10

Computational Quantum Field Theory

10.1 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 the physics of spin glasses, diluted magnets and other materials with quenched, random disorder, soft condensed matter physics (e.g., membranes and interfaces) and biologically motivated problems (e.g., protein folding and semiflexible polymers). Investigations of a geometrical approach to the statistical physics of topological defects with applications to superconductors and superfluids and research into fluctuating geometries with applications to quantum gravity (e.g., dynamical triangulations) are conducted within the EC-RTN Network "ENRAGE": *Random Geometry and Random Matrices: From Quantum Gravity to Econophysics*. Supported by a Development Host grant of the European Commission, also research into the physics of anisotropic quantum magnets and quantum phase transitions has been 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 new 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 and the European Science Foundation (ESF), 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

10.2 Monte Carlo Studies of Spin Glasses

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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. Since very large computing times of the order of many years are required for studies of spin glasses, we have adapted our computer codes to the special architecture of the recently installed supercomputer JUMP at NIC/ZAM Jülich.

We also extended our investigations 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. As a first step in this direction we investigated the finite-size scaling behaviour of the free-energy barriers in the SK model which are visible in the probability density of the Parisi overlap parameter. Assuming that the mean barrier height diverges with the number of spins N as N^{α}, our data showed good agreement with the theoretically expected value $\alpha = 1/3$ [8]. This is an important result since by applying precisely the same method of analysis to our data for the short-range EAI model, we obtained a significantly different exponent. As the second main result of our SK model study we found clear evidence that the tails of the barrier-height distribution can be described by the Fréchet extremal-value distibution [8].

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10.3 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.

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10.4 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 (see Fig. 10.1) 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.

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 [6]. For the 4-state Potts model in $d = 3$ dimensions [7], which in the

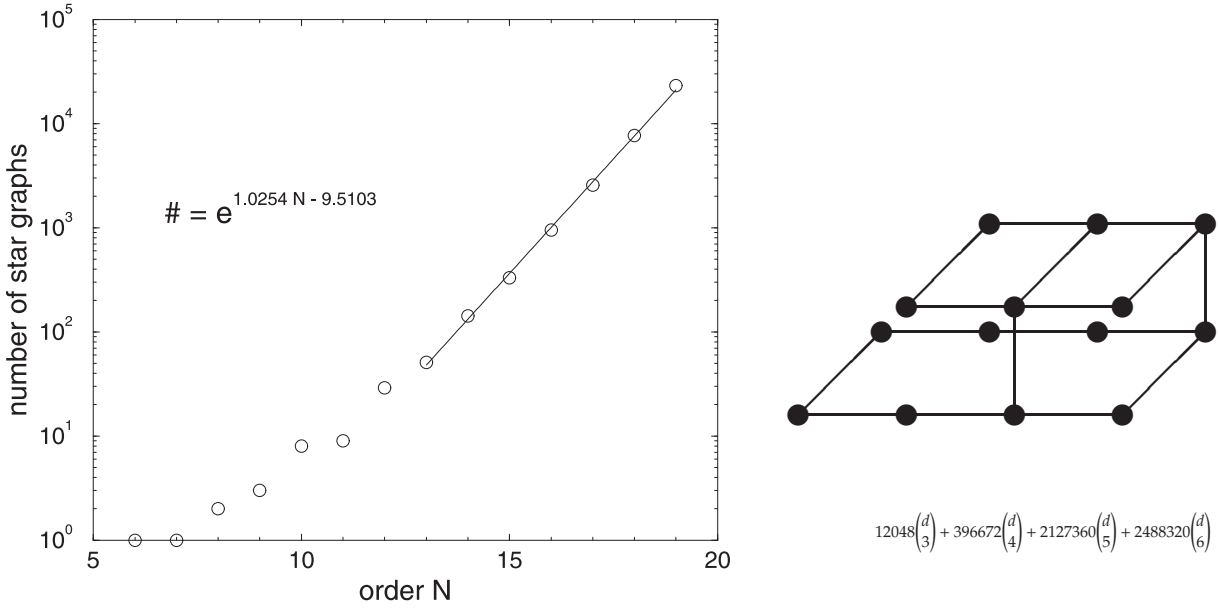

Figure 10.1: *Left*: Growth behaviour of the number of star graphs of order N that can be embedded in hypercubic lattices $\mathbb{Z}^d$. *Right*: A star graph of order 17 and its (weak) embedding number, carrying the dependence on the dimension (up to $d = 6$).

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 [8].

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10.5 Droplet/Strip and Evaporation/Condensation Transitions

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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".

In recent numerical work, Neuhaus and Hager [1] were able to identify such barriers in the magnetisation M of the much simpler two-dimensional Ising model. They first 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, which turned out to be in agreement with earlier analytical considerations of Leung and Zia [2]. 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 $\Delta_c(d)$, 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 (see Fig. 10.2). The fraction λ_Δ of excess particles forming the droplet is given explicitly.

