Computational Quantum Field Theory (CQT)
– Research Report 2004 –

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0.0.1 Computational Quantum Field Theory, Computerorientierte Quantenfeldtheorie

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0.1 Computational Quantum Field Theory

0.1.1 Introduction

The Computational Physics Group performs basic research into classical and quantum statistical physics with special emphasis on phase transitions and critical phenomena. In the centre of interest are currently spin glasses, diluted magnets and other physical systems with quenched, random disorder, a geometrical approach to the statistical physics of topological defects with applications to superconductors and superfluids, biologically motivated problems (e.g., protein folding and semiflexible polymers), fluctuating geometries with applications to quantum gravity (e.g., dynamical triangulations) and soft condensed matter physics (e.g., membranes and interfaces). Supported by a Development Host grant of the European Commission, currently also research into the physics of anisotropic quantum magnets is established.

The methodology is a combination of analytical and numerical techniques. The numerical tools are currently mainly Monte Carlo computer simulations and high-temperature series expansions. The computational approach to theoretical physics is expected to gain more and more importance with the future advances of computer technology, and will probably become the third basis of physics besides experiment and analytical theory. Already now it can help to bridge the gap between experiments and the often necessarily approximate calculations of analytical work. To achieve the desired high efficiency of the numerical studies we develop new algorithms, and to guarantee the flexibility required by basic research all computer codes are implemented by ourselves. The technical tools are Fortran, C, and C++ programs running under Unix or Linux operating systems and computer algebra using Maple or Mathematica. The software is developed and tested at the Institute on a cluster of PCs and workstations, where also most of the numerical analyses are performed. Large-scale simulations requiring vast amounts of computer time are carried out at the Institute on a recently installed Beowulf cluster with 40 Athlon MP1800+ CPUs and a brandnew Opteron cluster with 18 processors of 64-bit architecture, at the parallel computers of the University computing center, and upon grant application at the national supercomputing centres in Jülich and München on IBM and Hitachi parallel supercomputers. This combination of various platforms gives good training opportunities for the students and offers promising job perspectives in many different fields for their future career.

The research is embedded in a wide net of national and international collaborations funded by network grants of the European Commission, the European Science Foundation (ESF) and the German-Israel-Foundation (GIF), and by a binational research grant with scientists in Sweden. Close contacts and collaborations are also established with research groups in Armenia, Austria, China, France, Great Britain, Israel, Italy, Poland, Russia, Spain, Taiwan, Turkey, Ukraine, and the United States.

Wolfhard Janke

0.1.2 Monte Carlo Studies of Spin Glasses

B. A. Berg (Florida State University, Tallahassee, USA), A. Billoire (CEA/Saclay, Gif-sur- Yvette, France), E. Bittner, W. Janke, A. Nußbaumer and D. B. Saakian (Yerevan Physics Institute, Yerevan, Armenia)

Spin glasses are examples for the important class of materials with random, competing interactions [1]. This introduces so-called "frustration", since no unique spin configuration is favoured by all interactions, and consequently leads to a rugged free energy landscape with many minima separated by barriers. To cope with the problems of standard Monte Carlo simulations to overcome those barriers, we developed a multi-overlap Monte Carlo algorithm [2] which can be optimally tailored for the sampling of rare-events [3]. Employing this technique we first studied for the three-dimensional (3D) short-range Edwards-Anderson Ising (EAI) $\pm J$ model the scaling behaviour of the barrier heights [4] and the tails of the overlap-parameter distribution [5]. Recently we improved our methodology by combining it with parallel tempering and N-fold way ideas [6]. First tests with the new algorithm indicate [7] that it will enable us to push the studies of the spin-glass phase further towards the physically more interesting low-temperature regime. Currently we are extending our investigations also to the Sherrington-Kirkpatrick (SK) mean-field and random orthogonal models where particular focus is placed on studies of inherent structures and inhomogeneities in dynamical response functions. Since very large computing times of the order of several years are required, we have adapted our computer codes to the special architecture of the recently installed supercomputer JUMP at ZAM/NIC Jülich.

In a second, more analytically oriented subproject we consider the diluted generalized random-energy model (DGREM). This formulation provides an approximation to the ground-state energy of spin glasses whose exact computation belongs to the class of expensive NP problems of combinatoric optimization (the computation time grows exponentially with the size of the system). Besides applications to the 3D EAI model, we developed a generalization to q-state Potts spin glasses whose accuracy was tested against numerically determined ground-state energies for the two-dimensional models with $q = 3$ and 4 [8].

References

[1] K. H. Fischer and J. A. Hertz, *Spin Glasses* (Cambridge University Press, 1991).

[2] B. A. Berg and W. Janke, Phys. Rev. Lett. **80**, 4771 (1998).

[3] W. Janke, in: *Computer Simulations of Surfaces and Interfaces*, NATO Science Series, II. Mathematics, Physics and Chemistry – Vol. **114**, edited by B. Dünweg, D. P. Landau and A. I. Milchev (Kluwer, Dordrecht, 2003), p. 137.

[4] B. A. Berg, A. Billoire and W. Janke, Phys. Rev. B **61**, 12143 (2000); Physica A **321**, 49 (2003).

[5] B. A. Berg, A. Billoire and W. Janke, Phys. Rev. E **65**, 045102(R) (2002); *ibid.* **66**, 046122 (2002).

[6] A. Nußbaumer, E. Bittner and W. Janke, to be published.

[7] A. Nußbaumer, Diploma Thesis, University of Leipzig (2003).

[8] E. Bittner, W. Janke and D. B. Saakian, Phys. Rev. E **67**, 016105 (2003).

0.1.3 Monte Carlo Studies of Diluted Magnets

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The influence of quenched, random disorder on phase transitions has been the subject of exciting experimental, analytical and numerical studies over many years. Generically one expects that under certain conditions quenched disorder modifies the critical behaviour at a second-order transition (Harris criterion) and can soften a first-order transition to become second order (Imry-Wortis effect) [1]. In two dimensions these effects are fairly well understood [2]. In three dimensions (3D), numerical studies have mainly focused on the site-diluted Ising model [3], where good agreement with field theoretical predictions was obtained. For the case of a first-order transition in the pure model, large-scale simulations have only been performed for the 3-state Potts model with site-dilution [4].

In this project we have performed intensive Monte Carlo studies of the 3D Ising and 4-state Potts models with *bond*-dilution. The phase diagrams of the diluted models, starting from the pure model limit down to the neighbourhood of the percolation threshold, were found in very good agreement with the single-bond effective-medium approximation and our parallel high-temperature series expansions for the same models. For the estimation of critical exponents in the Ising case [5,6], we first performed finite-size scaling analyses at three different dilutions to check the stability of the disorder fixed point. We observe strong cross-over effects between the pure, disorder and percolation fixed points, leading to effective critical exponents apparently dependent on the dilution. In addition also the temperature behaviour of physical quantities was studied in order to characterize the disorder fixed point more accurately. This allowed us to determine critical amplitude ratios which are usually more sensitive to the universality class than critical exponents. Moreover, non-self-averaging properties at the disorder fixed point were found in good agreement with approximate analytical predictions. Overall our numerical results provide strong evidence for universality of bond and site dilution in the 3D Ising model. Similar simulations of the 3D bond-diluted 4-state Potts model [7] yield clear evidence for disorder induced softening to a second-order transition above a (tricritical) disorder strength. Here also the role of rare-event contributions was studied in great detail.

References

[1] A. B. Harris, J. Phys. C **7**, 1671 (1974); Y. Imry and M. Wortis, Phys. Rev. B **19**, 3580 (1979).

[2] B. Berche and C. Chatelain, in: *Order, Disorder, and Criticality*, edited by Yu. Holovatch (World Scientific, Singapore, 2004), p. 147 [cond-mat/0207421].

[3] S. Wiseman and E. Domany, Phys. Rev. Lett. **81**, 22 (1998); Phys. Rev. E **58**, 2938 (1998); H. G. Ballesteros, L. A. Fernández, V. Martín-Mayor, A. Muñoz Sudupe, G. Parisi and J. J. Ruiz-Lorenzo, Phys. Rev. B **58**, 2740 (1998).

[4] H. G. Ballesteros, L. A. Fernández, V. Martín-Mayor, A. Muñoz Sudupe, G. Parisi and J. J. Ruiz-Lorenzo, Phys. Rev. B **61**, 3215 (2000).

[5] P.-E. Berche, C. Chatelain, B. Berche and W. Janke, Eur. Phys. J. B **38**, 463 (2004).

[6] B. Berche, P.-E. Berche, C. Chatelain and W. Janke, Condens. Matter Phys. **8**, 47 (2005).

[7] C. Chatelain, B. Berche, W. Janke and P.-E. Berche, cond-mat/0501115.

0.1.4 High-Temperature Series Expansions for Spin Glasses and Disordered Magnets

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Systematic series expansions for statistical models defined on a lattice are a well-known alternative to large-scale numerical simulations for the study of phase transitions and critical phenomena [1]. For quenched disordered systems the extension of this method [2] requires especially adapted graph theoretical and algebraic algorithms. In this project we developed a computer package based on the "star-graph" method [3] which allows the generation of high-temperature series expansions for the free energy and susceptibility. We consider the class of disordered q-state Potts models on d-dimensional hypercubic lattices $\mathbb{Z}^d$ with bimodal probability distributions of quenched couplings parametrized by $P(J_{ij}) = p\delta(J_{ij}-J_0)+(1-p)\delta(J_{ij}-RJ_0)$, which includes spin glasses, diluted ferromagnets, random-bond models and transitions between them. The limiting case $p = 1$ describes the pure ferromagnetic ($J_0 > 0$) models. Even though the method is highly optimized for the problem at hand, it is extremely demanding since the number of contributing graphs grows exponentially with the order of the series and all intermediate calculations have to be performed by means of symbolic computer algebra, which we implemented ourselves in C++ since the available standard software products such as `Mathematica` or `Maple` are too slow and require too much memory.

