and Wolfhard Janke**[3]**)**
[1] IFF, Theorie II, Forschungszentrum Jülich, Germany
[2] JSC, Forschungszentrum Jülich, Germany
[3] Institut für Theoretische Physik, Universität Leipzig, Germany
bachmann@smsyslab.org

By means of sophisticated Monte Carlo methods, we investigate the conformational phase diagram of a simple model for flexible polymers with explicit thickness. The thickness constraint, which is introduced geometrically via the global radius of curvature of a polymer conformation, accounts for the excluded volume of the polymer and induces cooperative effects supporting the formation of secondary structures. We find that known secondary-structure segments like helices and turns, but also ringlike conformations and stiff rods are dominant intrinsic topologies governing the phase behavior of such cooperative tubelike objects. This shows that the thickness constraint is indeed a fundamental physical parameter that allows for a classification of generic polymer classes.

[1] T. Vogel, T. Neuhaus, M. Bachmann, and W. Janke, EPL **85** (2009) 10003.
[2] T. Vogel, T. Neuhaus, M. Bachmann, and W. Janke, Eur. Phys. J. E **30** (2009) 7.
[3] T. Vogel, T. Neuhaus, M. Bachmann, and W. Janke, Phys. Rev. E **80** (2009) 011802.

Spin glass on the hypercube

Beatriz Seoane Bartolomä
(with L.A. Fernandez, V. Martin Mayor, and G. Parisi)

Departamento de Fisica Teorica I, Universidad Complutense de Madrid, Spain
seoane@lattice.fis.ucm.es

We present a mean-field model for spin glasses with a natural notion of distance built in, namely,the Edwards-Anderson model on the diluted D-dimensional unit hypercube in the limit of large D. We show that finite D effects are strongly dependent on the connectivity, being much smaller for a fixed coordination number. We solve the non trivial problem of generating these lattices. Afterwards, we numerically study the nonequilibrium dynamics of the mean-field spin glass. Our two main findings are: (i) the dynamics is ruled by an infinite number of time-sectors, and (ii), the aging dynamics consists on the growth of coherent domains with a nonvanishing surface-volume ratio. We study as well finite D effects in the nonequilibrium dynamics, finnding that a naive finite-size scaling ansatz works surprisingly well.

Nonequilibrium phase transitions in finite arrays of globally coupled Stratonovich models: strong coupling limit (P)

Ulrich Behn
(with Fabian Senf and Philipp M. Altrock)

Institut für Theoretische Physik, Universität Leipzig, Germany
ulrich.behn@itp.uni-leipzig.de

A finite array of N globally coupled Stratonovich models exhibits a continous nonequilibrium phase transition. In the limit of strong coupling there is a clear separation of time scales of center of mass and relative coordinates. The latter relax very fast to zero and the array behaves as a single entity described by the center of mass coordinate. We compute analytically the stationary probability and the moments of the center of mass coordinate. The scaling behaviour of the moments near the critical value of the control parameter $a_c(N)$ is determined. We identify a crossover from linear to square root scaling with increasing distance from a_c. The crossover point approaches a_c in the limit $N \to \infty$ which reproduces previous results for infinite arrays. The results are obtained in both the Fokker-Planck and the Langevin approach and are corroborated by numerical simulations. For a general class of models we show that the transition manifold in the parameter space depends on N and is determined by the scaling behaviour near a fixed point of the stochastic flow.

[1] F. Senf, P.M. Altrock, and U. Behn, New J. Phys. **11** (2009) 063010 [arXiv:0903.2185].

Phase diagram of a mixed quantum spin chain with bond alternation and exchange anisotropy (P)

Rainer Bischof
(with Wolfhard Janke)

Institut für Theoretische Physik, Universität Leipzig, Germany
rainer.bischof@itp.uni-leipzig.de

The mixed spin chain with base cell setup $1/2 - 1/2 - 1 - 1$ is studied via continuous time quantum Monte Carlo simulations. In particular, the critical points in the two-parameter space of bond alternation and exchange anisotropy are located. A generalisation of the non-local disorder parameter [M. Nakamura and S. Todo, Phys. Rev. Lett. 89 (2002) 077 204] to mixed spin chains is proposed. By quantum reweighting [M. Troyer, F. Alet, and S. Wessel, Braz. J. Phys. 34 (2004) 377] of improved and unimproved estimators, precise estimates of pseudo-critical points of various observables could be obtained and put into finite-size scaling analyses.

Anisotropy of the interface tension of the three-dimensional Ising model (P)

Elmar Bittner
(with Andreas Nußbaumer and Wolfhard Janke)

Institut für Theoretische Physik, Universität Leipzig, Germany
elmar.bittner@itp.uni-leipzig.de

We determine the interface tension for the 100, 110 and 111 interface of the simple cubic Ising model with nearest-neighbour interaction using novel simulation methods. To overcome the droplet/strip transition and the droplet nucleation barrier we use a newly developed combination of the multimagnetic algorithm with the parallel tempering method. We investigate a large range of inverse temperatures to study the anisotropy of the interface tension in detail.

[1] E. Bittner, A. Nußbaumer, and W. Janke, Nucl. Phys. B **820** (2009) 694.

Polymers in crowded environment under stretching force: globule-coil transitions

Viktoria Blavatska[1]
(with Wolfhard Janke[2]**)**

[1] Institute for Condensed Matter Physics, Lviv, Ukraine
[2] Institut für Theoretische Physik, Universität Leipzig, Germany
viktoria@icmp.lviv.ua

We study flexible polymer macromolecules in a crowded (porous) environment, modelling them as self-attracting self-avoiding walks (SASAW) on site-diluted percolative lattices in space dimensions $d = 2, 3$. The influence of stretching force on the polymer folding and properties of globule-coil transitions are analyzed. Applying the pruned-enriched Rosenbluth chain-growth method (PERM), we estimate the transition temperature between collapsed and extended polymer configurations and construct the phase diagrams of the globule-coil coexistence when varying temperature and stretching force. The transition to a completely stretched state, caused by applying force, is discussed as well.