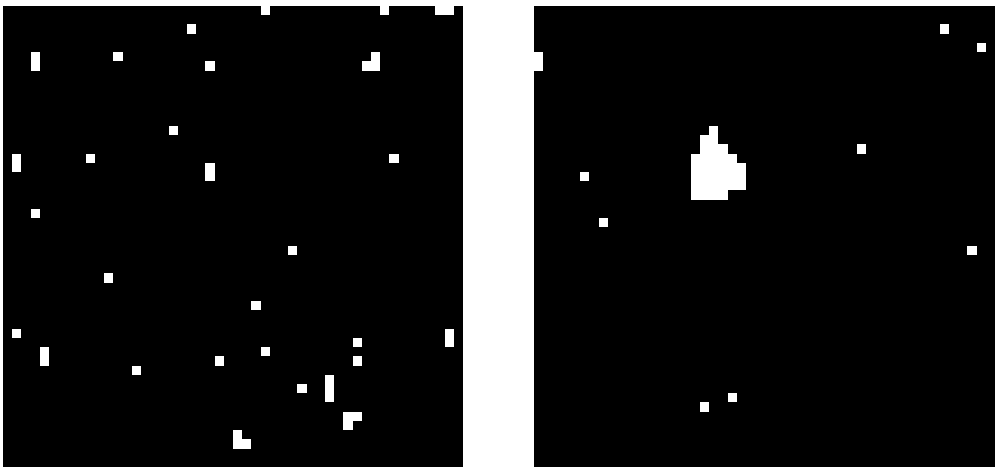

Figure 10.2: Two snapshots of a $L = 50$ Ising system at the same value of the magnetisation. *Left*: Evaporated system, a large number of very small bubbles exists (1 to 3 spins). *Right*: Condensed system, a single large droplet that has absorbed nearly all small bubbles.

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 ($L = 40, \ldots, 640$). Using analytic values for the spontaneous magnetisation m_0, the susceptibility χ and interfacial free energy τ_W for the infinite system, we were able to determine λ_Δ in very good agreement with the theoretical prediction [4, 5]. 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.

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10.6 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 determined 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].

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10.7 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, 8], 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 [3] as far as the order of the transition and the location of the transition point are concerned.

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10.8 Folding Kinetics and Thermodynamics of Coarse-Grained Protein Models

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Functional proteins in a biological organism are typically characterized by a unique three-dimensional molecular structure, which makes the protein selective for individual functions, e.g., in catalytic, enzymatic, and transport processes. In most cases, the free-energy landscape is believed to exhibit a rough shape with a large number of local minima and, for functional proteins, a deep, funnel-like global minimum. This assumed complexity is the reason, why it is difficult to understand how the random-coil conformation of covalently bonded amino acids – the sequence is generated in the ribosome according to a certain genetic sequence in the DNA – spontaneously folds into a well-defined stable "native" conformation within microseconds to seconds. Furthermore, it is expected that there is only a small number of folding paths from any unfolded conformation to this final fold.

Protein folding is hierarchical, i.e, the generation of the sequence (primary structure) is followed by the formation of secondary structures (α-helices, β-sheets, turns) by hydrogen bonding. Eventually, the folding into the "native" conformation, i.e., the tertiary structure, is accompanied by a global conformational transition, which requires

cooperativity of all amino acids in a tertiary protein domain [1]. Effectively, this process is due to the attraction of polar amino acids by the polar aqueous environment, and the resulting effective attractive interaction between hydrophobic amino acids. Therefore, in many cases, a folded protein domain possesses a compact hydrophobic core screened from the solvent by a shell of polar residues.

Computer simulations of protein folding are extremely exhaustive, if all atomic and molecular interactions are involved in the protein model. Since the hydrophobic interaction is expected to be the main driving force in the tertiary folding process, we have studied kinetic and statistical aspects employing and comparing simplified, coarse-grained models, such as the minimalistic hydrophobic-polar (HP) lattice model, different variants of similar off-lattice models (so-called AB-like models), as well as knowledge-based Gō-like C^{α} models. Sophisticated computational methods were applied, e.g., multicanonical chain-growth methods [2] for the lattice models, energy-landscape paving optimization, multicanonical sampling, parallel tempering, as well as molecular dynamics for the off-lattice models. The focus of the kinetic studies was on contact ordering in folding and unfolding events [3, 4], the thermodynamic aspects included the identification of folding channels and, in particular, free-energy landscapes as a function of a suitable system parameter [5, 6, 7].

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10.9 Conformational Transitions and Pseudo-Phase Diagrams of Nongrafted Flexible Polymers and Peptides in a Cavity

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In this project, we have investigated the temperature- and solubility dependence of polymer and peptide adsorption to planar solid substrates. The generalization of our multicanonical chain-growth algorithm [1] enabled us to determine qualitatively the *whole* temperature-solubility pseudo-phase diagram for such a hybrid system within a single simulation [2].

First, we studied the conformational transitions that flexible polymers of different, but finite lengths experience in the adsorption process [2, 3]. We found transitions between various (pseudo-)phases, but only a few of them are expected to be present in the thermodynamic limit of infinite chain length, i.e., the transitions between these phases are phase transitions in the thermodynamic sense. The main phases are separated into the adsorption phases of single-layer compact conformations (AC1), multiple-layer compact structures (AC2), globular, unstructured conformations (so-called surface-attached globules, AG), and expanded, random-coil conformations (AE). In the region

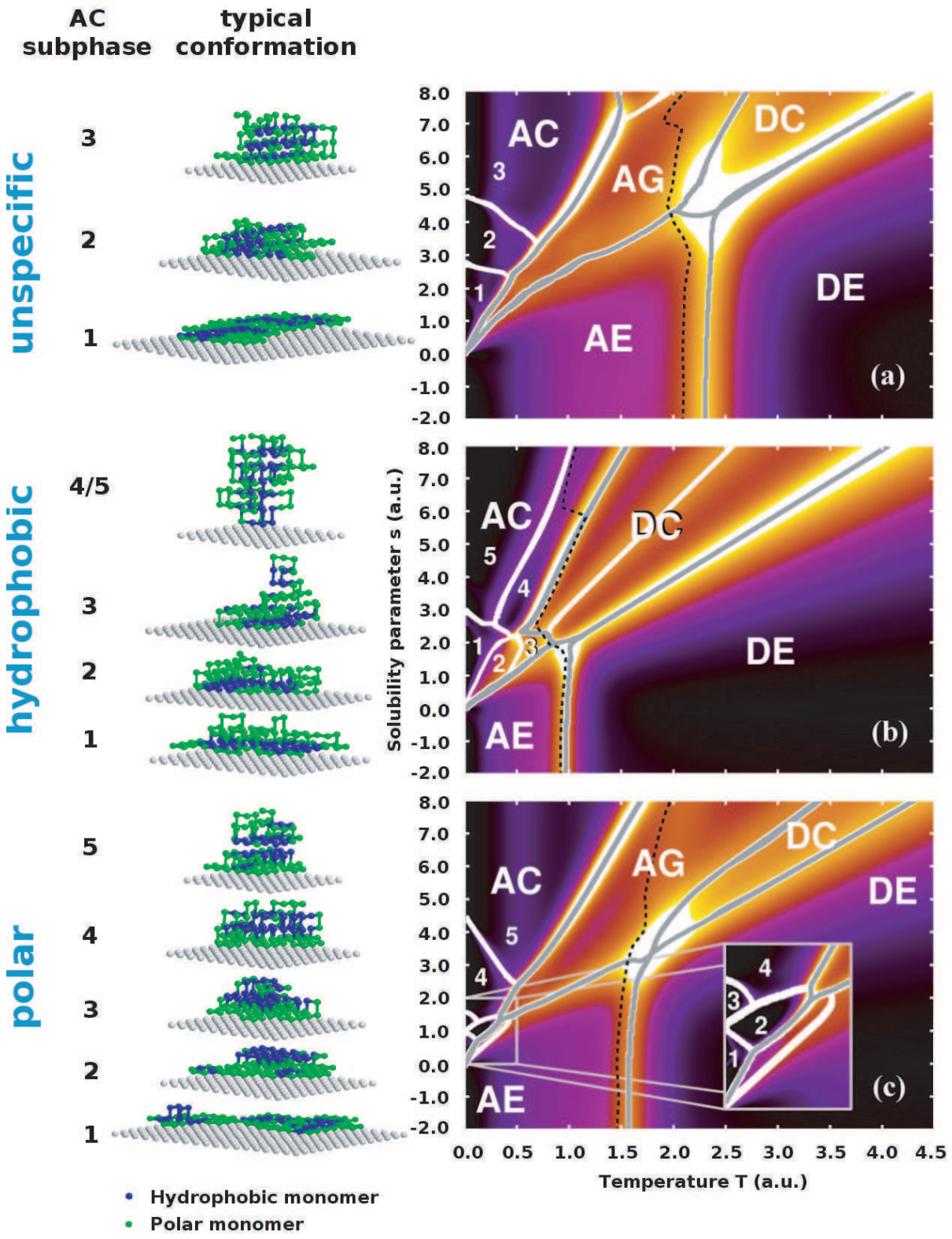

Figure 10.3: Shaded profiles of the specific heats as a function of temperature T and solubility s for a 103-mer in the vicinity of three substrates differing in their affinity to attract hydrophobic and/or polar monomers: (**a**) unspecific, i.e., type-independently attractive, (**b**) hydrophobic, and (**c**) polar. The ridges of this landscape indicate conformational transitions and separate pseudo-phases and subphases (gray and white lines, respectively). Also shown are typical conformations in the respective subphases of the adsorbed-compact (AC) pseudo-phases [4, 5, 6].

of desorbed conformations, we distinguish globular/compact (DC) and random-coil (DE) phases. Furthermore, we find a surprisingly rich structure of subphases, whose properties are highly dependent on the exact number of monomers. Although these subphases are unstable in the thermodynamic limit, they are not less interesting, because with today's high-resolution equipment it should be possible to detect them in experiments. In addition, these subphases might also be of relevance in certain nanotechnological applications.

We also studied the substrate-specificity of the pseudo-phase diagrams for the adsorption of peptides [4, 5, 6]. This project was stimulated by related experiments [7]. We investigated a hydrophobic-polar lattice protein with 103 monomers, whose bulk properties were subject of a recent study [8] in the vicinity of three different substrates. The first was equally attractive to hydrophobic and polar monomers, the second only for hydrophobic, and the third only for polar residues. The specific-heat profile as a function of temperature and solubility is shown in Fig. 10.3. Differences in the locations of the transition lines can be clearly identified as well as the absence of a globular pseudo-phase in the case of the hydrophobic substrate. The most prominent differences appear in the AC phases, where the type-dependence of the concurring forces (surface attraction and intrinsic monomer-monomer interaction) is particularly apparent.

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10.10 Adsorption Specificity of Semiconductor-Binding Synthetic Peptides

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The interest in understanding the mechanism of specific adsorption of polymers and peptides to solid substrates has enormously grown in the past years as the experimental equipment, biochemical structure analysis, and nanotechnology have reached such

a high level of resolution that the vision of practical biochemical and medical applications of hybrid organic-inorganic systems, such as nanoelectronic circuits, nanosensory devices, and pattern recognition by molecular substances, becomes more and more concrete.

The main inspiration for this joint project of theoretical and experimental physicists and biochemists came from recent adsorption experiments of short synthetic peptides with 12 amino acids to semiconductors [1, 2], where the specificity of binding properties was investigated in detail. In these experiments, it could be shown that the interplay of different specific properties of the solid (crystal orientation of the surface, electronic affinity, polarization), the peptide (amino acid content and, in particular, the sequence), and the surrounding solvent (solubility) strongly influence the adsorption of the peptide at the solid-fluid interface [3]. The binding or docking process, which is possibly accompanied by conformational transitions, is not yet understood. Therefore, the main objective of this interdisciplinary cooperation is the unravelling of the principles of peptide adsorption to solids, in particular semiconductors.

Since we expect that structural properties of the peptide fold and, in particular, conformational transitions in the fluid bulk as well as in the vicinity of the substrate have impact on the binding affinity, we have performed, in an inital step, exhaustive computer simulations investigating bulk properties of the peptides used in the experiment [2]. We found indications for helix-coil transitions employing an all-atom protein model based on the ECEPP/3 force field, extended by an implicit-solvent model [4]. As synthetic peptides are typically less stable than bioproteins selected by evolution, it is not yet clear whether these transitions can also be identified in biochemical analyses. Another reason is that the model used cannot predict precise, realistic transition temperatures. For this reason, these results are to be compared with outputs of other models, e.g., the simplified all-atom model with reduced parameter set developed by the Lund group [5]. A future task is to extend this model by an effective interaction between soft and solid matter to make it applicable for simulations of hybrid systems.

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10.11 Geometrical Approach to Phase Transitions

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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].

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10.12 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. Invoking duality arguments, this 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, which thus may play an important role in determining the properties of the λ-transition in liquid helium. 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, 3, 4, 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 obtains in general different percolation thresholds and critical exponents.

In three-dimensional, globally O(2) symmetric theories the percolating objects are vortex lines forming closed networks [6, 7, 8, 9]. 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 involves a certain ambiguity. We want to investigate the influence of the probability of treating such a branching point as a knot, see Fig. 10.4.

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 be-

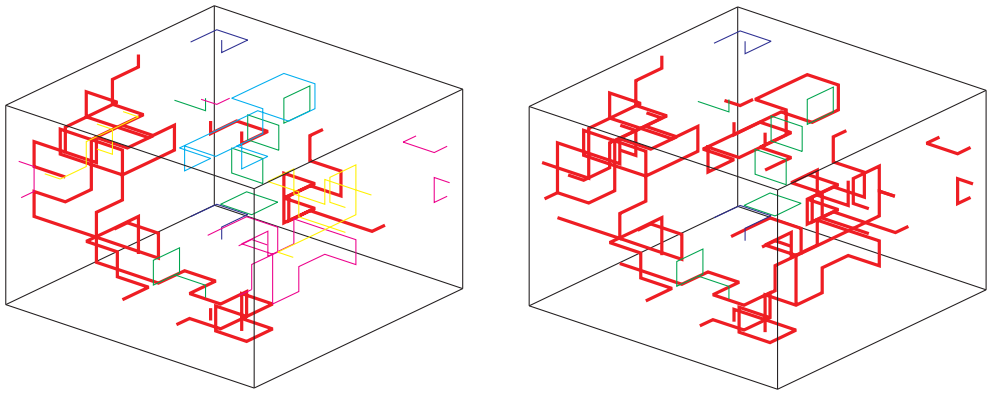

Figure 10.4: *Left*: Vortex-loop network generated at the thermodynamic critical point for lattice size $L = 8$ and probability $c = 0.4$ to treat a branching point as a knot. *Right*: Vortex-loop network generated treating *all* branching points as knots for the same spin configuration as in the left plot.

haviour 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.

The second part of this project concentrates on an extension of the three-dimensional complex Ginzburg-Landau model by adding a minimal coupling to an external compact U(1) gauge field (Abelian Higgs model) [10, 11], 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" (λ–κ) 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 [11], 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.

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10.13 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 performed Monte Carlo studies of the two-dimensional q-state Potts models with $q = 3$ and 8 states per spin which, in equilibrium, exhibit phase transitions of second and first order, respectively. We determined two-time correlators as well as the temporal and spatio-temporal behaviour of 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 results [3, 4] show very 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 [5]. 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 [6] 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 [7].

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10.14 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 susceptibility 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.

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10.15 Quantum Monte Carlo Studies

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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.

Furthermore, the thermodynamic properties (magnetization, isothermal magnetic susceptibility, specific heat) of one- and two-dimensional ferromagnets with arbitrary spin S in a magnetic field are investigated by second-order Green-function theory and compared with quantum Monte Carlo simulations for the $S = 1/2$ chain with $N = 128$ spins and the $S = 1$ ferromagnet on an $N = 64$ chain and an $N = 64 \times 64$ square lattice, employing the so-called stochastic series expansion (SSE) method [11]. Good agreement between the results of both approaches is found [12]. In one dimension and at low magnetic fields, two maxima in the temperature dependence of the specific heat of both the $S = 1/2$ and $S = 1$ ferromagnets are found. For $S > 1$ only one maximum occurs, as in the two-dimensional ferromagnets. This implies that the appearance of two specific-heat maxima is a distinctive effect of quantum fluctuations.

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10.16 Analyses of Partition Function Zeroes

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The distribution of partition function zeroes in the complex magnetic field plane (Lee-Yang zeroes) as well in the complex temperature plane (Fisher zeroes) encode the phase transition properties of statistical physics models. This fact is exploited in this project by developing suitable analyses methods.

Our recently developed technique for the determination of the density of partition function zeroes using data coming from finite-size systems [1] has been extended to deal with cases where the zeroes are not restricted to a curve in the complex plane and/or come in degenerate sets [2]. The efficacy of the approach was demonstrated by application to a number of models for which these features are manifest and the zeroes are readily calculable. Based on this approach properties of higher-order phase transitions could be derived [3].

In another subproject, a Lee-Yang zero approach was used to systematically analyse the exponents of multiplicative logarithmic corrections to scaling which are frequently encountered in the critical behaviour of certain statistical-mechanical systems. As one main result we proposed scaling relations between the exponents of the logarithmic corrections [4]. These proposed relations were then confronted with a variety of results from the literature.

