Final report of the project:
Ordering and dynamics in many body systems

The results of the project have been published in 50 publications, from which 43 are published in international journals having impact factors. The cumulative impact factor of the publications is 135.137. We have also disseminated our results in Hungarian journals, such as in *Fizikai Szemle* and *Magyar Kémikusok Lapja*. In connection with the project Gergő Roósz has written and defended a PhD Thesis.

In the final report we follow the structure of the research plan of the project and for publications in the given problem we refer to the citation list of the final report as [...].

Random quantum magnets

By means of a strong-disorder renormalization group (SDRG) method, we have shown that the (imaginary-time) spin-spin autocorrelation function of the random transverse-field Ising chain and the survival probability in the disordered contact process and in the problem of random walks in random environments exhibit multiscaling in the critical point, with an exponential distribution of scaling exponents in the case of a semi-infinite lattice.[6]

We considered the random transverse-field Ising model on a star-like network composed of M semi-infinite chains connected to a common central site. By the SDRG method, the scaling dimension $x(M)$ of the local order parameter at the junction has been calculated.[3] We have also calculated the entanglement entropy in the same geometry for the random transverse-field Ising model, the random XX model, and a random free-fermion model.[47]

We studied the low-energy properties of the long-range random transverse-field Ising chain with ferromagnetic interactions decaying as a power α of the distance. Using variants of the SDRG method, the critical behavior is found to be controlled by a strong-disorder fixed point with a finite dynamical exponent $z_c = \alpha$. Approaching the critical point, the correlation length is found to diverge exponentially. In the critical point, the magnetization shows a square-logarithmic finite-size scaling and the entanglement entropy satisfies the area law.[5] Similar observations are found numerically in the three-dimensional problem, too.[26] In the case of stretched exponentially decaying interactions, the critical behavior is controlled by infinite-disorder fixed points different from that of the short-range model.[4]

For the random transverse-field Ising model we have calculated the connected transverse-spin correlation function by a numerical implementation of the SDRG method in $d = 1, 2$ and 3 dimensions. At the critical point an algebraic decay with a decay exponent $\eta_t \approx 2 + 2d$ is found. In $d = 1$ the results are related to dimer-dimer correlations in the random AF XX-chain and have been tested by numerical calculations using free-fermionic techniques.[42]

We have written a review article about recent developments of the SDRG method[41] as well as a paper in Hungarian about infinite disorder critical behaviour and the use of the SDRG method.[2]

Nonequilibrium dynamics of closed quantum systems

We studied the time evolution of the local magnetization in the critical quantum Ising chain after a sudden change of the parameters at a defect. The relaxation of the defect magnetization is algebraic and the corresponding exponent, which is a continuous function of the defect parameters, is calculated exactly.[1]

We have considered the one-dimensional XX model in a quasiperiodic transverse field described by the Harper potential. For weak transverse field, $h < h_c$, the excitations are delocalized, but become localized for $h > h_c$. We studied the nonequilibrium relaxation of the system by a sudden change of h (quench dynamics) and a slow change of h in time (adiabatic dynamics). We have studied the time evolution of the entanglement entropy and the magnetization after a quench into the delocalized and the localized phases, as well as into the critical point. The density of defects after an adiabatic field change through the critical point is shown to scale with a power of the rate of field change.[13]

We have studied nonequilibrium dynamics of the quantum Ising chain at zero temperature when the transverse field is varied stochastically. In the fermion representation the problem is equivalent to a 1d continuous-time quantum random walk with stochastic transition amplitudes. In the quantum Ising chain, the average entanglement entropy grows in time as $\sqrt{t}$, and the logarithmic average magnetization decays in the same form. In the case of a dichotomous noise, when the transverse-field is changed in discrete time-steps, τ, there can be excitation modes, for which coherence is maintained, provided their energy satisfies $\epsilon(k)\tau \approx n\pi$ with $n = 1, 2, \ldots$. If the dispersion of $\epsilon(k)$ is quadratic, the long-time behavior of the entanglement entropy and the logarithmic magnetization is dominated by these ballistically traveling coherent modes and both will have $t^{3/4}$ dependence.[22]

