Quantum and classical phase transitions in electronic systems

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Preface

This Habilitation thesis collects and summarizes original research on classical and quantum phase transitions in electronic systems which the author performed in the years 1995 to 1999.

The thesis consists of two parts. The first, shorter part is intended to give an introduction to and a summary of the original research collected in the second part. It is organized as follows. Chapter 1 first gives a brief historical account of the key developments in the physics of phase transitions. Then the basic concepts are summarized, emphasizing the differences and similarities between classical and quantum phase transitions as well as those between equilibrium and non-equilibrium transitions. Chapters 2 to 5 introduce the phase transitions investigated in detail in this Habilitation thesis and summarize the main results. Specifically, in Chapter 2 a toy model for a quantum phase transition is considered, the so-called quantum spherical model. It can be solved exactly, providing an easily accessible example of a quantum phase transition. Chapter 3 contains a discussion of the ferromagnetic and antiferromagnetic quantum phase transitions of itinerant electrons. It is demonstrated that the coupling of the magnetization to additional soft modes in the zero-temperature electron system changes the properties of the transition profoundly. Moreover, it is shown that in the presence of disorder rare fluctuations can lead to a destruction of the conventional critical behavior at the magnetic quantum phase transition. In Chapter 4 the metal-insulator transition of disordered interacting electrons is investigated by means of large-scale numerical simulations. To do this, an efficient numerical method is developed, called the Hartree-Fock based diagonalization. It is shown that electron-electron interactions can lead to a considerable enhancement of transport in the strongly localized regime. The damage-spreading transitions considered in Chapter 5 are not quantum phase transitions but thermal non-equilibrium transitions. The basic properties of these transitions are discussed and a connection to the structure of the free-energy landscape and glassy behavior of disordered electrons is established. Finally, Chapter 6 is devoted to a short summary and outlook.

The second, larger part of the thesis is a collection of 17 reprints of original publications in refereed journals and 5 preprints available on the Los Alamos preprint server. Two of the papers are on the quantum spherical model, 7 on magnetic transitions of itinerant magnets, 7 on the metal-insulator transition and 6 on damage spreading transitions. During his Habilitation time, the author has also published four printed but unrefereed conference contributions on the topics covered here as well as five further refereed articles on topics only loosely connected with this thesis. These publications have not been reproduced here, their references are listed after the table of contents.

The work presented here would have been impossible without the contributions of many friends and colleagues. I am greatly indebted to Prof. Michael Schreiber from Chemnitz University of Technology for his continuing support and the opportunity to pursue an independent line of research. I am equally grateful to Prof. Dietrich Belitz from the University of Oregon from whom I learned quantum field theory and who was a great host during my repeated stays.
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## Contents

Preface iii

I Phase transitions in electronic systems 1

1 Classical and quantum phase transitions 3
   1.1 From critical opalescence to quantum criticality 3
   1.2 Basic concepts of phase transitions and critical behavior 5
   1.3 How important is quantum mechanics? 7
   1.4 Equilibrium versus non-equilibrium transitions 10

2 Quantum spherical model 13
   2.1 Classical spherical model 13
   2.2 Quantization of the spherical model 14
   2.3 Quantum phase transitions 15

3 Magnetic quantum phase transitions of itinerant electrons 17
   3.1 Itinerant ferromagnets 17
   3.2 Landau-Ginzburg-Wilson theory of the ferromagnetic quantum phase transition 19
   3.3 Influence of disorder and rare regions on magnetic quantum phase transitions 21

4 Metal-insulator transitions of disordered interacting electrons 25
   4.1 Localization and interactions 25
   4.2 Hartree-Fock approximation 27
   4.3 Hartree-Fock based diagonalization 29

5 Damage spreading transitions 33
   5.1 Introduction 33
   5.2 Mean-field theory 34
   5.3 Damage spreading simulations 36

6 Summary and outlook 39

Bibliography 43

II Reprints 47

Quantum spherical model 49

**Magnetic quantum phase transitions of itinerant electrons**


**Metal-insulator transitions of disordered interacting electrons**

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Part I

Phase transitions in electronic systems
Chapter 1

Classical and quantum phase transitions

Phase transitions have played, and continue to play, an essential role in shaping the world. The large scale structure of the universe is the result of a sequence of phase transitions during the very early stages of its development. Later, phase transitions accompanied the formation of galaxies, stars and planets. Even our everyday life is unimaginable without the never ending transformations of water between ice, liquid and vapor. Understanding phase transitions is thus a prime endeavor of physics.

Under normal conditions the phase transitions of water involve latent heat, i.e., a non-zero amount of heat is released while the material is cooled through an infinitesimally small temperature interval around the transition temperature. This type of phase transitions is usually called first-order transitions. Phase transitions that do not involve latent heat are called continuous transitions. They are particularly interesting since the typical length and time scales of fluctuations of, e.g., the density, diverge when approaching a continuous transition. These divergences and the resulting singularities of physical observables are called the critical behavior.

Understanding critical behavior has been a great challenge for theoretical physics. More than a century has gone by from the first discoveries until a consistent picture emerged. However, the theoretical concepts established during this development, viz., scaling and the renormalization group now belong to the central paradigms of modern physics.

