Infinitely Disordered Critical Behavior in Higher Dimensional Quantum Systems

Ph.D. Dissertation

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Introduction

Phase transitions are among the most striking phenomena of nature. While continuously changing the temperature, the system shows singular behavior at the transition point while a substantial change in the physical properties of the system is found. At a continuous phase transition the degrees of freedom become macroscopically correlated at the critical point, thus the emerging critical singularities are powerful manifestations of collective phenomena. In accordance, the \( \xi \) correlation length diverges as a power-law \( \xi \sim \delta^{-\nu} \) as the function of the \( \delta \) distance from the critical point. In this thesis we are going to study continuous quantum phase transitions, driven by quantum, rather than thermal fluctuations, originating from Heisenberg’s uncertainty principle. The most impressive property of continuous phase transitions is their universality: the critical behavior is insensitive to microscopic details, depending only on global characteristics, such as the number of spatial dimensions, the range of interactions and the symmetries of the system. Consequently, it is often sufficient to study a simplified model instead of a realistic system in order to obtain its critical properties. Spatial inhomogeneities, such as dislocations or impurities are inevitable features of realistic systems. In condensed matter systems the dynamics of disorder is slow compared to the time scale of the experiments, thus time-independent, quenched disorder can be used in the models. Naturally arises the following question: Do we have to incorporate also quenched disorder in the models to describe critical phenomena at large scales, or is it just one of the many unimportant microscopic details? In fact, quenched disorder may dramatically change the critical behavior known in the clean, disorder-free system. A paradigmatic example of this phenomena, is the quantum Ising model:

\[
\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij} \sigma_i^x \sigma_j^x - \sum_i h_i \sigma_i^z,
\]

where the \( J_{ij} \geq 0 \) ferromagnetic couplings between the \( S = 1/2 \) spins and the \( h_i > 0 \) magnetic fields are random variables. At zero temperature and small magnetic field, the system develops ferromagnetic order in the \( x \) direction, while by increasing the strength of the magnetic field — at a critical value — a second order phase transition is found into the paramagnetic phase. The model has numerous experimental realizations, among these the most important are the \( \text{K}(\text{H}_x \text{D}_{1-x})_2\text{PO}_4 \), \( \text{Rd}_{1-x}(\text{NH}_4)_x\text{H}_2\text{PO}_4 \) and \( \text{LiHo}_x\text{Y}_{1-x}\text{F}_4 \) systems, where also the strength of disorder is tunable with the \( x \) parameter. The most experimental results are available for the last system, where however not only slowly decaying, oscillating dipolar interaction is found, but also a longitudinal magnetic field. Consequently, the behavior of the system has still a lot of curiosities to study.

The clean, disorder-free, \( d \)-dimensional quantum Ising model belongs to the universality class of the \( d + 1 \)-dimensional classical Ising model. Although the critical behavior of the one-dimensional quantum chain is exactly known this way from Onsager’s solution, it is not appropriate to describe the phase transition under the more realistic, disordered conditions. The shocking result is, that in the presence of (even the weakest) quenched disorder, the critical behavior is completely different from the behavior of the clean model. The interplay between the emerging strong correlations and disorder fluctuations results in strong singularity of the
thermodynamic quantities, as well as the dynamical correlation functions. The profound effect of disorder extends also outside the critical point, in the so called Griffiths-phases, where the spatial correlations are already short-ranged.

Besides the quantum Ising model, there are many other physical systems, where quenched disorder plays an important role, such as the one-dimensional random walk, the one-dimensional Hubbard model, the Mott metal-insulator transition in 2D, localization of a random polymer at an interface, random exclusion process and trap models, driven lattice gases and reaction diffusion models, as well as several classical and quantum spin systems. In the understanding of the phenomena the strong disorder renormalization group (SDRG) method plays a crucial role, yielding exact analytical results in 1D.

As the most important finding, the critical point is described by infinitely disordered behavior, independently from the strength and form of the original disorder. During renormalization the strength of disorder grows without limits, thus becomes dominant over quantum fluctuations. At the critical point, the dynamics becomes extremely slow, resulting in a formally infinitely large $z$ dynamical exponent.

