1. Computational Quantum Field Theory (CQT)

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1.2. Research Projects 2003

The Computational Physics Group performs basic research in 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 PC's 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+ CPU's 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 T3E, 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 and the European Science Foundation, and by binational research grants with scientists in Great Britain, France, and Israel. Close contacts are also established with research groups in Armenia, Austria, China, Italy, Russia, Spain, Taiwan, and the United States.

Overview

1.2.1 Monte Carlo Studies of Spin Glasses

1.2.2 Monte Carlo Studies of Diluted Magnets

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

1.2.4 Harris-Luck Criterion and Potts Models on Random Graphs

1.2.5 The F Model on Quantum Gravity Graphs

1.2.6 Conformational Transitions of Lattice Heteropolymers

1.2.7 Thermodynamic Properties of Simple Off-Lattice Models for Proteins

1.2.8 Phase Transitions in Ginzburg-Landau Theory

1.2.9 Equilibrium Crystal Shapes in Three Dimensions

1.2.10 Geometrical Approach to Phase Transitions

1.2.11 Information Geometry and Phase Transitions

1.2.1. Monte Carlo Studies of Spin Glasses

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Spin glasses are examples for an important class of materials with random, competing interactions [1]. This leads to "frustration", since no unique spin configuration is favored by all interactions, and a rugged free energy landscape with many minima separated by barriers. Standard Monte Carlo simulations are very inefficient in such a case since they overcome the barriers only very rarely and hence run into ergodicity problems. To elucidate the scaling behaviour of the barriers with system size we therefore developed a multi-overlap Monte Carlo algorithm [2] which can be optimally tailored [3] for the sampling of rare-events. Recently we have further improved this method by combining it with parallel tempering and N-fold way ideas [4]. First tests indicate [5] that the new algorithm will enable us to push the studies of the spin-glass phase further towards the physically more interesting low-temperature regime. As in our previous work at higher temperatures [6] we focus on the free-energy barriers F_B^q in the probability density $P_{\mathcal{J}}(q)$ of the Parisi overlap parameter q [7] which can be defined in terms of the autocorrelation times τ_B^q of auxiliary Markov chains.

Along a second line of research we have also investigated the diluted generalized random-energy model (DGREM) which provides an approximation to the ground-state energy of spin glasses. Applications to two-dimensional q-state Potts models and a comparison with numerically determined ground-state energies are reported in Ref. [8]

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1.2.2. Monte Carlo Studies of Diluted Magnets

B. Berche (Université Nancy, France), P.-E. Berche (Université Rouen, France), C. Chatelain (Université Nancy, France) and W. Janke

The influence of quenched, random disorder on phase transitions has been the subject of exciting experimental, analytical and numerical studies in the past few years. To date most theoretical studies have concentrated on two-dimensional (2D) models with site- or bond-dilution or bond-disorder [1]. Generically one expects that quenched disorder, under certain conditions, will modify the critical behaviour at a second-order transition (Harris criterion) and can soften a first-order transition of the pure system to a second-order one [2]. In three dimensions (3D), numerical studies have mainly focused on the site-diluted Ising model [3] where good agreement with field theory 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 [5]. We have determined the phase diagrams of the diluted models, starting from the pure model limit down to the neighbourhood of the percolation threshold, in very good agreement with a single-bond effective-medium approximation. For the estimation of critical exponents in the Ising case [6], we have first performed a finite-size scaling study, where we concentrated on three different dilutions to check the stability of the disorder fixed point. We emphasize in this work the great influence of the cross-over phenomena between the pure, disorder and percolation fixed points which lead to effective critical exponents dependent on the concentration. In a second set of simulations, the temperature behaviour of physical quantities has been studied in order to characterize the disorder fixed point more accurately. In particular this allowed us to estimate universal ratios of some critical amplitudes which are usually more sensitive to the universality class than the critical exponents. Moreover, the question of non-self-averaging at the disorder fixed point is investigated and compared with recent results for the bond-diluted 4-state Potts model. We obtain very good agreement with approximate analytical calculations by Aharony and Harris. Overall our numerical results provide evidence that, as expected on theoretical grounds, the critical behaviour of the bond-diluted model is indeed governed by the same universality class as the site-diluted model.

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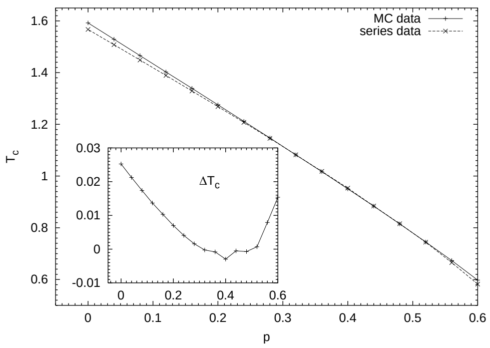
1.2.3. High-Temperature Series Expansions for Spin Glasses and Disordered Magnets

M. Hellmund (Fakultät für Mathematik und Informatik) and W. Janke

Despite considerable efforts there are still many open problems in the physics of disordered systems. One alternative to large-scale numerical simulations are systematic series expansions. Such expansions for statistical models defined on a lattice are a well-known method to study phase transitions and critical phenomena [1]. The extension of this method to disordered systems [2] demands the development of new graph theoretical and algebraic algorithms.