1.1 From critical opalescence to quantum criticality

130 years ago Andrews (1869) discovered a very special point in the phase diagram of carbon dioxide. At a temperature of about 31 °C and 73 atmospheres pressure the properties of the liquid and the vapor phases became indistinguishable. In the neighborhood of this point carbon dioxide strongly scattered light. Andrews called this point the critical point and the strong light scattering the critical opalescence. Four years later van der Waals (1873) presented his doctoral thesis ‘On the continuity of the liquid and gaseous states’ which contained one of the first theoretical explanations of critical phenomena based on the now famous van der Waals equation of state. It provides the prototype of a mean-field description of a phase transition by assuming that the individual interactions between the molecules are replaced by an interaction with a hypothetic global mean field. In the subsequent years similar behavior was found for many other materials. In particular, Pierre Curie (1895) noticed that ferromagnetic iron also shows such a critical point which today is called the Curie point. It is located at zero magnetic field and
a temperature of about 770 °C, the highest temperature for which a permanent magnetization can exist in zero field. At this temperature phases differing by the direction of the magnetization become obviously indistinguishable. Again it was only a few years later when Weiss (1907) proposed the molecular-field theory of ferromagnetism which qualitatively explained the experiments. As van der Waals theory of the liquid-gas transition the molecular-field theory of ferromagnetism is based on the existence of a hypotetic molecular (mean) field. The so-called classic era of critical phenomena culminated in the Landau theory of phase transitions (Landau 1937). Landau gave some very powerful and general arguments based on symmetry which suggested that mean-field theory is essentially exact. While we know today that this is not the case, Landau theory is still an invaluable starting point for the investigation of critical phenomena.

The modern era of critical phenomena started when it was realized that there was a deep problem connected with the values of the critical exponents which describe how physical quantities vary close to the critical point. Guggenheim (1945) realized that the coexistence curve of the gas–fluid phase transition is not parabolic, as predicted by van der Waals’ mean-field theory. At about the same time Onsager (1944) exactly solved the two-dimensional Ising model showing rigorously that in this system the critical behavior is different from the predictions of mean-field theory. After these observations it took about twenty years until a solution of the ’exponent puzzle’ was approached. Widom (1965) formulated the scaling hypothesis according to which the singular part of the free energy is a generalized homogeneous function of the parameters. A year later, Kadanoff (1966) proposed a simple heuristic explanation of scaling based on the argument that at criticality the system essentially ‘looks the same on all length scales’. The breakthrough came with a series of seminal papers by Wilson (1971). He formalized Kadanoff’s heuristic arguments and developed the renormalization group. For these discoveries, Wilson won the 1982 physics nobel price. The development of the renormalization group initiated an avalanche of activity in the field which still continues.

Today, it is probably fair to say that thermal equilibrium phase transitions are well understood in principle, even if new interesting transitions, e.g., in soft condensed matter systems, continue to be found. In recent years the scientific interest has shifted towards two new fields, viz. non-equilibrium phase transitions and quantum phase transitions. Non-equilibrium transitions can take place, e.g., in systems approaching equilibrium after a non-infinitesimal perturbation or in systems driven by external fields or non-thermal noise to a non-equilibrium (steady) state. Examples are provided by growing surfaces, chemical reaction-diffusion systems, or biological systems (see, e.g., Meakin 1993 or Marro and Dickman 1997). Non-equilibrium phase transitions are characterized by singularities in the stationary or dynamic properties of the non-equilibrium states rather than by thermodynamic singularities.

Another active avenue of research is the study of quantum phase transitions. These transitions occur at zero temperature when some non-thermal control-parameter (e.g., the pressure) is changed. The investigation of quantum phase transitions was pioneered by Hertz (1976). He developed a renormalization group approach to magnetic transitions of itinerant electrons and found that the ferromagnetic transition is mean-field like in all physical dimensions \( d = 2, 3 \). While Hertz’ general scaling scenario at a quantum critical point is valid, his specific predictions for the ferromagnetic quantum phase transition are incorrect, as will be explained in Chapter 3. In recent years quantum phase transitions in electronic systems have gained particular attention since some of the most exciting discoveries in contemporary condensed matter physics, viz. the integer and fractional quantum Hall effects and high-temperature superconductivity are often attributed to quantum critical points (see, e.g., Sachdev et al. 1995, Sondhi et al. 1997, and Zhang 1997).
1.2 Basic concepts of phase transitions and critical behavior

There are now quite a number of excellent textbooks available on the physics of phase transitions and critical behavior (see, e.g., Ma 1975 or Goldenfeld 1992). Therefore, in this section we only briefly collect the basic concepts which are necessary for the later chapters.

A continuous phase transition can usually be characterized by an order parameter, a concept first introduced by Landau. An order parameter is a thermodynamic quantity that is zero in one phase (the disordered) and non-zero and non-unique in the other (the ordered) phase. Very often the choice of an order parameter for a particular transition is obvious, e.g., for the ferromagnetic transition where the total magnetization is an order parameter. Sometimes, however, finding an appropriate order parameter is a complicated problem by itself, e.g., for the disorder-driven localization-delocalization transition of non-interacting electrons.