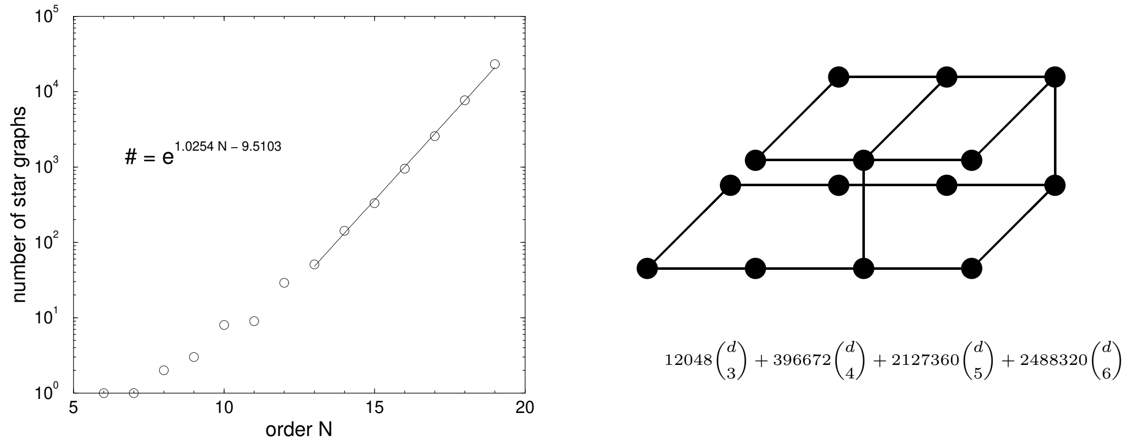

Figure 1: Left: Growth behaviour of the number of star graphs of order N that can be embedded in hypercubic lattices $\mathbb{Z}^d$. Right: A star graph of order 17 and its (weak) embedding number, carrying the dependence on the dimension (up to $d = 6$).

In the analysis we focused up to now mainly on the bond-diluted Ising model ($q = 2$) for which we used our computer package to generate high-temperature series up to order 21 in $d = 3$ dimensions [4,5] and up to order 19 in $d = 4, 5$ [5]. Applying various analysis tools we determined the phase diagrams in the temperature-dilution plane and estimated the critical exponent γ, parametrizing the singularity of the susceptibility at criticality, $\chi \sim (T-T_c)^{-\gamma}$. Depending on the dimension, our results can be compared with field-theoretic predictions and estimates from our Monte Carlo simulations performed in another project. For the 4-state Potts model in $d = 3$ dimensions [6], which in the pure case exhibits a first-order phase transition, we observed the expected softening by quenched disorder and estimated the critical exponent of the induced second-order transition.

Further new results were also obtained for the bond-percolation problem in various dimensions d, which is contained in the general formulation as the $q \to 1$ limit [7].

References

[1] C. Domb and M. S. Green, eds, *Phase Transitions and Critical Phenomena*, Vol. 3 (Academic Press, New York, 1974).

[2] R. R. P. Singh and S. Chakravarty, Phys. Rev. B **36**, 546 (1987).

[3] M. Hellmund and W. Janke, Condens. Matter Phys. **8**, 59 (2005).

[4] M. Hellmund and W. Janke, Comp. Phys. Comm. **147**, 435 (2002).

[5] M. Hellmund and W. Janke, Leipzig preprint (2005), to be published.

[6] M. Hellmund and W. Janke, Nucl Phys. B (Proc. Suppl.) **106/107**, 923 (2002); Phys. Rev. E **67**, 026118 (2003).

[7] M. Hellmund and W. Janke, Leipzig preprint (2005), to be published.

0.1.5 Droplet/Strip and Evaporation/Condensation Transitions

E. Bittner, W. Janke and A. Nußbaumer

The free energy of the three-dimensional Edwards-Anderson Ising spin-glass model exhibits in the low-temperature phase a rugged multi-valley structure. Consequently standard canonical Monte Carlo simulations are severely hampered by an exponential slowing down with increasing system size. This led to the application of multicanonical simulations, e.g. for the overlap parameter, which are designed by means of auxiliary weight factors to smooth out the energy landscape and thus to lead to uniform probability distributions. Given such a flat distribution, a much faster random walk behaviour in the corresponding observable is naively expected. In the actual simulations, however, one still observes jumps in the time series which can be attributed to so-called “hidden barriers”. Building up on early analytical considerations of Leung and Zia [1], in a recent numerical work Neuhaus and Hager [2] were able to identify such barriers in the magnetisation M of the much simpler two-dimensional Ising model. They observed a geometrically induced first-order phase transition from a droplet to a strip domain and showed that even a perfect multimagnetic simulation operating with the optimal weights still needs an exponential time to overcome the associated free energy barrier. To obtain more qualitative insights, we determined directly the anisotropy of a configuration during the transition by measuring its structure function. Simulating different system sizes with Kawasaki dynamics ($M =$ const.), the scaling of the anisotropy leads to a value for the barrier height in good agreement with the theoretical prediction. By generalising these considerations to the case of the three-dimensional Ising model, new transitions could be identified analytically and verified numerically. Also the various crystal shapes emerging during the transition could be visualised.

Another first-order like transition can be identified when the first large droplet forms out of the fluctuations around the equilibrium magnetization. Invoking the equivalent lattice-gas picture, Biskup *et al.* [3] recently studied the behaviour of d-dimensional finite-volume liquid-vapour systems at a fixed excess δN of particles above the ambient gas density. Identifiying a dimensionless parameter $\Delta(\delta N)$ and a universal constant $\Delta_{\rm c}(d)$, they were able to show that for $\Delta < \Delta_c$ a droplet of the dense phase occurs, while for $\Delta > \Delta_c$ the excess is absorbed in the background. The fraction λ_Δ of excess particles forming the droplet is given explicitly. To verify these results, we have simulated the spin-1/2 Ising model on a square lattice at constant magnetisation equivalent to a fixed particle excess. We measured the largest minority droplet, corresponding to the liquid phase, at various system sizes ($L = 40 \dots 640$). Using analytic values for the spontaneous magnetisation m_0, the susceptibility χ and interfacial free energy $\tau_{\rm W}$ for the infinite system, we were able to determine λ_Δ in very good agreement with the theoretical prediction. In order to test the universal aspects of this evaporation/condensation transition, the measurements were repeated for next-nearest neighbour interactions and on a triangular lattice, giving similarly good results.

References

[1] K. Leung and R. Zia, J. Phys. A **23**, 4593 (1990).

[2] T. Neuhaus and J. Hager, Stat. Phys. **113**, 47 (2003).

[3] M. Biskup, L. Chayes and R. Kotecký, Europhys. Lett. **60**, 21 (2002).

0.1.6 Harris-Luck Criterion and Potts Models on Random Graphs

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The Harris criterion judges the relevance of uncorrelated, quenched disorder for altering the universal properties of physical systems close to a continuous phase transition [1]. For this situation, as e.g., in the paradigmatic case of a quenched random-bond or bond diluted model, a change of universal properties is expected for models with a positive specific heat exponent α, i.e., the relevance threshold is given by $\alpha_c = 0$. For the physically more realistic case of spatially correlated disorder degrees of freedom, Harris' scaling argument can be generalised, yielding a shifted relevance threshold $-\infty < \alpha_c \leq 1$ known as Luck criterion [2]. The value of α_c depends on the quality and strength of the spatial disorder correlations as expressed in a so-called geometrical fluctuation or *wandering exponent*.

We consider the effect of a different, topologically defined type of disorder, namely the result of *connectivity disorder* produced by placing spin models on *random graphs*. As it turns out, the Harris-Luck argument can be generalised to this situation, leading to a criterion again involving a suitably defined wandering exponent of the underlying random graph ensemble. Using a carefully tailored series of finite-size scaling analyses, we precisely determine the wandering exponents of the two-dimensional ensembles of Poissonian Voronoï-Delaunay random lattices as well as the quantum gravity graphs of the dynamical triangulations model, thus arriving at explicit predictions for the relevance threshold α_c for these lattices [3]. As a result, for Poissonian Voronoï-Delaunay random graphs the Harris criterion $\alpha_c = 0$ should stay in effect, whereas for the dynamical triangulations the threshold is shifted to a negative value, $\alpha_c \approx -2$. The latter result is in perfect agreement with Monte Carlo simulations of the q-states Potts model [4] as well as an available exact solution of the percolation limit $q \to 1$ [5]. For the Voronoï-Delaunay triangulations, the Ising case $q = 2$ with $\alpha = 0$ is marginal and a change of universal properties cannot normally be expected. The $q = 3$ Potts model with $\alpha = 1/3$, on the other hand, should be shifted to a new universality class. Following up on a first exploratory study for small graphs [6], we performed high-precision cluster-update Monte Carlo simulations for rather large lattices of up to 80 000 triangles to investigate this model. Astonishingly, however, the (exactly known) critical exponents of the square-lattice $q = 3$ Potts model are reproduced to high precision [7]. To clarify this situation, we recently studied a generalised model introducing a distance dependence of the interactions [8].

References

[1] A. B. Harris, J. Phys. C **7**, 1671 (1974).

[2] A. Weinrib and B. I. Halperin, Phys. Rev. B **27**, 413 (1983); J. M. Luck, Europhys. Lett. **24**, 359 (1993).

[3] W. Janke and M. Weigel, Phys. Rev. B **69**, 144208 (2004).

[4] W. Janke and D. A. Johnston, Nucl. Phys. B **578**, 681 (2000).

[5] V. A. Kazakov, Mod. Phys. Lett. A **4**, 1691 (1989).

[6] F. W. S. Lima, U. M. S. Costa, M. P. Almeida and J. S. Andrade, Eur. Phys. J. B **17**, 111 (2000).

[7] W. Janke and M. Weigel, Acta Phys. Polon. B **34**, 4891 (2003).