Using the method of "star-graph expansion", we calculate, e.g., free energies and susceptibilities for disordered q-state Potts models on d-dimensional hypercubic lattices. The probability distribution of couplings is 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. First results for the random-bond Ising [3] and Potts [4] model demonstrate the feasibility of the method to complement Monte Carlo [5] and field theoretic studies of phase transitions in disordered systems.

For the bond-diluted 4-state Potts model in three dimensions, which exhibits a rather strong first-order phase transition in the undiluted case, we obtained results [6] for the transition temperature and the effective critical exponent γ as a function of p from analyses of susceptibility series up to order 18. A comparison with recent Monte Carlo data [5] shows signals for the softening to a second-order transition at finite disorder strength. Further new results were also obtained for the three-dimensional bond-diluted resp. random bond Ising model and the $q \to 1$ percolation limit for different dimensionalities d [7].



Critical temperature for different dilutions p as obtained from Monte Carlo (MC) simulations [5] and DLog-Padé series analyses [6]. The inset shows the difference between the two estimates.

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1.2.4. Harris-Luck Criterion and Potts Models on Random Graphs

W. Janke, G. Kähler and M. Weigel

The Harris criterion judges the relevance of uncorrelated, quenched disorder for altering the universal properties of systems of statistical mechanics 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 on the universal behaviour of coupled spin models, 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 Poissonian 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, a generalised model introducing a distance dependence of the interactions is currently under investigation.

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1.2.5. The F Model on Quantum Gravity Graphs

W. Janke, D. A. Johnston (Heriot-Watt University, Edinburgh, Scotland) and M. Weigel

As an alternative to various other approaches towards a theory of quantum gravity, the *dynamical triangulations* method has proved to be a successful discrete formulation of Euclidean quantum gravity in two dimensions. There, the necessary integration over all metric tensors as the dynamic variables of the theory, is performed as a discrete 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 gravity model in two dimensions. Furthermore, matrix models can be formulated for the coupling of spin models of statistical mechanics to the random graphs and some of them could be solved analytically. More generally, the "dressing" of the weights of $c < 1$ conformal matter on coupling it to quantum gravity in two dimensions is predicted by the KPZ/DDK formula [1], in agreement with all known exact solutions.

One of the most general classes of models in statistical mechanics is given by 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 as well as random lattices, 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 lattices and the presence of strong logarithmic corrections, leading to rather extreme finite-size effects. Nevertheless, a scaling analysis of the staggered polarizability yields results [6] 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.

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1.2.6. Conformational Transitions of Lattice Heteropolymers

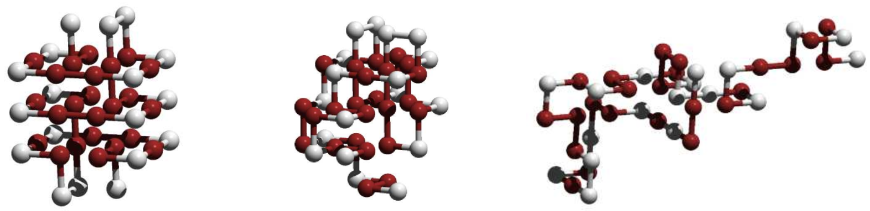
M. Bachmann, W. Janke, R. Schiemann and T. Vogel

The native conformation of a protein is strongly correlated with the sequence of amino acid residues building up the heteropolymer. The sequence makes the protein unique and assigns it a specific function within a biological organism. The reason is that the different types of amino acids vary in their response to the environment and in their mutual interaction. Since many diseases (e.g., Alzheimer's, Creutzfeld-Jacob, type II diabetes) are due to protein misfolds, it is an important task to reveal on what general principles the folding process of a protein is based. Models differ extremely in their level of abstraction, ranging from simple and purely qualitative lattice models to highly sophisticated all-atom off-lattice formulations with explicit solvent that partially yield results comparable with experimental data. Due to the enormous computational effort required for simulations of realistic proteins, usually characteristic properties of a protein with a given sequence are studied in detail. Much simpler, but by no means trivial, lattice models enjoy a growing interest, since they allow a more global view on, for example, the analysis of the relation between sequence and structure.

We focused ourselves on the study of thermodynamic properties of lattice proteins at all temperatures. In particular, this includes the investigation of the transitions between the different classes of states: lowest-energy (hydrophobic-core) states, compact globules, and random coils. Since the ground-state–globule transition occurs at rather low temperatures, a powerful algorithm is required that in particular allows a reasonable sampling of the low-lying energy states. To this end we combined multicanonical strategies [1] with chain growth algorithms [2] to a new method [3]. We applied this method to different lattice proteins, modeled by the simplest lattice formulation for heteropolymers, the HP model [4]. In this model, only two types of monomers enter, hydrophobic (H) and polar (P) residues. The model is based on the assumption that the hydrophobic interaction is one of the fundamental principles in protein folding. An attractive hydrophobic interaction provides for the formation of a compact hydrophobic core that is screened from the aqueous environment by a shell of polar residues.