[1] V. Blavatska and W. Janke, preprint arXiv:0907.2418, to appear in Phys. Rev. **E** (in print).

Product of random Gaussian matrices

Zdzisław Burda

Institute of Physics, Jagiellonian University, Krakow, Poland
zdzislaw.burda@uj.edu.pl

We calculate the eigenvalue density of a product $X = X_1 X_2 \dots X_M$ of M independent identically distributed N-by-N Gaussian matrices in the large-N limit.

Stochastic lattice gas model describing the dynamics of an epidemics (P)

Tania Tomé de Castro

Instituto de Física, Universidade de Sao Paulo, Brazil
ttome@if.usp.br

We analyze a stochastic dynamics to describe the onset of the spreading of an epidemic in a population composed by individuals of three classes: susceptible (S), infected (I), and recovered (R). The stochastic process

involves the cyclic process S → I → R → S (SIRS) which is investigated at different levels of description: by a stochastic lattice gas model and by a birth and death process. The open process S → I → R (SIR) is studied as a particular case of the SIRS process. Performing Monte Carlo simulations and dynamic mean-field approximations we show that the SIRS stochastic lattice model exhibit a line of critical points separating two phases: an absorbing phase where the lattice is completely full of S individuals and an active phase where the densities of S, I and R individuals are different from zero. The critical line, that corresponds to the onset of epidemic spreading, is shown to belong in the directed percolation universality class. By considering the birth and death process we observei thatthe active phase of the system may or may not present population cycles.

[1] T. Tomé and D.R. de Souza, preprint arXiv:0908.1296.

Exact results in the one-dimensional coagulation-diffusion process by the empty-interval method

Xavier Durang

Laboratoire de Physique des Matériaux, Université Henri Poincaré, Nancy, France
durang@lpm.u-nancy.fr

The long-time dynamics of reaction-diffusion processes in low dimensions is dominated by fluctuation effects. For the one-dimensional coagulation-diffusion process, the empty-interval method has been a convenient tool for the exact calculation of time-dependent particle densities. We generalise the empty-interval method by considering the probability distributions of two simultaneous empty intervals at a given distance. While the equations of motion of these probabilities reduce for the coagulation-diffusion process to a simple diffusion equation in the continuum limit, consistency with the single-interval distribution introduces several non-trivial boundary conditions which are solved for the first time. In this way, exact space-time-dependent correlation functions can be directly obtained.

Eggheads: shapes of embedded networks

Christian von Ferber

Applied Mathematics Research Centre, Coventry University, UK
c.vonferber@coventry.ac.uk

Many real world networks use space consuming links such as the human brain, printed circuits, or the system of tubes in a large scale refinery. We pose the question how the given statistical properties of a network such as the degree distribution and the occurrence of loops impact on their shape when embedded in two or three dimensions. Thus, what should be the shape of the skull, the circuit board or the refinery plant to embed the network if the network is scale free or rather not?

MD simulation of polymer brushes

Andre Galuschko

Institut Charles Sadron, ICS (UPR22-CNRS), Strasbourg, France
galuschko@ics.u-strasbg.fr

By means of molecular dynamics simulations and scaling theory we study the response of opposing polymer brushes to constant shear motion under good solvent conditions. Model systems that contain explicit solvent molecules (Lennard-Jones dimers) are compared to solvent-free systems while varying of the distance between the grafted layers and their molecular parameters, chain length and grafting density. Our study reveals a power-law dependence of macroscopic transport properties on the Weissenberg number, W, beyond linear response. For instance, we find that the kinetic friction constant scales as $\mu \sim W0.57$ for large values of W. We develop a scaling theory that describes our and previous numerical data including recent experiments.

Stability in continuous versus Boolean dynamics (P)

Fakhteh Ghanbarnejad
(with Konstantin Klemm)
Bioinformatik, Institut für Informatik, Universität Leipzig, Germany
fakhteh@bioinf.uni-leipzig.de

Boolean networks are time- and state-discrete models of dynamical systems with many variables and quenched disorder in the couplings. The use of such discrete models makes large systems amenable to detailed analysis. The discretization, however, may bring about "artificial" behaviour not found in the continuous (ODE) description. Especially the concept of stability of limit cycles is not reflected appropriately by the usual definition of attractor stability in Boolean dynamics. Here we have a fresh look at the correspondence between stability of continuous and discrete dynamics. We run extensive numerical simulations to test stability on various system architectures (networks). We establish a criterion for assessing stability of the continuous dynamics by probing the discrete counterpart.

Ising kinetic Monte Carlo simulations for investigating surface barriers in nanoporous materials

Lars Heinke
Abteilung Chemische Physik, Fritz-Haber-Institut Berlin and Abteilung Grenzflächenphysik, Universität Leipzig, Germany
heinke@fhi-berlin.mpg.de

The mass transfer of guest molecules in nanoporous materials is an important field of science with many applications, e.g., in the chemical and petrochemical industry. In recent investigations, it was found that the mass transfer is limited not only by diffusion in the nanopores but also by a transport resistance close to the crystal surface, called surface barriers. For unveiling the so far unexplored reasons of this transport resistance, a model of the pore space has been further developed: the entrances to most of the (one-dimensional) pores are blocked, and the pores are cross connected by crystal defects, which naturally occur. The mass transfer of the guest molecules is studied by means of a simple lattice-jump model using kinetic Monte Carlo simulations. The properties of this model have been extensively studied. All results reported in a detailed, experimental study of the surface barriers were reproduced, verifying this model.