[8] G. Kähler, Diploma Thesis, University of Leipzig (2004).

0.1.7 The F Model on Quantum Gravity Graphs

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As an alternative to various other approaches towards a theory of quantum gravity, the *dynamical triangulations* method has proved to be a successful discrete Euclidean formulation in two dimensions (2D). There, the integration over all metric tensors as the dynamic variables is performed by a summation over all possible gluings of equilateral triangles to form a closed surface of a given (usually planar) topology. The powerful methods of matrix integrals and generating functions allow for an exact solution of the pure 2D gravity model. Furthermore, matrix models can be formulated for spin models coupled to random graphs and some of them could be solved analytically. More generally, the "dressing" of the weights of $c < 1$ conformal matter coupled to 2D quantum gravity is predicted by the KPZ/DDK formula [1], in agreement with all known exact solutions.

One of the most general models in statistical mechanics is Baxter's 8-vertex model [2]. Thus its behaviour on coupling it to dynamical *quadrangulations*, i.e., surfaces built from simplicial squares, is of general interest. Although a solution of special slices of this model could recently be achieved [3], the general model could not yet be solved. Heading for computer simulations, one first has to ensure the correct handling of the (quite unorthodox) geometry of four-valent graphs or quadrangulations in the dual language. While simulations of three-valent graphs have already been extensively done, the code for ϕ^4 graphs had to be newly developed and tested [4]. Due to the fractal structure of the graphs being described as a self-similar tree of "baby universes", this local dynamics suffers from critical slowing down. To alleviate the situation, we adapted a non-local update algorithm known as "minBU surgery" [5].

Combining the developed techniques, we simulated the F model, a symmetric case of the 8-vertex model, coupled to planar random ϕ^4 graphs. On regular [6] as well as random lattices [7], this model is expected to exhibit a Kosterlitz-Thouless transition to an anti-ferroelectrically ordered state [2,3]. The numerical analysis of this model turned out to be exceptionally difficult due to the combined effect of the highly fractal structure of the graphs and the presence of strong logarithmic corrections. Still, a scaling analysis of the staggered polarizability yields results [7] in agreement with the predictions of Ref. [3] as far as the order of the transition and the location of the transition point are concerned.

References

[1] V. Knizhnik, A. Polyakov and A. Zamolodchikov, Mod. Phys. Lett. A **3**, 819 (1988); F. David, Mod. Phys. Lett. A **3**, 1651 (1988); J. Distler and H. Kawai, Nucl. Phys. B **321**, 509 (1989).

[2] R. Baxter, *Exactly Solved Models in Statistical Mechanics* (Academic Press, London, 1982).

[3] V. A. Kazakov and P. Zinn-Justin, Nucl. Phys. B **546**, 647 (1999); I. Kostov, Nucl. Phys. B **575**, 513 (2000); P. Zinn-Justin, Europhys. Lett. **50**, 15 (2000).

[4] M. Weigel and W. Janke, Nucl. Phys. B (Proc. Suppl.) **106–107**, 986 (2002); M. Weigel, Ph.D. Thesis, University of Leipzig (2002).

[5] J. Ambjørn *et al.*, Phys. Lett. B **325**, 337 (1994).

[6] M. Weigel and W. Janke, cond-mat/0501222, submitted to J. Phys. A.

[7] M. Weigel and W. Janke, hep-lat/0409028, submitted to Nucl. Phys. B.

0.1.8 Crystal Shapes and Sequence Dependence of Polymer and Heteropolymer Ground States

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It has not been clarified yet whether polymers and proteins form crystallline or amorphous global energy minimum conformations. Proteins are generally expected to possess a stable geometric structure which is strongly connected with its biological function, or at least a small number of metastable states being important for dynamical processes (a well-known example is the synthase of ATP). The study of this problem is interesting from different perspectives. First, the kinetics of the folding process through possibly well-defined folding channels in the free-energy landscape will strongly be influenced by the kind of transition towards the ground-state conformation. Second, from a purely pragmatic point of view, many complex analyses of polymer folding can only be performed by considering much simpler lattice models which are widely used for qualitative studies. If there would be, in fact, a relation between ground-state structures and crystal shapes, then lattice model studies could also give selective quantitative answers.

We have applied minimization algorithms to effective, coarse-grained lattice and off-lattice polymer and heteropolymer models in two and three dimensions. For the simple case of a pure Lennard-Jones polymer in two dimensions we could show the expected crystallization on a triangular lattice quite clearly. In three dimensions, the identification of the crystal shape, if any, is much more complicated, since surface effects affect the shape of the lowest-energy conformations more strongly. There are, however, some indications that the core could take face-centered cubic (fcc) or hexagonal closely packed (hcp) structures.

In a separate but related study we have investigated the thermodynamics of conformational transitions of lattice heteropolymers. We analysed short peptides, consisting only of two different types of amino acid classes (hydrophobic and polar), with up to 19 monomers extensively by exactly enumerating all possible sequences and conformations [1–3]. We identified all so-called designing sequences whose ground state is nondegenerate. One of the main results is that the ground-state conformations of heteropolymers with these sequences are not necessarily maximally compact, i.e., the radius of gyration of these structures is not the smallest possible. This is a consequence of the formation of a hydrophobic core, surrounded by a shell of polar monomers. Interestingly, many lattice heteropolymers experience two conformational transitions: the random-coil–globule collapse and the formation of the hydrophobic core. This was confirmed in our simulations of selected, much longer heteropolymers with up to 103 monomers [4], where we applied our recently developed multicanonical chain-growth algorithm [5].

References

[1] R. Schiemann, M. Bachmann and W. Janke, Comp. Phys. Comm. **166**, 8 (2005).

[2] R. Schiemann, M. Bachmann and W. Janke, J. Chem. Phys. **122**, 114705 (2005) [q-bio/0405009].

[3] T. Vogel, Diploma Thesis, University of Leipzig (2004).

[4] M. Bachmann and W. Janke, J. Chem. Phys. **120**, 6779 (2004).

[5] M. Bachmann and W. Janke, Phys. Rev. Lett. **91**, 208105 (2003).

0.1.9 Folding Channels in Coarse-Grained and All-Atom Peptide Models

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Notwithstanding enormous computational capacities, simulations of realistic protein models are still highly nontrivial and, with respect to studies of their folding dynamics, currently impossible. The reason is that the folding of a protein takes milliseconds to seconds, while the time scale of present molecular dynamics simulations is orders of magnitude smaller. As an alternative, Monte Carlo simulations are used to study the kinetics of folding transitions, although the dynamics of Markov chains, Monte Carlo methods are based upon, has no relation to Newtonian equations of motion. Therefore, kinetic studies by means of Monte Carlo methods are restricted to statements on ensemble properties, e.g., conformational phases. But, in fact, conformational transitions, where cooperative rearrangements of monomers happen, *could be* the key to understand folding kinetics even on this statistical level. Since more than a decade it has been known that some (short) proteins with less than 100 residues are two-state folder, i.e., the ensemble is dominated either by random conformations or by conformations which are structurally similar to the folded state. In this case the free energy is directly related with the Kramers rate and therefore, implicitly, with the dynamics of the folding process. Since these systems are too large to be simulated as all-atom models, however, the importance of so-called Gō models has drastically increased in the past years. The "energy" of an arbitrary conformation is determined by its structural deviation from the global energy minimum conformation (which is a priori unknown and enters into the model as experimental input). These models are, however, rather unsatisfying from the physical point of view as no natural forces appear in the model.

We investigate the main aspects of these general problems from different perspectives. One of the projects is the ongoing study of the 13-residue C-peptide of Ribonuclease A which has the nice property to only form an α-helix. Therefore it is a good example for studying two-state folding. We use a generalized-ensemble (multicanonical) method to perform the simulation and to study fluctuations of a helical order parameter to determine the characteristic folding transition and a structural order parameter to reconstruct the folding path. Another focus of our study is the comparison of simple coarse-grained (but physical) heteropolymer models and their Gō analogue. This is done by means of the replica exchange (parallel tempering) Monte Carlo method and molecular dynamics, where we are mostly interested in comparisons of dynamic components of the conformational transitions in these models. It is also important to understand how to modify coarse-grained models in order to make them capable to yield results being quantitatively competitive. Concerning two-state folding, for example, it is interesting to know how bending and torsion of successive covalent bonds influence the folding transition and to what extent these forces are responsible for the occurrence of intermediary states that slow down the folding dynamics [1,2].

References

[1] M. Bachmann and W. Janke, to appear in Comp. Phys. Comm. (in print).

[2] H. Arkın, M. Bachmann and W. Janke, Phys. Rev. E **71**, 031906 (2005).

0.1.10 Substrate Specificity of Peptide Adsorption

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From recent experiments of the adsorption of short peptides at semiconductor substrates it is known that different surface properties (materials such as Si or GaAs, crystal orientation, etc.) as well as different amino acid sequences strongly influence the binding of these peptides at the substrate [1,2]. This specificity will be of essential importance for future sensory devices and pattern recognition at the nanometer scale. The reasons for this binding specificity are far from being clear, and it is a big challenge from the experimental and theoretical point of view to understand the basic principles of substrate–peptide cooperativity. The experimental equipment has reached such a high resolution that it allows a precise identification of single molecule shapes at the substrate, and the available computational capacities and sophisticated algorithms necessary for probing appropriate models will make it possible to come closer to a solution of this problem in the near future.