For different sequences with lengths between 42 and 103 monomers, we analyzed in detail the temperature-dependent behavior of radius of gyration, end-to-end distance, as well as their fluctuations, and compared it with the specific heat in order to elaborate relations between characteristic properties of these curves (peaks, "shoulders") and conformational transitions not being transitions in a strict thermodynamic sense due to the impossibility to formulate a thermodynamic limit for proteins. Therefore, we identified temperature regions, where global changes of protein conformations occur. These transition regions separate "phases", where random coils, maximally compact globules, or states with compact hydrophobic core dominate. As an interesting by-product, we not only confirmed the known global-minimum energies for these examples, but we even found a new minimum for the 103mer being the longest sequence under consideration [3].

In another project [5] we exactly analyzed the combined space of sequences and conformations for proteins on the simple cubic lattice for HP-type models that differ in the contact energy between hydrophobic and polar monomers. Since there were only a few known exact results for heteropolymers in 3D, in particular on compact cuboid lattices, we generated by exact enumeration the sets of designing sequences (i.e. sequences with nondegenerate ground state) and native conformations on simple cubic lattices. We studied, how their properties, measured, e.g., in terms of quantities like end-to-end distance, radius of gyration, designability, etc., differ



bad solvent poor solvent good solvent

from the bulk of all possible sequences and all self-avoiding conformations, respectively. We confirmed that the ground-state conformations are very compact, but not necessarily maximal compact. We studied also energetic thermodynamic properties, in order to investigate how characteristic the low-temperature behavior of designing compared to non-designing sequences is and found that designing sequences show up a pronounced low-temperature peak in the specific heat being related to a conformational transition between low-energy states with hydrophobic core and highly compact globules. While designing sequences behave similarly for very low temperature, nondesigning sequences react quite differently on changes of the temperature, over the entire range of temperatures.

We also investigated the HP model on more general lattices, e.g. the triangular lattice in 2D and the face-centered cubic (fcc) lattice in 3D [6]. Comparing for given sequences the results obtained on the fcc lattice with results from considerations on the simple cubic lattice, it turned out that there was in most cases no qualitative coincidence. In particular, for exemplified sequences exhibiting a distinct "three-phase" behavior on the simple cubic lattice, we did not find a clear indication for the low-temperature transition between globules and hydrophobic-core conformations on the fcc lattice. Consequently, ground-state properties and thermodynamic properties for given sequences strongly depend on the type of the lattice used. This does not render lattice models completely irrelevant for qualitative studies of heteropolymers, but it shows that, just for this reason, HP proteins on the simplest lattices will not adequately describe properties of a realistic amino acid sequence that was translated into the corresponding HP sequence.

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1.2.7. Thermodynamic Properties of Simple Off-Lattice Models for Proteins

H. Arkın (Hacettepe University, Ankara, Turkey), M. Bachmann and W. Janke

The understanding of protein folding is one of the most challenging objectives in biochemically motivated research. Although the physical principles are known, the complexity of proteins as being macromolecules consisting of numerous atoms, the influence of quantum chemical details on long-range interactions as well as the role of the solvent, etc. makes an accurate analysis of the folding process of realistic proteins extremely difficult. Therefore, one of the most important questions in this field is how much detailed information can be neglected to establish effective models yielding reasonable, at least qualitative, results that allow for, e.g., a more global view on the relationship between the sequence of amino acid residues and the existence of a global, funnel-like energy minimum in a rugged free-energy landscape.

Within the past two decades much work has been done to introduce minimalistic models based on general principles that are believed to primarily control the structure formation of proteins. One of the most prominent examples is the HP model of lattice proteins [1] which has been exhaustively investigated without revealing all secrets, despite its simplicity. The only explicit interaction is between non-adjacent but next-neighbored hydrophobic monomers. This interaction of hydrophobic contacts is attractive to force the formation of a compact hydrophobic core which is screened from the (hypothetic) aqueous environment by the polar residues.

A manifest off-lattice generalization of the HP model is the AB model [2], where the hydrophobic monomers are labeled by A and the hydrophilic ones by B. The contact interaction is replaced by a distance-dependent Lennard-Jones type of potential accounting for short-range excluded volume repulsion and long-range interaction, the latter being attractive for AA and BB pairs and repulsive for AB pairs of monomers. An additional interaction accounts for the bending energy of any pair of successive bonds. This model was first applied in two dimensions [2] and generalized to three-dimensional AB proteins, partially with modifications taking into account the additional torsional degree of freedom of each bond [3].

We have studied thermodynamic and ground-state properties of known AB sequences for two representations [2,3] of the AB model. In order to more accurately resolve the low-temperature behavior we applied a multicanonical Monte Carlo algorithm with an appropriate update mechanism, which enabled us to sample the density of states over more than 70 *orders of magnitude* [4]. This allowed us to calculate fluctuating quantities such as the specific heat with very high accuracy for almost all temperatures. We also obtained with this method a very good estimate for the ground-state energies. These values are in very good agreement with results achieved by means of the energy landscape paving (ELP) minimizer [5], which was designed just for this purpose.