While the thermodynamic average of the order parameter is zero in the disordered phase, its fluctuations are non-zero. If the phase transition point, also called the critical point, is approached the spatial correlations of the order parameter fluctuations become long-ranged. Close to the critical point their typical length scale, the correlation length $\xi$, diverges as

$$\xi \propto t^{-\nu} \quad (1.1)$$

where $\nu$ is the correlation length critical exponent and $t$ is some dimensionless distance from the critical point. If the transition occurs at a non-zero temperature $T_c$ we can use $t = |T - T_c|/T_c$. In addition to the long-range correlations in space there are analogous long-range correlations of the order parameter fluctuations in time. The typical time scale for a decay of the fluctuations is the correlation (or equilibration) time $\tau_c$. As the critical point is approached the correlation time diverges as

$$\tau_c \propto \xi^z \propto t^{-\nu z} \quad (1.2)$$

where $z$ is the dynamical critical exponent. Close to the critical point there is no characteristic length scale other than $\xi$ and no characteristic time scale other than $\tau_c$ (in addition to the microscopic scales). As already noted by Kadanoff (1966), this is the physics behind Widom’s scaling hypothesis, which we will now discuss.

Let us consider a classical system, characterized by its Hamiltonian

$$H(p_i, q_i) = H_{\text{kin}}(p_i) + H_{\text{pot}}(q_i) \quad (1.3)$$

where $q_i$ and $p_i$ are the generalized coordinates and momenta, and $H_{\text{kin}}$ and $H_{\text{pot}}$ are the kinetic and potential energies, respectively. In such a system ‘statics and dynamics decouple’, i.e., the momentum and position sums in the partition function

$$Z = \int \prod dp_i e^{-H_{\text{kin}}/k_BT} \int \prod dq_i e^{-H_{\text{pot}}/k_BT} = Z_{\text{kin}}Z_{\text{pot}} \quad (1.4)$$

are completely independent from each other. The kinetic contribution to the free energy density $f = -(k_BT/V) \log Z$ will usually not display any singularities, since it derives from the product of simple Gaussian integrals. Therefore one can study the critical behavior using effective time-independent theories like the Landau-Ginzburg-Wilson theory. In this type of theories the free energy is expressed as a functional of the order parameter $m(r)$ only. All other degrees of freedom have been integrated out in the derivation of the theory starting from a microscopic

\footnote{Note that a microscopic cutoff scale must be present to explain non-trivial critical behavior, for details see, e.g., Goldenfeld (1992). In a solid such a scale is, e.g., the lattice spacing.}

\footnote{Velocity dependent potentials like in the case of charged particles in an electromagnetic field are excluded.}
Table 1.1: Definitions of the commonly used critical exponents in the 'magnetic language', i.e., the order parameter is the magnetization $m$, and the conjugate field is a magnetic field $B$. $t$ denotes the distance from the critical point and $d$ is the space dimensionality. (The exponent $y_B$ defined in (1.6) is related to $\delta$ by $y_B = d\delta/(1 + \delta)$.)

<table>
<thead>
<tr>
<th>exponent</th>
<th>definition</th>
<th>conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>specific heat</td>
<td>$\alpha$</td>
<td>$c \propto</td>
</tr>
<tr>
<td>order parameter</td>
<td>$\beta$</td>
<td>$m \propto (-t)^{\beta}$</td>
</tr>
<tr>
<td>susceptibility</td>
<td>$\gamma$</td>
<td>$\chi \propto</td>
</tr>
<tr>
<td>critical isotherm</td>
<td>$\delta$</td>
<td>$B \propto</td>
</tr>
<tr>
<td>correlation length</td>
<td>$\nu$</td>
<td>$\xi \propto</td>
</tr>
<tr>
<td>critical correlation function</td>
<td>$\eta$</td>
<td>$G(r) \propto</td>
</tr>
<tr>
<td>dynamical</td>
<td>$z$</td>
<td>$\tau_c \propto \xi^z$</td>
</tr>
</tbody>
</table>

Hamiltonian. In its simplest form (Landau 1937, Ginzburg 1960, Wilson 1971) valid, e.g., for an Ising ferromagnet, the Landau-Ginzburg-Wilson functional $\Phi[m]$ reads

$$\Phi[m] = \int d^d r \ m(r) \left(-\frac{\partial^2}{\partial r^2} + t\right) m(r) + \int d^d r \ m^4(r) - B \int d^d r \ m(r),$$

$$Z = \int D[m] e^{-\Phi[m]}$$

(1.5)

where $B$ is the field conjugate to the order parameter (the magnetic field in case of a ferromagnet).

Since close to the critical point the correlation length is the only relevant length scale, the physical properties must be unchanged, if we rescale all lengths in the system by a common factor $b$, and at the same time adjust the external parameters in such a way that the correlation length retains its old value. This gives rise to the homogeneity relation for the free energy density,

$$f(t, B) = b^{-d} f(t b^{1/\nu}, B b^y_B).$$

(1.6)

Here $y_B$ is another critical exponent. The scale factor $b$ is an arbitrary positive number. Analogous homogeneity relations for other thermodynamic quantities can be obtained by differentiating $f$. The homogeneity law (1.6) was first obtained phenomenologically by Widom (1965). Within the framework of the renormalization group theory it can be derived from first principles.