In order to reduce the complexity of the problem to a minimum, we study a heteropolymer with given sequence of only two types of monomers: hydrophobic (H) and polar (P). Another simplification is the restriction of the conformational space to self-avoiding walks in a cavity. The heteropolymer is modeled by the hydrophobic–polar (HP) model [3], which has become very popular for studies of the sequence and conformational space of lattice heteropolymers [4]. We use the simplest form, where only the hydrophobic force acts and the number of nearest-neighbour contacts between H monomers being nonadjacent along the chain is related to the energy of the heteropolymer. The interaction with the substrate is modeled in a like manner: The energy of the heteropolymer is reduced by the number of next-neighbor contacts between the substrate and those monomers that experience the attractive force of the substrate. For all other monomers the influence of the substrate is only entropic. In order to study the specificity of surface–binding, we investigate three attractive substrate models. In the first variant, all monomers, independent of their hydrophobic or polar character, are equally attracted by the substrate and the energy of the system is proportional to the total number of monomer–surface contacts. In the second and third model, the substrate is either hydrophobic or polar, i.e., only the hydrophobic or polar monomers in the heteropolymer sequence are attracted by the substrate, respectively.

For studying these systems, we have redesigned the multicanonical chain-growth algorithm [5] to sample the space of monomer–substrate and monomer–monomer contacts within a single simulation. This contact density method has already proven to be very efficient for a nongrafted homopolymer in solution near an adsorbing surface [6].

References

[1] S. R. Whaley, D. S. English, E. L. Hu, P. F. Barbara and A. M. Belcher, Nature **405**, 665 (2000).

[2] K. Goede, P. Busch and M. Grundmann, Nano Lett. **4**, 2115 (2004).

[3] K. F. Lau and K. A. Dill, Macromolecules **22**, 3986 (1989).

[4] R. Schiemann, M. Bachmann and W. Janke, J. Chem. Phys. **122**, 114705 (2005).

[5] M. Bachmann and W. Janke, Phys. Rev. Lett. **91**, 208105 (2003).

[6] M. Bachmann and W. Janke, cond-mat/0502138, submitted to Phys. Rev. Lett.

0.1.11 End-To-End Distribution of Stiff Polymers

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In this project we consider so-called Porod-Kratky wormlike chains which model stiff polymers [1]. By mapping the statistical physics problem onto an equivalent path-integral representation of quantum mechanics, it is possible to derive via the associated Schrödinger equation recursion relations for all even moments of the end-to-end distribution function [2]. By means of the algebraic computer software `Mathematica` these equations have been solved exactly to very high order in two and three dimensions.

The knowledge of these moments allows a very precise parametrization of the distribution function with uniform accuracy for all persistence lengths ξ of the polymer. This is a great advantage over earlier methods which could only be applied in limiting cases. We tested the accuracy of our analytical parametrization method by comparing it with extensive Monte Carlo simulations, see Fig. 2. With both methods we observed the interesting dip structure at intermediate values of the persistence length if one plots the radial distribution density for the two-dimensional system. Analogous analyses of the three-dimensional system are still in progress.

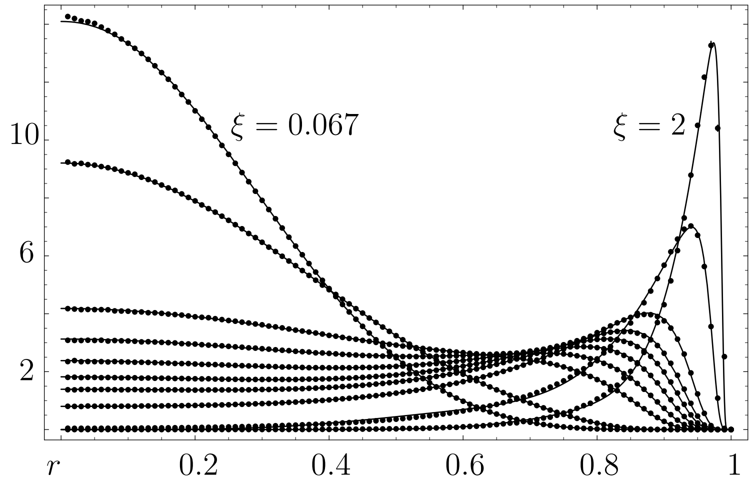

Figure 2: Comparison of analytical results (lines) and Monte Carlo data (dots) for the radial end-to-end distribution density of two-dimensional stiff polymers with persistence length ξ.

References

[1] H. Yamakawa, *Modern Theory of Polymer Solution* (Harper and Row, New York, 1971); *Helical Wormlike Chains in Polymer Solution* (Springer, Berlin, 1997).

[2] B. Hamprecht and H. Kleinert, cond-mat/0305226.

[3] B. Hamprecht, W. Janke and H. Kleinert, Phys. Lett. A **330**, 254 (2004).

0.1.12 Geometrical Approach to Phase Transitions

W. Janke and A. M. J. Schakel

This project aims at a geometrical description for a variety of phase transitions, ranging from thermal transitions in spin models over Bose-Einstein condensation in dilute gases to the deconfinement transition in gauge theories. Since many exact results are known in two dimensions, 2D models form the main focus of the present research. Using Monte Carlo simulations, the fractal structure of the spin configurations of the 2D Ising model was investigated [1], whose thermal critical behaviour can be equivalently described as percolation of suitably defined clusters of spins. The fractal dimension of these so-called Fortuin-Kasteleyn clusters, which encode the entire critical behaviour, and that of their boundaries have been determined numerically by applying standard finite-size scaling to observables such as the percolation probability and the average cluster size. The obtained results are in excellent agreement with theoretical predictions and partly provide significant improvements in precision over existing numerical estimates [2].

Also the naive "geometrical" spin clusters encode critical behaviour, namely that of the diluted model. Within this project, recently a one-to-one map between the two cluster types could be established. By numerically determining the fractal structure of the geometrical clusters and that of their boundaries, this map was verified to high precision [1]. Based on numerical results on the high-temperature representation of the 2D Ising model [3], a generalization of the famous de Gennes result, that connects the critical behaviour of the O(N) model in the limit $N \to 0$ to the configurational entropy of a polymer chain in a good solvent, to arbitrary $-2 \leq N \leq 2$ was given [4]. The high-temperature representation can be visualized by graphs on the lattice. In the high-temperature phase, where they have a finite line tension, large graphs are exponentially suppressed. Upon approaching the critical temperature, the line tension vanishes and the graphs proliferate. Their fractal structure was shown to encode the entire critical behaviour, so that a purely geometrical description of the phase transition in the O(N) model was obtained.

When including vacancies, it is generally believed that the O(N) model gives in addition to critical behaviour rise to also tricritical behaviour. By gradually increasing the activity of the vacancies, the continuous O(N) phase transition is eventually driven first order at a tricritical point. In the context of polymers ($N \to 0$), the latter obtains by lowering the temperature to the so-called Θ point where the increasingly important van der Waals attraction between monomers causes the polymer chain to collapse. Up to now, relatively little is known about the tricritical behaviour for $N \neq 0$. By arguing that the fractal dimensions of the high-temperature graphs close to the tricritical point are in one-to-one correspondence with those at the critical point, exact, albeit non-rigorous, predictions could be made for the tricritical exponent η and, through scaling relations, for the ratios β/ν and γ/ν [4].

References

[1] W. Janke and A. M. J. Schakel, Nucl. Phys. B [FS] **700**, 385 (2004).

[2] J. Asikainen, A. Aharony, B. B. Mandelbrot, E. M. Rauch and J.-P. Hovi, Eur. Phys. J. B **34**, 479 (2003); S. Fortunato, Phys. Rev. B **66**, 054107 (2002).

[3] W. Janke and A. M. J. Schakel, Phys. Rev. E **71**, 036703 (2005).

[4] W. Janke and A. M. J. Schakel, cond-mat/0502062, submitted to Phys. Rev. Lett.

0.1.13 Vortex-Line Percolation in a Three-Dimensional Complex Ginzburg-Landau Model

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The superfluid phase transition can be described either by a directional XY model or by an O(2) symmetric scalar field theory, whose Hamiltonian is commonly expressed with a complex field $\psi(\vec{r}) = |\psi(\vec{r})|e^{i\phi(\vec{r})}$ in the Ginzburg-Landau form. Therefore the model can also be represented by the partition function of an equivalent theory in which the spin configurations are replaced by configurations of closed lines. The loops of this equivalent theory can be identified with the vortex lines of the original theory, therefore they might play an important role in determining the properties of the phase transition. A seemingly natural approach to study the vortex degrees of freedom is to associate with every spin configuration generated in a lattice Monte Carlo simulation a number of vortex loops. The hope is then that the transition could be identified with a non-zero probability of finding vortex loops that extend through the whole system [1], a phenomenon which is usually called percolation.

Percolational studies of spin clusters in the Ising model showed that one has to handle this approach carefully. It only works, if one uses a proper stochastic definition of clusters [2–5]. The Fortuin-Kasteleyn (FK) clusters of spins can be obtained from the geometrical spin clusters, which consist of nearest neighbor sites with their spin variables in the same state, by laying bonds with a certain probability between the nearest neighbors. The resulting FK clusters are in general smaller than the geometrical ones and also more loosely connected. For the different cluster types one may find different percolation thresholds and critical exponents.

The work of this project concentrates on the three-dimensional complex Ginzburg-Landau model, which belongs to the O(2) universality class. Two experimentally important cases are studied: The pure complex Ginzburg-Landau model [6–8], relevant for the universal properties of the λ-transition in liquid helium, and its extension with a minimal coupling to an external compact U(1) gauge field (Abelian Higgs model) [9,10], relevant for the universal aspects of superconductors and also for elementary particle physics and cosmology. In the latter case, a first-order phase transition line ending at a critical point was found in the Higgs coupling – "hopping parameter" ($\lambda - \kappa$) plane for small λ at a fixed gauge coupling (β) which, similar to the liquid-gas phase diagram, separates the Higgs and "confinement" phase. Based on our data for the magnetic monopole density and other quantities we present arguments that this phase boundary continues for larger λ as a so-called Kertész line [10], across which no phase transition in a strict thermodynamic sense takes place, but percolation observables do exhibit singular behaviour. This picture is completely analogous to the scenario proposed by Kertész for the liquid-gas phase diagram.

