14.4. Computational Quantum Field Theory (CQT)

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 diluted magnets, spin glasses and other physical systems with random, quenched disorder, fluctuating geometries with applications to quantum gravity (e.g., dynamical triangulations), soft condensed matter physics (e.g., membranes and interfaces), and biologically motivated problems (e.g., lattice models for protein folding).

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 attacked at a recently installed Beowulf cluster with 40 Athlon MP1800+ CPU's and at national supercomputing centres on T3E and Hitachi parallel computers. This combination gives good training opportunities for the students and offers promising job perspectives 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, Italy, Russia, Spain, Taiwan, and the United States.

14.4.1. Multi-Overlap Monte Carlo Simulations of Spin Glasses

B. A. Berg (Florida State University, Tallahassee), A. Billoire (CEA/Saclay, Gif-sur-Yvette), W. Janke and A. Nußbaumer

Spin glasses are examples for an important class of materials with random and competing interactions between magnetic moments [1]. As a consequence, no unique spin configuration is favoured by all interactions ("frustration") and the free energy exhibits a rugged landscape with many minima and maxima separated by barriers. Among the main objectives of the project are investigations of the scaling behaviour of those barriers with system size using multi-overlap Monte Carlo simulations [2], which can be optimally tailored [3] for the sampling of rare-events. We focused first on the free-energy barriers F_B^q in the probability density $P_{\mathcal{J}}(q)$ of the Parisi overlap parameter q [4] which can be defined in terms of the autocorrelation times τ_B^q of auxiliary Markov chains. In both three and four dimensions [5] we found that the numerically obtained scaling behaviour is quite far off the $D \to \infty$ mean-field prediction.

We further analyzed the tails of the averaged probability density $P(q)$ in the limit $q \to \pm 1$. Again the consistency of the data with mean-field predictions is at best qualitative [6]. On the other hand, in 3D at and below the critical temperature, we obtained striking agreement over about 80 orders of magnitude with the statistics of extremes [7–9], which predicts a characteristic large x fall-off behaviour of the form $f(x) \sim \exp(-a\, e^x)$, $a > 0$ (Gumbel's law) for the tails. This result seems to be specific to spin glasses, since a completely analogous simulation study for the 3D Ising model (measuring also $P(q)$) [10] led to a much better description of the tails in terms of standard Boltzmann scaling.

Currently we are developing further improvements of the multi-overlap method which will eventually enable us to study the spin-glass phase at lower temperatures than previously.

Work partially supported by the German-Israel-Foundation (GIF) under grant No. I-653-181.14/1999, and by computer-time grants at NIC Jülich and CEA Grenoble.

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14.4.2. Monte Carlo Simulations of Disordered Magnets

B. Berche (Université Nancy), P.-E. Berche (Université Rouen), C. Chatelain (Université Nancy) 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 analytical and numerical studies have concentrated on two-dimensional (2D) models with site- or bond-dilution or bond-disorder [1]. Generically one expects that, under certain conditions, a first-order phase transition of the pure system is softened by quenched randomness to a second-order transition and that the critical behaviour associated with a second-order phase transition is modified (Harris criterion) [2]. The softening effect has been observed experimentally for the isotropic-nematic transition of liquid crystals confined into the pores of aerogels consisting of multiply connected internal cavities [3]. While experimentalists [3] tend to explain the softening by the influence of random fields or random uniaxial anisotropies, the random disorder chosen in an exploratory Monte Carlo (MC) simulation [4] is coupled to the energy density and thus more akin to bond-dilution.

In three dimensions (3D), numerically mainly the critical behaviour of the Ising model with site-dilution [5] has been studied and found in good agreement with extensive field theoretic calculations. For systems exhibiting a first-order phase transition in the pure case, large-scale simulations have only been performed for the 3-state Potts model with site-dilution [6]. In 3D one expects that the first-order nature persists for small dilutions up to a (tricritical) dilution from where on the softening to a second-order transition should be observed, until the transition completely vanishes at the percolation point.