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1.2.8. Phase Transitions in Ginzburg-Landau Theory

E. Bittner, W. Janke, A. Krinner and S. Wenzel

Scalar fields with n components and a fourth-order O(n)-symmetric quartic self-interaction are so far the best understood examples of systems, whose second-order phase transitions can be treated with field-theoretic techniques [1,2]. Universality ensures that spin models which describe only directional fluctuations show the same critical properties as scalar fields with $n \geq 2$ components, and the precise reason for this can easily be understood [3]. In particular, this equivalence holds for the superfluid phase transition which can be described either by a directional XY model or by an O(2)-symmetric scalar field theory, whose Hamiltonian is of the Ginzburg-Landau form with a complex field $\psi(\vec{r}) = |\psi(\vec{r})|e^{i\phi(\vec{r})}$. Therefore the model can equivalently be represented as a partition function of a dual theory where the elementary excitations are closed vortex lines, i.e. loops. The loops of the dual theory may therefore 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 decompose every spin configuration generated in a lattice Monte Carlo simulation [4] into a number of vortex loops. The hope is then that the transition will be signalized by a non-zero probability for finding vortex loops that extend through the whole system [5], a phenomenon which is often called percolation.

Percolation has been used to study phase transitions in various different theories. From studies of the Ising model, where a different kind of percolation may occur, related to spin clusters instead of vortex lines, it is known that one has to be quite careful with the interpretation [6]. 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.

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1.2.9. Equilibrium Crystal Shapes in Three Dimensions

E. Bittner, W. Janke and A. Nußbaumer

The free energy of the three-dimensional Edwards-Anderson Ising model in the low temperature phase shows a multi-valley structure. Multicanonical simulations, e.g. for the overlap parameter, were expected to remove these valleys and to lead to a random walk behaviour in the corresponding observable. In fact there are still jumps in the time series which were attributed to so-called "hidden barriers". Recently, Neuhaus and Hager [1] explained such barriers in the magnetisation M for the much simpler case of the two-dimensional Ising model. Based on the analytic work of Leung and Zia [2], they identified a geometrically induced first-order transition from a droplet to a strip domain and showed that even a perfect multimagnetic simulation operating with the optimal weights needs exponential time to overcome the associated free energy barrier. To obtain more qualitative insights, we determined directly the anisotropy of a configuration by measuring a 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 (see Fig. 1). By generalising these considerations to the case of the three-dimensional Ising model, new transitions could be identified analytically and verified numerically, and the crystal shapes emerging during the transition were visualised.

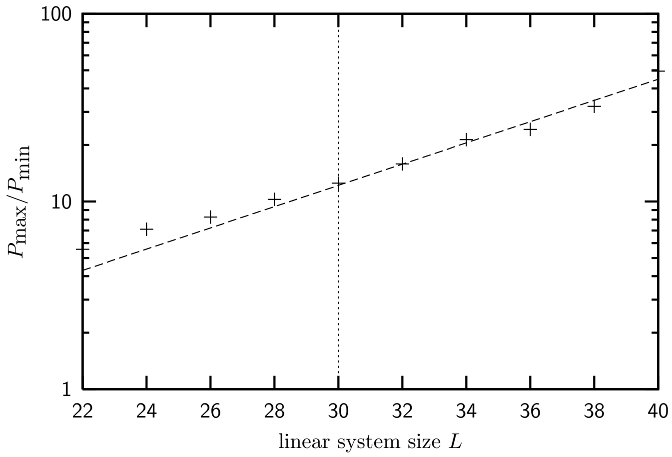

Figure 1. Linear fit to $\ln(P_{\max}/P_{\min})$ in the range $L = 30$ to $L = 40$. The measured value $\alpha = 1.30 \pm 0.01$ is to be compared with the analytic value [2] of $\alpha = 1.35$.

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1.2.10. Geometrical Approach to Phase Transitions

W. Janke and A. M. J. Schakel

The geometrical approach to phase transitions is an exciting research topic in contemporary physics. The prototype of this approach is percolation theory, describing clusters of (randomly) occupied sites on a lattice. The fractal structure of these geometrical objects and whether or not a cluster percolates the lattice are central topics addressed by the theory. Percolation theory is easily adapted to describe other geometrical objects such as lines and (hyper)surfaces as well. Typical line objects featuring in phase transitions that can be described in this way are, for example, (i) vortex lines in systems with spontaneously broken global U(1) or local gauge symmetries, (ii) worldlines in Bose-Einstein condensates, and (iii) graphs in high-temperature representations of spin models.

(i) Because of topological constraints, vortices generally form closed loops. Whereas in the broken-symmetry phase only finite vortex loops are present, at the critical point, loops of all sizes appear. This vortex proliferation is in complete analogy to what happens with clusters at the percolation threshold. The disordering effect of the proliferating vortices destroys superfluidity in superfluids, and leads to charge confinement in certain gauge theories.

(ii) Boson worldlines at finite temperature also form closed loops in imaginary time. Feynman's theory of Bose-Einstein condensation asserts that upon lowering the temperature, small loops describing single particles hook up to form larger exchange rings, so that the particles become indistinguishable. At the critical temperature, again as in percolation phenomena, worldlines proliferate and loops of arbitrary size appear, signalling the onset of Bose-Einstein condensation.

(iii) The high-temperature representation of spin models can be visualized by closed graphs on the lattice (see Fig. 1), making these models eligible to a geometrical description.