In three-dimensional, globally O(2) symmetric theories the percolating objects are vortex lines forming closed networks. One of the main questions we want to address is: Is there a similar clue in the case of vortex networks as for spin clusters, or do they display different features? Therefore we connect the obtained vortex-line elements to closed loops, which are geometrically defined objects. When a branching point, where $n \geq 2$ junctions are encountered, is reached, a decision on how to continue has to be made. This step

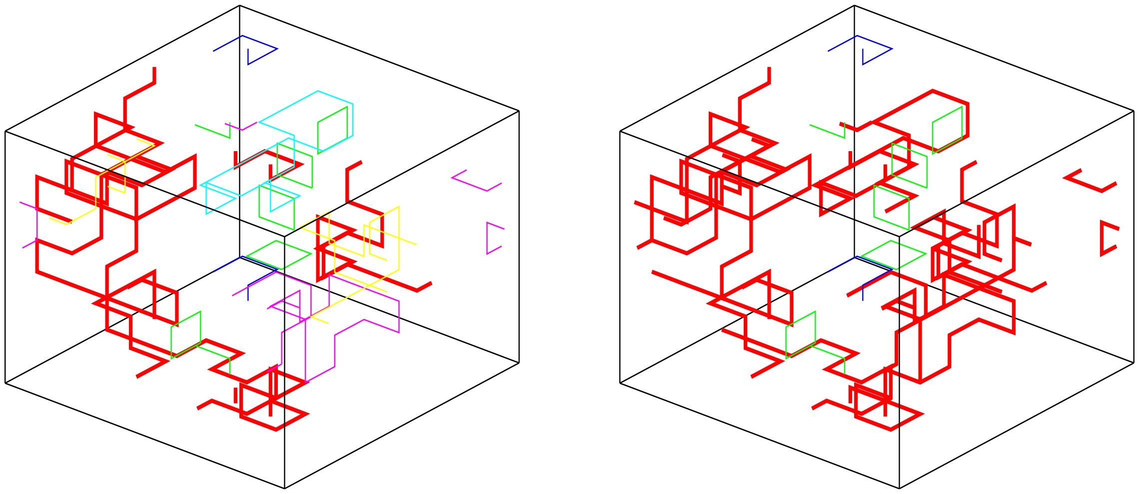

Figure 3: Left: Vortex-loop network generated at the thermodynamic critical point for lattice size $L = 8$ and probability $c = 0.4$ to treat a branching point as a knot. Right: Vortex-loop network generated treating *all* branching points as knots for the same spin configuration as in the left plot.

involves a certain ambiguity. We want to investigate the influence of the probability of treating such a branching point as a knot, see Fig. 3.

In discussing the phase transition of the Ginzburg-Landau theory, we study a geometrically defined vortex-loop network as well as the magnetic properties of the system in the vicinity of the critical point. Using high-precision Monte Carlo techniques we consider an alternative formulation of the geometrical excitations in relation to the global O(2) symmetry breaking, and check if both of them exhibit the same critical behaviour leading to the same critical exponents and therefore to a consistent description of the phase transition. Different percolation observables are taken into account and compared with each other.

References

[1] K. Kajantie, M. Laine, T. Neuhaus, A. Rajanie and K. Rummukainen, Phys. Lett. B **482**, 114 (2000).

[2] P. W. Kasteleyn and C. M. Fortuin, J. Phys. Soc. of Japan **26** (Suppl.), 11 (1969); C. M. Fortuin and P. W. Kasteleyn, Physica **57**, 536 (1972); C. M. Fortuin, Physica **58**, 393 (1972), *ibid.* **59**, 545 (1972).

[3] A. Coniglio and W. Klein, J. Phys. A **13**, 2775 (1980).

[4] S. Fortunato, J. Phys. A **36**, 4269 (2003).

[5] W. Janke and A. M. J. Schakel, Nucl. Phys. B **700**, 385 (2004).

[6] A. Krinner, Diploma Thesis, University of Leipzig (2004).

[7] E. Bittner and W. Janke, Phys. Rev. B **71**, 024512 (2005).

[8] E. Bittner, A. Krinner and W. Janke, Leipzig preprint (2005), to be published.

[9] S. Wenzel, Master Thesis, University of Leipzig (2003).

[10] S. Wenzel, E. Bittner, W. Janke, A. M. J. Schakel and A. Schiller, cond-mat/0503599, submitted to Phys. Rev. Lett.

0.1.14 Information Geometry and Phase Transitions

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Motivated by ideas in parametric statistics [1], various authors have recently discussed the advantages of taking a geometrical perspective on statistical mechanics [2]. The "distance" between two probability distributions in parametric statistics can be measured using a geodesic distance which is calculated from the Fisher information matrix for the system. To this end the manifold $\mathcal{M}$ of parameters is endowed with a natural Riemannian metric, the Fisher-Rao metric [1]. For the example of a spin model in a magnetic field h, $\mathcal{M}$ is a two-dimensional manifold parametrised by $(\theta^1, \theta^2) = (\beta, h)$, where $\beta = 1/k_B T$ is the inverse temperature. The components of the Fisher-Rao metric take the simple form $G_{ij} = \partial_i \partial_j f$ in this case, where f is the reduced free energy per site and $\partial_i = \partial/\partial\theta^i$. A natural object to consider in any geometrical approach is the scalar or Gaussian curvature $\mathcal{R}$ which in various two-parameter calculable models has been found to diverge at the phase transition point β_c according to the scaling relation $\mathcal{R} \sim |\beta - \beta_c|^{\alpha-2}$, where α is the usual specific heat critical exponent. For spin models the necessity of calculating in non-zero field has limited analytic consideration to 1D, mean-field and Bethe lattice Ising models [3].

In this project we used the exact solution in field of the Ising model on an ensemble of fluctuating planar random graphs (where $\alpha = -1,\ \beta = 1/2,\ \gamma = 2$) [4] to evaluate the scaling behaviour of the scalar curvature explicitly, and find $\mathcal{R} \sim |\beta - \beta_c|^{-2}$ [5]. The apparent discrepancy with the general scaling postulate is traced back to the effect of a *negative* α [5]. As anticipated, the same effect is found in exact calculations for the *three*-dimensional spherical model [6,7], which was solved (in field) in the classic Berlin and Kac paper [8] and shares the same critical exponents as the Ising model on *two*-dimensional planar random graphs. We mainly concentrated on the 3D case, but also discussed other dimensions [6,7], in particular the mean-field like behaviour which sets in at $D = 4$. Similar considerations have been used to explain a possible critical behaviour in families of solutions for black holes which we also briefly discuss [7].

References

[1] R. A. Fisher, Phil. Trans. R. Soc. Lond., Ser. A **222**, 309 (1922); C. R. Rao, Bull. Calcutta Math. Soc. **37**, 81 (1945).

[2] G. Ruppeiner, Rev. Mod. Phys. **67**, 605 (1995); D. Brody and N. Rivier, Phys. Rev. E **51**, 1006 (1995); D. Brody and L. Hughston, Proc. Roy. Soc. London A **455**, 1683 (1999).

[3] B. P. Dolan, D. A. Johnston and R. Kenna, J. Phys. A **35**, 9025 (2002).

[4] D. V. Boulatov and V. A. Kazakov, Phys. Lett. B **186**, 379 (1987).

[5] W. Janke, D. A. Johnston and R. P. K. C. Malmini, Phys. Rev. E **66**, 056119 (2002).

[6] W. Janke, D. A. Johnston and R. Kenna, Phys. Rev. E **67**, 046106 (2003); Physica **A336**, 181 (2004).

[7] D. A. Johnston, W. Janke and R. Kenna, Acta Physica Polonica B **34**, 4923 (2003).

[8] T. Berlin and M. Kac, Phys. Rev. **86**, 821 (1952).

0.1.15 Ageing Phenomena in Ferromagnets

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When a ferromagnet is suddenly quenched from the disordered into the ordered phase at a temperature below the Curie point, its temporal relaxation exhibits ageing phenomena similar to the behaviour of glasses and spin glasses. For ferromagnets this effect could recently be described in quite some detail with the help of dynamical symmetry arguments [1]. While the assumptions underlying these theoretical considerations are very plausible, their validity is not proven and it is hence important to test the predictions by means of alternative methods such as Monte Carlo simulations. Recent studies of the Ising model in two and three dimensions showed indeed good agreement [2]. Still, to ensure the general applicability of the theoretical framework, typical representative models of other universality classes should be investigated. In this project we therefore perform a Monte Carlo study of the two-dimensional 3-state Potts model and determine two-time correlators as well as the thermoremanent response function. In order to achieve the necessary accuracy, one has to prepare many independent random start configurations and monitors for each copy its stochastic time evolution after the quench into the low-temperature phase. The final results are obtained by averaging over the copies. Also for this model our preliminary results [3] show good agreement with the analytical predictions.

Quite similar phenomena can be observed in the so-called gonihedric lattice spin model which was orginally constructed as a discretized string (or, equivalently, self-avoiding surface) model [4]. Generically it consists of nearest-neighbour, next-nearest neighbour and plaquette interactions with fine-tuned coupling constants. In its original formulation the spins are taken to be of Ising type, i.e., $s = \pm 1$. It was soon recognized that this type of model exhibits a very intricate temporal relaxation behaviour in Monte Carlo simulations reminiscent of ageing phenomena in structural glasses. The analogy is, in fact, closer to (off-lattice) structural than to (lattice) spin glasses since *no* quenched disorder is involved in gonihedric models. The gonihedric model is hence a rare example for lattice models *without* quenched disorder that display ageing phenomena, and from this point of view it has attracted considerable interest also in the statistical physics community. After reproducing the quite intricate relaxation behaviour for the Ising case [5] and refining some of the measurement prescriptions with further input from our experiences with the properties of glasses and spin glasses, we also performed first exploratory computer experiments with suitable generalizations to Potts and $O(n)$ symmetric spin models with $n \geq 2$, in particular the O(2) or XY model [6].