Non-Markovian global persistence in phase-ordering kinetics

Malte Henkel
Laboratoire de Physique des Matériaux, Université Nancy I, France
henkel@lpm.u-nancy.fr

The persistence probability $P_g(t)$ of the global order-parameter of a simple ferromagnet undergoing phase-ordering kinetics is analysed. It is argued that the persistence probability decays algebraically with time, in the entire low-temperature phase. For a Markov process, one has the global persistence exponent $\theta_g = (2\lambda_C - d)/2z$, where λ_C is the autocorrelation exponent. While this relationship is confirmed in the 1D Glauber-Ising model and the D-dimensional spherical model, it fails for the 2D Glauber-Ising model, where $\theta_g = 0.063(2)$ is found. The non-Markovian nature of the dynamics of the global order-parameter is also confirmed by the form of the normalised global autocorrelator.

[1] M. Henkel and M. Pleimling, preprint arXiv:0907.1642.

Structure analysis of bottle-brush polymers: simulation and experiment

Hsiao-Ping Hsu

Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany
hsu@uni-mainz.de

We present extensive Monte Carlo simulations for bottle-brush polymers under good solvent conditions by using the bond fluctuation model on the simple cubic lattice [1, 2]. In order to speed up the simulation, the algorithm which combines "L26"-move and "pivot moves" is applied. Varying the backbone length N_b as well as the side chain length N, for a physically reasonable grafting density of one chain per backbone monomer, we find that the structure factor describing the total scattering from the bottle-brush provides an almost perfect match for some combinations of (N_b, N) to experimental data of Rathgeber *et al.* [J. Chem. Phys. 122 (2005) 124904], when we adjust the length scale of the simulation to reproduce the experimental gyration radius of the bottle-brush. While in the experiment other length scales (gyration radius of side chains, backbone persistence length, scale characterizing the radial monomer density profile in the plane normal to the backbone) can be extracted only via fitting to a complicated and approximate theoretical expression derived by Pedersen and Schurtenberger, all these properties can be extracted from the simulation directly. In this way, quantitatively more reliable estimates for the persistence length and side chain gyration radius of the experimental systems can be extracted. Finally we show that by suitable mappings between simulation and experiment on length scales of the local concentration fluctuations (here < 2 nm) the analysis of experimental data can be systematically refined.

[1] H.-P. Hsu, K. Binder, and W. Paul, Phys. Rev. Lett. **103** (2009) 198301.
[2] H.-P. Hsu, W. Paul, S. Rathgeber, and K. Binder, preprint (2009).

Nonequilibrium phase transition in an exactly solvable driven Ising model with friction

Alfred Hucht

Fakultät für Physik, Universität Duisburg-Essen, Duisburg, Germany
fred@thp.uni-due.de

A driven Ising model with friction due to magnetic correlations has recently been proposed by Kadau *et al.* [Phys. Rev. Lett. 101 (2008) 137205]. The nonequilibrium phase transition present in this system is investigated in detail using analytical methods as well as Monte Carlo simulations. In the limit of high driving velocities v the model shows mean-field behavior due to dimensional reduction and can be solved exactly for various geometries. The simulations are performed with three different single spin flip rates: the common Metropolis and Glauber rates as well as a multiplicative rate. Due to the nonequilibrium nature of the model all rates lead to different critical temperatures at $v > 0$, while the exact solution matches the multiplicative rate. Finally, the crossover from Ising to mean-field behavior as function of velocity and system size is analysed in one and two dimensions.

[1] A. Hucht, preprint arXiv:0909.0533.

Ab initio study of Fe-porphyrin, Fe-phthalocyanine and carbon nanotubes with FeN4 defects (P)

Ingrid Ibagon

Departamento de Física, Universidade Federal de Minas Gerais, Belo Horizonte, Brazil
ingrid@fisica.ufmg.br

We studied the electronic structure and the relationship between the electronic charge and the oxidation state for the iron atom in Fe-porphyrin, Fe-phthalocynine and carbon nanotubes with FeN4 defects by using ab initio calculations based on the Density Functional Theory (DFT). We observed that the Mulliken Population of the valence orbitals of the iron atom in the molecules does not change more than 0.2e when a electron is added to or removed from the system while the total spin of the molecule goes from 1 to 3/2 when an electron is removed and from 1 to 1/2 when a electron is added. Similar results are obtained for the carbon nanotubes when the charge for carbon atom is equivalent to the molecules.

Disordered Potts model on the diamond hierarchical lattice

Ferenc Iglói
Research Institute for Solid State Physics and Optics, Budapest, Hungary
igloi@szfki.hu

We consider the critical behavior of the random q-state Potts model in the large-q limit with different types of disorder leading to either the nonfrustrated random ferromagnet regime or the frustrated spin-glass regime. The model is studied on the diamond hierarchical lattice for which the Migdal-Kadanoff real-space renormalization is exact. It is shown to have a ferromagnetic and a paramagnetic phase and the phase transition is controlled by four different fixed points. The state of the system is characterized by the distribution of the interface free energy $P(I)$ which is shown to satisfy different integral equations at the fixed points. By numerical integration we have obtained the corresponding stable laws of nonlinear combination of random numbers and obtained numerically exact values for the critical exponents.

Simulation study on nonequilibrium transport phenomena

Nobuyasu Ito
Department of Applied Physics, Graduate School of Engineering, The University of Tokyo, Japan
ito@ap.t.u-tokyo.ac.jp

Computer is now powerful enough to reproduce various nonequilibrium behaviors of macroscopic materials with molecular dynamics simulation. For example, linear nonequilibrium transport phenomena like the Fourier's law of thermal conduction, the Ohmic electoric resistance and the Newtonean fluid viscosity have been directly confirmed based on microscopic dynamics of molecules. Now two directions are in our front: one is a challenge to the more complex problems like strongly nonlinear nonequilibrum phenomena, and the other is to elucidate simulated nonequilibrium state. In this talk, results of thermal conduction problem are shown after a overview of simulation statistical physics. Dimensionality dependence of thermal conduction phenomena, especially a cross-over behavior between microscopic reversible dynamics and the Fourier's law, are confirmed. Nonequilibrium distribution function with thermal flow is characterized by a direction-dependence of velocity distribution function. Finally, a perspective of future computers of exa-flops-scale and more is discussed. Statistical physics models are to be advantageous in wider fields of computational sciences than now. Agent models with short-range interaction will work efficiently on future supercomputers with millions of cores or more for simulating from material with molecules to society with individuals.