The relation between the $\tau$ time- and $L$ length-scale is usually described by a power-law as $\tau \sim L^z$, which is replaced by a completely different, so called activated scaling form, described by the new $\psi$ exponent:

$$\log \tau \sim L^{\psi}$$

At the critical point the system is heterogeneous even at large scales, and the distributions of the physical quantities are broadening while the system size is increased. The average and typical values significantly differ from each other, even their ratio is singular. The average values are dominated by rare regions and realizations, thus a huge number of random realizations is needed to correctly estimate them. The critical behavior is characterized by 3 different critical exponents, besides the $\nu$ and $\psi$ exponents, it is practical to choose the $x$ exponents describing the $m \sim L^{-x}$ size dependence of the $m$ magnetization. In one dimension, the critical exponents are exactly known, due to the works of Daniel Fisher from 1994:

$$\nu(1D) = 2, \quad x(1D) = \frac{3 - \sqrt{5}}{4}, \quad \psi(1D) = \frac{1}{2}.$$  \hspace{1cm} (3)

Unfortunately, in higher dimensional systems the method is only numerically applicable, requiring expensive calculations. In 2D this enabled to study only relatively small systems with size $L \sim 100$, with a limited accuracy, as shown in Table 1. Although the results show clear evidence of infinitely disordered behavior (with $\psi > 0$ and $\nu > 1$), a large error in the value of the $\psi$ exponent is observable.

In the experimentally important three dimensional case no quantitative results have been achieved before us. Analysis of the numerical RG trajectories led to the conclusion in 2000 (Motrunich et al.) that the critical behavior is probably also in this case controlled by an IDFP, but no estimates about the critical exponents were obtained. According to the Harris-criterion in 4 and higher dimensions weak disorder is irrelevant, this however does not exclude the existence of infinitely disordered critical behavior for stronger initial disorder. Although in
Table 1: Estimates for the critical exponents of the 2D disordered quantum Ising model together with or results extrapolated from the behavior of ladders with increasing width. QMC: Quantum Monte Carlo simulation; MC: Monte Carlo simulation of the 2D random Contact Process, which belongs to the same universality class.

<table>
<thead>
<tr>
<th>$\psi$</th>
<th>$\nu$</th>
<th>$x$</th>
<th>method</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.4(1)</td>
<td>1.0</td>
<td>QMC</td>
<td>Pich et al. (1998)</td>
</tr>
<tr>
<td>0.42(6)</td>
<td>1.07(15)</td>
<td>SDRG</td>
<td>Motrunich et al. (2000)</td>
</tr>
<tr>
<td>0.5</td>
<td>0.94</td>
<td>SDRG</td>
<td>Lin et al. (2000)</td>
</tr>
<tr>
<td>0.6</td>
<td>1.25</td>
<td>SDRG</td>
<td>Karevski et al. (2001)</td>
</tr>
<tr>
<td>0.51(6)</td>
<td>1.20(15)</td>
<td>MC</td>
<td>Vojta et al. (2009)</td>
</tr>
<tr>
<td>0.51(2)</td>
<td>1.25(3)</td>
<td>SDRG</td>
<td>our work [5] (2009)</td>
</tr>
</tbody>
</table>

4 and higher dimensions no numerical studies have been performed so far, theoretically it is an important open question, whether there is a finite upper critical dimension, above which the infinite disorder behavior is absent. The high dimensional limit is also experimentally interesting in the case of long-ranged interactions, such as the dipolar interaction in LiHo$_x$Y$_{1-x}$F$_4$.

In addition, a major challenge in the theory of quantum phase transitions is to understand the characteristics, which are absent in classical physics. The entanglement of the subsystems is a prominent example, being extensively studied in the literature. For the time being, it is also an interesting open question, how to quantify the entanglement in a general quantum state. However, in a pure state, described by a unique wave function — e.g. in a non-degenerate ground state — the entanglement entropy is known to be a good choice. In contrast to classical physics, the subsystem — containing for example only one spin — may be in multiple states also if the whole system has a unique wave function. We can imagine the entanglement entropy as the log-number of possible states of the subsystem (with a significant probability). In the case of finite correlation length, the general expectation states that the entanglement entropy is proportional to the subsystems surface area, known as the area law. However, at the critical point the correlation length diverges, which may cause a deviation from the area law.

