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ABSTRACTS

of contributions to the

20th International NTZ-Workshop on *New Developments in Computational Physics*

CompPhys19

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Institut für Theoretische Physik,
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Preface

Welcome to the 20th International NTZ-Workshop *CompPhys19* on *New Developments in Computational Physics*. As in previous years, also this year's Workshop will cover a broad spectrum of different fields ranging from general aspects of computational and statistical physics over computer simulation studies in condensed and soft matter physics, including applications to biological systems, and random networks to the intriguing properties of quantum systems and high-energy physics. Following the traditional setup of the Workshop, it is also this year designed to provide a forum for an informal exchange of ideas and to meet in a relaxed atmosphere in Leipzig at the beginning of Christmas time.

The main part of the Workshop takes place from 28 – 29 November 2019 in the Theory Lecture Hall ("Hörsaal für Theoretische Physik") and the "Aula" of the Experimental Physics building in Linnéstr. 5. We are very grateful to all colleagues who helped moving their regular lecture courses to another location or date, and in particular to Ms. Isabell Schulthoff for coordinating this difficult task. We also wish to thank our secretary of the Computational Physics Group at the Institute for Theoretical Physics, Ms. Gabriele Menge, for her invaluable help with all administrative matters. As in previous years, the Saturday, 30 November 2019, is devoted to various discussion rounds and collaborative meetings which will take place in the seminar rooms of the Theoretical Physics building in "Brüderstr. 16".

Finally, we and the Centre for Theoretical Sciences (NTZ) gratefully acknowledge financial support of the Workshop from Doctoral College "$\mathbb{L}^4$" of Deutsch-Französische Hochschule (DFH-UFA), DFG Collaborative Research Centre SFB/TRR 102 "Polymers under Multiple Constraints", Research Academy Leipzig (RALeipzig), and Leipzig Graduate School of Natural Sciences "BuildMoNa".

Leipzig,
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Abstracts

Off-equilibrium computation of the dynamic critical exponent of the three-dimensional Heisenberg model

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Working in the out-of-equilibrium regime and using state-of-the-art techniques we have computed the dynamic critical exponent of the three-dimensional Heisenberg model. We have run very large lattices ($L < 250$) in CPUs and GPUs obtaining $z = 2.041(16)$ from the growth of the correlation length and $z = 2.034(22)$ for the decay of the energy. We compare our values with that previously computed at equilibrium with relatively small lattices ($L < 24$), with that provided by means a three-loops calculation using perturbation theory and with experiments. Finally we have checked previous estimates of the static critical exponents, η and ν, in this out-of-equilibrium regime.

Statistical mechanics and phase transitions of semiflexible polymers

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Semiflexible polymers are basic constituents of living matter (DNA, actin, etc.) and also important building blocks for liquid-crystalline devices. Their statistical mechanics still is incompletely understood. By large-scale computer simulations theoretical concepts on semiflexible polymers are tested. When the chain stiffness varies, crossover scaling of the polymer radius occurs in bulk dilute solutions. For contour lengths L exceeding the persistence length ℓ, gaussian coils occur only in $d = 3$ dimensions: in $d = 2$ coil swelling due to excluded volume begins for $L > \ell$. The initial decay of orientational correlations in $d = 2$ is twice as large as in $d = 3$; but adsorbed chains do not behave strictly two-dimensional, perpendicular excursions occur on a lateral scale of the deflection length, and a gradual crossover of the decay length of orientational correlations is found. The adsorption threshold scales with the minus 1/3 power of ℓ. In concentrated lyotropic solutions, nematic order occurs; the transition depends on both ratios L/ℓ and D/ℓ (D = chain thickness). The effect of collective deflection fluctuations on nematic order is elucidated, and the transition to smectic order is studied.

[1] A. Milchev and K. Binder, Phys. Rev. Lett. **123** (2019) 128003.