Since the undiluted 3D 3-state Potts model exhibits a very *weak* first-order transition [7], the observed softening from a certain dilution threshold on did not appear very stringent. We therefore chose the 4-state Potts model where the transition is known to be *strongly* of first order in the pure case. And in order to be able to compare with other techniques such as series expansions applied to the same model, we considered bond-dilution instead of site-dilution. In a first step the phase diagram in the dilution-temperature ($p-T$) plane was determined from the location of the susceptibility maxima for a moderate system size (16^3) [8], in good agreement with complementary analyses of high-temperature series expansions [9] and with an "effective medium" approximation [10]. A more detailed comparison with the series expansions as well as analyses of autocorrelation times gave a first estimate of the boundary between the regimes of first- and second-order phase transitions, i.e., the location of the tricritical point. By using multicanonical resp. multibondic simulations the regime of first-order transitions was studied quantitatively by determining the latent heat and interface tension. In the regime of second-order transitions the Swendsen-Wang cluster MC update algorithm was used for FSS analyses at two selected dilutions. Since the fluctuations between different disorder realizations turned out to be quite large (see Fig. 1), many different realizations (1 000 – 5 000) had be be averaged. The properties of the disorder distributions (average vs. medium values, long-tail behaviour, (non-) self-averaging etc.) have also been studied and compared with scaling predictions. Presently we are investigating the correlations of thermodynamic quantities such as the susceptibility with the clustering properties of the underlying random bond configurations.

Preliminary results of a comparative MC study of the bond-diluted 3D Ising model are reported in Ref. [11].

The project is partially supported by the DAAD through a collaborative PROCOPE re-

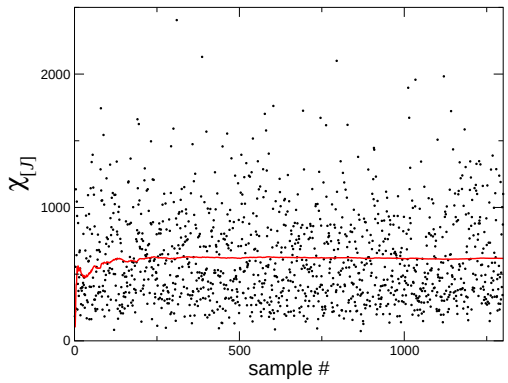

Figure 1. Distribution of susceptibility measurements on a 96^3 lattice at $T_{\rm sim} \approx T_{\chi_{\rm av}^{\rm max}}$ for dilution $p = 0.56$.

search grant, by the German-Israel-Foundation (GIF) under grant No. I-653-181.14/1999, the EU-Network HPRN-CT-1999-000161 "Discrete Random Geometries: From Solid State Physics to Quantum Gravity", the ESF-Network "Challenges in Molecular Simulations: Bridging the Length- and Time-Scale Gap (SIMU)", and the computer-time grants hlz061 of NIC, Jülich, h0611 of LRZ München, C2000-06-20018 of CINES and C2000015 of CRIHAN.

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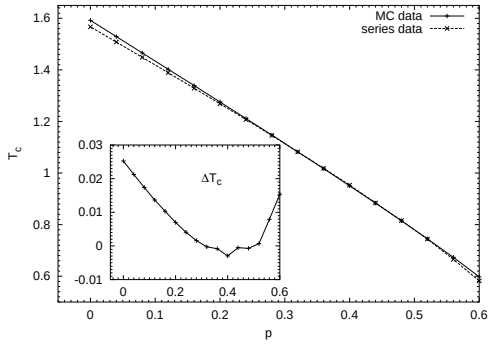
14.4.3. Series Expansions for Random-Bond Models and Spin Glasses

M. Hellmund 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.



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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14.4.4. Effects of Connectivity Disorder on the Potts Model

W. Janke, M. Weigel and A. Wernecke

In the context of quenched disorder, the influence of uncorrelated, geometrically regular types of disorder such as the random dilution of bonds or sites or the random variation of coupling strengths found in spin glasses has been extensively explored, see, e.g., [1,2]. On the other hand, systems subject to *geometrical* disorder, which differs from the former type of randomness first of all in the strong correlation of the disorder degrees of freedom, have not received comparable attention.

In the case of quasi-crystals, the relevance of these types of disorder for the (critical) behaviour of matter models coupled to such random lattices can be judged by means of the so-called Harris-Luck criterion [3,4]. We consider two types of lattices with connectivity disorder, so-called Voronoï-Delaunay random lattices and the planar ϕ^3 random graphs occurring in discrete approaches to quantum gravity. By means of numerical methods, we determine the *wandering exponent* [4] of these lattice types, which is an essential input of the Harris-Luck criterion.

For the three-state Potts model, this analysis implies that disorder of the Voronoï-Delaunay type should be relevant, which is in contrast to previous observations [5]. Extensive investigations of this system by means of Monte Carlo simulations show that the predictions of the Harris-Luck criterion are correct. The contradiction to the prior results of Ref. [5] are tracked down to the much smaller lattices used there, since in this system the crossover from the pure to the disorder fixed point occurs only very close to the critical point.