As a basic result in 1D, the entanglement entropy diverges logarithmically with the $\ell$ size of the subsystem at the critical point, with a universal prefactor. Among several consequences, the most impressive is, that this singularity can be directly used to locate the critical points of quantum systems. Thus, the phase transition may be detected just by studying the entanglement entropy, even without knowing the nature of the phases and the correct order parameters characterizing them. Unfortunately, due to technical difficulties, there is almost complete lack of results on the entanglement entropy in higher dimensional interacting quantum systems. An exception is the disordered quantum Ising model, where the SDRG method also permits the calculation of the entanglement entropy. So far, the application of the method only succeeded up to two spatial dimensions, providing however conflicting interpretations about the validity of the area law due to small achievable system sizes.

Although the dissertation uses the notions of the RTIM, a large class of other random quantum and classical systems are in the same universality class. An extensively studied example is the nonequilibrium phase-transition of the Contact Process — a simple model of
infection spreading — between the macroscopically infected and healthy states. Due to the similarity of the SDRG equations, our results can be readily applied also for this case.

Aims of the present work

- The study of the disordered quantum Ising model at the critical point in higher dimensions:
  - principally the refinement and completion of the 2D results,
  - as well as the study of the practically important 3D case, for which there are no quantitative results,
  - and the question of the upper critical dimension;
- the study of the higher dimensional disordered quantum Ising model outside the critical point, in the Griffiths-phase, where there is a lack of complete numerical analysis;
- the study of dimensional cross-overs, especially ladders between 1 and 2 dimensions;
- the study of disordered topologies, specifically the infinite dimensional Erdős-Rényi random graphs, which are particularly important also for the Contact Process on social and other networks, besides the long-ranged quantum Ising model;
- the study of the entanglement in the ground state based on the SDRG results:
  - to clarify the critical scaling of the entanglement entropy in 2 (and possibly even higher) dimensions, where the available results contradict in the validity of the area law;
  - to study the general expectation, that the entanglement entropy is maximal at the critical point, in accordance to the diverging correlation length.

Applied method: strong disorder renormalization group technique

In the study of the consequences of quenched disorder, a prominent role is played by the strong disorder renormalization group technique, first applied for the disordered quantum Ising model by Daniel Fisher in 1994. Fisher showed, that the critical point displays infinitely disordered behavior, which leads to the asymptotic exactness of the obtained results. On the contrary of usual renormalization group approaches, which treat the system in a homogeneous way (e.g. by building up regular blocks), the SDRG method handles the system in a spatially completely heterogeneous way. During the method, the maximal $J$ and $h$ coupling is found and ‘decimated out’ in each renormalization step, corresponding to its elimination from the system, while new effective couplings are perturbatively generated. This corresponds to the step-by-step elimination of the excitations having a maximal energy, more and more focusing on the
low energy behavior alone. In the numerical application of the SDRG method for an $N$-spin system, the number of spins decreases in each step by one, until the whole system is described by only one, effective spin. The size of this effective spin gives the value of the magnetization in the system, while its external field yields the smallest energy gap.

Figure 1: Snapshots of the naïve and our improved SDRG algorithm. While in the naïve algorithm numerous new couplings are generated, leading to a running time of $t \sim O(N^3)$, in the improved algorithm we merely delete sites, which leads to an order of magnitudes faster, $t \sim O(N \log N)$, running time for $N$ spins.

In higher dimensional systems numerous effective couplings are generated during the method, which leads to an $O(N^3)$ running time and $O(N^2)$ memory consumption for $N$ spins.