Steric effects and hydrophobic interactions determine one-dimensional self-assembly

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C_3 symmetric amphiphilic peptides in water have been successfully applied for the construction of supramolecular aggregates and polymers of defined size and shape. Prospect of controlling the polymerization via external stimuli like temperature and pH enhances their importance in several biomedical applications. These compounds typically contain a hydrophobic core and three amphiphilic arms, each containing hydrophobic and hydrophilic chains. In water, due to combined effects of hydrophobic interactions, hydrogen bonding and shielding effects of flexible hydrophilic chain, the monomers stack over one another to form one-dimensional nanorods. We present a minimal model for efficient simulations of such unidirectional self-assembly without the requirement of an explicit solvent. Composites of the monomers interact among themselves via simple pair potentials to invoke hydrophobic and steric effects. We show that these two factors are sufficient to obtain self-assembly of the monomers into elongated, defect-free, filament-like structures from highly dilute, disordered initial state. This assembly kinetics

have been linked to the rates of microscopic processes governing the polymerization. The understanding thus obtained has been used to draw comparison with the experiments. Further, study of the structure of the filaments reveals that beyond a threshold value of hydrophobic interactions among the achiral building blocks, there is a transition to helical structure.

Extraordinary adsorption/reaction selectivity of NO_x from N_2 by combined adsorption and reaction on MIL-127 (P)

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For the first time the strong enhancement effect of the recombination reaction $N_2O_4 \leftrightarrow 2\ NO_2$ (see, e.g., I. Matito-Martos *et al.*, Phys. Chem. Chem. Phys. 20 (2018) 4189) inside the restricted geometry of the Metal-Organic-Framework (MOF) MIL-127 is used for the separation of NO_2 and N_2O_4 from N_2 (air). The number of N atoms in the nitrogen oxides NO_x and that in N_2 is used to define a selectivity of the combined adsorption and chemical reaction process that can reach values of about 1000. This result is obtained from extensive computer simulations. The equilibrium between a gas phase in simulation box A and molecules adsorbed in MIL-127 in simulation box B has been examined by Gibbs Ensemble Monte Carlo simulations (GEMC) employing the home-made software "Gibbon". The chemical reaction equilibrium between NO_2 and N_2O_4 has been treated by simulations using RxMC, a special version of Monte Carlo simulations. The basic idea of RxMC is that the chemical equilibrium (like usual equilibrium without chemical reaction) can be described by the grand canonical partition function. In the classical version of the grand canonical partition function its integrand is the probability density of the possible states of the system. Thus a Monte Carlo random walk using this probability density can be carried out.

Tuning interaction in long-range models changes dynamical scaling during aging

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The understanding of the aging phenomenon, even though being manifested for a range of nonequilibrium processes, is still predominantly limited to short-range systems. To bridge this gap we, here, via Monte Carlo simulations, explore aging during coarsening of the power-law interacting long-range Ising model in two spatial dimensions. We show that the dynamical scaling of the spin-spin two-time autocorrelation function is best described via sub-aging in the long-range regime $\sigma \leq 1$ with the sub-aging exponent μ depending on the power-law exponent σ of the model. In the effectively short-range regime $\sigma > 1$ we recover the simple aging behavior. From our analyses, we also conjecture that the autocorrelation decay exponent $\lambda = \sigma$ in the long-range and $\lambda = 1.25$ in the short-range regime.

[1] H. Christiansen, S. Majumder, M. Henkel, and W. Janke, preprint `arXiv:1906.11815` (2019).

Molecular theory of liquid crystals with inhomogeneous distribution of order parameters (P)

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In the framework of molecular-statistical theory [1] the causes of spontaneous polarization in synclinic and anticlinic smectic liquid crystals were discussed. The effect of the interaction of molecules and of the bent of molecules on the magnitude of the polarization were studied. The polar order parameter is introduced as $p = P/(\rho\mu)$, where P is the polarization, μ is the molecular transverse electric dipole and ρ is the concentration of molecules. We have shown that piezoelectric spontaneous polarization should generally be related to the bent shape of molecules (even for the molecules which are not normally considered as bent-shaped), while both chirality and polarization appear due to the presence of the electric dipole in the direction perpendicular to the plane of molecular bend. The molecular origin of the flexoelectric effect in tilted smectic phases and the influence of the dipole-dipole interaction on the polar order parameter was also studied. The principal result of the work is elaboration of a self-consistent mean theory for the description of polarization in Sm-C^* and Sm-C_A^* phases [2]. Nematic-Isotropic and Smectic-Nematic-Isotropic transitions in case of inhomogeneous distribution function were also studied.

