B 3882

Disorder Dominated Singular Behaviour in Random Quantum and Classical Systems

PhD thesis

Róbert Juhász

Institute for Theoretical Physics University of Szeged 2002

1. Preliminaries

The bulk of substances and processes in nature is often characterized by certain degree of inhomogeneity: one might say, it is rather the rule than the exception. The theoretical description of this kind of feature of real systems established the concept of *disorder*, and started on its way of the-nowadays investigation wide-spreadthe disordered models, which is gently developing to be an independent discipline. Among disordered models special attention was paid for models which exhibit a phase transition, where the obvious question arises, what consequences the introduction of disorder has on the properties of the pure system. According to the experiences quenched disorder has effects on the nature of phase transitions in varying degrees. It may lead to the elimination of the transition by smearing out singularities. Or it may cause the change of order of the transition: a first order transition can turn to a continuous one. In case of a continuous transition a basic question was, how the universal properties, such as critical exponents are influenced by disorder.

For systems which undergo a continuous phase transition in their pure form, a general heuristic relevance-irrelevance criterion is known. It was firstly formulated by Harris for diluted systems, and it was later generalized to other kinds of random models. After this result intensive numerical and analytical work has started in order to clarify the universality class of various disordered models. Besides transitions in classical systems, also zero-temperature *quantum phase transitions* attracted much interest. Here, there is no heat bath and activated dynamics is replaced by quantum

tunneling through energy barriers, which leads to an entirely different mechanism of phase transition. The random quantum critical behaviour is formed by the interplay between disorder and quantum fluctuations instead of thermal ones. In low-dimensional random quantum systems, such as spin chains, a remarkable progress was achieved by an asymptotically exact real-space renormalization group scheme, which was firstly developed for the random Heisenberg chain by Ma, Dasgupta and Hu. This method was later extended by Fisher to other random quantum spin chains including the random transverse-field Ising spin chain (RTIC) and the XX chain. The procedure was applied in the critical region of the above models and it was believed to lose its asymptotic exactness in the off-critical region. In these systems an unconventional coarse-grained behaviour appeared. It turned out, that the distributions of parameters in the Hamiltonian become arbitrarily broad on a logarithmic scale as the fixed point is approached. The ratio of parameters is typically infinite or zero and the system is governed by a so called infinite-randomness fixed point. The broad distributions involve the lack of self-averaging and average quantities are dominated by the extreme contribution of a vanishing fraction of rare samples.

Disorder influences however not only the critical behaviour. Griffiths and McCoy pointed out in the random classical and quantum Ising model, respectively, that there exists an extended region around the critical point, where several physical quantities are singular. The origin of *Griffiths phase* is the presence of such rare domains, which are locally in the opposite phase. In the quantum Ising model, where the Griffiths-McCoy singularities are much

more enhanced than in the classical one, the average temporal correlations have a power-law decay, which is reminiscent of criticality, while in the spatial direction there is short-range order. For this reason the Griffiths phase is termed as a line of "semicritical fixed points". By a phenomenological scaling theory the power-law tail of the distribution of the energy gap was related to the dynamical exponent of the system. Thus the singular behaviour of quantities related to the energy gap were reduced to a common ground and the corresponding exponents were given in terms of the dynamical exponent. This latter was found to be a continuous function of the control parameter in the Griffiths phase.

Contrary to continuous transitions, there is no general relevance criterion concerning the stability of first order transitions against disorder. An exception is the criterion by Aizenman and Wehr, which rigorously states that in two dimensions any amount of disorder softens the transition into a continuous one. This result induced much numerical work, the most of which was devoted to the q-state randombond Potts model (RBPM). Finite-q Monte Carlo simulations and transfer matrix calculations consistently reported a correlation length exponent showing weak q-dependence, and a q-dependent magnetization exponent, which tends to a finite limiting value in the large-q limit.

2. Aims and methods

Concerning the Griffiths phase of the RTIC one might ask the question whether the dynamical exponent is sufficient to characterize all singular quantities including those which do not have a trivial connection to the energy gap, such as the higher gaps, the nonlinear susceptibility and the energydensity autocorrelation function. Our aim was to clarify the behaviour of these quantities in the paramagnetic Griffiths phase. The free-fermion representation of the RTIC served as a basis of our investigations. We used the free-fermion expressions of the above quantities obtained by analytic calculations in order to predict their singular behaviour in the framework of a phenomenological scaling theory of the strongly coupled domains. Another relevance of the freefermion picture is that it reduces the dimensionality of the problem, therefore it is a good starting point for numerical calculations. We performed an extensive numerical analysis of the above quantities, by diagonalising chains of maximum length 128. The number of samples was several 10000.

Another method we applied was the Ma-Dasgupta-Hu RG scheme, which we extended to the Griffiths phase. We performed an analytical study of the RG flow equations of the RTIC, but also used phenomenological scaling arguments in order to obtain general results. In case of the one-dimensional random quantum Potts model (RQPM) we could not find an analytical solution to the coupled integrodifferential equations governing the RG flow, therefore we solved them in a numerical way, and also performed a direct simulation of the RG procedure.

Considering the random XY- and random dimerized XX chain, which are closely related to the RTIC, our aim was to determine the lacking critical exponents of these models and the temporal correlations, which are not accessible by the RG procedure. Moreover we aimed at the exploration of the Griffiths-phase. The basis of the investigations was the freefermion representation of the above models again, and an exact mapping into decoupled RTIC-s. We have developed a phenomenological scaling theory of average quantities based on the properties of rare events. We have identified the rare events by using a connection of the problem to an elementary stochastic process, the random walk. Afterwards we have employed the properties of surviving random walks in order to obtain the scaling behaviour of average quantities. In the Griffiths phase we obtained exact results by establishing a connection between the XX and XY models and the Sinai walk model. Furthermore we have performed an exhaustive numerical analysis of the operator profiles at criticality and spin-spin autocorrelations both at criticality and in the paramagnetic Griffiths phase. The largest system size we considered was 512, and the typical number of samples was 10^4 . The critical exponents were determined from the operator profiles by finite-size scaling, and by making use of the predictions of conformal invariance.

Concerning the two-dimensional RBPM our aim was to determine the critical properties of the model directly in the $q \rightarrow \infty$ limit. For this purpose we used a graph representation of the model, the so called *random cluster representation*. We applied two numerical optimization methods in order to obtain the dominant graph. One of them was a stochastic one, the standard simulated annealing, whereas the other was a combinatorial optimization method, which is based on the notion of *minimum-cut* coming from the theory of network flow. For the purpose of cluster analysis we have

implemented the standard Hoshen-Kopelman algorithm. We have determined the critical exponents by finite-size scaling, and by measuring correlations in strip geometry. The latter method exploits the conformal invariance of the model.

3. Results

Our main results are summarized as follows.

-We pointed out that the second- and higher energy gaps, the non-linear susceptibility and the energy-density autocorrelation function have power-law singularities in the Griffiths phase of the RTIC, and we have given the corresponding exponents in terms of the dynamical exponent of the model [1].

-We have solved the Ma-Dasgupta-Hu RG flow equations in the Griffiths phase of the RTIC and have shown that the method becomes asymptotically exact here [4].

-We have have proven that the dynamical exponent of the RTIC remains invariant during the above procedure, and we have given an independent derivation for the exact expression of the dynamical exponent in the Griffiths phase [4].

-We have generally shown for random quantum spin chains governed by a critical infinite-randomness fixed point, that the Ma-Dasgupta-Hu RG method is asymptotically exact in the Griffiths phase and the dynamical exponent remains invariant under the procedure [4].

-We have numerically estimated the q-dependent dynamical exponents of the one-dimensional RQPM in several points of the Griffiths phase [4].

-We have determined the complete set of bulk- and surface critical exponents of the random XY- and random dimerized XX chain [2,3].

-We have determined the distribution and the average asymptotic behaviour of the spin-spin autocorrelation function at the critical point and in the Griffiths phase of the random XY- and random dimerized XX chain [2,3].

-We have obtained an exact expression for the dynamical exponent of the random XY- and random dimerized XX chain in the Griffiths phase [2,3].

-We have shown that the RBPM in the large-q limit can be formulated as a non-trivial optimization problem [5].

-We have given numerical estimates on the critical exponents of the two-dimensional RBPM in the large-q limit and constructed its phase diagram [5].

References

1.F. Iglói, R. Juhász, and H. Rieger Griffiths-McCoy Singularities in the Random Transverse Ising Spin Chain Phys. Rev. B 59, 11308 (1999).

2. H. Rieger, R. Juhász, and F. Iglói Critical Exponents of Random XX and XY Chains: Exact Results via Random Walks Europ. Phys. J. B 13, 409 (2000).

3. F. Iglói, R. Juhász, and H. Rieger Random Antiferromagnetic Quantum Spin Chains: Exact Results from Scaling of Rare Regions Phys. Rev. B 61, 11552 (2000).

4. F. Iglói, R. Juhász, and P. Lajkó Griffiths-McCoy Singularities in Random Quantum Chains: Exact Results through Renormalisation Phys. Rev. Lett. **86**, 1343 (2001).

5. R. Juhász, H. Rieger, and F. Iglói Random-Bond Potts Model in the Large-q Limit Phys. Rev. E 64, 56122 (2001).