Results

1. During my work, I considerably improved the strong disorder renormalization group method:

   - I proved, that the routinely applied technical step of the SDRG method, known as the maximum rule, enables the significant simplification of the method [4]. Based on the proofs of my conjectures about the method, I worked out a series of different, increasingly efficient algorithm, providing equivalent results with the usual SDRG method. Finally, the $O(N^3)$ running time of the naïve algorithm was kept down to $O(N \log N)$ for an arbitrary dimensional system [2,3].

   - This way much larger systems became available than previously, for instance in 2D a linear size of $L = 2048$ [4] instead of the earlier $L \sim 100$, but also in higher dimensions several million spins became available, with more than ten thousand realizations.
• I also extended the efficient SDRG algorithm for further models [2], such as the quantum Potts model and the quantum rotor model, which is also used to describe superconducting materials.

• In higher dimensional systems one of the first problems to face with, is the sufficiently precise location of the critical point. During my work, I extended the doubling method for higher dimensional systems, which enabled to define a sample dependent pseudo-critical point. From the size dependence of the distribution of the pseudo-critical points it became possible to calculate also the correlation length critical exponent besides the precise location of the critical point [4,5].

• First time in the field, I applied two kinds of specially chosen disorder distributions, which besides illustrated the disorder independence of the obtained results at the critical point, also enabled to obtain more accurate estimates, principally due to the opposite sign of the finite-size corrections present.

2. I found infinitely disordered critical behavior in the quantum Ising model for ladders and 2, 3 and 4 dimensional lattices, as well as for the infinite dimensional Erdős-Rényi random graphs. I determined in all cases the numerical values of the critical exponents, as indicated in Table 1.

• For ladders between 1 and 2 dimensions I found that these ladders behave as one dimensional objects up to a width of \( w = 20 \) — similarly to the known \( w = 2 \) case in the literature —, despite of the SDRG algorithm is more complicated. From the scaling of the scaling parameters with \( w \) it was possible to extrapolate for the 2D case.

• In 2D, the new method enabled to obtain precisely the critical exponents and the form of the scaling functions. The obtained results are the most accurate known estimates [4], including the results obtained for the Contact Process by a Monte Carlo simulation of 40000 CPU days.

• After locating the critical point in 3D, the first estimates for the critical exponents were obtained [3], demonstrating the infinitely disordered behavior.

• The new renormalization method also made it possible to locate the critical point and obtain the critical exponents in 4D, which was the first demonstration of infinitely disordered critical behavior in 4 dimensions [3].

• In even higher dimensional systems the mean difficulty of the direct studies lies in the hardness of precisely locating the critical point. In order to overcome the difficulties, instead of finite dimensional lattices, I studied Erdős-Rényi random graphs, directly corresponding to the infinite dimensional limit. I showed, that the distribution of the effective log-couplings broadens also in this case, as an indication of the infinitely disordered behavior. As shown in Fig. 2, the critical exponents fit to the trend of the finite dimensional results [2,3].
3. By applying my method outside the critical point, in the Griffiths-phase, I presented the first systematic study of the scaling expectations in higher dimensions.

- In higher dimensional systems the scaling behavior is significantly different in the ordered and disordered Griffiths-phase, leading to much stronger singularities in the latter case. My results agree in all cases with the scaling predictions.
- Furthermore, I showed, that the distribution of the log-gaps follows the Fréchet distribution in 2, 3 and 4 dimensions as well.

4. I also studied the scaling of the critical entanglement entropy with a new, effective algorithm, and showed the validity of the area law in 2, 3 and 4 dimensions, supplemented by a universal logarithmic correction, coming from the corners of the subsystem. The obtained universal values of the $b$ prefactor of the $b \ln \ell$ correction are shown in Table 1.