The study was partially supported by Russian Science Foundation (RSF) under research project No. 16-43-03010.

[1] A. V. Emelyanenko, Eur. Phys. J. E **28** (2009) 441.
[2] A. V. Emelyanenko and E. S. Filimonova, Phase Transitions **91** (2018) 984.

Clarifying the case of zero-temperature coarsening in the $d = 3$ Ising model (P)

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For coarsening to any temperature below the critical temperature of the non-conserved Ising model in three spatial dimensions theory predicts a power-law growth of domains of like spins with exponent 1/2. For the last 30 years, also including very recent work, it was not possible to clearly observe this growth law when the quench temperature was set to absolute zero. We here perform nonequilibrium simulations on GPUs with more than 1 billion spins, allowing us to finally beyond question confirm the theory.

Structural transitions in protein folding and amyloid formation

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A detailed knowledge of the processes by that proteins fold, change their structure and function, or self-assemble and aggregate, is crucial for an understanding of disease pathways and the working of drugs at the level of cells. In the present talk we show how advanced computer simulations can complement experiments in tracing these processes. We will focus on fold switching in proteins, and their role in regulating protein activity and amyloid formation.

Large-deviation simulation of height distribution for the KPZ equation: Dependence on initial conditions and morphologies of extreme configurations

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The distribution of relative free energies H of directed polymers in disordered media is studied, which is in the KPZ universality class. We study the distribution at large temperatures, corresponding to short times in KPZ. Using a statistical mechanics-based *large-deviation approach*, the distribution can be obtained over a large range of the support, down to a probability density as small as 10^{-1000}. We compare with analytical predictions for different types of initial conditions and for full as well as for half space. A very good agreement is found for $H < 0$ and a strong convergence is visible for $H > 0$. Furthermore, we study the morphology of atypical fluctuations, compare with analytical results from the *optimal fluctuation method*, and find again a good agreement.

Monte Carlo study of an improved clock model in three dimensions

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We study a modified clock model on the simple cubic lattice. In the main part of the study we simulate the model with Z_8 symmetry. At the transition, $O(2)$ symmetry is restored. Our motivation to study this model is mainly of technical nature. The field variable requires less memory to be stored and the updates are faster than for a model with a $O(2)$ symmetric Hamiltonian. We perform Monte Carlo simulations using a hybrid of local Metropolis and cluster algorithms. Our finite-size scaling analysis yields accurate estimates for the critical exponents of the three-dimensional XY universality class.

Meta-conformal invariance in directed kinetic spin models

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Meta-conformal transformations are time-space transformations which are not angle-preserving but contain time and space translations and time-space dilatations with dynamical exponent $z = 1$. Their Lie algebras contain conformal Lie algebras as sub-algebras. They act as dynamical symmetries of the linear transport equation in d spatial dimensions. Infinite-dimensional Lie algebras of meta-conformal transformations exist for $d = 1$ and $d = 2$ and are isomorphic to the direct sum of either two or three Virasoro algebras, respectively. The form of meta-conformally co-variant two-point correlators is derived. An application to the directed Glauber-Ising chain with spatially long-ranged initial conditions is described.

New development of a coarse-grained model for studying the glass transition of polymer melts

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For studying the generic properties of large and highly entangled polymer melts in bulk, in confinement, and with free surfaces as a function of temperature, with accessible computing times, a new coarse-grained model based on a standard bead-spring model with purely repulsive interaction at the monomer density $\rho = 0.85\sigma^{-3}$ is developed. Adding a new short-range attractive potential between non-bonded monomers, and a new bond-bending potential, the pressure of the system is tuned to zero and the local conformational properties of semiflexible chains are kept as the system undergoes cooling. We show that our model captures the major features of glass-forming polymers that the viscosity dramatically increases close to the glass transition temperature T_g in a non-Arrhenius way from the study of a small entangled polymer melt in bulk [1]. Applying this new model to large and highly entangled polymer melts choosing the same cooling rate, we observe that T_g determined from the change in volume slightly increases with increasing chain size N for fully equilibrated polymer melts while the estimate of T_g for disentangled polymer melts is lower than that for entangled polymer melts of $N = 1000$. This is in agreement with the experimental studies [2] which were motivated by the simulations.