[1] S. Yukawa, T. Shimada, F. Ogushi, and N. Ito, *Nonequilibrium microscopic distribution of thermal current in particle systems*, J. Phys. Soc. Jpn. **78** (2009) 023002; awarded as the Papers of Editors' Choice.
[2] S. Yukawa and N. Ito, *The Avogadro challenge – nanodynamics study on nonequilibrium problems*, Prog. Theor. Phys. Suppl. **178** (2009) 24–32.
[3] F. Ogushi, T. Shimada, S. Yukawa, and N. Ito, *Energy transport in Lennard-Jones particle system*, Prog. Theor. Phys. Suppl. **178** (2009) 92–99.
[4] T. Shimada, F. Ogushi, S. Yukawa, and N. Ito, *Microscopic energy flux in particle systems and nonlinear lattices*, Prog. Theor. Phys. Suppl. **178** (2009) 100–106.

Versatile object-oriented toolkit for coarse-graining applications

Christoph Junghans
Max-Planck-Institut für Polymerforschung (MPI-P), Mainz, Germany
junghans@mpip-mainz.mpg.de

Coarse-graining is a systematic way of reducing the number of degrees of freedom representing a system of interest. Several coarse-graining techniques have so far been developed, such as iterative Boltzmann inversion, force-matching, and inverse Monte Carlo. However, there is no unified framework that implements these methods and allows their direct comparison. We present a versatile object-oriented toolkit for coarse-graining applications that implements these techniques and provides a flexible modular platform for the further development of coarse-graining techniques. All methods are illustrated and compared by coarse-graining the SPCE water model, liquid methanol, liquid propane, and a single molecule of hexane.

Cutting the energy range in multicanonical Monte Carlo simulations (P)

Steffen Karalus[1]
(with Michael Bachmann[2] **and Wolfhard Janke**[1]**)**
[1] Institut für Theoretische Physik, Universität Leipzig, Germany
[2] IFF, Theorie II, Forschungszentrum Jülich, Germany
steffen.karalus@itp.uni-leipzig.de

By means of a bead-and-spring polymer model, we investigated the dependence of several observables on the energy boundaries in a multicanonical Monte Carlo simulation. As expected the results of the inverse reweighting to a certain temperature deviate seriously if a substantial part of the corresponding energy distribution lies outside the predefined energy range. However structural quantities like the mean end-to-end distance seem to be effected less than the mean energy itself.

Critical quench dynamics in confined systems

Dragi Karevski
IJL, Université Henri Poicaré, Nancy, France
karevski@lpm.u-nancy.fr

We study the loading/deloading in time of a power law confining potential in a quantum critical system. The amplitude of the confining potential follows a non-linear ramp which drives the system across its critical point. For a slow driving rate, we develop a scaling theory which predicts a power law behavior of the density of defects with the ramping rate with an exponent which depends on the space-time properties of the potential. The scaling theory is supported by first order adiabatic calculation and exact results on an inhomogeneous transverse field Ising chain where the full time-evolution of the density of defects is derived.

The site-diluted Ising model in 2 and 4 dimensions (P)

Ralph Kenna
Applied Mathematics Research Centre, Coventry University, UK
r.kenna@coventry.ac.uk

The Ising model with uncorrelated, quenched random-site or random-bond disorder has been controversial in both two and four dimensions. In these dimensions, the leading exponent α, which characterizes the specific-heat critical behaviour, vanishes and no Harris prediction for the consequences of quenched disorder can be made. In the two-dimensional case, the controversy is between the strong universality hypothesis which maintains that the leading critical exponents remain the same as in the pure case and the weak universality hypothesis, which favours dilution-dependent leading critical exponents. Here the random-site version of the model is subject to a finite-size scaling analysis, paying special attention to the implications for multiplicative logarithmic corrections. The analysis is fully supportive of the scaling relations for logarithmic corrections and of the strong scaling hypothesis in the 2D case. In the four-dimensional case unusual corrections to scaling characterize the model, and the precise nature of these corrections has been debated. Progress made in determining the correct 4D scenario is outlined.

On the mass in fundamental theories of physics and its computation and measurement (P)

Harald Markum
Atominstitut, Vienna University of Technology, Austria
markum@tuwien.ac.at

In Classical Newtonian Mechanics the Hamiltonian function consists of a sum of kinetic and potential energy, where the mass of a body enters as a parameter. Within gravity one does not distinguish between gravitational

mass in the attraction of bodies in contrast to the inertial mass of objects in empty space; experimentally no difference can be found. In Special Theory of Relativity there appears the energy-momentum relation, where the value of the mass depends on the velocity; the rest mass is the same parameter as in Classical Mechanics. In Quantum Mechanics the mass stays as a parameter in the Hamiltonian; excited states in the Hydrogen atom are proportional to the rest mass. In Quantum Field Theory the mass becomes a (divergent) parameter, which has to be fixed to the experimental value via a renormalisation procedure. In the Standard Model of Particle Physics the masses depend on the vacuum expectation value of the Higgs Field. The fermions are additionally influenced from a Yukawa Coupling, being an open parameter.
In the Three Body Problem the mass of the interating particles plays a decisive role. In general such systems are chaotic. A stability criterion is given by the Kolmogorow-Arnold-Moser Theorem. Approximate solutions can be derived if one mass of the bodies is small. It is also exactly solvable if the two heavy bodies are in equilibrium with respect to gravity. There exists an analytic solution for the special case of identical masses of the three bodies travelling on a special loop. We give an overview of the different definitions and measurements.