By means of free fermionic techniques combined with multiple precision arithmetic we studied the time evolution of the average magnetisation, $m(t)$, of the random transverse-field Ising chain after global quenches. We observed different relaxation behaviours for quenches starting from different initial states to the critical point. Starting from a fully ordered initial state, the relaxation is logarithmically slow and in a finite sample the average magnetisation saturates at a size-dependent plateau. Starting from a fully disordered initial state, the magnetisation stays at zero for a period of time and then starts to increase until it saturates to an asymptotic value. For both quenching protocols, finite-size scaling is satisfied in terms of scaled variables. Furthermore, the distribution of long-time limiting values of the magnetisation shows that the typical and the average values scale differently and the average is governed by rare events. The non-equilibrium dynamical behaviour of the magnetisation is explained through semi-classical theory.[31]

The coupling of cold atoms to the radiation field within a high-finesse optical resonator, an optical cavity, induces long-range interactions which can compete with an underlying optical lattice. To model this situation we have introduced a model of hard-core bosons with competing short- and long-range interactions and solved exactly in $1d$ in the thermodynamic limit. The ground-state phase diagram is shown to contain Mott-insulator, density wave (DW) and superfluid (SF) phases. Remanent DW order is observed for quenches from a DW ground state into the SF phase below a dynamical transition line. After sufficiently strong SF to DW quenches beyond a static metastability line DW order emerges on top of remanent SF order, giving rise to a dynamically generated supersolid state.[40] A similar model, the quantum XX-chain with competing short- and long-range interactions is solved exactly both in equilibrium and in nonequilibrium quench dynamics.[43]

Entanglement entropy of quantum systems

The entanglement entropy, $\mathcal{S}$, is an indicator of quantum correlations in the ground state of a many body quantum system. At a second-order quantum phase-transition point in 1d $\mathcal{S}$ generally has a logarithmic singularity. We considered quantum spin chains with a first-order quantum phase transition, the prototype being the Q-state quantum Potts chain for $Q > 4$ and calculated $\mathcal{S}$ across the transition point. According to numerical, density matrix renormalisation group results, at the first-order quantum phase transition point, $\mathcal{S}$ shows a jump, which is expected to vanish for $Q \to 4^+$. This jump was calculated in leading order of $1/Q$.[36]

We considered a composite, antiferromagnetic XX chain that consists of a clean and a random part, and found a double- logarithmic scaling of the half-chain entanglement entropy: $\mathcal{S} \sim \ln\ln(L)$, L being the length of the chain. We also considered the case, when the disorder penetrates into the homogeneous part in such a way that its strength decays with the distance as $l^{-\kappa}$. For $\kappa < 1/2$, the entropy scales logarithmically with a modified prefactor as $\mathcal{S}(\kappa) \simeq (1-2\kappa)\mathcal{S}(\kappa=0)$, while for $\kappa \geq 1/2$, we recover the double-logarithmic scaling. These results were explained by SDRG arguments.[39] We also studied the half-chain entanglement entropy across a symmetric, extended random defect, where the strength of disorder decays algebraically on both sides of the interface. In the whole regime $\kappa \geq 0$, we found a logarithmic scaling of the entropy, but the variation of the prefactor with κ is non-monotonic and discontinuous at $\kappa = 1/2$.[37]

Ground states of classical and quantum systems of interacting particles

We clarified the meaning of Galilean invariance of N-particle quantum systems in confined geometries, and proved some interesting spectral consequences of this invariance. Implications for ground state superfluidity and periodic ordering were also discussed.[14]

The probability distribution of the total momentum P is studied in N-particle interacting homogeneous quantum systems at positive temperatures. Using Galilean invariance we prove that in one dimension the asymptotic distribution of P, normalised with the square root of N is normal at all temperatures and densities, and in two dimensions the tail distribution of the normalised P is normal. We introduce the notion of the density matrix reduced to the center of mass, and show that its eigenvalues are N times the probabilities of the different eigenvalues of P. A series of results is presented for the limit of sequences of positive definite atomic probability measures, relevant for the probability distribution of both the single-particle and the total momentum.[15]

Alternating-projection-type dual-space algorithms have a clear construction, but are susceptible to stagnation and, thus, inefficient for solving the phase problem ab initio. To improve this behavior a perturbation is introduced, which consists in deleting some predetermined subvolume of the unit cell without searching for atomic regions or analyzing the electron density in any other way. The basic algorithms of positivity, histogram matching and low-density elimination are tested and found to work well with this kind of perturbation.[21]

Critical behaviour of classical many-body systems

We considered the Q-state Potts model as well as the percolation process at criticality and study the number of Fortuin-Kasteleyn (and spin) clusters, N, which intersect a given contour. To leading order, N is proportional to the area of the contour, however, there occur logarithmic contributions related to the corners. These are found to be universal and their size in two dimensional systems can be calculated employing techniques from conformal field theory.[8] For three-dimensional percolation the prefactors are calculated numerically and our results indicate that there are logarithmic finite-size corrections in the free-energy of three-dimensional critical systems, too.[9] In the random-bond Potts model in the large-Q limit N represents the excess entropy and its prefactor is proportional to the central charge of the model. This has been calculated numerically with high precision.[7]

Modelling long-range epidemic spreading in a random environment, we have considered a quenched disordered, d-dimensional contact process with infection rates decaying with distance as $r^{-(d+\sigma)}$. We have studied the dynamical behavior of the model at and below the epidemic threshold by a variant of the SDRG method and by Monte Carlo simulations in $d = 1$ and $d = 2$. The system exhibits a nonequilibrium phase-transition point and we have calculated the associated critical exponents with high numerical precision.[18]

The contact process is also considered in a multiple junction geometry, which is composed of M semi-infinite chains having a common starting site. For $M > 2$ the local order parameter is found to be discontinuous, but the temporal correlation length diverges algebraically at the critical point, thus the transition is of mixed order. We proposed a scaling theory, which is compatible with the numerical results and explains the exponent asymmetry found in the numerical simulations.[38]

The contact process is also studied in the presence of a smooth inhomogeneity, when the local control parameter deviates from the bulk value as Al^{-s}, l being the distance from the surface. In the marginal case, $s = 1/\nu_\perp$, where $\nu_\perp$ is the correlation-length critical exponent, Monte Carlo simulations show a rich surface critical behavior. For weaker perturbations, $A < A_c$, the transition is continuous and the order-parameter critical exponent varies continuously with A. For $A > A_c$, the phase transition is of mixed order, which behaviour was explained in the frame of a scaling theory.[45]

We studied phase transitions of the ferromagnetic Q-state Potts chain with random nearest-neighbour couplings having a variance Δ^2 and with homogeneous long-range interactions, which decay with the distance as $r^{-(1+\sigma)}$, $\sigma > 0$. In the large-Q limit the free-energy of random samples of length $L \leq 2048$ was calculated exactly by a combinatorial optimisation algorithm. The phase transition stays first order for $\sigma < \sigma_c(\Delta) \leq 0.5$, while it is mixed order for $\sigma_c(\Delta) < \sigma < 1$.[23]

We investigated how the dimensionality of the embedding space affects the microscopic crackling dynamics and the macroscopic response of heterogeneous materials. Using a fiber bundle model with localized load sharing, computer simulations are performed from one to eight dimensions slowly increasing the external load up to failure. We found a gradual crossover from the universality class of localized behavior to the mean field class of fracture as the embedding dimension increases. The average temporal profile of crackling avalanches evolves with the dimensionality of the system from a strongly asymmetric shape (localized stresses) to a symmetric parabola (homogeneous stress fields).[49]

Nonequilibrium models defined on general networks

Representation of large data sets became a key question of many scientific disciplines. We developed an information theoretic data representation approach as a unified solution of network visualization, data ordering and coarse-graining. The representation of network nodes as probability distributions provides an efficient visualization method and, in one dimension, an ordering of network nodes and edges. Coarse-grained representations of the input network enable both efficient data compression and hierarchical visualization to achieve high quality representations of larger data sets.[17]

We have showed that non-Markovian, bursty behavior can emerge in models at the critical point, or in Griffiths phases (GPs) as the consequence of diverging auto-correlation of Markovian variables.[10] We have performed spectral analysis of the susceptible-infected-susceptible SIS) models and the contact process on different networks. We showed that a localization transition occurs in scale-free networks for $g > 3$ degree exponents. Furthermore we studied the Lifschitz tails of these models, pointing out an accordance with the emergence of GPs.[11]

We studied effects of heterogeneities in network models. We analyzed large human brain networks generated by the Open Connectome project and showed that although they are heavy tailed, small-world graphs, their graph dimension is below 4, thus rare-region phenomena can be relevant[27]. Simple spreading models, like the threshold model defined on such networks does not exhibit Griffiths Effects owing to the hubs with large incoming weights. When the sensitivity of nodes is equalized or when inhibitory links are allowed nonuniversal critical dynamical behavior emerges even on single connectomes as the consequence of modular structure[20]. We generated hierarchical modular networks, similar to brain connectomes and found numerical evidence for Griffiths effects, localization and slow bursty dynamics of threshold models defined on them[16]. We also studied the dynamics of the SIS model on finite scale-free networks. Extensive simulations revealed the existence of slow dynamics in large sample averages around the critical point, but this smeared transition region and the Griffiths effects disappear in the thermodynamic limit[28].

We investigated the dynamical behavior of an activity spreading model evolving in heterogeneous random networks with highly modular structure, organized non-hierarchically. We observed that loosely coupled modules act as effective rare regions slowing down the extinction of activation, in the same way as in a real GP. The avalanche size distributions of spreading events exhibit robust power-law tails. Our findings relax the requirement of a hierarchical organization of the modular structure, paving more solid path to rationalize the criticality of the brain and other social, technological, and biological modular systems in the framework of GPs.[48]

We have compared the phase synchronization transition of the second-order Kuramoto model on 2d lattices and on large, synthetic power grid networks, generated from real data. Due to the inertia the synchronization transitions are of first-order, which occur in the in the thermodynamic limit, unlike in the mean-field model. The temporal behavior of desynchronization avalanches after a sudden quench to low parameter values has been followed and duration distributions with power-law tails have been detected. This suggests rare region effects, caused by frozen disorder, resulting in heavy-tailed distributions, even without a self-organization mechanism as a consequence of a catastrophic drop event in the couplings.[44]

We provided numerical evidence for the robustness of the GP reported previously in dynamical threshold model simulations on a large human brain network with N=836733 connected nodes. We have shown that the nonuniversal power-law dynamics in an extended control parameter region survives, if the model is extended by a short refractory state and by weak disorder. In case of temporal disorder the GP shrinks and for stronger heterogeneity disappears, leaving behind a mean-field type of critical transition.[50]

Surface growth phenomena and ageing

We have performed large scale simulations to investigate the aging properties of the (2+1)-dimensional Kardar-Parisi-Zhang (KPZ) model. In particular we have determined the auto-correlation and auto-response functions and showed that the fluctuation-dissipation relation is weakly broken.[12]

Extensive dynamical simulations of restricted solid-on-solid models in 2+1 dimensions have been done using parallel multi-surface algorithms implemented on graphics cards. Numerical evidence is presented that these models exhibit KPZ surface growth scaling, irrespective of the step heights N. We showed that by increasing N the corrections to scaling increase, thus smaller step-sized models describe better the asymptotic, long-wave-scaling behaviour[24].

Local Scale-Invariance (LSI) theory has also been tested by dynamical simulations of the driven dimer lattice gas model on graphics cards[25], describing the surface growth of KPZ. Very precise measurements of the universal auto-response function enabled us to perform nonlinear fitting with the scaling forms, suggested by LSI. While the simple LSI ansatz does not seem to work, forms based on logarithmic extension of LSI provide satisfactory description of the full (measured) time evolution of the auto-response function[33].

We studied dynamical universality classes of simple growth and lattice gas models in 2+1 dimensions, in particular KPZ type of models. We compared the effects of random serial (RS) vs. parallel (SCA) update dynamics, both from algorithmical[34] and from statistical physics point of view[45]. SCA updates proved to be much more efficient, but resulted in different autocorrelations than that of the serial model. Surface growth and autoresponse function scaling is the same for both cases. On the other hand the ordered update alters the dynamics of the lattice gas variables, by increasing (decreasing) the memory effects for nonlinear (linear) models with respect to RS. Additionally, we support the KPZ ansatz and the Kallabis-Krug conjecture in $2 + 1$ dimensions and provide a precise growth exponent value $\beta = 0.2414(2)$. We show the emergence of finite size corrections, which occur long before the steady state roughness is reached.