[1] H.-P. Hsu and K. Kremer, J. Chem. Phys. **150** (2019) 091101; *ibid.* 159902.
[2] M. K. Singh, M. Hu, Y. Cang, H.-P. Hsu, H. Therien-Aubin, K. Koynov, G. Fytas, K. Landfester, and K. Kremer, preprint (2019).

Bond-flip Monte Carlo based on exact results for the square-lattice Ising model

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We present preliminary results on a Monte Carlo method with single *bond* flip dynamics in the square-lattice Ising model with $\pm J$ couplings and arbitrary boundary conditions. Using a recently derived exact expression for the free energy of a system with arbitrary nearest-neighbor couplings J_{ij} on the torus, we derive an efficient update scheme for the calculation of the free energy change under a bond flip. We numerically calculate the density of states of the bond ensemble and discuss advantages and disadvantages of the method.

Reentrant random quantum Ising antiferromagnet

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We consider the quantum Ising chain with uniformly distributed random antiferromagnetic couplings ($1 \leq J_i \leq 2$) and uniformly distributed random transverse fields ($\Gamma_0 \leq \Gamma_i \leq 2\Gamma_0$) in the presence of a homogeneous longitudinal field, h. Using different numerical techniques (DMRG, combinatorial optimisation and strong disorder RG methods) we explore the phase diagram, which consists of an ordered and a disordered phase. At one end of the transition line ($h = 0$, $\Gamma_0 = 1$) there is an infinite disorder quantum fixed point, while at the other end ($h = 2$, $\Gamma_0 = 0$) there is a conventional classical random fixed point. Close to this fixed point, for $h > 2$ and $\Gamma_0 > 0$ there is a reentrant ordered phase, which is the result of quantum fluctuations through an order through disorder phenomenon.

Lattice SUSY and the DiSSEP

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We discuss whether the dynamical lattice supersymmetry which exists for various Hamiltonians, including some one-dimensional quantum spin chains, might also exist for the Markov matrix of one-dimensional exclusion processes. One such example is provided by the DiSSEP (the Dissipative, Symmetric Simple Exclusion Process).

Critical exponents of the long-range correlated disordered Ising model in three dimensions

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We study the Ising model in three dimensions with site dilution with the help of Monte Carlo techniques. The dilution is long-range correlated and the correlation function decays proportional to a power law $\propto r^{-a}$. We derive the critical exponent of the correlation length ν in dependence of a by combining different defect concentrations $0.1 \leq p_d \leq 0.4$ and by applying finite-size scaling techniques to the derivative of the logarithm of the magnetization $\partial_\beta \ln |m|$. We study a wide range of correlation exponents $1.5 \leq a \leq 3.5$ as well as the uncorrelated case $a = \infty$. Finally, we compare our results to known estimates from other works and to the conjecture of Weinrib and Halperin: $\nu = 2/a$.

Monte Carlo simulations of chiral colloidal membranes

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Inspired by the zoo of self-assembled objects formed by viruses in polymer solutions, we study the shape and structure of colloidal membranes composed of chiral rod-like particles. The particles are hard spherocylinders and the chirality is induced by a Goossens-like interaction potential between the rods. As depleting agents we use Asakura-Oosawa spheres (non-selfinteracting, but hard core repulsion with the rods). The resulting membrane (single layer of rods) is disk-shaped and twisted. The exact shape and structure follows from minimizing elastic and surface free energy. We discuss the influence of the different terms and how one might use a few snapshots to determine elastic constants.

Critical behavior and approximate ground states in the random-field Potts model via graph cuts

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Finding ground state in a system of the random-field Potts model (RFPM) is a multi-terminal flow problem that is known to be NP-hard. Thus, an efficient exact algorithm is extremely unlikely to exist for an RFPM system. With the use of a graph-cut approach we obtain approximate ground states of the RFPM in polynomial time by embedding binary degrees of freedom into the Potts spins. Then these approximate solutions have been benchmarked using a set of quasi-exact ground states found for small enough systems from long parallel tempering runs. We find that the graph-cut method is a promising algorithm for the RFPM for a not-too-large q. We employ this heuristic algorithm to study the critical behavior of the RFPM in three dimensions.