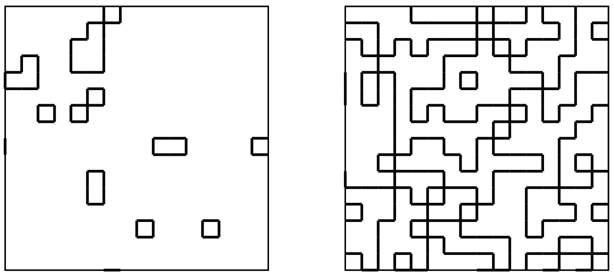

Figure 1. Typical graph configurations generated on a 16×16 square lattice with periodic boundary conditions in the high- (left panel) and low-temperature (right panel) phase of the two-dimensional Ising model.

In this project, the fractal structure of two-dimensional spin models was investigated and a close connection between different models established. To support our theoretical findings, the high-temperature representation of the Ising model was simulated by means of a Metropolis plaquette update. It was shown that (a) large graphs are exponentially suppressed in the high-temperature phase, and that (b) graphs percolate the lattice and proliferate precisely at the thermal critical point. From the percolation strength (defined as the number of bonds in the largest graph) and the average graph size, the fractal dimension of the graphs is extracted through finite-size scaling [1]. The resulting value was found to agree with theoretical predictions [2].

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1.2.11. Information Geometry and Phase Transitions

W. Janke, D. A. Johnston (Heriot-Watt University, Edinburgh, Scotland), R. Kenna (Coventry University, England) and R. P. K. C. Malmini (University of Sri Jayewardenepura, Sri Lanka)

Various authors, motivated by ideas in parametric statistics [1], have 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 a spin model in field, $\mathcal{M}$ is a two-dimensional manifold parametrised by $(\theta^1, \theta^2) = (\beta, h)$. 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 [6] in exact calculations for the *three*-dimensional spherical model, which was solved (in field) in the classic Berlin and Kac paper [7] 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], in particular the mean-field like behaviour which sets in at $D = 4$.

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1.3. Funding 2003

1. *Discrete Random Geometries: From Solid State Physics to Quantum Gravity.*
   W. Janke.
   EU-Network "EUROGRID".
   Grant No. HPRN-CT-1999-000161.

2. *Statistical Physics of Random Structures with Applications to Life and Material Sciences.*
   W. Janke.
   German-Israel-Foundation (GIF).
   Grant No. I-653-181.14/1999.

3. *Hochtemperaturreihen für Random-Bond-Modelle und Spingläser.*
   W. Janke.
   Deutsche Forschungsgemeinschaft (DFG).
   Grant Nos. JA 483/17-1 and 17-3.

4. *Two-Dimensional Magnetic Systems with Anisotropy.*
   W. Janke.
   EU-Marie Curie Development Host Fellowship.
   Grant No. IHP-HPMD-CT-2001-00108.

5. *Quantenfeldtheorie: Mathematische Struktur und Anwendungen in der Elementarteilchen- und Festkörperphysik.*
   Dozenten der Theoretischen Physik und Mathematik (Sprecher B. Geyer).
   Deutsche Forschungsgemeinschaft (DFG).
   Graduiertenkolleg, Grant No. 52.

6. *Geometry and Disorder: From Membranes to Quantum Gravity.*
   W. Janke.
   ESF-Network.

7. *Challenges in Molecular Simulations: Bridging the Length and Time-Scale Gap.*
   W. Janke.
   ESF-Programme "SIMU".

8. *Statistical Physics of Glassy and Non-Equilibrium Systems.*
   W. Janke.
   ESF-Programme "SPHINX".

9. *Multi-Overlap Simulationen von Spingläsern.*
   W. Janke.
   NIC Jülich (computer time grant).
   Grant No. hmz09.

10. *Ungeordnete Ferromagnete.*
    W. Janke.
    NIC Jülich (computer time grant).
    Grant No. hlz06.

11. *Disordered Ferromagnets*.
    W. Janke.
    LRZ München (computer time grant).
    Grant No. h0611.

12. *Studentenstipendium*.
    R. Schiemann.
    Studienstiftung des deutschen Volkes.

13. *Studentenstipendium*.
    S. Wenzel.
    Studienstiftung des deutschen Volkes.

1.4. Organizational Activities 2003

Wolfhard Janke:

1. Member of Advisory Committee, *YALELAT03 – 13. Workshop on Lattice Field Theory*, Yale University, New Haven, USA, May 1–3, 2003.

2. Organizer of the Workshop *CompPhys03 – 4. NTZ-Workshop on Computational Physics*, ITP, University of Leipzig, December 4–5, 2003.

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

4. Member of Scientific Organizing Committee, *Fourth Eurogrid Meeting – Random Geometry: Theory and Applications*, Les Houches, March 22–26, 2004.

5. Director of the Naturwissenschaftlich-Theoretisches Zentrum (NTZ) at the Zentrum für Höhere Studien (ZHS), University of Leipzig.