Large-scale equilibrium simulation of the 3D Edwards-Anderson model

Victor Martin-Mayor
Departamento de Fisica Teorica I, Universidad Complutense de Madrid, Spain
victor@lattice.fis.ucm.es

Using the dedicated computer Janus, we have studied the low-temperature phase of the 3D Edwards-Anderson model for spin glasses. We have thermalized 1000 samples of $L = 32$ systems down to temperature $T = 0.64\,T_c$. A detailed study of the random walk in temperature space during the Parallel Tempering simulation was needed to check for thermalization on a sample-by-sample basis. We present our results for the distribution of the spin-overlap, infinite volume extrapolations for the order parameter $q_{\rm EA}$, and a study of the spatial correlation functions in the spin-glass phase.

Effects of spillover and particle size in a kinetic model of catalyzed reactions

Thiago Mattos
Instituto de Física, Universidade Federal Fluminense, Niterói, Brazil
tgmattos@if.uff.br

We study a model for unimolecular reaction on a supported catalyst including reactant diffusion, desorption and a constant reactant flux, using analytical methods and scaling concepts. The turnover frequency (TOF), which is the rate of production of the reaction product, is calculated exactly as function of the diffusion coefficient, desorption rate and external flux of reactants, and also as function of size and coverage of catalytic particles. We analyze the effects of diffusion and geometry on the TOF, identifying whether spillover (reactant flux from the catalyst to the support) or backspillover (the reverse process) is dominant. With an Arrhenius model for the several rates, we also study the effects of temperature on the TOF. The exact results for the model, associated with scaling concepts, can be extended to interpret experimental data and results of more complex models.

Critical behavior of bond-diluted negative-weight percolation

Oliver Melchert
Institut für Physik, Universität Oldenburg, Germany
melchert@theorie.physik.uni-oldenburg.de

We investigate the geometric properties of loops on two dimensional lattice graphs, where edge weights are drawn from a distribution that allows for positive and negative weights. We are interested in the appearance of lattice spanning loops of total negative weight. The resulting negative-weight percolation (NWP) problem is fundamentally different from conventional percolation [O. Melchert and A.K. Hartmann, New J. Phys. 10 (2008) 043039]. Here, we investigate how the percolation transition is affected by dilution that has an impact on the topology of the underlying lattice. We further characterize the model in the limit of densely packed

loop configurations and study the transition in higher dimensions. We study these systems numerically using exact combinatorial optimization techniques based on suitable transformations of the lattice graphs and applying sophisticated matching algorithms. We use observables from percolation theory and perform finite-size scaling analyses, e.g. two-dimensional square systems with side length up to $L = 512$ sites, in order to obtain the phase diagram and determine the critical properties of the phase boundary in the disorder-dilution plane. We find that bond-dilution leads to a change in the universality class of NWP. As disorder increases, the correlation length exponent changes from $\nu = 1.49(7)$ for the undiluted model to the value $\nu = 1.33(5)$ of usual percolation. In the limit of maximal disorder, the critical exponents fit those of fully packed loop models with fractal dimension $d_f = 1.751(5)$ and loop-length distribution exponent $\tau = 2.14(2)$. In higher dimensions, the results are compatible with $\nu = 3/d$ for the correlation length exponent.

Critical behavior of the Coulomb-glass model in the zero-disorder limit: Ising universality in a system with long-range interactions

Arnulf Möbius

Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden, Germany
a.moebius@ifw-dresden.de

The ordering of charges on half-filled hypercubic lattices is investigated numerically, where electroneutrality is ensured by background charges. This system is equivalent to the $s = 1/2$ Ising lattice model with antiferromagnetic $1/r$ interaction. The temperature dependences of specific heat, mean staggered occupation, and of a generalized susceptibility indicate continuous order-disorder phase transitions at finite temperatures in two- and three-dimensional systems. In contrast, the susceptibility of the one-dimensional system exhibits singular behavior at vanishing temperature. For the two- and three-dimensional cases, the critical exponents are obtained by means of a finite-size scaling analysis. Their values are consistent with those of the Ising model with short-range interaction, and they imply that the studied model cannot belong to any other known universality class. Samples of up to 1400, 112^2, and 22^3 sites are considered for dimensions 1 to 3, respectively.

[1] A. Möbius and U.K. Roessler, preprint arXiv:0904.3723.

Systematic microcanonical analyses of polymer adsorption transitions

Monika Möddel[1]

(with Michael Bachmann[2] **and Wolfhard Janke**[1]**)**

[1] Institut für Theoretische Physik, Universität Leipzig, Germany
[2] IFF, Theorie II, Forschungszentrum Jülich, Germany
monika.moeddel@itp.uni-leipzig.de

The understanding of the cooperative effects of structure formations at substrates requires systematic studies of mesoscopic aspects of adsorption transitions. Such an understanding is particularly desirable regarding the advances in processing and manipulating molecules at solid substrates on the nanometer scale. After we recently derived the complete phase structure of a single polymer near an attractive substrate of varying adsorption strengths [1], we now focus on the adsorption transition. This is conveniently and to our knowledge for the first time done by a detailed microcanonical analysis of densities of states obtained by extensive multicanonical Monte Carlo computer simulations. For short chains and strong surface attraction, the microcanonical entropy turns out to be a convex function of energy in the transition regime, indicating that surface-entropic effects are relevant. Albeit known to be a continuous transition in the thermodynamic limit of infinitely long chains, the adsorption transition of polymers with finite length thus exhibits a clear signature of a first-order-like transition, with coexisting phases of adsorbed and desorbed conformations. Another remarkable consequence of the convexity of the microcanonical entropy is that the transition is accompanied by a decrease of the microcanonical temperature with increasing energy. Since this is a characteristic physical effect it might not be ignored in analyses of cooperative macrostate transitions in finite systems.

[1] M. Möddel, M. Bachmann, and W. Janke, J. Phys. Chem. B **113** (2009) 3314.

Statistical analysis of quantum adiabatic computations

Thomas Neuhaus
JSC, Forschungszentrum Jülich, Germany
t.neuhaus@fz-juelich.de

The quantum adiabatic algorithm is conjectured to solve NP hard optimization problems in possibly polynomial time, if the algorithm is implemented on a quantum device. We discuss some principles of the algorithm and present exploratory first numerical results for the 3 SAT satisfiability problem. Our preliminary findings do not support the optimistic point of view as expressed in the conjecture.