Monomer density profiles dependence on polymer chain topology and temperature (P)

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Dilute polymer solution in confined geometries present interesting critical behaviour due to entropic reasons [1, 2, 3, 4]. Some properties can be altered by change of the boundary conditions of the confining walls, temperature, geometry of surfaces and topological structure of polymers. Polymers might have very complicated structure as they are flexible and long, which increases the probability of self entanglement. The more complicated topological structure of polymer the less degrees of freedom is left for movement. The behaviour of polymers change when they are confined in the slit of two parallel walls. Such systems present interesting features like arising of depletion forces [2, 3] Taking those properties into account one might find interesting to investigate the critical behavior of ring polymer chains with different topologies in confined geometries like slit geometry of two parallel walls with mixed boundary conditions (b.c.). Boundary conditions are responsible for defining different types of interactions between the wall and polymer. For example, in the mixed case it corresponds to the situation when one surface is repulsive to polymer chain (Dirichlet b.c.) and another one is attractive (Neumann b.c.). Using molecular dynamics simulations we obtained results for the monomer density profiles for linear polymers and ring polymer chains of $N = 360$ monomers with different topologies such as: 0 1, 3 1, 6 1, 7 1 and 9 1 in a slit. The obtained results suggest that with increasing degree of entanglement of polymer chain the number of adsorbed monomers on the surface decrease with increasing relative number of monomers in between the walls. Thanks to more complicated structure polymers can penetrate deeper the space between the walls. For higher temperatures polymer chains start desorbing from the surface of the wall which might be explained intuitively by increased fluctuations of the polymers. These results are important for better understanding nature of the depletion forces which arise in a slit geometry of two parallel walls with mixed b.c.

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[4] Z. Usatenko, P. Kuterba, H. Chamati, and D. Romeis, Eur. Phys. J. – Special Topics **226** (2017) 651.

Additional topological effect imposed by ring-shaped aggregates in supramolecular polymer melts

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This work investigates structures and dynamics of supramolecular polymer (SMP) melts comprising polyethylene glycols end-functionalized by hydrogen bonding stickers via molecular dynamics simulations of a coarse-grained SMP model. Our sticker preferably forms a pairwise H-bond due to its strict directionality, thus the system involves ring and linear aggregates. The average length of both aggregates increases with the increasing strength of the association, leading to a slowing down of the dynamics of the system. An exponentially increasing structure relaxation time of the precursor end-to-end vectors indicates a topological effect other than the entanglements between linear aggregates. We show that small ring aggregates induce additional entanglements of the linear aggregates, proven by the reduced entanglement length of linear aggregates with increasing ring fraction. The exponential slowing down of the structure relaxation can be explained, however, not only by the elongated primitive paths of linear aggregates but also by the rings themselves slowly diffusing in space due to the threading configuration. This can be shown by the lifetime of ring aggregates which increases by the same rate as the structure relaxation time. This work provides the first direct evidence of the ring topology affecting the dynamics of SMPs, which would further broaden the possibility of tailoring novel SMP properties taking into account ring-topological effect.

Pearl-necklace-like local ordering drives polypeptide collapse (P)

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Collapse of the polypeptide backbone is an integral part of protein folding. Using polyglycine as a probe, we explore the nonequilibrium pathways of protein collapse in water. We find that the collapse depends on the competition between hydration effects and intra-peptide interactions. Once intra-peptide van der Waal interactions dominate, the chain collapses along a nonequilibrium pathway characterized by formation of pearl-necklace-like local clusters as intermediates that eventually coagulate into a single globule. By describing this coarsening through the contact probability as a function of distance along the chain, we extract a time-dependent length scale that grows in linear fashion. The collapse dynamics is characterized by a dynamical critical exponent $z = 0.5$ that is much smaller than the values of $z = 1 - 2$ reported for non-biological polymers. This difference in the exponents is explained by the instantaneous formation of intra-chain hydrogen bonds and local ordering that may be correlated with the observed fast folding times in proteins.