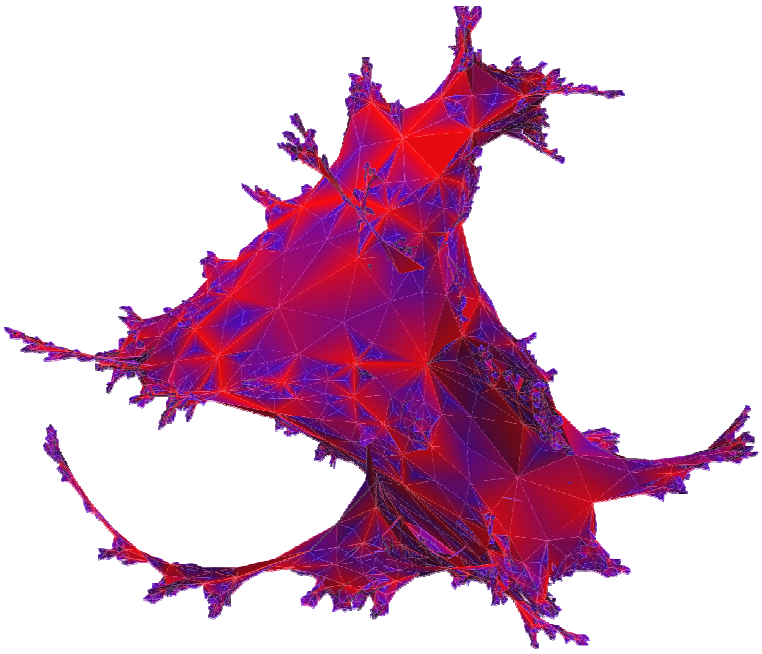

Figure 1. Example of a triangulation dual to the planar ϕ^3 random graphs.

Parallel to the study of the Voronoï-Delaunay case we have also investigated the three-state Potts model on quenched, random ϕ^3 graphs (see Fig. 1), where the Harris-Luck criterion sug-

gests a stronger influence of the connectivity disorder. This expectation is clearly supported by the simulational results [6]. Already for moderate system sizes we obtain significantly altered critical exponents as compared to the pure case. In addition self-averaging properties of geometric and thermodynamic quantities are carefully measured and analyzed within the framework of recent finite-size scaling theories.

This work was supported through the EC network HPRN-CT-1999-000161 "Discrete Random Geometries: From Solid State Physics to Quantum Gravity" and the ESF network "Geometry and Disorder: From Membranes to Quantum Gravity". MW was supported by the DFG through the Graduiertenkolleg "QFT".

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14.4.5. Ising Model on "Fat" and "Thin" Random Graphs

B. P. Dolan (National University of Ireland, Maynooth), W. Janke, D. A. Johnston (Heriot-Watt University, Edinburgh) and M. Stathakopoulos (Heriot-Watt University, Edinburgh)

For the Ising model on fluctuating planar ("fat") ϕ^4 random graphs and their dual quadrangulations we show that in the thermodynamic limit the locus of Fisher zeroes [1] can be determined exactly [2,3] by matching up [4] the analytically known [5] real part of the high- and low-temperature branches of the free energy. We also point out that results for the zeroes on finite graphs may be obtained with rather less effort than might appear necessary at first sight [6] by simply reverting the series expansion of a function $g(z)$ which appears in the solution [5] and taking a logarithm [2]. Unlike regular 2D lattices where numerous unphysical critical points exist with non-standard exponents, on planar ϕ^4 graphs the Ising model displays only the physical transition at $c = \exp(-2\beta) = 1/4$ and a mirror transition at $c = -1/4$ both with KPZ/DDK exponents ($\alpha = -1, \beta = 1/2, \gamma = 2$). The relation between the ϕ^4 locus and that of the dual quadrangulations is akin to that between the (regular) triangular and honeycomb lattices since there is no self-duality. By exploiting the fact that the Ising model on dynamical "fat" graphs has also been solved in the presence of an external magnetic field [5], we furthermore discuss the so-called Kertész line [7].

Moreover, using a similar approach, we calculated the Fisher zeroes for Ising and Potts models on non-planar ("thin") random graphs and noted that the locus of Fisher zeroes is identical to that on a Bethe lattice [8]. Since the number of states q of the Potts model appears as a parameter in the solution, the limiting locus of chromatic zeroes is accessible as well [8]. And along similar lines also the Lee-Yang zeroes have recently been discussed [9].

Work partially supported by the DAAD grant 313-ARC-XII-98/41, the EU-Network HPRN-CT-1999-000161 "Discrete Random Geometries: From Solid State Physics to Quantum Gravity", and the ESF-Network "Geometry and Disorder: From Membranes to Quantum Gravity".