1.5. External Cooperations 2003

1. EU-Network “EUROGRID” – *Discrete Random Geometries: From Solid State Physics to Quantum Gravity* with 11 teams throughout Europe.
2. 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).
3. Prof. Dr. Bernd A. Berg, Dept. of Physics, Florida State University, Tallahassee, USA.
4. Dr. Alain Billoire, CEA/Saclay, Service de Physique Théorique, France.
5. Prof. Dr. Desmond A. Johnston, School of Mathematical and Computer Sciences, Heriot-Watt University, Edinburgh, Scotland.
6. Dr. Ralph Kenna, School of Mathematical and Information Sciences, Coventry University, England.
7. Prof. Dr. Bertrand Berche and Dr. Christophe Chatelain, Laboratoire de Physique des Matériaux (UMR CNRS No 7556), Université Henri Poincaré, Nancy, France.
8. Dr. Pierre-Emmanuel Berche, Groupe de Physique des Matériaux (UMR CNRS No 6634), Université de Rouen, France.
9. Dr. Handan Arkın, Dept. of Physics, Hacettepe University, Ankara, Turkey.
10. Prof. Dr. Peter Grassberger and Dr. Hsiao-Ping Hsu, NIC, Forschungszentrum Jülich.
11. Prof. Dr. Hagen Kleinert and Prof. Dr. Bodo Hamprecht, Inst. für Theoretische Physik, FU Berlin.
12. Prof. Dr. Harald Markum and Dr. Rainer Pullirsch, Atominstitut, TU Wien, Austria.
13. Priv.-Doz. Dr. Rudolf Hilfer, IAC-1, Universität Stuttgart.
14. Dr. Simon Hands, Dept. of Physics, University of Wales Swansea, Swansea, Wales.
15. Priv.-Doz. Dr. Thomas Neuhaus, Inst. für Theoretische Physik, Universität Bielefeld.
16. Prof. Dr. Lev N. Shchur, Landau Institute for Theoretical Physics, Chernogolovka, Russia.
17. Prof. Dr. David B. Saakian, Yerevan Physics Institute, Yerevan, Armenia.
18. Prof. Dr. Bo Zheng and Prof. Dr. He-Ping Ying, Zhejiang University, Hangzhou, P.R. China.

1.6. Publications

1.6.1. Published in 2003

[1] Bachmann, M.; Janke, W.
Density of States for HP Lattice Proteins.
Acta Physica Polonica **B34** (2003) 4689–4697.

[2] Bachmann, M.; Janke, W.
Multicanonical Chain Growth Algorithm.
Phys. Rev. Lett. **91** (2003) 208105-1–4.

[3] Berche, P.-E.; Chatelain, C.; Berche, B.; Janke, W.
Monte Carlo Studies of Three-Dimensional Bond-Diluted Ferromagnets.
In: Wagner, S.; Hanke, W.; Bode, A.; Durst, F. (Eds.): *High Performance Computing in Science and Engineering, Munich 2002.*
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Nucl. Phys. **B** (Proc. Suppl.) **119** (2003) 924–926.

[7] Bittner, E.; Janke, W.
Generalized Complex $|\Psi^4|$ *Model.*
Acta Physica Polonica **B34** (2003) 4727–4737.

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Star-Graph Expansions for Bond-Diluted Potts Models.
Phys. Rev. **E67** (2003) 026118-1–9.

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Multicanonical Monte Carlo Study and Analysis of Tails for the Order-Parameter Distribution of the Two-Dimensional Ising Model.
Phys. Rev. **E68** (2003) 046123-1–9.

[10] Janke, W.; Johnston, D.A.; Kenna, R.
The Information Geometry of the Spherical Model.
Phys. Rev. **E67** (2003) 046106-1–4.

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Nucl. Phys. **B** (Proc. Suppl.) **119** (2003) 882–884.

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Nucl. Phys. **B** (Proc. Suppl.) **119** (2003) 867–899.

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Effects of Connectivity Disorder on the Potts Model.
Acta Physica Polonica **B34** (2003) 4891–4907.

[14] Janke, W.; Berg, B.A.; Billoire, A.
Simulating Rare Events in Spin Glasses.
Acta Physica Polonica **B34** (2003) 4909–4921.

[15] Janke, W.
First-Order Phase Transitions.
In: Dünweg, B.; Landau, D.P.; Milchev, A.I. (Eds.): *Computer Simulations of Surfaces and Interfaces.*
NATO Science Series, II. Mathematics, Physics and Chemistry – Vol. **114**, Proceedings of the NATO Advanced Study Institute, Albena, Bulgaria, 9 – 20 September 2002.
Dordrecht: Kluwer, 2003; pp. 111–135.

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Histograms and All That.
In: Dünweg, B.; Landau, D.P.; Milchev, A.I. (Eds.): *Computer Simulations of Surfaces and Interfaces.*
NATO Science Series, II. Mathematics, Physics and Chemistry – Vol. **114**, Proceedings of the NATO Advanced Study Institute, Albena, Bulgaria, 9 – 20 September 2002.
Dordrecht: Kluwer, 2003; pp. 137–157.

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Information Geometry, One, Two, Three (and Four).
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1.6.2. Published in 2004

[19] Bachmann, M.; Janke, W.
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J. Chem. Phys. **120** (2004) 6779–6791.

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Information Geometry and Phase Transitions.
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1.6.3. To appear in 2004 (in print)

[22] Berche, P.-E.; Chatelain, C.; Berche, B.; Janke, W.
Bond Dilution in the 3D Ising Model: A Monte Carlo Study.
e-print cond-mat/0402596, to appear in Eur. Phys. J. **B** (in print).