[1] S. Majumder, U. H. E. Hansmann, and W. Janke, Macromolecules **52** (2019) 5491.

Non-flat histogram techniques for spin glasses (P)

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Simulation of systems with rugged free-energy landscapes such as spin glasses and polymers are intrinsically difficult and algorithmic improvements for such systems are still needed to enlighten the nature of their low-temperature phase. We developed Monte Carlo non-flat histogram methods, which base on parametric optimization of well-known flat histogram techniques in generalized ensembles, tailored explicitly for systems with complex free-energy landscapes.

Collapse dynamics of a flexible polymer with active beads

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Many biologically active systems can effectively be understood within the framework of active matter models in statistical physics. In this regard, even modeling a single-component Lennard-Jones-type fluid with Vicsek-like activity shows both rich phase and dynamical behavior. Motivated by this we construct a flexible bead-spring polymer model with Vicsek-like activity of the monomer beads. We pay particular emphasis on exploring the pathways of its collapse, following a quench from a high-temperature random-coil state into a low-temperature phase where the equilibrium phase is a compact globule in the passive limit of the model. In the active case, however, our results from molecular dynamics simulations reveal that depending upon the strength of activity there is a rich phase behavior of the model that ranges from compact globule to dumbbells. On the nonequilibrium dynamics front, we compare our results with the passive polymer case, from the perspective of various scaling laws related to the collapse time, cluster coarsening, etc.

Interacting Majorana modes on surfaces of noncentrosymmetric superconductors

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Noncentrosymmetric superconductors with line nodes are expected to possess topologically protected flat zero-energy bands of surface states. These flat bands can be understood as being composed of Majorana modes. We here investigate their fate if residual interactions, beyond BCS mean-field theory, are included. Due to the vanishing of their kinetic energy, the Hamiltonian starts with quartic terms in Majorana operators. Considering a minimal real-space model of Majorana modes on a square lattice with a plaquette interaction, we find string-like integrals of motion that form a Clifford algebra and lead to exact degeneracies of all states. These degeneracies strongly depend on whether the lattice dimensions are even or odd and are robust against disorder in the plaquette interactions. We show that the mapping of the interacting Majorana model onto two decoupled spin compass models and decoupled degrees of freedom [Kamiya *et al.*, Phys. Rev. B 98 (2018) 161409] only works for open boundary conditions. The mapping is used to show that the three-leg and four-leg Majorana ladders are integrable. In addition, the mapping maximally reduces the effort for exact diagonalization, which is utilized to obtain the gap above the ground state as one of the linear dimensions is sent to infinity. Turning to the thermodynamic limit, we compare the interacting Majorana model to the toric-code model with regard to their topological properties. The Majorana model has long-range entangled ground states that differ by Z2 fluxes through the system put on a torus. The ground states exhibit string condensation similar to the toric code but the topological order is not robust. While the spectrum is gapped – due to conventional spontaneous symmetry breaking inherited from the compass models – states with different values of the Z2 fluxes end up in the ground-state sector in the thermodynamic limit. Hence, the gap does not protect the ground states against small perturbation.

Collapse transition of a long polymer with and without periodic boundary conditions

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The collapse transition of polymers and the behavior at the Θ-point are qualitatively well understood. In the collapsed regime the segments interact attractively and form a dense globule, while in the opposite phase excluded volume leads to a swollen coil with the characteristics of a self-avoiding walk. At the transition the polymer is thought to behave like an ideal Gaussian chain. However, no coherent picture with regard to the scaling of the critical temperature has emerged. Experimental and numerical results are not confirming theoretical predictions. Here, we explore the impact of the polymer's inherent inhomogeneity. Although the units of the polymer are generally identical, monomers close to a polymer's ends experience different conditions than those in the center. This can be changed with the introduction of periodic boundary conditions, i.e., by connecting the polymer to a copy of itself. We present results of simulations of a bead-stick model with long-range 12-6 Lennard-Jones interactions with and without periodic boundary conditions for sizes $N \leq 32768$.