Trading leads to scale-free self-organization

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

Financial markets display scale-free behavior in many different aspects. The power-law behavior of part of the distribution of individual wealth has been recognized by Pareto as early as the nineteenth century. Heavy-tailed and scale-free behavior of the distribution of returns of different financial assets have been confirmed in a series of works. The existence of a Pareto-like distribution of the wealth of market participants has been connected with the scale-free distribution of trading volumes and price-returns. The origin of the Pareto-like wealth distribution, however, remained obscure. I will discuss that it is the process of trading itself that under two mild assumptions spontaneously leads to a self-organization of the market with a Pareto-like wealth distribution for the market participants and at the same time to a scale-free behavior of return fluctuations. These assumptions are (i) everybody trades proportional to his current capacity and (ii) supply and demand determine the relative value of the goods.

[1] M. Ebert and W. Paul, preprint arXiv:0905.4815.

Wilson loops at very high order of lattice pertubation theory

Holger Perlt
Institut für Theoretische Physik, Universität Leipzig, Germany
holger.perlt@itp.uni-leipzig.de

We calculate Wilson loops of various sizes up to loop order $n = 20$ for lattice sizes of $L^4 (L = 4, 6, 8, 12)$ using the technique of Numerical Stochastic Perturbation Theory in quenched QCD. This allows to investigate the behaviour of the perturbative series at high orders. We discuss three models to estimate the perturbative series: a renormalon inspired fit, a heuristic fit based on an assumed power-law singularity and boosted perturbation theory. We have found differences in the behavior of the perturbative series for smaller and larger Wilson loops at moderate n. A factorial growth of the coefficients could not be confirmed up to $n = 20$. From Monte Carlo measured plaquette data and our perturbative result we estimate a value of the gluon condensate $\langle \frac{\alpha}{\pi} GG \rangle$.

[1] E.-M. Ilgenfritz, Y. Nakamura, H. Perlt, P.E.L. Rakow, G. Schierholz, and A. Schiller, preprint arXiv:0910.2795.

Translational diffusion in two-component lipid membranes close to phase transition

Eugene Petrov
Biophysics, BIOTEC, Technische Universität Dresden, Germany
petrov@biotec.tu-dresden.de

The intriguing phenomenon of subdiffusion frequently observed in cell membranes by single-molecule techniques is usually ascribed to the presence of membrane heterogeneities with dimensions below the optical res-

olution limit. In order to understand how the submicrometer-scale phase separation in the cell membrane can affect the lipid diffusion and manifest itself experimentally, we carry out dynamic Monte Carlo simulations of a two-component (DMPC/DSPC) lipid membrane with the size on the micrometer scale over time intervals of order of a second. To be able to do that with reasonable computational efforts, we represent the membrane as a square lattice of lipid molecules. By comparing our simulation results with differential scanning calorimetry data for DMPC/DSPC membranes, we demonstrate that our model correctly reproduces the thermodynamic properties, as well as the phase diagram of the lipid mixture. For certain ranges of the membrane compositions and temperatures we find that the Brownian motion of lipid molecules shows strong deviations from the normal diffusion law. In cases where the membrane shows critical fluctuations, simulated single particle tracking and fluorescence correlation spectroscopy experiments show transient subdiffusion behavior spanning about three orders of magnitude in time.

From an atomistic to a path integral representation of molecules in adaptive simulation (P)

Adolfo Poma

Max-Planck-Institut für Polymerforschung (MPI-P), Mainz, Germany
poma@mpip-mainz.mpg.de

In this contribution, our aim is to explore a suitable representation of atomistic molecules with the help of the path-integral formalism. Further studies will open the possibility to treat realistically the process of bond breaking in classical system, so far, we despict a possible way to be carried out using the Adaptive Resolution Scheme (AdResS).

Influence of chain stiffness and sequence on knottedness in polymer globules

Daniel Reith

Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany
reithd@uni-mainz.de

Although globular homopolymers display an abundance of knots, little is known about the effect of chain stiffness on topology, and the degree of entanglement in copolymer globules. To this end we investigate a bead-spring polymer model with varying persistence length in a spherical capsid, and globular phases of the HP model. For this purpose we have implemented three efficient bridging Monte Carlo moves to assure an efficent sampling of phase space despite of high densities, self entanglements and knots. Our results shed some light on the influence of stiffness on the packing of viral DNA, and the longstanding controversy why only few knots have been observed in experimentally determined protein structures.

The stochastic nature of predator-prey cycles (P)

Áttila Rodrigues

Institute of Physics, University of Sao Paulo, Brazil
attila@if.usp.br

We study by numerical simulations the time correlation function of a stochastic lattice model describing the dynamics of coexistence of two interacting biological species that present time cycles in the number of species individuals. Its asymptotic behavior is shown to decrease in time as a sinusoidal exponential function from which we extract the dominant eigenvalue of the evolution operator related to the stochastic dynamics showing that it is complex with the imaginary part being the frequency of the population cycles. The transition from the oscillatory to the nonoscillatory behavior occurs when the asymptotic behavior of the time correlation function becomes a pure exponential, that is, when the real part of the complex eigenvalue equals a real eigenvalue. We also show that the amplitude of the undamped oscillations increases with the square root of the area of the habitat as ordinary random fluctuations.

Critical loop gases and the worm algorithm

Adriaan M.J. Schakel[1]
(with Thomas Neuhaus[2] **and Wolfhard Janke**[1]**)**

[1] Institut für Theoretische Physik, Universität Leipzig, Germany
[2] JSC, Forschungszentrum Jülich, Germany
schakel@itp.uni-leizpig.de

The loop gas approach to lattice field theory provides an alternative, geometrical description in terms of fluctuating loops. Statistical ensembles of random loops can be efficiently generated by Monte Carlo simulations using the worm update algorithm. In this talk, concepts from percolation theory and the theory of self-avoiding random walks are used to describe estimators of physical observables that utilize the nature of the worm algorithm. The fractal structure of the random loops as well as their scaling properties are studied. To support this approach, the O(1) loop model, or high-temperature series expansion of the Ising model, is simulated on a honeycomb lattice, with its known exact results providing valuable benchmarks.

[1] W. Janke, T. Neuhaus, and A.M.J. Schakel, preprint arXiv:0910.5231.

The lattice ghost propagator in Landau gauge up to three loops using numerical stochastic perturbation theory (P)

Arwed Schiller
Institut für Theoretische Physik, Universität Leipzig, Germany
arwed.schiller@itp.uni-leipzig.de

We complete our high-accuracy studies of the lattice ghost propagator in Landau gauge in Numerical Stochastic Perturbation Theory up to three loops. We present a systematic strategy which allows to extract with sufficient precision the non-logarithmic parts of logarithmically divergent quantities as a function of the propagator momentum squared in the infinite-volume and $a \to 0$ limits. We find accurate coincidence with the one-loop result for the ghost self-energy known from standard Lattice Perturbation Theory and improve our previous estimate for the two-loop constant contribution to the ghost self-energy in Landau gauge. Our results for the perturbative ghost propagator are compared with Monte Carlo measurements of the ghost propagator performed by the Berlin Humboldt university group which has used the exponential relation between potentials and gauge links.

[1] F. Di Renzo, E.-M. Ilgenfritz, H. Perlt, A. Schiller, and C. Torrero, preprint arXiv:0910.2905.

The modified sharpened index h_ms and other variants in the Hirsch index zoo

Michael Schreiber
Institut für Physik, Technische Universität Chemnitz, Germany
schreiber@physik.tu-chemnitz.de

The Hirsch index or h-index is widely used to quantify the impact of an individual's scientific research output, determining the highest number h of a scientist's papers that received at least h citations. I present an analysis of two case studies, one for 8 famous physicists and another for 26 not-so-prominent colleagues. Difficulties with the determination of the index and its interpretation are discussed. Fractionalised counting of the publications is an appropriate way to distribute the impact of a paper among all the coauthors of a multi-authored manuscript in an easy way, leading to a simple modification hm of the h-index. On the other hand the exclusion of self-citations allows one to sharpen the index, what is appropriate, because self-citations are usually not reflecting the significance of a publication. Self-citations can significantly reduce the sharpened index hs compared to the original index in contrast to Hirsch's expectations. Combining the two procedures gives the modified sharpened index hms. The correlations between the indices are rather strong, but nevertheless the positions of some datasets change, in a few cases significantly, depending on whether they are put into order according to the values of h, hm, hs, or hms. This leads to the conclusion that the additional effort in determining the modified sharpened index hms is worth performing in order to obtain a fairer evaluation of the citation records. In order to take into account the highly skewed frequency distribution of citations, Egghe proposed the g-index as an improvement

of the h-index. I compare the h and g values for the two case studies. It is demonstrated that the g-index discriminates better between different citation patterns. This can also be achieved by evaluating Jin's A-index which reflects the average number of citations in the h-core (i.e. the h-defining set), but only by interpreting it in conjunction with the h-index. h and A can be combined into the R-index to measure the h-core's citation intensity. In contrast to A and R the g-index can stand alone, measuring both the productivity of a scientist by the number of papers in the core and the impact by the number of citations of the papers in the core. Fractionalised counting of the multi-authored manuscripts leads again to a simple modification gm. As for the h-index the exclusion of self-citations allows one to sharpen the index yielding gs. In my opinion the modified sharpened index gms is the most appropriate way to estimate the visibility of a scientist's research. Whether this is a measure of importance and significance is a debatable and debated question.

Structural synthesis of operational parameters of tribocoupling (P)

Leonid Semishev
Volgograd State Technical University, Russia
7leon@list.ru

This research is connected with studying strength properties of dynamic systems with variable structure, their synthesis and control. Two effective methods for optimizing technological parameters and the structure of tribocoupling are offered, one of which bases on the simplex algorithm, and another uses neural networks.

The ball-model of an early stage of nucleation of the globular protein crystals with the use of fulleren-like mapping of the surface properties (P)

Jacek Siódmiak
Department of Modeling of Physicochemical Processes, Institute of Mathematics and Physics, University of Technology and Life Sciences, Bydgoszcz, Poland
siedem@utp.edu.pl

The mesoscopic ball-model of the globular protein assumes that the biomolecule is represented by the hard ball covered by the "fulleren-geometry-map" of an attractive regions. These regions reflect the hydrophobic and hydrophilic properties of aminoacids constituting the protein and its location in the tertriary structure of the biomolecule. In this way, modeled protein manifests anisotropy of its interacting properties. The positions of the attractive patches can be controlled in some (limited) way and are determined by the geometry of the unit cell of the protein crystal. In the case of the lysozyme (PDB ID: 193L), the protein under consideration, the space group of the crystal is P43212 and is the same like in the silicon crystal. For this structure the coordinate number is four, what means that each ball makes four contacts with surrounding balls, and therefore, the optimal number of attractive patches on the surface of the central ball should be four. In the most-dense-packing case, when the number of attractive patches is twelve, the positions of the attractive patches match with the position of the pentagons in the fullerene (or in the football). For the coordinate number twelve, obtained structure is one of the close packed structures with packing factor of 0.74. In our modeling, corresponding to the physico-chemical properties of the protein solution (pH, ionic strength, dielectric constant) we are going to find the most effective method to distribute four attractive patches on the modeled protein-ball, which will lead to the P43212 symmetry.

All-or-none protein-like folding of a homopolymer chain

Mark Taylor
Department of Physics, Hiram College, Hiram, OH, USA
taylormp@hiram.edu

Many small proteins fold via a first-order "all-or-none" transition directly from an expanded coil to a compact native state. Here we report an analogous direct freezing transition from an expanded coil to a compact crystallite for a simple flexible homopolymer. Wang-Landau sampling is used to construct the complete density of states for square-well chains up to length 256. Analysis within both the microcanonical and canonical ensembles shows

that, for a chain with sufficiently short-range interactions, the usual polymer collapse transition is preempted by a direct freezing transition. Despite the non-unique homopolymer ground state, the thermodynamics of this direct freezing transition are identical to the thermodynamics of two-state protein folding. A free energy barrier separates a high-entropy ensemble of unfolded states from a low-entropy set of crystallite states and the transition proceeds via the formation of a transition-state folding nucleus. An Arrhenius analysis of the folding/unfolding free energy barrier yields a Chevron plot characteristic of proteins and the model chain satisfies the van't Hoff calorimetric criterion for two-state folding.

Exact solution of the stochastic SIR model

Steffen Trimper

Institut fürPhysik, Naturwissenschaftliche Fakultät II, Martin-Luther Universität Halle, Germany
steffen.trimper@physik.uni-halle.de

The susceptible-infectious-recovered (SIR) model describes the evolution of three species of individuals which are subject to an infection and recovery mechanism. A susceptible can become infectious with an infection rate by an infectious type provided that both are in contact. The I–type may recover with another rate. Due to the coupling between the different individuals, the model is nonlinear and out of equilibrium. We adopt a stochastic individual-based description where individuals are represented by nodes of a graph and contact is defined by the links of the graph. Mapping the underlying Master equation into a quantum formulation in terms of spin operators, the hierarchy of evolution equations can be solved exactly for arbitrary initial conditions on a linear chain. The exact results for the ensemble averaged population size are compared with simulations for single realizations of the process and also with standard mean-field theory which is expected to be valid on large fully-connected graphs.

Tuning the shape of the condensate in spontaneous symmetry breaking

Bartłomiej Wacław[1]

(with J. Sopik[2]**, W. Janke**[3]**, and H. Meyer-Ortmanns**[2]**)**

[1] Department of Physics & Astronomy, University of Edinburgh, UK
[2] School of Engineering and Science, Jacobs University Bremen, Germany
[3] Institut für Theoretische Physik, Universität Leipzig, Germany
bwaclaw@googlemail.com

We investigate the conditions which determine the shape of a particle condensate in situations when it emerges as a result of spontaneous breaking of translational symmetry. We consider a model with particles hopping between sites of a one-dimensional grid and interacting if they are at the same site or at neighboring sites. We predict the envelope of the condensate and the scaling of its width with the system size for various interaction potentials and show how to tune the shape from a delta-peak to a rectangular or a parabolic-like form.

[1] B. Wacław, J. Sopik, W. Janke, and H. Meyer-Ortmanns, Phys. Rev. Lett. **103** (2009) 080602; J. Phys. A **42** (2009) 315003; J. Stat. Mech.: Theor. Exp. P10021 (2009).

Numerical investigation of the aging of the fully-frustrated XY model

Jean-Charles Walter

Laboratoire de Physique des Matériaux, Université Henri Poincaré, Nancy I, France
walter@lpm.u-nancy.fr

We study the out-of-equilibrium dynamics of the fully-frustrated XY model. At equilibrium, this model undergoes two phase transitions at two very close temperatures: a Kosterlitz-Thouless topological transition and a second-order phase transition between a paramagnetic phase and a low-temperature phase where the chiralities of the lattice plaquettes are anti-ferromagnetically ordered. We compute by Monte Carlo simulations two-time spin-spin and chirality-chirality autocorrelation and response functions. From the dynamics of the spin waves in the low-temperature phase, we extract the temperature-dependent exponent η. We provide evidences for logarithmic corrections above the Kosterlitz-Thouless temperature and interpret them as a manifestation of free

topological defects. Our estimates of the autocorrelation exponent and the fluctuation-dissipation ratio differ from the XY values, while $\eta(T_{\mathrm{KT}})$ lies at the boundary of the error bar. Indications for logarithmic corrections at the second-order critical temperature are presented. However, the coupling between angles and chiralities is still strong and explains why autocorrelation exponent and fluctuation-dissipation ratio are far from the Ising values and seems stable.

Evaporation/condensation transition of 3D Ising droplets (P)

Micha Wiedenmann

(with Andreas Nußbaumer, Elmar Bittner, and Wolfhard Janke)

Institut für Theoretische Physik, Universität Leipzig, Germany
micha.wiedenmann@itp.uni-leipzig.de

This work studies the evaporation/condensation transition of Ising droplets in three dimensions. We performed Monte Carlo simulations of the Ising model with nearest-neighbor couplings on a simple cubic lattice with periodic boundary conditions at a fixed magnetization, corresponding to a certain amount v_L of overturned spins. The volume v_d of the largest droplet was measured at constant magnetization employing a flood-fill algorithm. For values of the magnetization $m < m_c$ there exists no droplet in the system and the fraction of overturned spins above the equilibrium magnetization m_0 in the largest droplet $\lambda = v_d/v_L$ is zero. At $m = m_c$ one half of the overturned spins form a droplet which grows for larger values of the magnetization. This behavior can be compared to analytical results given by Biskup *et al.* [Europhys. Lett. 60 (2002) 21]. In order to do so we measured the spontaneous magnetization m_0, the magnetic susceptibility χ and the planar surface tension τ (which is a good approximation of a Wulff shaped droplet).

A cluster Monte Carlo algorithm with a conserved order parameter

David Yllanes

Universidad Complutense de Madrid, Spain
yllanes@lattice.fis.ucm.es

We propose a cluster simulation algorithm for statistical ensembles with fixed order parameter. We use the tethered ensemble, which features Helmholtz's effective potential rather than Gibbs's free energy, and in which canonical averages are recovered with arbitrary accuracy. For the $D = 2, 3$ Ising model our method's critical slowing down is comparable to that of canonical cluster algorithms. Yet, we can do more than merely reproduce canonical values. As an example, we obtain a competitive value for the 3D Ising anomalous dimension from the maxima of the effective potential.