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Discretization and Continuum Limit of Quantum Gravity on a Four-Dimensional Space-Time Lattice.
e-print hep-lat/0311031, to appear in: *Difference Equations and Special Functions*, International Conference "Bexbach Colloquium on Science", Bexbach, Germany, October 26–30, 2002 (in print).

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Quantum Chaos in Supersymmetric QCD at Finite Density.
e-print hep-lat/0402015, to appear in Progress of Theoretical Physics Supplement (in print).

[25] Janke, W.; Berche, P.-E.; Chatelain, C.; Berche, B.
Quenched Disorder Distributions in Three-Dimensional Diluted Ferromagnets.
To appear in: Landau, D.P.; Lewis, S.P.; Schüttler H.-B. (Eds.): *Computer Simulation Studies in Condensed-Matter Physics XVI*.
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e-print cond-mat/0310269, to appear in Phys. Rev. **B** (in print).

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e-print cond-mat/0311624, to appear in Nucl. Phys. **B** (in print).

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Monte Carlo Studies of Connectivity Disorder.
To appear in: *High Performance Computing in Science and Engineering, Munich 2004*, proceedings of the *Second Joint HLRB and KONWIHR Result and Reviewing Workshop* (in print).

1.6.4. Talks and Posters 2003

Michael Bachmann:

1. *Energy Density of HP Lattice Proteins*,
(with Janke, W.) 28th Conference of the Middle European Cooperation in Statistical Physics (MECO28), Saarbrücken, March 20–22 (P).

2. *Energy Density of Heteropolymers*,
DPG-Frühjahrstagung Dresden, March 24–28 (T).

3. *Multicanonical Chain Growth Algorithm*,
Seminar *Theory of Complex Systems*, John von Neumann Institute for Computing (NIC), Forschungszentrum Jülich, April 24 (T).

4. *Density of States for HP Lattice Proteins*,
(with Janke, W.) Workshop on *Random Geometry* and EU-Network Meeting, Krakow, Poland, May 15–17 (P).

5. *Energetic Properties of Heteropolymers*,
(with Janke, W.) 2nd Day of Biotechnology, Leipzig, May 21 (P).

6. *Exact Analysis of Designing Sequences*,
(with Schiemann, R.; Janke, W.) 2nd Day of Biotechnology, Leipzig, May 21 (P).

7. *Generalized-Ensemble Simulations of Off-Lattice Heteropolymers*,
Computational Physics Workshop (CompPhys03), Leipzig, December 4–5 (T).

Elmar Bittner:

1. *Nature of Phase Transitions in a Generalized Complex* $|\psi|^4$ *Model*,
(with Janke, W.) 28th Conference of the Middle European Cooperation in Statistical Physics (MECO28), Saarbrücken, March 20–22 (P).

2. *Zum Phasenübergang in der komplexen* $|\psi^4|$ *Theorie*,
DPG-Frühjahrstagung, Arbeitskreis Festkörperphysik, TU Dresden, March 24–28 (T).

3. *Generalized Comlex* ψ^4 *Model*,
(with Janke, W.) Workshop on *Random Geometry* and EU-Network Meeting, Krakow, Poland, May 15–17 (P).

4. *Phase Structure of a Generalized* ψ^4 *Model*,
Computational Physics Workshop (CompPhys03), Leipzig, December 4–5 (T).

Meik Hellmund:

1. *Star-Graph Expansions for Bond-Diluted Potts Models*,
(with Janke, W.) DPG-Frühjahrstagung, Arbeitskreis Festkörperphysik, TU Dresden, March 24–28 (P).

Wolfhard Janke:

1. *Phasenübergänge in ungeordneten Ferromagneten*,
Theorie-Kolloquium, Universität Mainz, January 16 (T).

2. *Partition Function Zeroes for Fluctuating Graphs*,
Seminaire LPM, Université Henri Poincaré, Nancy, France, January 23 (T).

3. *Quenched Disorder in Three-Dimensional Ferromagnets*,
16th Workshop on *Recent Developments in Computer Simulation Studies in Condensed Matter Physics*, The University of Georgia, Athens, Georgia, USA, February 24–28 (T).

4 *Information Geometry and Phase Transitions*,
(with Johnston, D.A.; Kenna, R.; Malmini, R.P.K.C.) 28th Conference of the Middle European Cooperation in Statistical Physics (MECO28), Saarbrücken, March 20–22 (P).

5. *Phase Transitions of the Diluted 3D 4-State Potts Model*,
DPG-Frühjahrstagung, Arbeitskreis Festkörperphysik, TU Dresden, March 24–28 (T).

6. *Quenched Disorder in Ferromagnets*,
invited talk, *Yalelat03* – 13. Workshop on Lattice Field Theory, Yale University, New Haven, USA, May 1–3 (T).

7. *Simulating Rare Events in Spin Glasses*,
invited talk, Workshop on *Random Geometry* and EU-Network Meeting, Krakow, Poland, May 15–17 (inv. T).

8. *Quenched Connectivity Disorder*,
invited talk, Atelier Nancy, Université Henri Poincaré, Nancy, Frankreich, May 21–22 (inv. T).

9. *Ground States of Lattice Proteins*,
invited talk, Dagstuhl-Seminar on *New Optimization Algorithms in Physics*, Wadern, September 14–19 (inv. T).

10. *Overcoming Slow Dynamics in Generalized Ensemble Simulations*,
invited talk, Workshop NesPhy03, MPI-PKS Dresden, September 22 – October 10 (inv. T).

Andreas Nußbaumer:

1. *Parallel Tempering at Second-Order Phase Transitions*,
(with Bittner, E.; Janke, W.) DPG-Frühjahrstagung, Arbeitskreis Festkörperphysik, TU Dresden, March 24–28 (P).

2. *Ising Droplets in Action*,
Computational Physics Workshop (CompPhys03), Leipzig, December 4–5 (T).

Adriaan Schakel:

1. *Physics in Geometrical Potts Clusters*,
Computational Physics Workshop (CompPhys03), Leipzig, December 4–5 (T).

Reinhard Schiemann:

1. *Exact Statistical Analysis of Native Ground States of Lattice Proteins*, (with Bachmann, M.; Janke, W.) DPG-Frühjahrstagung, Arbeitskreis Festkörperphysik, TU Dresden, March 24–28 (P).

Thomas Vogel:

1. *Monte Carlo Simulations of the 2D Ising Model with Brascamp-Kunz Boundary Conditions*, (with Krinner, A.; Janke, W.) DPG-Frühjahrstagung, Arbeitskreis Festkörperphysik, TU Dresden, March 24–28 (P).

Martin Weigel:

1. *Effects of Connectivity Disorder on the Potts Model*, (with Janke, W.) 28th Conference of the Middle European Cooperation in Statistical Physics (MECO28), Saarbrücken, March 20–22 (P).

2. *Effects of Connectivity Disorder on the Potts Model*, (with Janke, W.) DPG-Frühjahrstagung, Arbeitskreis Festkörperphysik, TU Dresden, March 24–28 (P).

3. *Effects of Connectivity Disorder on the Potts Model*, (with Janke, W.) Workshop on *Random Geometry* and EU-Network Meeting, Krakow, Poland, May 15–17 (P).

4. *The Harris-Luck Criterion for Random Lattices*, Institute for Theoretical Physics, University of Leipzig, October 8 (T).

5. *The Harris-Luck Criterion for Random Lattices*, Condensed Matter Theory Seminar, University of Waterloo, Canada, November 4 (T).

6. *Harris Criterion and Correlated Disorder from Random Graphs*, Emerging Materials Knowledge Meeting, University of Waterloo, Canada, December 18 (T).

Andreas Wernecke:

1. *Q-state Potts Models on Quenched Random Planar ϕ^3 Graphs*, (with Janke, W.) DPG-Frühjahrstagung, Arbeitskreis Festkörperphysik, TU Dresden, March 24–28 (P).

1.7. Graduations 2003

Diploma and Master Theses:

1. Andreas Nußbaumer, *Rare-Event Sampling of Spin Glasses*, Diploma Thesis, April 2003.
2. Reinhard Schiemann, *Exact Enumeration of 3D Lattice Proteins*, Diploma Thesis, September 2003.
3. Sandro Wenzel, *Monte Carlo Simulations of the 3D Ginzburg-Landau Model with Compact U(1) Gauge Field*, Master Thesis, December 2003.
4. Thomas Vogel, *HP-Proteine auf verallgemeinerten Gittern und Homopolymerkollaps*, Diploma Thesis, January 2004.
5. Axel Krinner, *Nature of Phase Transitions in a Generalized Complex Ginzburg-Landau*, Diploma Thesis, March 2004.

1.8. Guests 2003

Short-term guests:

1. Dr. Pai-Yi Hsiao, Laboratoire de Physique Théorique de la Matière Condensée, University Paris 7, France,
   NTZ-Kolloquium, January 9, 2003: *Critical Behavior of the Ferromagnetic Ising Model on the Fractals*,
   Period: January 8–11, 2003.

2. Prof. Dr. Yuko Okamoto, Dept. of Theoretical Studies, Institute for Molecular Science, Okazaki, Aichi 444-8585, Japan,
   TKM-Seminar, May 20, 2003: *Protein Folding Simulations by Generalized-Ensemble Algorithms*,
   Period: May 19–21, 2003.

3. Prof. Dr. Royce Zia, Virgina Tech. Univ., USA,
   NTZ-Kolloquium, November 27, 2003: *Non-Equilibrium Statistical Mechanics*,
   Period: November 26–28, 2003.

4. Prof. Dr. Bernd A. Berg, Florida State University, Tallahassee, USA,
   NTZ-Kolloquium, December 18, 2003: *A Biased Metropolis Sampling Method for Peptides*,
   Period: December 16–19, 2003.

Long-term guests:

1. Adriaan Schakel (FU Berlin): June–July 2003.

2. Handan Arkın (Hacettepe University, Ankara, Turkey): July–October 2003.

3. Thomas Neuhaus (Univ. Bielefeld): November–December 2003.

4. Adriaan Schakel (FU Berlin): November–December 2003.

5. Thomas Neuhaus (Univ. Bielefeld): January–February 2004.