Crystallisation in melts of short, semi-flexible hard-sphere polymer chains: The role of the non-bonded interaction range

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In contrast to the flexible pure hard-sphere chains, the semi-flexible ones have an intrinsic stiffness energy scale, which determines the natural temperature scale of the system and determines the ordering transition temperature. We consider the effect of weak additional non-bonded interaction on the phase transition temperature. We study

the system using the stochastic approximation Monte Carlo (SAMC) method to estimate the density of states (DOS) of the system. Since DOS in the purely hard-sphere non-bonded interaction case already covers 5600 orders of magnitude, we consider the effect of weak interactions as a perturbation. In this case, the system undergoes the same ordering transition with a temperature shift non-uniformly depending on the additional interaction. Short-range attractions impede ordering of the melt of semi-flexible polymers and decrease the transition temperature, whereas relatively long-range attractions assist ordering and shift the transition temperature to higher values, whereas weak repulsive interactions demonstrate an opposite effect on the transition temperature.

Excluded volume studies on a single semi-flexible polymer chain (P)

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Long-range interactions of distant segments of the same polymer due to the finite spatial volume of these segments, which are known as excluded volume effect or self-avoidance, were first discussed by Kuhn [1] and in a very successful theoretical approach subsequently described by Flory [2] in a mean-field-type calculation. Flory's theory derives an exponent which describes among other things the scaling of the equilibrium size of a polymer on the number of its monomers within an accuracy of one percent compared to the best simulation results although profiting from an amazing cancellation of two errors [2]. A whole bunch of theoretical work was done on excluded volume effects subsequently spanning perturbation calculations, mean field theories and renormalization group theories pursuing better theoretical predictions also for charged chains where Flory's approach fails. Within the frame of renormalization group theory, Schfer and Krger derived a probability distribution of the total segment density about the center of mass (COM) for an isolated polymer involving these long-range interactions [2]. Using our previously introduced thermophoretic trap [2] we have the possibility to cancel the Brownian motion of single DNA molecules which are homogeneously labeled with an intercalating fluorescent dye giving direct access to the density distribution of the molecule. Mean images calculated from a whole measurement thus allow for testing the theory by Schfer and Krger for the first time to figure out the impact of volume exclusion of different types of single DNA molecules in free diffusion and in a compressed state.

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Ring polymer chains in confined geometries

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Investigation of a dilute solution of ring polymer chains with excluded volume interaction in a good solvent immersed in a confined geometry like slit of two parallel walls with different boundary conditions are performed analytically using the massive field theory approach and numerically using molecular dynamic simulations. The monomer density profiles are obtained in the framework of both methods for different topological structures. The obtained results have practical application in production of nano- and micro-electromechanical devices and gyroscopes of new generation and are important from a biological point of view.

Multifractality in aperiodic quantum spin chains

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Recently, it has been investigated that the ground-state wavefunction of the one dimensional quantum spin-1/2 chain models is multifractal in general with non-trivial fractal dimension. We are studying this phenomena for the quantum Ising chain with aperiodic perturbation. By performing a block real-space renormalization approach, we obtain the ground-state wave function and we extract the generalized multifractal dimension and the multifractal spectrum. For a spin chain with negative wandering exponent the multifractal quantities have the same behavior with the unperturbed chain while for a spin chain with a vanishing wandering exponent, are dependent on the coupling ratio. Finally, for a spin chain with a positive wandering exponent, the multifractal quantities present a different non-linear behavior.

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Breath figures: How universal is its scaling exponent?

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Breath figures have been explored in the late 20th century as an example of a self-organized, far from equilibrium system where a sustained mass flux leads to self-similar droplet distributions. Family and Meakin (1989) provided detailed simulations on the scaling behavior for different substrate and droplet dimensions. Their analysis involves a single non-trivial exponent τ. Its dependence on the dimensions was predicted by Blackman and Brochard (2000). Careful numerical and experimental studies of my group (2012, 2015) obtained values for the exponent, however, that are in variance with the prediction. Here, I will revisit the status of the theoretical understanding of the exponent, and I will present a new approach for the data analysis that faithfully describes our data.

One less parameter least-square fitting (P)

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Following a recent propoal by Berg [1], we analyse how by excluding one (multiplicative) parameter the number of iterations of least-square fitting can be reduced.

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