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W. Janke
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W. Janke
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Investigation of Thermodynamic Properties of Lattice and Off-Lattice Models for Proteins and Polymers
M. Bachmann and W. Janke
Deutsche Forschungsgemeinschaft (DFG), Grant No. JA 483/24-1/2

Phasenübergänge in Systemen mit einschränkender Geometrie
W. Janke
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Dozenten der Theoretischen Physik und Mathematik (Sprecher B. Geyer)
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Numerical Simulations of Protein Folding
G. Gökoğlu
Fellowship of TÜBITAK (The Scientifc and Technical Research Council of Turkey)

Spin Glass Physics
D. Yang, A. Nußbaumer and W. Janke
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Physics of Protein Folding P.E. Green, T. Vogel and W. Janke
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W. Janke
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Protein and Polymer Models
M. Bachmann and W. Janke
NIC Jülich (computer time grant for *JUMP*), Grant No. hlz11

Quantum Monte Carlo Simulations
W. Janke
NIC Jülich (computer time grant for *JUMP*), Grant No. hlz12

10.18 Organizational Duties

M. Bachmann

- Scientific Secretary of the Workshop *CompPhys05 – 6. NTZ-Workshop on Computational Physics*, ITP, Universität Leipzig, 1–2 December 2005

E. Bittner

- Scientific Secretary of the Workshop *CompPhys05 – 6. NTZ-Workshop on Computational Physics*, ITP, Universität Leipzig, 1–2 December 2005

W. Janke

- Director of the Naturwissenschaftlich-Theoretisches Zentrum (NTZ) at the Zentrum für Höhere Studien (ZHS), Universität Leipzig
- Chairperson of the Programme Committee "Scientific Computing" of Forschungszentrum Jülich and member of the Scientific-Technical-Council of the Supervisory Board ("Aufsichtsrat") of the Forschungszentrum Jülich GmbH
- Organizer of the CECAM Workshop *Rugged Free Energy Landscapes: Common Computational Approaches in Spin Glasses, Structural Glasses and Biological Macromolecules*, Lyon, France, 6–8 June 2005
- Organizer of the Workshop *ProtFold05 – NTZ-Workshop on Protein Folding and Substrate Specificity: Computational and Experimental Approaches for Studying Biological Macromolecules*, ITP, Universität Leipzig, 16 June 2005
- Organizer of the Workshop *CompPhys05 – 6. NTZ-Workshop on Computational Physics*, ITP, Universität Leipzig, 1–2 December 2005
- Permanent Member of International Advisory Board, *Conference of the Middle European Cooperation in Statistical Physics (MECO)*
- Member of Advisory Committee, *VIELAT05 – 15. Workshop on Lattice Field Theory*, Vienna, Austria, 6–8 October 2005
- Member of Advisory Committee, *COVLAT06 – 16. Workshop on Lattice Field Theory*, Coventry, England, 29 Juni – 1 July 2006
- Member of Local Organizing Committee, international Conference *MG11 – 11th Marcel Grossmann Meeting*, FU Berlin, 23–29 July 2006
- Member of International Program Committee, international Conference *Mathematical Modeling and Computational Physics 2006*, High Tatra Mountains, Slovakia, 28 August – 1 September 2006
- Referee: Phys. Rev. Lett., Phys. Rev. B, Phys. Rev. E, Europhys. Lett., Phys. Lett. A, Phys. Lett. B, Eur. Phys. J. B, Physica A, J. Phys. A, Comp. Phys. Commun., J. Stat. Mech. Theor. Exp., New J. Phys.

10.19 External Cooperations

Academic

- EU RTN-Network *ENRAGE – Random Geometry and Random Matrices: From Quantum Gravity to Econophysics* with 13 teams throughout Europe
- Dept. of Physics, Florida State University, Tallahassee, USA
  Prof. Dr. B.A. Berg
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- Department of Physics, University of Waterloo, Canada
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  Prof. Dr. U. Hansmann, Prof. Dr. P. Grassberger, PD Dr. T. Neuhaus, Dr. S. Mohanty
- Institut für Physik, Universität Mainz
  Prof. Dr. K. Binder, Dr. H.-P. Hsu
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  Prof. Dr. H.-P. Ying, Prof. Dr. B. Zheng

10.20 Publications

Journals

G. Akemann, E. Bittner: *Two-Colour Lattice QCD with Dynamical Fermions at Non-Zero Density versus Matrix Models*, PoS LAT2005, 197 (2005)

G. Akemann, E. Bittner, M.-P. Lombardo, H. Markum, R. Pullirsch: *Density Profiles of the Lowest Eigenvalues of the Dirac operator for Two-Color QCD at Non-Zero Chemical Potential Compared to Matrix Models*, Nucl. Phys. B (Proc. Suppl.) **140**, 568 (2005)

M. Bachmann, H. Arkin, W. Janke: *Multicanonical Study of Coarse-Grained Off-Lattice Models for Folding Heteropolymers*, Phys. Rev. E **71**, 031 906 (2005)

M. Bachmann, W. Janke: *Conformational Transitions of Non-Grafted Polymers Near an Adsorbing Substrate*, Phys. Rev. Lett. **95**, 058 102 (2005)

M. Bachmann, W. Janke: *Conformational Transitions of Heteropolymers*, Comp. Phys. Comm. **169**, 111 (2005)

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

E. Bittner, W. Janke: *Nature of Phase Transitions in a Generalized Complex $|\psi|^4$ Model*, Phys. Rev. B **71**, 024 512 (2005)

E. Bittner, A. Krinner, W. Janke: *Vortex-Line Percolation in the Complex $|\psi|^4$ Model* Phys. Rev. B **72**, 094 511 (2005)

E. Bittner, A. Krinner, W. Janke: *Vortex-Line Percolation in the Three-Dimensional Complex Ginzburg-Landau Model*, PoS LAT2005, 247 (2005)

L. Bogacz, Z. Burda, W. Janke, B. Waclaw: *A Program Generating Homogeneous Random Graphs with Given Weights*, Comp. Phys. Comm. **173**, 162 (2005)

L. Bogacz, W. Janke: *QMC Simulations of Heisenberg Ferromagnet*, PoS LAT2005, 241 (2005)

C. Chatelain, B. Berche, W. Janke, P.-E. Berche: *Monte Carlo Study of Phase Transitions in the Bond-Diluted 3D 4-State Potts Model*, Nucl. Phys. B **719**, 275 (2005)

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

K. Goede, M. Grundmann, K. Holland-Nell, A.G. Beck-Sickinger, M. Bachmann, W. Janke: *Peptide auf neuen Wegen*, BIOforum **10**, 53 (2005)

H. Hellmund, W. Janke: *High-Temperature Series Expansions for Random Potts Models*, Cond. Matter Phys. **8**, 59 (2005)

R. Hilfer, B. Biswal, H.-G. Mattutis, W. Janke: *Multicanonical Simulations of the Tails of the Order-Parameter Distribution of the 2D Ising Model*, Comp. Phys. Comm. **169**, 230 (2005)

W. Janke, B. Berche, C. Chatelain, P.-E. Berche, M. Hellmund: *Quenched Disordered Ferromagnets*, invited plenary talk, PoS LAT2005, 018 (2005)

W. Janke, D.A. Johnston, R. Kenna: *Critical Exponents from General Distributions of Zeroes*, Comp. Phys. Comm. **169**, 457 (2005)

W. Janke, D.A. Johnston, R. Kenna: *Properties of Phase Transitions of Higher Order*, PoS LAT2005, 244 (2005)

W. Janke, A.M.J. Schakel: *Fractal Structure of Spin Clusters and Domain Walls in the Two-Dimensional Ising Model*, Phys. Rev. E **71**, 036 703 (2005)

W. Janke, A.M.J. Schakel: *Geometrical Phase Transitions*, Comp. Phys. Comm. **169**, 222 (2005)

W. Janke, A.M.J. Schakel: *Fractal Structure of High-Temperature Graphs of O(N) Models in Two Dimensions*, Phys. Rev. Lett. **95**, 135 702 (2005)

W. Janke, M. Weigel: *Simulations of the F Model on Planar* ϕ^4 *Feynman Diagrams*, PoS LAT2005, 251 (2005)

A. Nußbaumer, E. Bittner, W. Janke: *Evaporation/Condensation of Ising Droplets*, PoS LAT2005, 252 (2005)

R. Schiemann, M. Bachmann, W. Janke: *Exact Sequence Analysis for Three-Dimensional Hydrophobic-Polar Lattice Proteins*, J. Chem. Phys. **122**, 114 705 (2005)

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

M. Weigel, W. Janke: *The F Model on Dynamical Quadrangulations*, Nucl. Phys. B **719**, 312 (2005)

M. Weigel, W. Janke: *The Square-Lattice F Model Revisited: A Loop-Cluster Update Scaling Study*, J. Phys. A **38**, 7067 (2005)

S. Wenzel, E. Bittner, W. Janke, A.M.J. Schakel, A. Schiller: *Kertész Line in the Three-Dimensional Compact U(1) Lattice Higgs Model*, Phys. Rev. Lett. **95**, 051 601 (2005)

S. Wenzel, E. Bittner, W. Janke, A.M.J. Schakel, A. Schiller: *Vortex Proliferation and the Dual Superconductor Scenario for Confinement: The 3D Compact U(1) Lattice Higgs Model*, PoS LAT2005, 248 (2005)

Journals January–March 2006

M. Bachmann, W. Janke: *Substrate Specificity of Peptide Adsorption: A Model Study*, Phys. Rev. E **73**, 020 901(R) (2006)

M. Bachmann, W. Janke: *Chain-Growth Simulations of Lattice-Peptide Adsorption to Attractive Substrates*, in *Proc. NIC Symp. 2006*, ed. by G. Münster, D. Wolf, M. Kremer, NIC Series, Vol. **32** (John von Neumann Institute for Computing, Jülich 2006) p 245

M. Bachmann, W. Janke: *Substrate Adhesion of a Nongrafted Polymer in a Cavity*, Phys. Rev. E **73**, 041 802 (2006)

E. Bittner, W. Janke: *Free-Energy Barriers in the Sherrington-Kirkpatrick Model*, Europhys. Lett. **74**, 195 (2006), arXiv:cond-mat/0603526

W. Janke, E. Bittner: *Phase Transitions in a Generalized $|\psi|^4$ Model*, Proc. 8th Int. Conf. *Path Integrals from Quantum Information to Cosmology*, Prague, Czech Republic, 6–10 June 2005, ed. by Č. Burdik, O. Navrátil, S. Pošta (JINR Press, Dubna 2006) (www.jinr.ru/publish/Proceedings/Burdik-2005/index.html)

W. Janke, D.A. Johnston, R. Kenna: *Properties of Higher-Order Phase Transitions*, Nucl. Phys. B **736**, 319 (2006)

R. Kenna, D.A. Johnston, W. Janke: *Scaling Relations for Logarithmic Corrections*, Phys. Rev. Lett. **96**, 115 701 (2006)

In press

W. Janke: *Introduction to Monte Carlo Simulations*, Leipzig preprint (February 2006), Lecture Notes, to appear in: *Ageing and the Glass Transition*, Summer School, University of Luxembourg, September 2005 (in press)

W. Janke, A.M.J. Schakel: *Two-Dimensional Critical Potts and its Tricritical Shadow World*, Leipzig/FU Berlin preprint (October 2005), to appear in Braz. J. Phys. (in press)

Talks

G. Akemann, E. Bittner: *Two-Colour Lattice QCD with Dynamical Fermions at Non-Zero Density versus Matrix Models*, XXIII Int. Symp. Latt. Field Theory, Dublin, July 25–30

M. Bachmann: *Thermodynamic Aspects of Coarse-Grained Heteropolymer Folding*, CECAM Workshop *Rugged Free Energy Landscapes: Common Computational Approaches in Spin Glasses, Structural Glasses and Biological Macromolecules*, Lyon, June 6–8

M. Bachmann: *Minimalistic Models for Substrate Adsorption of Polymers and Peptides*, Workshop ProtFold05, Leipzig, June 16

M. Bachmann: *Polymers Astray: Folding and Binding Near Attractive Substrates*, Theory Seminar of the Computational Biology & Biological Physics Group, Lund University, September 19

M. Bachmann: *Conformational Transitions of Polymers and Peptides near Attractive Substrates*, Workshop CompPhys05, Leipzig, December 1–3

E. Bittner, A. Krinner, W. Janke: *Vortex Line Percolation in the Three-Dimensional Complex Ginzburg-Landau Model*, DPG-Frühjahrstagung, Berlin, March 4–9

E. Bittner, W. Janke: *Free-Energy Barriers in the Sherrington-Kirkpatrick Model*, CECAM Workshop, Lyon, June 6–8

E. Bittner, A. Krinner, W. Janke: *Vortex-Line Percolation in a Three-Dimensional Complex Ginzburg-Landau Model*, XXIII Int. Symp. Latt. Field Theory, Dublin, July 25–30

E. Bittner, A. Krinner, W. Janke: *Phase Transitions in a Generalized Complex Ginzburg-Landau Model*, VIELAT05, 15. Workshop Latt. Field Theory, TU Wien, October 6–8

E. Bittner: *Complex Eigenvalues of the Dirac Operator in Two-Color QCD with Chemical Potential*, Brunel University, London, November 20–23

E. Bittner, W. Janke: *Free-Energy Barriers in a Mean-Field Spin-Glass Model*, Workshop CompPhys05, Leipzig, December 1–3

L. Bogacz, W. Janke: *QMC Simulations of Heisenberg Ferromagnet*, XXIII Int. Symp. Latt. Field Theory, Dublin, July 25–30

L. Bogacz, W. Janke: *Quantum Monte Carlo Simulations of Ferromagnetic Chains*, Workshop CompPhys05, Leipzig, December 1–3

P. Crompton, R. Bischof, W. Janke, S. Wenzel: *Quantum Phase Transitions in Inhomogeneous Spin Chains*, DPG-Frühjahrstagung, Berlin, March 4–9

W. Janke: *Monte Carlo Simulations of the 3D Bond-Diluted Potts Model*, DPG Frühjahrstagung, Berlin, March 4–9

W. Janke: *High-Temperature Series Expansions for Diluted Magnets*, 30th Conf. Middle Eur. Coop. Stat. Phys. (MECO30), Cortona, Italy, April 3–6

W. Janke: *Lecture Series on Monte Carlo Simulations in Statistical Physics, Ising Lectures*, Lecture I: *Introduction to Monte Carlo simulations*, Lecture II: *Improved algorithms and generalised ensembles*, Lecture III: *Applications to disordered systems*, Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, University of Lviv, Ukraine, May 17–20

W. Janke: *Phase Transitions in a Generalized $|\psi|^4$ Model*, 8th Int. Conf. *Path Integrals: From Quantum Information to Cosmology*, Prague, Czech Republic, June 6–10

W. Janke: *2D Quantum Gravity: Fluctuating Graphs and Quenched Connectivity Disorder*, series of three lectures, Mochima Theoretical Physics Spring School, Joint CEA-IVIV-SFP-Workshop on *Foundations of Statistical and Mesoscopic Physics*, Mochima, Venezuela, June 20–24

W. Janke: *The F Model on Dynamical Quadrangulations*, *Lattice 2005*, Trinity College, Dublin, Ireland, July 25–30

W. Janke: *Quenched Disordered Ferromagnets*, plenary talk, *Lattice 2005*, Trinity College, Dublin, Ireland, July 25–30

W. Janke: *Geometrical Approach to Phase Transitions*, IV Brazilian Meeting on Simulational Physics, Ouro Preto, Brasil, August 10–12

W. Janke: *Introduction to Computer Simulations*, series of lectures, Summer School *Ageing and the Glass Transition*, University of Luxembourg, September 18–24

W. Janke: *Multicanonical Chain Growth Simulations and Exact Enumerations of Lattice Proteins*, VIELAT05 15th Workshop Latt. Field Theory, Vienna University of Technology (VUT), Austria, October 6–8

W. Janke: *Percolating Geometrical Excitations – Critical vs. Tricritical*, VIELAT05 15th Workshop Latt. Field Theory, Vienna University of Technology (VUT), Austria, October 6–8

A. Nußbaumer, E. Bittner, W. Janke: *Evolution of Equilibirum Droplets*, DPG-Frühjahrstagung, Berlin, March 4–9

A. Nußbaumer, E. Bittner, W. Janke: *Evaporation/Condensation of Ising Droplets*, XXIII Int. Symp. Latt. Field Theory, Dublin, July 25–30

A.M.J. Schakel, W. Janke: *Fractal Structure and Critical Properties of Planar Loops*, DPG Frühjahrstagung, Berlin, March 4–9

S. Wenzel, E. Bittner, W. Janke, A.J.M. Schakel, A. Schiller: *Kertész Line in the 3D U*(1) *Abelian Higgs Model*, XXIII Int. Symp. Latt. Field Theory, Dublin, July 25–30

Poster

M. Bachmann, K. Goede, W. Janke, M. Grundmann: *Bindungsspezifität von Peptiden auf Halbleiteroberflächen*, DPG-Frühjahrstagung Berlin, March 4–9

M. Bachmann, W. Janke: *Conformational Phase Diagram of Nongrafted Polymer near Adsorbing Substrate*, 30th Conf. Middle Eur. Coop. Stat. Phys. (MECO30), Cortona, April 3–6

M. Bachmann, K. Goede, W. Janke, M. Grundmann: *Bindungsspezifität von Peptiden auf Halbleiteroberflächen*, 4th Biotechnol. Symp., Leipzig, June 3

E. Bittner, A. Krinner, W. Janke: *Vortex-Line Percolation in a Three-Dimensional Complex $|\psi|^4$ Model*, 30th Conf. Middle Eur. Coop. Stat. Phys. (MECO30), Cortona, April 3–6

W. Janke, M. Hellmund: *Series Expansions for Disordered Potts Models*, DPG Frühjahrstagung, Berlin, March 4–9

A. Kallias, M. Bachmann, W. Janke: *Crystallization of Two-Dimensional Off-Lattice Lennard-Jones Polymers*, DPG-Frühjahrstagung Berlin, March 4–9

E. Lorenz, W. Janke: *Phase-Ordering and Aging Phenomena in Potts Models*, DPG-Frühjahrstagung Berlin, March 4–9

A. Nußbaumer, W. Janke, T. Neuhaus: *Evaporation/Condensation of Ising Droplets*, 30th Conf. Middle Eur. Coop. Stat. Phys., Cortona, April 3–6

A. Nußbaumer, E. Bittner, W. Janke, T. Neuhaus; *Evaporation/Condensation of Ising Droplets*, Workshop CompPhys05, Leipzig, December 1–3

S. Schnabel, M. Bachmann, W. Janke: *Folding Channels in Coarse-Grained Heteropolymer Models*, DPG-Frühjahrstagung Berlin, March 4–9

T. Vogel, M. Bachmann, W. Janke: *Coarse-Grained Heteropolymer Models: On-Lattice vs. Off-Lattice*, DPG-Frühjahrstagung Berlin, March 4–9

T. Vogel, M. Bachmann, W. Janke: *Coarse-Grained Lattice and Off-Lattice Heteropolymer Models*, 30th Conf. Middle Eur. Coop. Stat. Phys. (MECO30), Cortona, April 3–6

T. Vogel, M. Bachmann, W. Janke: *Coarse-Grained Heteropolymer Models: On-Lattice vs. Off-Lattice*, 4th Biotechnol. Symp., Leipzig, June 3

T. Vogel, M. Bachmann, W. Janke: *HP Proteins on Generalized Lattices*, 3rd Day of Biotechnology, Leipzig, May 19

10.21 Graduations

Diploma

- Eric Lorenz
  Aeging Phenomena in Phase-Ordering Kinetics in Potts Models
  07/2005

- Stefan Schnabel
  Thermodynamische Eigenschaften und Faltungskanäle von Coarse-Grained Heteropolymeren
  07/2005
- Anna Kallias
  Thermodynamics and Folding Kinetics of Coarse-Grained Protein Models
  09/2005
- Jakob Schluttig
  Molecular Mechanics of Coarse-Grained Protein Models
  10/2005

10.22 Guests

- Dipl.-Phys. Sebastian Brandt
  Washington University, St. Louis, USA
  January 06–07, 2005
- Prof. Dr. Yurij Holovatch
  Lviv, Ukraine
  January 17–19, 2005
- Prof. Dr. Hans-Jörg Hofmann
  Institut für Biochemie, Universität Leipzig
  January 20, 2005
- Prof. Dr. Bo Zheng
  Zhejiang University, Hangzhou, P.R. China
  February 03, 2005
- Dr. Christiane P. Koch
  Orsay, France
  March 31 – April 04, 2005
- Thomas Weikl
  MPI Golm
  April 21, 2005
- Prof. Dr. Bernd A. Berg
  Florida State University, Tallahassee, USA
  May – August 2005
- Prof. Dr. Anders Irbäck
  Lund University, Sweden
  June 14–17, 2005
- Dr. Sandipan Mohanty
  Lund University, Sweden
  June 14–17, 2005
- Patrick E. Green
  Ohio University, Athens/Ohio, USA
  June – August 2005

- David Yang
  Simon Fraser University, Canada
  June – August 2005
- Prof. Dr. Hans Gerd Evertz
  TU Graz, Österrreich
  July 06–08, 2005
- Prof. Dr. Tarik Celik
  Ankara, Turkey
  June – July 2005
- Prof. Dr. David P. Landau
  University of Georgia, Athens, GA, USA
  July 20–22, 2005
- Dr. Flavio Nogueira
  FU Berlin
  November 11, 2005
- Prof. Dr. Bernd A. Berg
  Florida State University, Tallahassee, USA
  November 21–25, 2005
- Prof. Dr. Anders Irbäck
  Lund University, Sweden
  November 29 – December 2
- Simon Mitternacht
  Lund University, Sweden
  November 29 – December 2
- Prof. Dr. Desmond A. Johnston
  Heriot-Watt University, Edinburgh, UK
  November 30 – December 4, 2005
- Dr. Ralph Kenna
  Coventry University, UK
  November 30 – December 4, 2005
- Prof. Dr. Kurt Binder
  Universität Mainz
  December 1–2, 2005
- Prof. Dr. Harald Markum
  TU Wien, Österreich
  December 1–4, 2005
- Dr. Martin Weigel
  University of Waterloo, Canada
  December 1–7, 2005