References

[1] M. Henkel, Nucl. Phys. B **641**, 405 (2002).

[2] M. Henkel and M. Pleimling, Phys. Rev. E **68**, 065101(R) (2003); M. Henkel, A. Picone and M. Pleimling, Europhys. Lett. **68**, 191 (2004).

[3] E. Lorenz, Diploma Thesis, University of Leipzig (in preparation).

[4] G. K. Savvidy and K. G. Savvidy, Phys. Lett. B **337**, 333 (1994).

[5] P. Dimopoulos, D. Espriu, E. Jané and A. Prats, Phys. Rev. E **66**, 056112 (2002).

[6] R. Megaides, Master Thesis, University of Leipzig (2004).

0.1.16 Critical Amplitude Ratios in the Baxter-Wu Model

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At a second-order phase transition not only critical exponents but also certain amplitude ratios are universal, i.e., do not depend on the details of the considered statistical system. A typical example is provided by the scaling relation for the magnetic suceptibility χ which in the vicinity of the critical temperature T_c behaves according to $\chi \sim \Gamma_{\pm}|T/T_c - 1|^{-\gamma}$, where γ is a critical exponent and Γ_+ and Γ_- denote the critical amplitudes in the high- and low-temperature phase, respectively. The ratio Γ_+/Γ_- is then such a universal amplitude ratio, whose value could recently be predicted analytically for the two-dimensional q-state Potts model with $q = 2$, 3 and 4 states [1,2]. While for $q = 2$ and 3 this prediction could subsequently be confirmed with numerical techniques (Monte Carlo simulations and high-temperature series expansions) [3], the situation for $q = 4$ remained controversial. The resason for the disagreement lies probably in relatively strong logarithmic corrections of the leading scaling behaviour [4]. In order to test this conjecture, we considered the two-dimensional Baxter-Wu model [5] (a model with three-spin interaction on a triangular lattice) which is known from its exact solution to belong to the $q = 4$ universality class, but does *not* exhibit logarithmic corrections. By employing a special cluster-update algorithm [6] we have performed extensive Monte Carlo simulations of this model which are currently analysed.

References

[1] G. Delfino and J. L. Cardy, Nucl. Phys. B [FS] **519**, 551 (1998).

[2] G. Delfino, G. T. Barkema and J. L. Cardy, Nucl. Phys. B **565**, 521 (2000).

[3] L. N. Shchur, P. Butera and B. Berche, Nucl. Phys. B **620**, 579 (2002).

[4] J. Salas and A. D. Sokal, J. Stat. Phys. **88**, 567 (1997).

[5] R. J. Baxter and F. Y. Wu, Phys. Rev. Lett. **31**, 1294 (1973); Aust. J. Phys. **27**, 357 (1974).

[6] M. A. Novotny and H. G. Evertz, in: *Computer Simulation Studies in Condensed Matter Physics*, Vol. VI, edited by D. P. Landau, K. K. Mon and H.-B. Schüttler (Springer, Berlin, 1993), p. 188.

0.1.17 Quantum Monte Carlo Studies of Spin-Wave Superconductivity

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The Valence Bond Solid picture of spin-wave superconductivity developed following Haldane's conjecture [1] gives a precise framework for determining the critical properties of a variety of quasi-one dimensional ferromagnetic spin applications exploiting low-temperature superconductivity phenomena currently being fabricated for use in the computing and recording industries. We investigate valence bond state quantum phase transitions by means of the continuous time Quantum Monte Carlo loop cluster algorithm [2]. The algorithm has allowed for numerical investigation in regimes previously limited by algorithmic development, and also of the analytic conjecture itself (recently generalised for our inhomogeneous-spin cases of interest [3]) with now indications of novel quantum interference effects [4]. The proposal of Haldane was essentially for single-spin chains but the numerical testing of the ideas has subsequently pushed forward the boundaries of potential quantum interference solutions [5,6]. Making for a closing mapping into experimental systems through the inclusion of higher spin representations and off-diagonal Hamiltonian contributions such as spin-ladder models, treatable via numerical study [7].

Specifically, we are determining the critical exponents that govern the scaling of numerical results to allow both for a closer experimental mapping and to further investigate the range of applicability of the central algorithmic technique [8]. An investigation of the short-time dynamics exponents of this method further establishes the credibility of this approach for the novel states we would intend to investigate [9,10]. Providing also a means to further develop both improved estimators for the superconducting gap states by means of new cross-correlated statistical measures, and to also gain a deeper understanding of the effect of applying and removing magnetic fields to these systems and magnetic impurities.

References

[1] F. D. M. Haldane, Phys. Rev. Lett. **61**, 8 (1988).

[2] B. B. Beard and U.-J. Wiese, Phys. Rev. Lett. **77**, 5130 (1996).

[3] K. Takano, Phys. Rev. B **61**, 13 (2000).

[4] P. Zhang, Z. X. Xu, H. P. Ying and J. H. Dai, to appear in Mod. Phys. Lett. A (2005).

[5] Z. Xu, J. Dai, H. Ying and B. Zheng, Phys. Rev. B **67**, 214426 (2003).

[6] P. R. Crompton, W. Janke, Z. X. Xu and H. P. Ying, Nucl. Phys. B (Proc. Suppl.) **140**, 817 (2005).

[7] S. Todo, M. Matsumoto, C. Yasuda and H. Takayama, Phys. Rev. B **64**, 224412 (2001); M. Nakamura and S. Todo, Phys. Rev. Lett. **89**, 077204 (2002).

[8] R. Bischof, P. R. Crompton and W. Janke, Leipzig preprint (in preparation).

[9] W. Janke and R. Villanova, Phys. Rev. B **66**, 134208 (2002).

[10] H. P. Ying and K. Harada, Phys. Rev. E **62**, 1 (2000).

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W. Janke
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M. Bachmann and W. Janke
NIC Jülich (computer time grant for "JUMP")
Grant No. hlz11

0.1.19 Organizational Duties

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Permanent Member of International Advisory Board, *Conference of the Middle European Cooperation in Statistical Physics (MECO)*

Member of Advisory Committee, *TIRLAT05 – 15. Workshop on Lattice Field Theory*, Tirana, Albania (2005)

Referee: Physical Review Letters, Physical Review B, Physical Review E, Europhysics Letters, Physics Letters A, Physics Letters B, The European Physical Journal B, Physica A, Journal of Physics A, Computer Physics Communications, JSTAT, New Journal of Physics

0.1.20 External Cooperations

Academic

EU-Network "EUROGRID" – *Discrete Random Geometries: From Solid State Physics to Quantum Gravity* with 11 teams throughout Europe

GIF-Network *Statistical Physics of Random Structures with Applications to Life and Material Sciences* with Joan Adler (Technion, Haifa), Amnon Aharony (Tel Aviv Univ.), Eytan Domany (Weizmann Inst., Rehovot), Kurt Binder (Mainz), Peter Grassberger (Jülich and Wuppertal), Thomas Nattermann (Köln) and Dietrich Stauffer (Köln)

Dept. of Physics, Florida State University, Tallahassee, USA
Prof. Dr. Bernd A. Berg

CEA/Saclay, Service de Physique Théorique, France
Dr. Alain Billoire

Laboratoire de Physique des Matériaux (UMR CNRS No 7556), Université Henri Poincaré, Nancy, France
Prof. Dr. Bertrand Berche, Dr. Christophe Chatelain

Groupe de Physique des Matériaux (UMR CNRS No 6634), Université de Rouen, France
Dr. Pierre-Emmanuel Berche

School of Mathematical and Computer Sciences, Heriot-Watt University, Edinburgh, Scotland
Prof. Dr. Desmond A. Johnston

School of Mathematical and Information Sciences, Coventry University, England
Dr. Ralph Kenna

Dept. of Physics, Hacettepe University, Ankara, Turkey
Dr. Handan Arkın

Complex Systems Division, Department of Theoretical Physics, Lund University, Lund, Sweden
Prof. Dr. Anders Irbäck

NIC, Forschungszentrum Jülich
Prof. Dr. Peter Grassberger, Dr. Hsiao-Ping Hsu

Atominstitut, TU Wien, Austria
Prof. Dr. Harald Markum, Dr. Rainer Pullirsch

Dept. of Physics, University of Wales Swansea, Swansea, Wales
Dr. Simon Hands

Service de Physique Théorique, CEA/DSM/SPhT Saclay, France
Dr. Gernot Akemann

Inst. für Theoretische Physik, FU Berlin
Prof. Dr. Bodo Hamprecht, Prof. Dr. Hagen Kleinert

IAC-1, Universität Stuttgart
Priv.-Doz. Dr. Rudolf Hilfer

Inst. für Theoretische Physik, Universität Bielefeld
Priv.-Doz. Dr. Thomas Neuhaus

Institute of Physics, Jagellonian University, Kraków, Poland
Prof. Dr. Zdzisław Burda

Landau Institute for Theoretical Physics, Chernogolovka, Russia
Prof. Dr. Lev N. Shchur

Yerevan Physics Institute, Yerevan, Armenia
Prof. Dr. David B. Saakian

University of Sri Jayewardenepura, Sri Lanka
Dr. Ranasinghe P. K. C. Malmini

Department of Physics, Sri Venkateswara College, University of Delhi, New Delhi, India
Dr. Bibudhananda Biswal

Department of Mechanical Engineering and Intelligent Systems, Tokyo University of Electro-communications, Chofu, Tokyo, Japan
Prof. Dr. Hans-Georg Mattutis

Zhejiang Institute of Modern Physics, Zhejiang University, Hangzhou, P.R. China
Prof. Dr. He-Ping Ying, Prof. Dr. Bo Zheng

Industry

0.1.21 Publications

Journals

Bachmann, M.; Janke, W.
Thermodynamics of Lattice Heteropolymers
J. Chem. Phys. **120** (2004) 6779–6791

Berche, P.-E.; Chatelain, C.; Berche, B.; Janke, W.
Bond Dilution in the 3D Ising Model: A Monte Carlo Study
Eur. Phys. J. **B38** (2004) 463–474

Bittner, E.; Hands, S.; Markum, H.; Pullirsch, R.
Quantum Chaos in Supersymmetric QCD at Finite Density
Proceedings of the Workshop on *Finite Density QCD*, Nara, Japan, July 10–12, 2003, Prog. Theor. Phys. Suppl. **153** (2004) 295–300

Blythe, R.A.; Janke, W.; Johnston, D.A.; Kenna, R.
The Grand-Canonical Asymmetric Exclusion Process and the One-Transit Walk
J. Stat. Mech.: Theor. Exp. (2004) P06001-1–10

Blythe, R.A.; Janke, W.; Johnston, D.A.; Kenna, R.
Dyck Paths, Motzkin Paths and Traffic Jams
J. Stat. Mech.: Theor. Exp. (2004) P10007-1–22

Hamprecht, B.; Janke, W.; Kleinert, H.
End-to-End Distribution Function of Two-Dimensional Stiff Polymers for all Persistence Lengths
Phys. Lett. **A330** (2004) 254–259

Janke, W.; Berche, P.-E.; Chatelain, C.; Berche, B.
Quenched Disorder Distributions in Three-Dimensional Diluted Ferromagnets
In: Landau, D.P.; Lewis, S.P.; Schüttler, H.-B. (Eds.): *Computer Simulation Studies in Condensed-Matter Physics XVI*
Berlin, Springer, 2004; pp. 89–94

Janke, W.; Johnston, D.A.; Kenna, R.
Phase Transition Strength through Densities of General Distributions of Zeroes
Nucl. Phys. **B682** (2004) 618–634

Janke, W.; Johnston, D.A.; Kenna, R.
Information Geometry and Phase Transitions
Physica **A336** (2004) 181–186

Janke, W.; Schakel, A.M.J.
Geometrical vs. Fortuin-Kasteleyn Clusters in the Two-Dimensional q-State Potts Model
Nucl. Phys. **B700** (2004) 385–406

Janke, W.; Weigel, M.
The Harris-Luck Criterion for Random Lattices
Phys. Rev. **B69** (2004) 144208-1–12

Janke, W.; Weigel, M.
Monte Carlo Studies of Connectivity Disorder
In: Wagner, S.; Hanke, W.; Bode, A.; Durst, F. (Eds.): *High Performance Computing in Science and Engineering, Munich 2004*, transactions of the *Second Joint HLRB and KONWIHR Result and Reviewing Workshop*
Berlin, Springer, 2004; pp. 363–374

Journals January–March 2005

Akemann, G; Bittner E.; Lombardo, M.-P.; Markum, H.; Pullirsch R.
Density Profiles of Small Dirac Operator Eigenvalues for Two Color QCD at Nonzero Chemical Potential Compared to Matrix Models
Nucl. Phys. **B** (Proc. Suppl.) **140** (2005) 568–570

Bittner, E.; Janke, W.
Nature of Phase Transitions in a Generalized Complex $|\psi|^4$ Model
Phys. Rev. **B71** (2005) 024512-1–11

Crompton, P.R.; Janke, W.; Xu, Z.X.; Ying, H.P.
Finite-Size Scaling, Fisher Zeroes and N=4 Super Yang-Mills
Nucl. Phys. **B** (Proc. Suppl.) **140** (2005) 817–819

Schiemann, R.; Bachmann, M.; Janke, W.
Exact Enumeration for Three-Dimensional Lattice Proteins
Comp. Phys. Comm. **166** (2005) 8–16

Bachmann, M.; Arkın, H.; Janke, W.
Multicanonical Study of Coarse-Grained Off-Lattice Models for Protein Folding
Phys. Rev. **E71** (2005) 031906-1–11

Berche, B.; Berche, P.-E.; Chatelain, C.; Janke, W.
Random Ising Model in Three Dimensions: Theory, Experiment and Simulation – a Difficult Coexistence
Condens. Matter Phys. **8** (2005) 47–58

Hellmund, M.; Janke, W.
High-temperature Series Expansions for Random Potts Models
Condens. Matter Phys. **8** (2005) 59–74

Janke, W.; Schakel, A.M.J.
Fractal Structure of Spin Clusters and Domain Walls in 2D Ising Model
Phys. Rev. **E71** (2005) 036703-1–8

Schiemann, R.; Bachmann, M.; Janke, W.
Exact Sequence Analysis for Three-Dimensional HP Lattice Proteins
J. Chem. Phys. **122** (2005) 114705-1–10

In press

Bachmann, M.; Janke, W.
Conformational Transitions of Heteropolymers
Leipzig preprint (August 2004), to appear in Proceedings *CCP2004*, Genoa, Italy, 1 – 4 September, 2004 (in press)

Hilfer, R.; Biswal, B.; Mattutis, H.-G.; Janke, W.
Multicanonical Simulations of the Tails of the Order-Parameter Distribution of the 2D Ising Model
Stuttgart/New Delhi/Tokyo/Leipzig preprint (August 2004), e-print cond-mat/0502408, to appear in Proceedings *CCP2004*, Genoa, Italy, 1 – 4 September, 2004 (in press)

Janke, W.; Johnston, D.A.; Kenna, R.
Phase Transition Strength from General Distributions of Zeroes
Leipzig/Edinburgh/Coventry preprint (August 2004), to appear in Proceedings *CCP2004*, Genoa, Italy, 1 – 4 September, 2004 (in press)

Janke, W.; Schakel, A.M.J.
Geometrical Phase Transitions
Leipzig preprint (August 2004), e-print cond-mat/0409267, to appear in Proceedings *CCP2004*, Genoa, Italy, 1 – 4 September, 2004 (in press)

0.1.22 Talks and Posters

Michael Bachmann

Statistical Properties of Off-Lattice Heteropolymers
(with Janke, W.; Arkın, H.) Winter School on Computational Soft Matter, Bonn, February 29 – March 6 (P)

Thermodynamics of Off-Lattice Heteropolymers
DPG-Frühjahrstagung Regensburg, March 8–12 (T)

Off-Lattice Heteropolymers
Seminar on Complex Systems, John von Neumann Institut für Computing (NIC), Forschungszentrum Jülich, March 16–20 (T)

Multicanonical Study of Effective Off-Lattice Models for Heteropolymers
(with Janke, W.; Arkın, H.) 29th Conference of the Middle European Cooperation in Statistical Physics (MECO29), Bratislava, Slovakia, March 28 – April 1 (P)

Thermodynamics of Heteropolymers
Statistical Physics Workshop, Technische Universität Wien, Austria, April 1–3 (T)

Conformational Transitions of Heteropolymers
Theorie-Seminar, Hahn-Meitner-Institut, Berlin, April 29 (T)

Thermodynamics of Simple Heteropolymer Models
Theorie-Seminar, Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Golm, May 10 (T)

Statistical Properties of Off-Lattice Heteropolymers
(with Janke, W.; Arkın, H.) 3rd Day of Biotechnology, Leipzig, May 19 (P)

Conformational Transitions of Lattice Heteropolymers
14th Workshop on Lattice Field Theory (LEILAT04), Leipzig, June 3–5 (T)

Conformational Transitions of Heteropolymers
Conference on Computational Physics (CCP04), Genoa, Italy, September 1–4 (T)

Multicanonical Simulations of Heteropolymers
(with Janke, W.; Arkın, H.) Conference on Computational Physics (CCP04), Genoa, Italy, September 1–4 (P)

Elmar Bittner

Phase Diagram of the Generalized Complex $|\psi|^4$ Model
DPG-Frühjahrstagung, Arbeitskreis Festkörperphysik, Universität Regensburg, March 8–12 (T)

Phase Diagram of the Generalized Ginzburg-Landau Model
(with Janke, W.) 4th EUROGRID Conference on Random Geometry: Theory and Applications, Les Houches, France, March 22–26 (T)

Generalized Complex $|\psi|^4$ Model in Two and Three Dimensions
(with Janke, W.) 29th Conference of the Middle European Cooperation in Statistical Physics (MECO29), Bratislava, Slovakia, March 28–April 1 (P)

Phase Diagram of a Generalized $|\psi|^4$ Model in Two and Three Dimensions
14th Workshop on Lattice Field Theory (LEILAT04), Leipzig, June 3–5 (T)

Vortex Line Percolation in a Complex ψ^4 Model
(with Krinner, A.; Janke, W.) Conference on Computational Physics (CCP04), Genoa, Italy, September 1–4 (P)

Leszek Bogacz

Dirac Operator Coupled to 2D Lorentzian Quantum Gravity
4th EUROGRID Conference on Random Geometry: Theory and Applications, Les Houches, France, March 22–26 (P)

Peter Crompton

Quantum Phase Transitions and the Nonlinear Sigma Model
14th Workshop on Lattice Field Theory (LEILAT04), Leipzig, June 3–5 (T)

Partition Function Zeroes of Quantum Phase Transitions
Conference on Exotic Order and Criticality in Quantum Matter, KITP, Santa Barbara, USA, June 7–11 (P)

Finite Size Scaling, Fisher Zeroes, and $\mathcal{N}=4$ Super Yang-Mills
The XXII International Symposium on Lattice Field Theory (Lattice 2004), Fermi National Accelerator Laboratory, Batavia, USA, June 21–26 (T)

A Fisher Zeroes Analysis of Valence Bond Solid Transitions in Quantum Spin Chains
Conference on Computational Physics (CCP 2004), Genoa, Italy, September 1–4 (T)(P)

Valence Bond Solid Transitions in Inhomogeneous Spin Chains
WE-Heraeus-Seminar on Quantum Phase Transitions, Physikzentrum, Bad Honnef, 11–14 October (P)

A Fisher Zeroes Analysis of the Continuous-time Quantum Monte Carlo Method
International Workshop Hangzhou 2004 on Simulational Physics, Zhejiang University, Hangzhou, China, November 5–7 (T)

Nonequilibrium Quantum Dynamics
5th NTZ-Workshop on Computational Physics (CompPhys04), Leipzig, December 25–26 (T)

Wolfhard Janke

Thermodynamics of Lattice Proteins using Multicanonical Chain Growth
Theoretisch-Physikalisches Kolloquium, Freie Universität Berlin, January 5 (T)

Monte Carlo Simulations of Complex Physical Systems
Physics Colloquium, Zhejiang University, Hangzhou, China, February 27 (T)

"Optimal Paths" Through Computer Simulations
Physics Seminar, Zhejiang University, Hangzhou, China, February 28 (T)

Monte Carlo Study of the Bond-Diluted 3D Ising Model
(with Berche, P.-E.; Chatelain, C.; Berche, B.) DPG-Frühjahrstagung, Arbeitskreis Festkörperphysik, Universität Regensburg, March 8–12 (P)

Multicanonical Chain Growth Method for Folding Lattice Proteins
Workshop on Markov Chain Monte Carlo, Institute for Mathematical Sciences, National University of Singapore, Singapore, March 1–28 (inv. T)

Multicanonical Chain Growth Simulations of Lattice Protein Folding
4th EUROGRID Conference on Random Geometry: Theory and Applications, Les Houches, France, March 22–26 (T)

Monte Carlo Simulations of 3D Bond-Diluted Potts Models
29th Conference of the Middle European Cooperation in Statistical Physics (MECO29), Bratislava, Slovakia, March 28 – April 1 (T)

Relevance of Quenched Disorder
Statistical Physics Workshop, Technische Universität Wien, Austria, April 1–3 (T)

Multicanonical Chain Growth Method for Folding Lattice Proteins
Physikalisches Kolloquium, Universität Erlangen-Nürnberg, April 26 (T)

Folding Lattice Proteins
Atelier Nancy, Université Henri Poincaré, Nancy, France, May 26–28 (inv. T)

Multicanonical Simulations of the Tails of the Order-Parameter Distribution of the 2D Ising Model
Conference on Computational Physics (CCP2004), Genoa, Italy, September 1–4 (T)

Moments of Stiff Polymer Chains
Mathematica-Aktionstag, Universität Leipzig, October 29 (T)

Folding Lattice Proteins: Multicanonical Chain Growth and Exact Enumerations
Statistik-Seminar, Universität Göttingen, November 10 (T)

Axel Krinner

Vortex-Loop Percolation in XY and Ginzburg-Landau Model
DPG-Frühjahrstagung, Arbeitskreis Festkörperphysik, Universität Regensburg, March 8–12 (T)

Andreas Nußbaumer

Equilibrium Crystal Shapes in Three Dimensions
DPG-Frühjahrstagung, Arbeitskreis Festkörperphysik, Universität Regensburg, March 8–12 (T)

Ising Droplets in Action
(with Bittner, E.; Janke, W.) 29th Conference of the Middle European Cooperation in Statistical Physics (MECO29), Bratislava, Slovakia, March 28 – April 1 (P)

Ising Droplets in Action
Statistical Physics Workshop, Technische Universität Wien, Austria, April 1–3 (T)

Ising Droplets in Action
14th Workshop on Lattice Field Theory (LEILAT04), Leipzig, June 3–5 (T)

Equilibrium Crystal Shapes in Three Dimension
(with Bittner, E.; Janke, W.) Conference on Computational Physics (CCP04), Genoa, Italy, September 1–4 (P)

Wulff Shapes of Ising Droplets
Mathematica-Aktionstag, Universität Leipzig, October 29 (T)

Ising Droplets in Action
(with Bittner, E.; Janke, W.) 5th NTZ-Workshop on Computational Physics (CompPhys04), Leipzig, November 25–26 (P)

Adriaan Schakel

Physics in Geometrical Potts Clusters
Seminar, March 19, 2004, Institute of Physics, Jagellonian University, Krakow, Poland, March 19 (T)

Geometrical Approach to Phase Transitions
8th Annual Workshop on Phase Transitions and Critical Phenomena, Lviv, Ukraine, March 23–25 (T)

Physics in Geometrical Potts Clusters
(with Janke, W.) 29th Conference of the Middle European Cooperation in Statistical Physics (MECO29), Bratislava, Slovakia, March 28 – April 1 (P)

Fractal Structure of Field Theories
14th Workshop on Lattice Field Theory (LEILAT04), Leipzig, June 3–5 (T)

Vortex Network Generation in Superfluid Turbulence
COSLAB Workshop on Turbulence and Vacuum Instability in Condensed Matter and Cosmology, Lammi, Finland, August 17–22 (T)

Loops in the 2D XY Model
Conference on Computational Physics (CCP2004), Genoa, Italy, September 1–4 (T)

Fractal Structure of Critical and Collapsing Loops in 2D
5th NTZ-Workshop on Computational Physics (CompPhys04), Leipzig, November 25–26 (T)

Reinhard Schiemann

Exact Sequence Analysis of HP Lattice Proteins
(with Bachmann, M.; Janke, W.) DPG-Frühjahrstagung, Arbeitskreis Festkörperphysik, Universität Regensburg, March 8–12 (P)

Thomas Vogel

HP Proteins on Generalized Lattices
(with Bachmann, M.; Janke, W.) Winter School on Computational Soft Matter, Bonn, February 29 – March 6 (P)

Hydrophobic-Polar Lattice Heteropolymers on Generalized Lattices
(with Bachmann, M.; Janke, W.) DPG-Frühjahrstagung, Arbeitskreis Festkörperphysik, Universität Regensburg, March 8–12 (P)

Collapse of Long Lattice Polymers
DPG-Frühjahrstagung, Arbeitskreis Festkörperphysik, Universität Regensburg, March 8–12 (T)

HP Proteins on Generalized Lattices
(with Bachmann, M.; Janke, W.) 3rd Day of Biotechnology, Leipzig, May 19 (P)

0.1.23 Graduations

PhD

Diploma

Thomas Vogel
HP-Proteine auf verallgemeinerten Gittern und Homopolymerkollaps
Diploma Thesis, January 2004

Axel Krinner
Nature of Phase Transitions in a Generalized Complex Ginzburg-Landau
Diploma Thesis, March 2004

Goetz Kähler
The 3-State Potts-Model on 2-Dimensional Delaunay Random Lattices
Diploma Thesis, August 2004

M.Sc.

Rodrigo Megaides
Autocorrelation Measurements of the Gonihedric Model
Master Thesis, September 2004

0.1.24 Guests

Priv.-Doz. Dr. Axel Pelster
Freie Universität Berlin
NTZ-Kolloquium, January 29, 2004: *Quantum phase diagram for Bose gases*
January 29–30, 2004

Priv.-Doz. Dr. Rudolf Hilfer
ICA-1, Universität Stuttgart
NTZ-Kolloquium, February 5, 2004: *Anomalous diffusion, fractional calculus and Mittag-Leffler functions*
February 5–6, 2004

Priv.-Doz. Dr. Thomas Neuhaus
Universität Bielefeld
NTZ-Kolloquium, February 12, 2004: *Duality and scaling in 3d scalar electrodynamics*
January – February 2004

Prof. Dr. He-Ping Ying
Zhejiang University, Hangzhou, China
NTZ-Kolloquium, February 19, 2004: *Monte Carlo simulations of quantum mixed-spin chains*
February 19, 2004

Priv.-Doz. Dr. Christian Holm
MPI für Polymerforschung, Mainz
NTZ-Kolloquium, April 15, 2004: *Geladene weiche Materie: Bio – Nano – Techno*
April 14–15, 2004

Prof. Dr. Sigismund Kobe
TU Dresden
NTZ-Kolloquium, June 17, 2004: *Exact ground states of finite Ising spin glasses obtained by "branch-and-bound"*
June 17, 2004

Prof. Dr. Zdzislaw Burda
Jagellonian University, Krakow, Poland
NTZ-Kolloquium, July 8, 2004: *Statistical mechanics of random graphs*
July 7–9, 2004

Priv.-Doz. Dr. Boris Kastening
FU Berlin
NTZ-Kolloquium, July 15, 2004: *Bose-Einstein condensation temperature of a weakly interacting Bose gas*
July 15, 2004

Prof. Dr. Lev N. Shchur
Landau Institute, Chernogolovka, Russia
NTZ-Kolloquium, July 22, 2004: *On the evolution of time horizons in parallel discrete*

event simulations
July – August 2004

Dr. Martin Weigel
University of Waterloo, Canada
September 2004

Dr. Handan Arkin
Hacettepe University, Beytepe, Ankara, Turkey
NTZ-Kolloquium, October 14, 2004: *Generalized-ensemble simulations of peptides and proteins*
June – October 2004

Prof. Dr. Ulrich H.E. Hansmann
Michigan Technological University, Houghton, USA
NTZ-Kolloquium, November 4, 2004: *Protein folding in silico*
November 4–5, 2004

Prof. Dr. Hans-Gert Gräbe
Institut für Informatik, Universität Leizpig
NTZ-Kolloquium, November 11, 2004: *Trends und Entwicklungen in der Computeralgebra*
November 11, 2004.

Prof. Dr. Roman Kotecky
Charles University, Prague, Tschechien
TKM/NTZ-Kolloquium, November 30, 2004: *Birth of equilibrium droplet*
November 30, 2004

Priv.-Doz. Dr. Michel Pleimling
Universität Erlangen/Nürnberg
NTZ-Kolloquium, December 9, 2004: *Alterungsphänomene in Systemen fern vom Gleichgewicht*
December 9–10, 2004

Prof. Dr. Bernd A. Berg
Florida State University, Tallahassee, USA
NTZ-Kolloquium, December 16, 2004: *A tutorial lecture on Markov chain Monte Carlo simulations*
December 16–17, 2004

Prof. Dr. Lev N. Shchur
Landau Institute, Chernogolovka, Russia
October – December 2004