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14.4.6. The 6-Vertex Model on Quantum-Gravity Graphs

W. Janke, D. A. Johnston (Heriot-Watt University, Edinburgh) 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 [1]. There, the necessary integration over all metric tensors as the dynamic variables of the theory occurring in the path-integral ansatz, 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 [2] and generating functions [3] allow for an exact solution of the pure gravity model in two dimensions. Furthermore, matrix models can be formulated for the coupling of classic spin models of statistical mechanics, such as the Ising, Potts or O(n) models, to the random graphs and some of them could be solved analytically [4]. More generally, the transformation or "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 [5], in agreement with all known exact solutions.

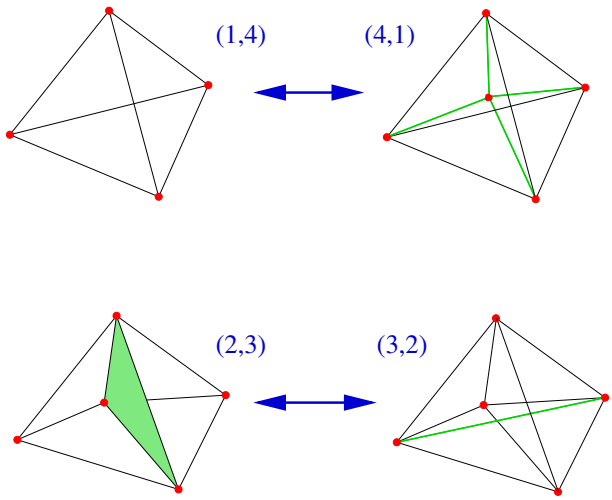

Figure 1. Illustration of the so-called Pachner moves employed for updating triangulated geometries.

One of the most general classes of models in statistical mechanics is given by Baxter's 8-vertex model [6], which includes as limiting cases most of the more well-known models such as the Ising and Potts models and exhibits an exceptionally rich phase diagram with lines of first- and second-order transitions as well as critical and multi-critical points. 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 coupled to quantum gravity could recently be achieved [7], the general model could not yet be solved. Thus, one has to revert to numerical techniques, especially Monte Carlo simulations of the combined system.

Heading for the simulation of 6- and 8-vertex models, one first has to ensure the correct

functioning of a dynamics for the (quite unorthodox) geometry of four-valent graphs, corresponding to 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 against available exact solutions for the case of the Ising model. While for the 3-valent case the so-called Pachner moves, depicted in Figure 1 above, are known to be an ergodic set of updates [8], it is found that for the case of the ϕ^4-graphs one has to add a special "two-link flip" along self-energy insertions to ensure ergodicity there also [9]. Due to the fractal structure of the underlying 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 set of update moves known as minBU surgery algorithm [10].

Combining the developed techniques, we study the F model, a symmetric case of the 6-vertex model, coupled to planar random ϕ^4 graphs by means of a set of Monte Carlo simulations. On regular as well as random lattices, this model is expected to exhibit a Kosterlitz-Thouless type phase transition to an anti-ferroelectrically ordered state [6,7]. We find the numerical analysis of this model to be exceptionally difficult due to the combined effect of the highly fractal structure of the lattices and the presence of strong logarithmic corrections. Thus, the analysis is hampered by rather extreme finite-size effects, the expected asymptotical behaviour not quite being reached with the accessible system sizes. Nevertheless, a scaling analysis of the staggered polarizability yields results in agreement with the predictions of Ref. [7] as far as the order of the transition and the location of the transition point are concerned.

This work was supported by the DAAD through the research grant 313-ARC-XII-98/41, the EC network HPRN-CT-1999-000161 "Discrete Random Geometries: From Solid State Physics to Quantum Gravity" and the ESF network "Geometry and Disorder: From Membranes to Quantum Gravity". MW was supported by the DFG through the Graduiertenkolleg "QFT".

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14.4.7. Quantum Gravity with Matter Fields in Four Dimensions

E. Bittner, W. Janke and H. Markum (TU Wien)

A very efficient method for numerical studies of general relativity was suggested by Regge [1]. In this method a simplicial approximation is applied to a space-time manifold. The underlying lattice has fixed connectivities and the link lengths are taken as gravitational degrees of freedom. The Discrete Regge Model [2] employed in this work is structurally and computationally much simpler than the Standard Regge Calculus. Here the squared link lengths are restricted to only two possible values, both always compatible with the triangle inequalities.