- The calculation of the entanglement entropy usually takes $O(N^2)$ time, which enables to study only much smaller system sizes, than the SDRG algorithm, producing the underlying cluster structure. In order to solve this problem, I derived an exact analytical expression for the entanglement entropy as the function of the structure of the clusters [1]. However, the time needed to evaluate the expression grows exponentially with the cluster size, thus I worked out a combined analytical-numerical method, with which it became already achievable to study the same system sizes as with the improved SDRG algorithm.
- In the case of ladders, the entanglement entropy does not grow in leading order as the width increases, but remains the same as in 1D. By studying the additional corrections to this logarithmic divergence, in 2D the validity of the area law is expected [5].
- Calculating the entanglement entropy in 2D, I clarified, that the area law is satisfied in leading order, and the first correction diverges logarithmically at the critical point. I showed, that the logarithmic correction appears through the corners of the subsystem and its prefactor is a disorder independent, universal quantity [1].
- I also showed the validity of the area law in the previously unexplored 3 and 4 dimensional cases, as well as the fact, that the corners of the subsystem lead to a universal logarithmic correction also in these cases.
- I demonstrated, that the $0 < E < d - 1$-dimensional edges of the subsystem lead to an $\ell^E$ correction to the area law, but these corrections are nonuniversal and do not show a divergence while approaching the critical point.
- By studying the entanglement entropy outside the critical point, I showed, that instead of the entanglement entropy, only the corner contribution diverges at the critical point and this divergence is a consequence of the diverging correlation length.
- Finally, by using the properties of the SDRG algorithm, I gave a qualitative derivation for the logarithmic shape of the corner contribution, which also predicts the alternating sign of the prefactor with the dimensionality.
Table 2: Our results for the universal critical parameters in higher dimensional disordered quantum Ising model together with the exactly known values in 1D. $N_{\text{max}}$ denotes the number of spins in the largest finite systems used in the calculations.

<table>
<thead>
<tr>
<th>$N_{\text{max}}$</th>
<th>1D</th>
<th>2D</th>
<th>3D</th>
<th>4D</th>
<th>E.-R. graphs</th>
</tr>
</thead>
<tbody>
<tr>
<td>(exact)</td>
<td>$2048^2 \approx 4.2 \times 10^6$</td>
<td>$128^4 \approx 2.1 \times 10^6$</td>
<td>$48^4 \approx 5.3 \times 10^6$</td>
<td>$2^{22} \approx 4.2 \times 10^6$</td>
<td></td>
</tr>
<tr>
<td>$d\nu_w$</td>
<td>2</td>
<td>2.48(4)</td>
<td>2.90(15)</td>
<td>3.30(15)</td>
<td>7.8(20)</td>
</tr>
<tr>
<td>$d\nu_s$</td>
<td>(no shift)</td>
<td>2.50(6)</td>
<td>2.96(5)</td>
<td>2.96(15)</td>
<td>4.5(15)</td>
</tr>
<tr>
<td>$x/d$</td>
<td>$\frac{3-\sqrt{5}}{4} \approx 0.191$</td>
<td>0.491(8)</td>
<td>0.613(5)</td>
<td>0.68(3)</td>
<td>0.83(5)</td>
</tr>
<tr>
<td>$\psi$</td>
<td>0.5</td>
<td>0.48(2)</td>
<td>0.46(2)</td>
<td>0.46(2)</td>
<td>-</td>
</tr>
<tr>
<td>$b$</td>
<td>$1/6 \approx 0.1667$</td>
<td>$-0.029(1)$</td>
<td>0.012(2)</td>
<td>$-0.006(2)$</td>
<td>-</td>
</tr>
</tbody>
</table>

Conclusions

From my results the conclusion can be drawn, that the infinitely disordered critical behavior exists in arbitrary high dimensional lattices, without an upper critical dimension. As a consequence, the SDRG method yields asymptotically exact values for the critical exponents.

The entanglement entropy of the disordered quantum Ising model satisfies the area law in arbitrary dimensions, supplemented by a singular logarithmic correction at the critical point, the prefactor of which being universal. The singularity is a consequence of the diverging correlation length and appears through the corners of the subsystem. In higher dimensional systems the directly obtainable corner entropy can be used to locate the critical point rather than the entanglement entropy.

Figure 2: Critical exponents of the random transverse-field Ising model as a function of $1/d$, where $d$ stands for the number of spatial dimensions. At $1/d = 0$ there are results of the infinite dimensional Erdős-Rényi random graph, fitting to the trend of the finite dimensional results.
The thesis is based on the following publications:


Further publications in the field:
