ABSTRACTS

of talks at the

5th NTZ-Workshop on

Computational Physics

CompPhys04

Institut für Theoretische Physik,
Universität Leipzig, Germany

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http://www.physik.uni-leipzig.de/~janke/CompPhys04

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List of contributions

CompPhys04 Timetable

November 25, 2004 - Vor dem Hospitaltore 1, Large (‘‘Grosser’’) Seminar Room 1L12/13

9:00-12:50		**- COPIRA/NTZ-Workshop ANet04 -**
12:50-14:00		**- Lunch Break at "Das Fass" -**
14:00-14:15		**- Welcome Coffee -**
14:15-14:45	**Zdzislaw Burda**	Statistical mechanics of complex networks
14:45-15:15	**Marian Brandau**	Delay effects in the SIR-model on small world networks
15:15-15:45	**Alexander Hartmann**	Partition functions and distributions of connected components: the q-state Potts model
15:45-16:00	**Adriaan Schakel**	Fractal structure of critical and collapsing loops in 2D
16:00-16:30		**- Coffee Break -**
16:30-17:00	**Thomas Neuhaus**	Loop updates in 3D compact QED
17:00-17:30	**Andrei Fedorenko**	Stability of critical behavior of weakly disordered spin systems with respect to the replica symmetry breaking
17:30-17:45	**Meik Hellmund**	Series expansions for disordered Potts models
17:45-18:15	**Knud Zabrocki**	Reaction and diffusion in glasses
19:00-20:00		**- Glühwein at Christmas Market -**
20:00		**- Dinner at "Thüringer Hof" -**

November 26, 2004 - Vor dem Hospitaltore 1, Large (‘‘Grosser’’) Seminar Room 1L12/13

9:00- 9:30		**- Wake-up Coffee -**
9:30-10:00	**Christian von Ferber**	Simulation of charged polymers: self-assembly of ionic surfactants with a polyelectrolyte
10:00-10:30	**Hsiao-Ping Hsu**	Simulations of lattice animals
10:30-11:00	**Frank Dressel**	Exact ground state of model proteins
11:00-11:30		**- Coffee Break -**
11:30-12:00	**Bernd Burghardt**	Dependence of the RNA secondary structure on the energy model
12:00-12:15	**Horst L. Vörtler**	Efficient simulation of chemical potentials: gradual particle insertion versus ‘‘monomer/dimer’’ insertion
12:15-12:45	**Michael Schreiber**	A multi-parameter Ising model for the adsorption of molecules on structured surfaces
12:45-14:30		**- Lunch Break at "Blaue Adria" (Johannisallee) -**

14:30-15:00	**Peter Grassberger**	MILCA (Mutual Information based Least dependent Component Analysis) is sweet
15:00-15:30	**Lev Shchur**	Ensemble of cat maps is hard to decipher: periodic orbits and random number generator
15:30-16:00	**Ralph Kenna**	Properties of higher-order phase transitions
16:00-16:15	**Peter Crompton**	Nonequilibrium quantum dynamics
16:15-17:00		**- Posters & Coffee -** 
17:00-17:30	**Malte Henkel**	Local scale-invariance in ageing phenomena
17:30-18:00	**Christophe Chatelain**	On universality in ageing ferromagnets
18:00-18:15	**Ulrich Behn**	Generation of spatiotemporal correlated noise in 1+1 dimensions
18:15-18:45	**Desmond Johnston**	Dyck paths, Motzkin paths and traffic jams
18:45-19:45		**- Posters & Fare-Well Beer/Wine -** 

20:30 **- Dinner at ??? ("democratic decision") -** 

November 27, 2004 - Vor dem Hospitaltore 1

10:00-17:00 **- Open Discussions of Project Groups -**
- Summary & Future Perspectives -

Generation of spatiotemporal correlated noise in 1+1 dimensions

Ulrich Behn
(with A. Traulsen and K. Lippert)

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We propose a generalization of the Ornstein-Uhlenbeck process in 1+1 dimensions which is the product of a temporal Ornstein-Uhlenbeck process with a spatial one and has exponentially decaying autocorrelation. The generalized Langevin equation of the process, the corresponding Fokker-Planck equation, and a discrete integral algorithm for numerical simulation is given.

Delay effects in the SIR–model on small world networks

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Epidemiological processes on a hierarchical network model are studied by using the susceptible–infective–refractory model (SIR) which is extended by including delay effects. A feature of the network model is the characterization by H independent hierarchies or dimensions at which each of them stands for a grouping of individuals. Detailed numerical simulations reveal that for $H > 1$, the global spreading results regardless of the degree of homophily α of the individuals forming a social circle. For $H = 1$, a transition from a global to a local spread occurs as the population becomes decomposed into increasingly homophilous groups. Multiple dimensions in classifying individuals (nodes) thus make a society (computer network) highly susceptible to large scale outbreaks of infectious diseases (viruses). The SIR–model can be extended by the inclusion of waiting times resulting in modified distribution function of the recovered.

Statistical mechanics of complex networks

Zdzislaw Burda

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Statistical approach to complex networks is discussed. Random networks are defined through the concept of statistical ensemble with a given probability measure. Physical quantities like for instance fractal dimension or node degree distribution, correlations, etc. are defined not on an individual network but on the whole ensemble. This approach is a natural generalization of the Erdös-Rényi ideas for the case of correlated networks or networks with arbitrary degree distribution.

Dependence of the RNA secondary structure on the energy model

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In the literature mainly two different types of energy models are considered for RNA secondary structures: On the one hand side every paired base pair is assigned an energy, on the other hand only so called stacked base pairs, e.g. two or more consecutive base pairs, are assigned an energy. We examined a model that uses both types of energy contributions, and therefore we were able to study the transition from one type of the above mentioned energy models to the other one. We have done numerical studies on statistical quantities, where we used algorithms that are able to calculate the partition function and the ground-state energy exactly in polynomial time.

On universality in ageing ferromagnets

Christophe Chatelain

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We will discuss in this talk the issue of universality in the context of ageing homogeneous ferromagnets. We consider lattice models undergoing a second-order phase transition at equilibrium that are quenched at their critical temperature. Two quantities that are believed to take universal values are investigated by means of Monte Carlo simulations : the exponent λ/z obtained from the decay of autocorrelation functions and the asymptotic value X_∞ of the fluctuation-dissipation ratio $X(t,s)$. This protocol was applied to the Ising model, the 3-state clock model and the 4-state Potts model on square, triangular and honeycomb lattices and to the Ashkin-Teller model at the point belonging at equilibrium to the 3-state Potts model universality class and to a multispin Ising model and the Baxter-Wu model both belonging to the 4-state Potts model universality class at equilibrium.

Nonequilibrium quantum dynamics

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Inhomogeneous AF spin chains offer us the opportuntity to extend the definition of Haldane's conjecture: gaps occur above the ground state in integer spin systems at low temperatures. These inhomogeneous chains model the effect of the experimentally relevant doping of quasi-metalic systems used in investigations of spin-wave superconductivity. We report on our recent analyses developments of the Quantum Monte Carlo scheme for simulations of these models, and discuss now new perspectives for tackling the algorithmic issues associated with implementing frustation and quantum "glassy" dynamics from our new results.

Exact ground state of model proteins

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(with S. Kobe)

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Lattice models are used to investigate the energy landscape, folding properties and thermodynamics of proteins. The main disadvantage of such up to now considered rigid models is the disability to characterize the real structure. We propose a model, which is more appropriate to deal with biological conformations. The real positions of the amino acids are dynamically simulated using fixed bond lengths between the atoms and an angle distribution taken from Ramachandran plots. Data of the pairwise interactions between the amino acids are based on results of biological investigations [1]. The exact ground state (energy and conformation) is calculated using methods of optimization algorithms with respect to the global energy. Results for proteins up to a chain length of 25 amino acids are obtained and compared with the biological native states.

References

[1] R.I. Dima, G. Settanni, C. Micheletti, J.R. Banavar, A. Maritan, J. Chem. Phys. **112**, 9151 (2000).

Stability of critical behavior of weakly disordered spin systems with respect to the replica symmetry breaking

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We consider the critical behavior of weakly disordered spin systems. In dealing with the quenched disorder the standard method is the replica trick, and in terms of replicas all the results obtained for the weakly disordered spin systems correspond to the so-called replica-symmetric (RS) solutions. Physically it means that only the unique ground state is assumed to be relevant for the observable thermodynamics. However, as was suggested by Dotsenko *et al.* [1], the existence of numerous local minimal energy configurations in weakly disordered spin systems may give rise to

the replica symmetry breaking (RSB) and to the subsequent instability of the RS fixed points which are usually considered to describe the disorder-induced universal critical behavior. Using the renormalization group methods we investigate the critical behavior of a model with RSB potentials of a general type in the two-loop approximation. We show that in this approximation the RS fixed points are stable with respect to 1-step RSB [2] and with respect to the continuous RSB [3], confirming the realization of the former scenario of disorder influence on the critical behavior.

References

[1] V.S. Dotsenko *et al.*, J. Phys. A **28**, 3093 (1995).

[2] V.V. Prudnikov, P.V. Prudnikov, and A.A. Fedorenko, Phys. Rev. B **63**, 184201 (2001).

[3] A.A. Fedorenko, J. Phys. A **36**, 1239 (2003).

MILCA (Mutual Information based Least dependent Component Analysis) is sweet

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We propose to use precise estimators of mutual information (MI) to find least dependent components in a linearly mixed signal. On the one hand this seems to lead to better blind source separation than with any other presently available algorithm. On the other hand it has the advantage, compared to other implementations of "independent" component analysis (ICA) some of which are based on crude approximations for MI, that the numerical values of the MI can be used for: (i) estimating residual dependencies between the output components; (ii) estimating the reliability of the output, by comparing the pairwise MIs with those of re-mixed components; (iii) clustering the output according to the residual interdependencies. For the MI estimator we use a recently proposed k-nearest neighbor based algorithm. For time sequences we combine this with delay embedding, in order to take into account non-trivial time correlations. After several tests with artificial data, we apply the resulting MILCA (Mutual Information based Least dependent Component Analysis) algorithm to a real-world dataset, the ECG of a pregnant woman.

Partition functions and distributions of connected components: the q-state Potts model

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A new algorithm is presented, which allows to calculate numerically the partition function Z_q of the d-dimensional q-state Potts models for arbitrary real values $q > 0$ at any given temperature T with high precision. The basic idea is to measure the distribution of the number of connected components in the corresponding Fortuin-Kasteleyn representation and to compare with the distribution of the case $q = 1$ (graph percolation), where the exact result $Z_1 = 1$ is known. As application, $d = 2$ and $d = 3$-dimensional ferromagnetic Potts models are studied, and the critical values q_c, where the transition changes from second to first order, are determined. Large systems of sizes $N = 1000^2$ respectively $N = 100^3$ are treated. The critical value $q_c(d = 2) = 4$ is confirmed and $q_c(d = 3) = 2.35(5)$ is found.

Series expansions for disordered Potts models

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We derive high-temperature series expansions for the free energy and the susceptibility of random-bond q-state Potts models on hypercubic lattices using a star-graph expansion technique. This method enables the exact calculation of quenched disorder averages for arbitrary uncorrelated coupling distributions. Moreover, we can keep the disorder strength p as well as the dimension d as symbolic parameters. By applying several series analysis techniques to the new series expansions, one can scan large regions of the (p, d) parameter space for any value of q.

We present results for the transition temperature and the effective critical exponent γ as a function of p for the diluted Ising model in three dimensions and discuss the observed crossover behaviour.

As a by-product we get high-temperature series in the parameter q for pure q-state Potts models up to order 19 which allow us to analyze the different $q \to 0$ limits (percolation, tree percolation) in various dimensions.

Local scale-invariance in ageing phenomena

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The time-dependent scaling of the two-time correlation and response functions of systems undergoing ageing is studied. An important special case of this is furnished by systems undergoing phase-ordering kinetics. We propose to extend the standard dynamical scaling to a local scale-invariance. For phase-ordering kinetics, the dynamical exponent $z = 2$ and we show that local scale-invariance is a new version of conformal invariance. Then the form of the scaling functions of correlators and response functions can be predicted. These predictions are in excellent agreement with simulational data, in particular from the kinetic Glauber-Ising model. We compare our results with previous attempts to obtain closed-form expressions for the autocorrelator.

Simulations of lattice animals

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The scaling behaviour of randomly branched polymers in a good solvent is studied in two to nine dimensions, using as microscopic models lattice animals on simple hypercubic lattices. As a stochastic sampling method we use a biased sequential sampling algorithm with re-sampling, similar to the pruned-enriched Rosenbluth method (PERM) used extensively for linear polymers. Essentially we start simulating percolation clusters (either site or bond), re-weigh them according to the animal ensemble, and prune or branch the further growth according to a heuristic fitness function. In contrast to previous applications of PERM, this fitness function is *not* the weight with which the actual configuration would contribute to the partition sum, but is closely related to it. We obtain high statistics of animals with up to several thousand sites in all dimension $2 \leq d \leq 9$. In addition to the partition sum (number of different animals) we estimate gyration radii and numbers of perimeter sites. In all dimensions we verify the Parisi-Sourlas prediction, and we verify all exactly known critical exponents in dimensions 2, 3, 4, and ≥ 8. In addition, we present the hitherto most precise estimates for growth constants in $d \geq 3$. For clusters with one site attached to an attractive surface, we verify for $d \geq 3$

the superuniversality of the cross-over exponent ϕ at the adsorption transition predicted by Janssen and Lyssy, but not for $d = 2$. There, we find $\phi = 0.480(4)$ instead of the conjectured $\phi = 1/2$. Finally, we study two-dimensional animals grafted to the tips of wedges with a wide range of angles α, to the tips of cones (wedges with the sides glued together), and to branching points of Riemann surfaces. The latter can either have k sheets and no boundary, generalizing in this way cones to angles $\alpha > 360$ degrees, or can have boundaries, generalizing wedges. We obtain precise values for the entropic exponent θ ($Z_N \sim \mu^N N^{-\theta}$) and we find that $\theta \sim 1/\alpha$ for small angles ($\alpha \ll 2\pi$), while $\theta \approx const - \alpha/2\pi$ for $\alpha \gg 2\pi$. These scalings hold both for wedges and cones. A heuristic argument for the behaviour at large α (which clearly shows that conformal invariance does not hold in the standard way) is given, and comparison is made with critical percolation.

Dyck paths, Motzkin paths and traffic jams

Desmond A. Johnston

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It has recently been observed that the normalization of a one-dimensional out-of-equilibrium model, the Asymmetric Exclusion Process (ASEP), is exactly equivalent to the partition function of a two-dimensional lattice path model of one-transit walks, or equivalently Dyck paths. We discuss the equivalence for various update dynamics.

Properties of higher-order phase transitions

Ralph Kenna

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It has long been suspected that phase transitions of order greater than two do not exist in nature. However, there is no physical reason that this should be the case. Recent experimental observations of a certain cubic superconductor have been ascribed to its possessing a fourth order discontinuous transition. Further claims have been made that higher order transitions may conceivably have been observed in other physical systems in the past, but that they were wrongly interpreted as belonging to the second order framework. A theory for higher order transitions has recently been developed and found to be consistent with the limited experimental results available. Here, such higher order transitions are analysed through the

medium of partition function zeroes. Certain scaling relations are recovered, new ones are found and some new results concerning the distributions of zeroes are derived.

Loop updates in 3D compact QED

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We update closed loops of gauge fields in 3D compact QED and determine the mass gap as well as Wilson's string tension. The algorithm is as efficient as comparable local updates. Nevertheless scaling is studied up to β values 3 in the theory with the Wilson action.

Fractal structure of critical and collapsing loops in 2D

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The high-temperature graphs of the two-dimensional O(N) model naturally form a loop gas whose fractal structure encodes the entire critical behavior of the model. In this talk, results are reported on the study of these loops close to their tricritical point, corresponding to the Θ point in the context of polymers, where they collapse. A close connection between the fractal structures of the critical and collapsing loops and thus the two critical behaviors is established.

A multi-parameter Ising model for the adsorption of molecules on structured surfaces

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(with S. Gemming, K. Morawetz, C. Olbrich, R. Scholz)

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Several modifications of the standard two-parameter Ising model are necessary for the mesoscopic modelling of a realistic adsorbate ensemble on a non-ideal substrate. Depending on the shape of the molecule, the nearest-neighbours coupling exhibits a directionality, and also additional coupling terms with next nearest neighbour are taken into account. Structured or defective surfaces are modelled by local modifications of the magnetisation term. Several sets of coupling parameters were derived from first-principles calculations on PTCDA monomer, dimer, and adsorbate systems. The adsorbate distribution on the surface was investigated by Metropolis-Monte-Carlo simulations and cluster statistics employing the Hoshen-Kopelman cluster recognition algorithm. It was observed that surface defects like steps influence the pattern formation mainly close to the critical temperature of the order-disorder transition. It could be shown that all adsorbate-adsorbate interactions are connected by a straightforward scaling in the critical temperature, whereas the adsorbate-substrate interaction is of a more complicated nature, especially in the presence of surface defects.

Ensemble of cat maps is hard to decipher: periodic orbits and random number generator

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We discuss the construction of the random number generator based on the parallel evolution of the ensemble of cat maps (Sinai-Arnold cat maps). Each cat map provides just one bit, so to construct s-bit random number we have to evaluate s cat maps. We analyse the period of the generator using Percival-Vivaldi theory. We discuss the correlations in the single cat map and propose the way to diminish them. The proposed generator is successfully tested using the standard bench of statistical tests. Output of the generator is hard to decipher because most of the information on the state of the ensemble of cat maps is hidden.

Efficient simulation of chemical potentials: gradual particle insertion versus "monomer/dimer" insertion

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The problem of efficient simulation of chemical potentials in dense complex fluids is of high importance since classical Widom test particle method usually fails on such conditions. Recently we have shown the applicability of gradual particle insertion to chemical potential simulations of highly associating primitive water models. Here we extended these studies to a new particle insertion approach of Tripathi and Chapman (TC) which divides the water molecules in "bonded" and "unbonded" particles and counts only test particles which stay "unbonded" after insertion. We implemented the method to primitive models of water and compared the results with gradual particle insertion. The original TC (using "monomers", i.e. free water molecules, as unbonded particles) provides a clear improvement over the classical Widom method but it yet fails for low temperatures and high densities. Therefore we modified the TC method using "monomers + dimers" as "unbonded" particles. This algorithm provides accurate chemical potentials for the entire temperature and density range which we studied previously by gradual insertion. The very good mutual agreement of both methods serves as an independent check of the accuracy of our simulation results. For low densities and supercritical temperatures the efficiency of modified TC is superior to gradual insertion while in the low temperature/high density range gradual insertion is more efficient.

Simulation of charged polymers: self-assembly of ionic surfactants with a polyelectrolyte

Christian von Ferber
(with F. Jasch and A. Blumen)

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We study the structure of complexes formed between ionic surfactants (SF) and a single oppositely charged polyelectrolyte (PE) chain. For our computer simulation

we use the primitive electrolyte model: while the polyelectrolyte is modeled by a tethered chain of charged hard sphere beads, the surfactant molecules consist of a single charged head bead tethered to a tail of tethered hard spheres. A hydrophobic attraction between the tail beads is introduced by assuming a Lennard-Jones potential outside the hard-sphere diameter. As a function of the strengths of both the electrostatic and the hydrophobic interactions, we find characteristic transitions in the geometry and the internal structure of the self assembled complex formed by the PE and SF. Switching on and increasing the electrostatic forces first leads to a stretching of the PE and then by condensation of SF to the formation of a complex. For vanishing hydrophobic forces this complex has the architecture of a molecular bottle-brush cylindrically centered around the stretched PE molecule. Upon increasing the hydrophobic attraction between the SF tails, a transition occurs inverting this structure to a spherical micelle with a neutral core of SF tails and a charged corona of SF heads with the PE molecule wrapped around. At intermediate hydrophobicity there is a competition between the two structures indicated by a non-monotonic dependence of the shape as function of the Coulomb strength, favoring the cylindrical shape for weak and the spherical micellar complex for strong interaction.

Reaction-diffusion in glasses

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(with S. Trimper)

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The formalism of reaction-diffusion rate equations is applied to an experimental measured phenomenon of particle creation in glasses. The description of the kinetic growth is major task of our investigation. There are three partial processes, which are proceeding in parallel: (i) Reduction of silver ions to silver atoms; (ii) Nucleation of the silver atoms; (iii) Creation of silver particles. Most of the known theoretical models are using homogeneous distribution of the silver ions in the first step. In our case we take a possible mobility of the silver ions into account resulting in a system of partial differential equation instead of ordinary ones. Whereas an effective linear theory is solved exactly in form of Fourier series, the complete non-linear system of equations is performed numerically. After the implementation of the other two steps of the kinetics, first in sequential manner and then in a parallel one we find the spatial distribution of the silver particles as well as the size distribution of them which influence the macroscopic properties of the glass like the colour and the rigidity.