Spin systems coupled to d-dimensional manifolds are studied as a simple example for matter fields coupled to gravity. To access the accuracy of the simplified formulation, we considered both versions of quantum Regge calculus and coupled these manifolds with Z_2 (Ising) spins [3]. We used the path-integral quantization of the theory and studied the partition function

$$Z = \sum_s \int \mathcal{D}\mu(q) \exp\left[-I(q) - KE(q,s)\right], \tag{1}$$

where the path-integral measure $\mathcal{D}\mu(q)$ was chosen as in our pure gravity simulations [4]. The Einstein-Hilbert action of gravitation

$$I(q) = -\beta_g \sum_t A_t \delta_t + \sum_i (\lambda V_i + a\frac{\delta_i^2}{A_i}) \tag{2}$$

consists of a curvature term with the gravitational coupling β_g, a volume term with the cosmological constant λ, and a squared curvature with coupling a. The deficit angle is denoted by δ_t, and A_t and A_i are triangular and barycentric areas, respectively. The energy of the matter field

$$E(q,s) = \frac{1}{2} \sum_{\langle ij \rangle} A_{ij} \frac{(s_i - s_j)^2}{q_{ij}} \tag{3}$$

results from the Ising spins $s_i = \pm 1$, which are located at the vertices i of the lattice. Here A_{ij} are barycentric areas associated with the edges $\langle ij \rangle$.

In our Monte Carlo simulations, the gravitational degrees of freedom of the partition function (1) were updated with the heat-bath algorithm. For the Ising spins we employed the single-cluster algorithm [5]. Between measurements we performed $n = 10$ Monte Carlo steps consisting of one lattice sweep to update the squared link lengths q_{ij}, followed by two single-cluster flips to update the spins s_i. The simulations were done for cosmological constant $\lambda = 0$, $a = 0$ and gravitational coupling $\beta_g = -4.665$. This β_g-value corresponds to a phase transition of the pure Discrete Regge Model [6]. The lattice topology is given by triangulated tori of size $N_0 = L^4$ with $L = 3$ up to 10. From short test runs we estimated the location of the phase transition of the spin model and set the spin coupling $K_0 = 0.024 \approx K_c$ in the long runs. After an initial equilibration time we took about 100 000 measurements for each lattice size. Analyzing the time series we found integrated autocorrelation times for the energy and the magnetization in the range of unity for all lattice sizes. To extract the critical exponent ratio γ/ν we used a finite-size scaling ansatz according to mean-field theory with logarithmic corrections

$$\chi \propto (L(\log L)^{\frac{1}{4}})^{\gamma/\nu} \tag{4}$$

of the susceptibility χ at its maximum as well as at K_c, yielding in the range $L = 4-10$ estimates of $\gamma/\nu = 2.039(9)$ and $\gamma/\nu = 2.036(7)$, respectively, being consistent with the mean-field value of $\gamma/\nu = 2$. In Fig. 1 this is demonstrated graphically by comparing the scaling of $\chi_{\max}$ with a constrained one-parameter fit of the form $\chi_{\max} = c(L(\log L)^{\frac{1}{4}})^2$ with $c = 4.006(10)$.

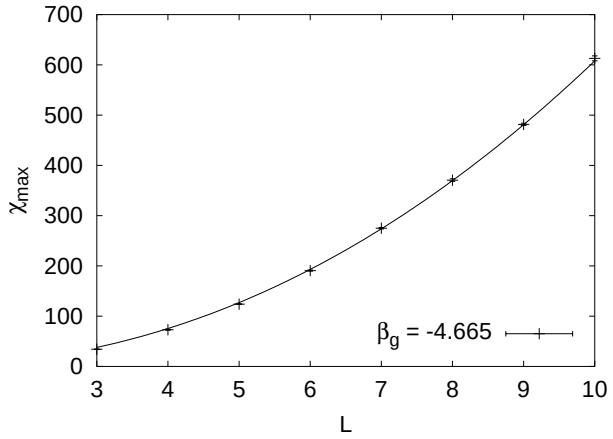

Figure 1. Finite-size scaling of the susceptibility maxima $\chi_{\max}$. The exponent entering the curve is set to the mean-field value $\gamma/\nu = 2$ for regular static lattices.

In two dimensions [7] we could measure the critical exponents α, β, γ, and ν whereas in four dimensions [8] only γ and ν could be determined. To get an estimate or bound for the remaining critical exponents we will need data for larger lattices and with higher statistical accuracy.

Work supported by the EU-Network HPRN-CT-1999-000161 "Discrete Random Geometries: From Solid State Physics to Quantum Gravity" and the ESF-Network "Geometry and Disorder: From Membranes to Quantum Gravity".

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14.4.8. Quantum Monte Carlo Simulations

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The past few years have shown a rapidly growing interest in the properties of low-dimensional structures with pronounced quantum character. One of the main reasons for this interest is the availability of many novel materials, already having or promising for the future important technological applications, whose physical properties appear strictly connected to their layered structure and dominant two-dimensional (2D) character. From the scientific point of view, magnetic monolayers appear particularly attractive since, being truly 2D systems, they allow significant verifications of the proposed models.

With this project we wish to contribute to this line of research, especially for the quantum simulation part. In particular we shall study the XXZ model whose Hamiltonian is given by $H = -J \sum_{\langle ij \rangle} \left[\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y + \lambda \hat{S}_i^z \hat{S}_j^z \right]$, where $\hat{S}_i^\alpha$ denotes the α-component of the spin operator $\hat{\boldsymbol{S}}_i$ at site i of a square lattice with periodic boundary conditions. The spins are three-component quantum objects obeying the $\mathcal{SU}(2)$-group commutation relations $[\hat{S}_i^\alpha, \hat{S}_j^\beta] = i\,\delta_{ij}\,\epsilon^{\alpha\beta\gamma}\hat{S}_i^\gamma$ and belonging to the spin-S representation, $|\hat{\boldsymbol{S}}_i|^2 = S(S{+}1)$. The parameter $J > 0$ describes ferromagnets, and $J < 0$ yields anti-ferromagnets. The latter case is of particular interest and can be further classified into the cases of easy-*plane* ($|\lambda| < 1$) and easy-*axis* ($|\lambda| > 1$) magnets. Guided by their spin symmetries, one expects phase transitions of the Kosterlitz-Thouless respectively Ising type in these models.

We investigate above quantum systems with Monte Carlo (MC) simulations which are much more involved than in the classical case, and many new problems arise. One difficulty of quantum MC (QMC) simulations lies in the dramatic growth of the number of quantum states with the size of the simulated sample and with the value of the spin. In recent years this problem has partially been overcome by the discovery of efficient *non-local* QMC algorithms [1–5] based on clustering ideas (discrete and continuous loop algorithms). The theoretical formulation of these algorithms is highly non-trivial and, even with extensive experience in classical MC studies, their practical and efficient implementation is a major research project [6]. This is particularly pronounced for higher spin values and external magnetic fields, where the proposals made in the literature appear so complicated that innovative formulations are clearly called for.

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14.4.9. Aspects of Protein Folding on the Lattice

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

Proteins are essential constituents within a biological cell system, performing numerous functions, e.g. controlling transport processes of organells, stabilization of the cell structure, enzymatic catalyzation of chemical reactions, etc. Chemically, proteins are built up of sequences of amino acid residues linked by peptide bonds. Usually, proteins consist of 50–3000 of such residues. 20 different amino acids are known, most of them can be arranged in two groups, polar and hydrophobic. It is known that the sequence (also called primary structure), i.e. the consecutiveness of the amino acids within the chain, is responsible for the conformation (or the secondary, tertiary, and quartery structure), and this three-dimensional geometrical shape itself determines the biological function of a protein. Thus, the interplay between sequence and function can only be understood, if it is found out how the protein folds into its unique shape [1]. This is, however, an extremely difficult task, since the complex electrostatic and van der Waals interactions between atoms, molecules, and the aqueous environment inhibit an exact theoretical description of the folding process. For a qualitative understanding, computer simulations of quite simple effective models constrained upon a lattice are most promising.

The simplest model that allows a qualitative study of the folding of sequences of hydrophobic (H) and hydrophilic or polar (P) residues is known as the HP model [2], where the energy function is given by

$$E = \sum_{\langle i,j<i-1\rangle} \mathbf{s}_i^T C_{ij} \mathbf{s}_j. \tag{1}$$

Here $\langle i, j < i-1\rangle$ symbolizes that only contributions of monomers at i and at j are taken into account if they are next neighbours on the lattice but non-adjacent along the chain, i.e. they are not linked by a chemical bond. In this case, these monomers form a *contact* and the elements of the so-called contact matrix

$$C = \begin{pmatrix} c_{HH} & c_{HP} \\ c_{HP} & c_{PP} \end{pmatrix}$$

describe the strength of the interaction between the different types of residues. The components of the state vector of the ith monomer, $\mathbf{s}_i^T = (s_{iH}, s_{iP})$, contain the hydrophobic and the hydrophilic content of the corresponding residue, respectively. For pure HP sequences, only two states are used, $\mathbf{s}^T = (1, 0)$ for hydrophobic monomers and $\mathbf{s}^T = (0, 1)$ for hydrophilic ones.

It is anticipated that a qualitatively correct fold of the lattice protein is obtained, when the hydrophobic residues form an approximately compact core, i.e. a maximum of HH contacts is established. In that case the hydrophilic residues separate the hydrophobic core from the aqueous environment and the protein has folded into its native state with lowest possible energy. In order to primarily study this aspect of folding, the HP model (1) is often simplified by setting $c_{HH} = -1$ and $c_{HP} = c_{PP} = 0$. We analyze the properties of HP lattice proteins from different point of views. On the one hand we perform exact enumerations for chains with up to 18 monomers in the complete space of sequences and conformations, allowing for a statistical analysis of the interplay between sequences and conformations for the mostly interesting case of native, i.e. unique ground states. On the other hand, there is a great interest in the development of fast algorithms for finding low-energy states of HP sequences of lengths > 50 that render a more realistic image of natural proteins. Most-promising computational methods are based on chain growth algorithms like PERM and its extensions [3] which we apply to more generalized, e.g. triangular, lattices. Another important question we are dealing with is what we can learn

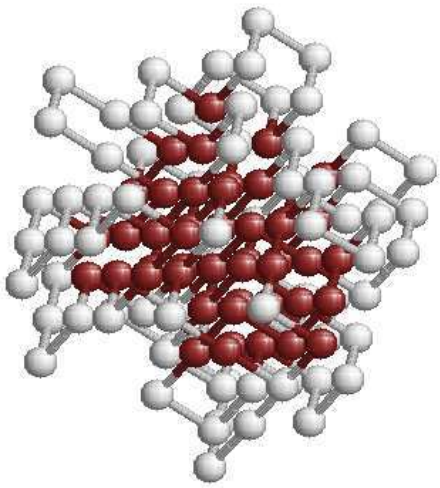

Figure 1. Low-energy conformation of a HP lattice protein with 124 monomers ($E = -70$ a.u.). The core of hydrophobic residues (dark spheres) is well-separated from the environment by the polar molecules (light spheres).

from the thermodynamics of lattice proteins. It is well known that maxima in the specific heat indicate collective conformational changes within the protein. In order to study these effects with reasonable accuracy it is necessary to apply an efficient conformational search algorithm that is applicable over a wide range of temperatures. Therefore "flat histogram" methods like the multicanonical Monte Carlo algorithm [4] and a related method by Wang and Landau [5] that directly simulates the density of states of the system, are preferable choices. In this regard, particular interest is devoted to the detection of conformational "barriers" that strongly influence the efficiency and applicability of Monte Carlo algorithms.

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14.4.10. The 2D Ising Model with Brascamp-Kunz Boundary Conditions

E. Bittner, W. Janke, R. Kenna (Coventry University), A. Krinner and T. Vogel

The two-dimensional Ising model in zero external field is the simplest, exactly solvable statistical physics model displaying critical behaviour [1]. Exploiting the exactly known partition function for finite toroidal $L \times L$ lattices [2], the specific heat finite-size scaling (FSS) has been analytically determined to order L^{-1} a long time ago [3]. At the infinite volume critical point $\beta_c \equiv J/k_B T_c$ this was recently extended to order L^{-3} [4,5], demonstrating that only integer powers of L^{-1} occur.

In this project we studied lattices with Brascamp-Kunz boundary conditions [6,7] which can be depicted as a cylinder of length M with $2N$ boundary spins all pointing up at the one end and alternating between up and down at the other end. With these boundary conditions the partition function consists of only one product term (instead of a sum of four such terms in the toroidal case), and hence in particular the Fisher zeroes are almost trivial to obtain [7]. The product form also allowed for the detailed investigation of the FSS properties of the specific heat reported in Ref. [8] which was later confirmed and partially generalized in a more formalized way [9]. Recently we extended previous analyses of the singular part of the specific heat at T_c and at its maximum for aspect ratios $\rho = N/(M+1)$ to the full specific heat for aspect ratios $\sigma = 2N/M$, which now also includes the square lattice case.

In order to test the analytical results numerically, we adapted the single-cluster Monte Carlo algorithm to the special fixed boundary conditions at hand. To this end the boundary values are considered as part of the clusters and flipped as well ($\ldots + + + \ldots \to \ldots - - - \ldots$ and $\ldots + - + \ldots \to \ldots - + - \ldots$), thereby creating four different cases which are equivalent by symmetry. We furthermore extracted the exact density of states from the partition function which, due to its comparatively simple product form, can be driven to larger system sizes than for toroidal boundary conditions. The latter result was compared with multicanonical and Wang-Landau flat histogram Monte Carlo simulations.

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14.4.11. Information Geometry and Phase Transitions

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Various authors, motivated by ideas in parametric statistics [1], have discussed the advantages of taking a geometrical perspective on statistical mechanics [2,3]. 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 [4].

In this project we used the solution in field of the Ising model on an ensemble of planar random graphs (where $\alpha = -1,\ \beta = 1/2, \gamma = 2$) [5] to evaluate the scaling behaviour of the scalar curvature explicitly, and find $\mathcal{R} \sim |\beta - \beta_c|^{-2}$ [6]. The apparent discrepancy with the general scaling postulate is traced back to the effect of a *negative* α [6].

As anticipated the same effect is found [7] in exact calculations for the three-dimensional spherical model, which was solved (in field) in the classic Berlin and Kac paper [8] and shares the same critical exponents as the Ising model on two-dimensional planar random graphs. We mainly concentrated on the 3D case, but also discussed other dimensions [7], in particular the mean-field like behaviour which sets in at $D = 4$.

Work partially supported by the EU-Network HPRN-CT-1999-000161 "Discrete Random Geometries: From Solid State Physics to Quantum Gravity" and the ESF-Network "Geometry and Disorder: From Membranes to Quantum Gravity".

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14.4.12. Functional Closure of Schwinger-Dyson Equations in Quantum Electrodynamics

M. Bachmann, H. Kleinert (Freie Universität Berlin) and A. Pelster (Freie Universität Berlin)

In quantum field theory, the calculation of physical quantities usually relies on evaluating Feynman integrals which are pictured by diagrams. Each diagram is associated with a certain weight depending on its topology. In contrast to various convenient combinatorial computer programs (e.g. *FeynArts* or *QGRAF* [1]) and the star-graph generation [2], we use a more systematic and physical approach to construct all Feynman diagrams of a quantum field theory [3,4]. It is based on the observation that the complete knowledge of the vacuum energy implies the knowledge of the entire theory ("the vacuum is the world") [5]. In this spirit, all vacuum diagrams are initially generated by a recursive graphical procedure, which is derived from a functional differential equation involving functional derivatives with respect to free propagators and interactions. In a subsequent step, the n-point functions are found graphically by applying the functional derivatives to the vacuum energy [6]. In contrast to the conventional generating functional technique no external currents coupled to single fields are used, such that there is no need for introducing Grassmann sources for fermion fields. An additional advantage is that the number of derivatives necessary to generate a certain correlation function is half as big as with external sources.

The Feynman diagrams of n-point functions obey an infinite hierarchy of coupled Schwinger-Dyson equations which can be closed functionally by using functional derivatives with respect to the free propagators and the interaction. In this way we obtain a closed set of equations determining the connected electron and photon two-point function, the connected three-point function as well as the electron and photon self-energy and the one-particle irreducible three-point function [7]. A further advantage is that in these cases the closed set of Schwinger-Dyson equations can be converted into graphical recursion relations for the connected and one-particle irreducible Feynman diagrams. From these follow the corresponding vacuum diagrams by short-circuiting external legs.

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14.4.13. Z_2-Spins on Dynamical 4D Z_2-Regge Lattices

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This project is devoted to numerical studies of a non-perturbative formulation of (Euclidean) quantum gravity using Regge calculus [1]. In this path-integral approach the fluctuating space-time metric is modeled by varying edge lengths of the Regge skeleton. In contrast to the dynamical triangulation approach, here the connectivity of the skeleton is kept fixed. Spin models defined on such dynamical manifolds are often used to mimic the interaction of gravity with matter fields. In particular the Ising model may be viewed as the minimal representation of a scalar field, sharing the same Z_2 symmetry.

Numerical studies of the coupled system are extremely time demanding [2,3] and one therefore seeks for suitable approximations. One such candidate is the Discrete Regge Model [4] where the squared link lengths of the discretized manifold are constrained to take on only two different values. As a first step we qualitatively compared the two versions of pure quantum Regge calculus by means of Monte Carlo simulations, using in both models the same (local) functional integration measure, chosen such that the Z_2-Regge Model becomes particularly simple [5]. We also investigated an Ising spin system coupled to the two-dimensional Discrete Regge Model and compared it with the results of the Standard Regge Calculus [6]. Particular emphasis was placed on the phase transition of the spin system and the associated critical exponents, employing finite-size scaling analyses. Overall we can summarize that our numerical estimates agree with the Onsager exponents for regular static lattices and are thus fully consistent with the Standard Regge Calculus results [2,3].

In the current project we extended these studies to an Ising spin system coupled to a four-dimensional Z_2-Regge lattice [7,8] and compared with simulations of the Ising model on a regular four-dimensional hypercube where, being at the upper critical dimension, multiplicative logarithmic corrections play an important role and had to be considered with great care. As the main result of our finite-size scaling analyses, similar to two dimensions, the critical properties in the Regge case turn out to be compatible with those of the regular lattice model [7,8].

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