In addition to the critical exponents $\nu, y_B$ and $z$ defined above, a number of other exponents is in common use. They describe the dependence of the order parameter and its correlations on the distance from the critical point and on the field conjugate to the order parameter. The definitions of the most commonly used critical exponents are summarized in Table 1.1. Note that not all the exponents defined in Table 1.1 are independent from each other. The four thermodynamic exponents $\alpha, \beta, \gamma, \delta$ can all be obtained from the free energy (1.6) which contains only two independent exponents. They are therefore connected by the so-called scaling relations

$$2 - \alpha = 2\beta + \gamma,$$

(1.7)

$$2 - \alpha = \beta(\delta + 1).$$

(1.8)
1.3. How important is quantum mechanics?

Analogously, the exponents of the correlation length and correlation function are connected by two so-called hyperscaling relations

\[ 2 - \alpha = d \nu , \]
\[ \gamma = (2 - \eta) \nu . \]

Since statics and dynamics decouple in classical statistics the dynamical exponent $z$ is completely independent from all the others.

The critical behavior at a particular phase transition is completely characterized by the set of critical exponents. One of the most remarkable features of continuous phase transitions is universality, i.e., the fact that the critical exponents are the same for entire classes of phase transitions which may occur in very different physical systems. These classes, the so-called universality classes, are determined only by the symmetries of the Hamiltonian and the spatial dimensionality of the system. This implies that the critical exponents of a phase transition occurring in nature can be determined exactly (at least in principle) by investigating any simplistic model system belonging to the same universality class, a fact that makes the field very attractive for theoretical physicists. The mechanism behind universality is again the divergence of the correlation length. Close to the critical point the system effectively averages over large volumes rendering the microscopic details of the Hamiltonian unimportant.

The critical behavior at a particular transition is crucially determined by the relevance or irrelevance of order parameter fluctuations. It turns out that fluctuations become increasingly important if the spatial dimensionality of the system is reduced. Above a certain dimension, called the upper critical dimension $d^+_{\text{c}}$, fluctuations are irrelevant, and the critical behavior is identical to that predicted by mean-field theory (for systems with short-range interactions and a scalar or vector order parameter $d^+_{\text{c}} = 4$). Between $d^+_{\text{c}}$ and a second special dimension, called the lower critical dimension $d^-_{\text{c}}$, a phase transition still exists but the critical behavior is different from mean-field theory. Below $d^-_{\text{c}}$ fluctuations become so strong that they completely suppress the ordered phase.

1.3 How important is quantum mechanics?

The question of to what extent quantum mechanics is important for understanding a continuous phase transition is a multi-layered question. One may ask, e.g., whether quantum mechanics is necessary to explain the existence and the properties of the ordered phase. This question can only be decided on a case-by-case basis, and very often quantum mechanics is essential as, e.g., for superconductors. A different question to ask would be how important quantum mechanics is for the asymptotic behavior close to the critical point and thus for the determination of the universality class the transition belongs to.

It turns out that the latter question has a remarkably clear and simple answer: Quantum mechanics does not play any role for the critical behavior if the transition occurs at a finite temperature. It does play a role, however, at zero temperature. In the following we will first give a simple argument explaining these facts.

We have seen in the preceding section that the typical time scale $\tau_c$ of the fluctuations diverges as the transition is approached. Correspondingly, the typical frequency scale $\omega_c$ goes to zero and with it the typical energy scale

\[ \hbar \omega_c \propto |t|^{\nu z} . \]
Quantum mechanics will be important as long as this typical energy scale is larger than the thermal energy $k_B T$. If the transition occurs at some finite temperature $T_c$, quantum mechanics will thus become unimportant for $|t| < t_x$ with the crossover distance $t_x$ given by

$$t_x \propto T_c^{1/z}.$$  \hfill (1.12)

We thus find that the critical behavior asymptotically close to the transition is entirely classical if the transition temperature $T_c$ is nonzero. This justifies to call all finite-temperature phase transitions classical transitions, even if the properties of the ordered state are completely determined by quantum mechanics as is the case, e.g., for the superconducting phase transition of, say, mercury at $T_c = 4.2$ K. In these cases quantum fluctuations are obviously important on microscopic scales, while classical thermal fluctuations dominate on the macroscopic scales that control the critical behavior. If, however, the transition occurs at zero temperature as a function of a non-thermal parameter like the pressure $p$, the crossover distance $t_x = 0$. (Note that at zero temperature the distance $t$ from the critical point cannot be defined via the reduced temperature. Instead, one can define $t = |p - p_c|/p_c$.) Thus, at zero temperature the condition $|t| < t_x$ is never fulfilled, and quantum mechanics will be important for the critical behavior. Consequently, transitions at zero temperature are called quantum phase transitions.

Let us now generalize the homogeneity law (1.6) to the case of a quantum phase transition. We consider a system characterized by a Hamiltonian $H$. In a quantum problem kinetic and potential part of $H$ in general do not commute. In contrast to the classical partition function (1.4) the quantum mechanical partition function does not factorize, i.e., 'statics and dynamics are always coupled'. The canonical density operator $e^{-H/k_B T}$ looks exactly like a time evolution operator in imaginary time $\tau$ if one identifies

$$1/k_B T = \tau = -i\Theta/\hbar$$ \hfill (1.13)

where $\Theta$ denotes the real time. This naturally leads to the introduction of an imaginary time direction into the system. An order parameter field theory analogous to the classical Landau-Ginzburg-Wilson theory (1.5) therefore needs to be formulated in terms of space and time dependent fields. The simplest example of a quantum Landau-Ginzburg-Wilson functional, valid for, e.g., an Ising model in a transverse field, reads

$$\Phi[m] = \int_0^{1/k_B T} d\tau \int d^4 r \ m(r, \tau) \left( \frac{\partial^2}{\partial r^2} - \frac{\partial^2}{\partial \tau^2} + t \right) m(r, \tau) + \int_0^{1/k_B T} d\tau \int d^4 r \ m^4(r, \tau) - B \int_0^{1/k_B T} d\tau \int d^4 r \ m(r, \tau), \hfill (1.14)$$

\[ Z = \int D[m] e^{-\Phi[m]} \]

Let us note that the coupling of statics and dynamics in quantum statistical dynamics also leads to the fact that the universality classes for quantum phase transitions are smaller than those for classical transitions. Systems which belong to the same classical universality class may display different quantum critical behavior, if their dynamics differ.

The classical homogeneity law (1.6) for the free energy density can now easily be adopted to the case of a quantum phase transition. At zero temperature the imaginary time acts similarly to an additional spatial dimension since the extension of the system in this direction is infinite. According to (1.2), time scales like the $z$th power of a length. (In the simple example (1.14) space and time enter the theory symmetrically leading to $z = 1$.) Therefore, the homogeneity
law for the free energy density at zero temperature reads

\[ f(t, B) = b^{-(d+z)} f(t^{b^{1/\nu}}, B^{b^{\mu_N}}). \]  

(1.15)

Comparing (1.15) and (1.6) directly shows that a quantum phase transition in \(d\) dimensions is equivalent to a classical transition in \(d + z\) spatial dimensions. Thus, for a quantum phase transition the upper critical dimension, above which mean-field critical behavior becomes exact, is reduced by \(z\) compared to the corresponding classical transition.

Now the attentive reader may ask: Why are quantum phase transitions more than an academic problem? Any experiment is done at a non-zero temperature where, as we have explained above, the asymptotic critical behavior is classical. The answer is again provided by the crossover condition (1.12): If the transition temperature \(T_c\) is very small quantum fluctuations will remain important down to very small \(t\), i.e., very close to the transition. At a more technical level, the behavior at small but non-zero temperatures is determined by the crossover between two types of critical behavior, viz. quantum critical behavior at \(T = 0\) and classical critical behavior at non-zero temperatures. Since the 'extension of the system in imaginary time direction' is given by the inverse temperature \(1/k_B T\) the corresponding crossover scaling is equivalent to finite size scaling in imaginary time direction. The crossover from quantum to classical behavior will occur when the correlation time \(\tau_c\) reaches \(1/k_B T\) which is equivalent to the condition (1.12). By adding the temperature as an explicit parameter and taking into account that in imaginary-time formalism it scales like an inverse time (1.13), we can generalize the quantum homogeneity law (1.15) to finite temperatures,

\[ f(t, B, T) = b^{-(d+z)} f(t^{b^{1/\nu}}, B^{b^{\mu_N}}, T^{b^z}). \]  

(1.16)

The resulting phase diagram close to a quantum critical point is illustrated in Fig. 1.1. Here \(p\) stands for the (non-thermal) parameter which tunes the quantum phase transition. According to (1.12) the vicinity of the quantum critical point can be divided into regions with predominantly classical or quantum fluctuations. The boundary, marked by the dashed lines in Fig. 1.1, is not sharp but rather a smooth crossover line. At sufficiently low temperatures these crossover lines are inside the critical region (i.e., the region where the critical power laws can be observed). An experiment performed along path (a) will therefore observe a crossover from quantum critical behavior away from the transition to classical critical behavior asymptotically close to it. At very low temperatures the classical region may become so narrow that it is actually unobservable in an experiment.

In addition to the critical behavior at very low temperatures, the quantum critical point also controls the behavior in the so-called quantum critical region (Chakravarty, Halperin, and Nelson 1989). This region is located at the critical \(p\) but, somewhat counter-intuitively, at comparatively high temperatures (where the character of the fluctuations is classical). In this region the system 'looks critical' with respect to \(p\) but is driven away from criticality by the temperature (i.e., the critical singularities are exclusively protected by \(T\)). An experiment carried out along path (b) will therefore observe the temperature scaling at the quantum critical point.

In recent years quantum phase transitions have attracted considerable attention from theoretical as well as experimental physicists. Among the transitions investigated are magnetic transitions in metals, the anti-ferromagnetic transition associated with high-temperature superconductivity, metal-insulator transitions, superconductor-insulator transitions, and the plateau transition in quantum Hall systems. This list is certainly incomplete and is likely to be expanded in the future.
Chapter 1. Classical and quantum phase transitions

Figure 1.1: Schematic phase diagram in the vicinity of a quantum critical point (QCP). The solid line marks the boundary between ordered and disordered phase. The dashed lines indicate the crossover between predominantly quantum or classical character of the fluctuations, and the shaded area denotes the critical region where the leading critical singularities can be observed. Paths (a) and (b) are discussed in the text.

For a more comprehensive coverage of quantum phase transitions and their appearance in different physical contexts the reader is referred to the excellent review articles by Sachdev (1996), Kirkpatrick and Belitz (1997), Sondhi et al. (1997), or Belitz and Kirkpatrick (1998).

1.4 Equilibrium versus non-equilibrium transitions

Strictly speaking, there are no true equilibrium phenomena in nature since they would require infinite relaxation times and infinite thermal reservoirs. Unfortunately, non-equilibrium statistical mechanics has by far not reached the same level of development as equilibrium statistical mechanics. This general statement is also true for the study of phase transitions and critical phenomena. The critical dynamics of small fluctuations around the equilibrium state is generally well understood today. It has been classified according to the different dynamical universality classes in the well-known review article by Hohenberg and Halperin (1977). In contrast, a corresponding classification for phase transitions far from equilibrium still waits in a distant future.

Two classes of non-equilibrium phenomena have been intensively discussed in the literature during the last two decades. First, there are systems approaching equilibrium after a non-infinitesimal displacement from the equilibrium state. Second, there are systems which are driven by external fields or non-thermal noise to a non-equilibrium steady state.

The prime example for the first class is the problem of phase separation in a binary alloy. At high temperatures the two species are uniformly mixed in the alloy. Below a certain critical temperature $T_c$ the uniform state becomes unstable and the new equilibrium state consists of two domains containing phases of different compositions. The question is now, how will the system evolve from the homogeneous to the inhomogeneous state after quenching from a
1.4. Equilibrium versus non-equilibrium transitions

Figure 1.2: Schematic comparison of conventional and directed percolation. The thick lines symbolize resistors while the arrows symbolize diodes. In the example shown a spanning cluster exists for conventional percolation but the same cluster is not a spanning cluster for directed percolation. The grey circle marks the bond which breaks the cluster.

Percolation

Directed Percolation

temperature above the critical temperature into the two-phase region. There are two principal mechanisms for phase separation: nucleation and spinodal decomposition. Nucleation occurs if the homogeneous state is metastable and can thus be destroyed only by a finite perturbation. In this case phase separation occurs through the formation of droplets of one of the stable phases which will grow if they are larger than a certain critical radius. If, in contrast, the homogeneous state is unstable towards arbitrarily small composition fluctuations then the homogeneous state will decay via the formation and growth of small-amplitude long-wavelength fluctuations. In both cases the later stages of the phase separation are dominated by processes on long length and time scales. They can therefore be analyzed using scaling and the renormalization group. For reviews see, e.g., Gunton et al. (1983), Furukawa (1985), or Langer (1991).

Systems having non-equilibrium steady states, the second class mentioned above, arise in a large variety of externally driven systems, ranging from growing surfaces (Meakin 1993), moving interfaces in random media (Kardar 1998, Fisher 1998), and reaction-diffusion processes (Schmittmann and Zia 1995, Marro and Dickman 1997) to biological systems and population dynamics (Murray 1989). The steady states of such systems constantly gain energy from the external field. At the same time they constantly lose energy to a heat bath. Therefore, even if the states are time-independent, they are by no means equilibrium states. Instead they are non-equilibrium steady states with an unknown non-Boltzmann probability distribution in general. Using the intuition acquired from studying equilibrium states, the properties of non-equilibrium steady states often appear to be very surprising. One example is the appearance of long-range spatial correlations away from criticality which do not exist in classical equilibrium systems. Note, however, that they can also exist in quantum systems at zero temperature (an example is discussed in Chapter 3).

The prototypical dynamical universality class for driven systems is the one known as the directed-percolation universality class. It is as ubiquitous in non-equilibrium critical phenomena as is the Ising universality class in equilibrium critical phenomena. Directed percolation is similar to conventional percolation (Stauffer and Aharony 1992), see Fig. 1.2. Conventional percolation can be visualized by a network of bonds which are randomly occupied by resistors or empty. If the portion $p$ of occupied bonds is small no current will flow between the bottom
and top electrodes. If $p$ exceeds a critical $p_c$ so that a cluster of occupied bonds connects the top and bottom electrodes a current starts to flow. For directed percolation, diodes are used instead of the resistors so that the current can only flow in a preferred direction (upwards in Fig. 1.2). It is obvious that directed percolation has a larger $p_c$ than conventional percolation. Moreover, it turns out that the critical behavior is different, defining the directed-percolation universality class. In order to establish the connection between directed percolation and non-equilibrium phase transitions, the time dimension in the non-equilibrium problem is identified with the 'directed' space dimension (the upward direction in Fig. 1.2) in the percolation problem.

In addition to the references already given, a number of review articles on non-equilibrium phase transitions and non-equilibrium critical behavior can be found in van Beijeren (1998).
Chapter 2

Quantum spherical model

2.1 Classical spherical model

In the process of understanding a novel physical problem it is often very useful to consider a simple model which displays the phenomena in question in their most basic form. In the field of classical equilibrium critical phenomena such a model is the so-called classical spherical model which is one of the very few models in statistical physics that can be solved exactly but show non-trivial (i.e., non mean-field) critical behavior. The spherical model was conceived by Kac in 1947 in an attempt to simplify the Ising model. The basic idea was to replace the discrete Ising spins having only the two possible values $S_i = \pm 1$ by continuous real variables between $-\infty$ and $\infty$ so that the multiple sum in the partition function of the Ising model is replaced by a multiple integral which should be easier to perform. However, the multiple integral turned out to be not at all simple, and for a time it looked as if the spherical model was actually harder to solve than the corresponding Ising model. Eventually Berlin and Kac (1952) solved the spherical model by using the method of steepest descent to perform the integrals over the spin variables. Stanley (1968) showed that the spherical model, though created to be a simplification of the Ising model, is equivalent to the $n \to \infty$ limit of the classical $n$-vector model. Therefore, it can be used as the starting point for a $1/n$-expansion of the critical behavior.

In the following years the classical spherical model was solved exactly not only for nearest neighbor ferromagnetic interactions but also for long-range power-law interactions, random interactions, systems in random magnetic fields, and disordered electronic systems with localized states. Moreover, the model has been used as a test case for the finite-size scaling hypothesis. Reviews on the classical spherical model were given by Joyce (1972) and Khorunzhy et al. (1992).

Because the classical spherical model possesses such a wide variety of applications in the field of classical critical phenomena, it seems natural to look for a quantum version of the model in order to obtain a toy model for quantum critical behavior. Actually, the history of quantum spherical models dates back at least as far as the history of quantum critical behavior. Obermair (1972) suggested a canonical quantization scheme for a dynamical spherical model. However, this and later studies focused on the classical finite temperature critical behavior of the quantum model and did not consider the properties of the zero temperature quantum phase transition.

1In the classical $n$-vector model the dynamical variables are $n$-dimensional unit vectors. Thus, the Ising model is the 1-vector model, the classical XY-model is the 2-vector model and the classical Heisenberg model is the 3-vector model.
2.2 Quantization of the spherical model

The classical spherical model consists of \( N \) real variables \( S_i \in (-\infty, \infty) \) that interact with an external field \( h_i \) and with each other via a pair potential \( U_{ij} \). The Hamiltonian is given by

\[
H_{cl} = \frac{1}{2} \sum_{i,j} U_{ij} S_i S_j + \sum_i h_i S_i .
\]  

(2.1)

In order to make the model well-defined at low temperatures, i.e., in order to prevent a divergence of \( S_i \) in the ordered phase, the values of \( S_i \) are subject to an additional constraint, the so-called spherical constraint. Two versions of the constraint have been used in the literature, the strict and the mean constraints, defined by

\[
\sum_i S_i^2 = N ,
\]

(2.2)

\[
\sum_i \langle S_i^2 \rangle = N ,
\]

(2.3)

respectively. Here \( \langle \ldots \rangle \) is the thermodynamic average. Both constraints have been shown to give rise to the same thermodynamic behavior while other quantities like correlation functions differ. In the following we restrict ourselves to the mean spherical constraint which is easier to implement in the quantum case. The Hamiltonian (2.1) has no internal dynamics. According to the factorization (1.4) it can be interpreted as being only the configurational part of a more complicated problem. Therefore, the construction of the quantum model consists of two steps: First we have to add an appropriate kinetic energy to the Hamiltonian which defines a dynamical spherical model which can be quantized in a second step.

In order to construct the kinetic energy term we define canonically conjugate momentum variables \( P_i \) which fulfill the Poisson bracket relations \( \{ S_i, P_j \} = \delta_{ij} \). The simplest choice of a kinetic energy term is then the one of Obermair (1972), \( H_{kin} = \frac{g}{2} \sum_i P_i^2 \), where \( g \) can be interpreted as inverse mass. In this case, the complete Hamiltonian of the dynamical spherical model

\[
H = H_{kin} + H_{cl} = \frac{g}{2} \sum_i P_i^2 + \frac{1}{2} \sum_{i,j} U_{ij} S_i S_j + \sum_i h_i S_i + \mu \left( \sum_i S_i^2 - N \right)
\]

(2.4)

is that of a system of coupled harmonic oscillators. Here we have also added a source term for the mean spherical constraint (2.3). (The value of \( \mu \) has to be determined self-consistently so that (2.3) is fulfilled.)

In order to quantize the dynamical spherical model (2.4) we use the usual canonical quantization scheme: The variables \( S_i \) and \( P_i \) are reinterpreted as operators. The Poisson bracket relations are replaced by the corresponding canonical commutation relations

\[
[S_i, S_j] = 0, \quad [P_i, P_j] = 0, \quad \text{and} \quad [S_i, P_j] = i\hbar \delta_{ij} .
\]

(2.5)

Equations (2.3), (2.4), and (2.5) completely define the quantum spherical model. At large \( T \) or \( g \) the model is in its disordered phase \( \langle S_i \rangle = 0 \). The transition to an ordered state can be triggered by lowering \( g \) and/or \( T \).

It must be emphasized that this model does not mimic (or even describe) Heisenberg-Dirac spins. Instead it is equivalent to the \( n \to \infty \) limit of a quantum rotor model which can be seen as a generalization of an Ising model in a transverse field. Of course, the choices of the kinetic energy and quantization scheme are not unique. In agreement with the general discussion in Sec. 1.3 different choices will lead to different critical behavior at the quantum phase transition, while the classical critical behavior is the same for all these models. For a more detailed discussion of these questions see reprint 1.
2.3 Quantum phase transitions

The quantum spherical model defined in eqs. (2.3), (2.4), and (2.5) can be solved exactly since it is equivalent to a system of coupled harmonic oscillators.

In the reprint 1 this was done for a model with arbitrary translationally invariant interactions (long-range as well as short-range) in a spatially homogeneous external field. As expected, the resulting critical behavior at finite temperatures is that of the classical spherical model (2.1). In contrast, we find that the critical behavior at the zero-temperature quantum phase transition is different. If the interaction $U_{ij}$ in the Hamiltonian is short ranged, the dynamical exponent turns out to be $z = 1$. For a power-law interaction, parameterized by the singularity of the Fourier transform of the interaction, $U_k \propto |k|^x$ for $k \to 0$, we obtain $z = x/2$. In both cases the quantum critical behavior of the $d$-dimensional quantum spherical model is the same as the classical critical behavior of a corresponding $d + z$-dimensional model.

In order to describe the crossover between the quantum and classical critical behaviors we also derive the crossover scaling form of the equation of state. This is only possible below the upper critical dimension. Above, crossover scaling breaks down. This is analogous to the breakdown of finite-size scaling in the spherical model above the upper critical dimension. It can be attributed to a dangerous irrelevant variable.

In reprint 2 we consider the influence of a quenched random field on the quantum phase transition in the quantum spherical model. The model can be solved exactly even in the presence of a random field without the necessity to use the replica trick. We find that the quantum critical behavior is dominated by the static random field fluctuations rather than by the quantum fluctuations. Since the random field fluctuations are identical at zero and finite temperatures it follows that in the presence of a random field quantum and classical critical behavior are identical.
Chapter 3

Magnetic quantum phase transitions of itinerant electrons

3.1 Itinerant ferromagnets

In the normal metallic state the electrons form a Fermi liquid, a concept introduced by Landau (1956, 1957). In this state the excitation spectrum is very similar to that of a non-interacting Fermi gas. The basic excitations are weakly interacting fermionic quasiparticles which behave like normal electrons but have renormalized parameters like an effective mass. However, at low temperatures the Fermi liquid is potentially unstable against sufficiently strong interactions, and some type of a symmetry-broken state may form. This low-temperature phase may be a superconductor, a charge density wave, or a magnetic phase, e.g., a ferromagnet, an anti-ferromagnet, or a spin glass, to name a few possibilities. In general, it will depend on the microscopic parameters of the material under consideration what the nature of the low-temperature phase and, specifically, of the ground state will be. Upon changing these microscopic parameters at zero temperature, e.g., by applying pressure or an external field or by changing chemical composition, the nature of the ground state may change, i.e., the system may undergo a quantum phase transition.

In this chapter we will discuss the universal properties of a particular class of quantum phase transitions in metallic systems, viz. magnetic quantum phase transitions. Most of the chapter will be devoted to the ferromagnetic quantum phase transition of clean itinerant electrons but we will also briefly consider the influence of disorder on the ferromagnetic and antiferromagnetic transitions of itinerant electrons.

The experimentally best studied example of a ferromagnetic quantum phase transition of itinerant electrons is probably provided by the pressure-tuned transition in MnSi (Pfleiderer et al. 1997 and references therein). MnSi belongs to the class of so-called nearly or weakly ferromagnetic materials. This group of metals, consisting of transition metals and their compounds such as ZrZn2, TiBe2, Ni3Al, and YCO2 in addition to MnSi are characterized by strongly enhanced spin fluctuations. Thus, their ground state is close to a ferromagnetic instability which makes them good candidates for actually reaching the ferromagnetic quantum phase transition in experiment by changing the chemical composition or applying pressure.

At ambient pressure MnSi is paramagnetic for temperatures larger than \( T_c = 30 \, \text{K} \). Below \( T_c \) it orders magnetically. The order is, however, not exactly ferromagnetic but a long-wavelength (190 Å) helical spin spiral along the (111) direction of the crystal. The ordering wavelength depends only weakly on the temperature, but a homogeneous magnetic field of about 0.6 T
suppresses the spiral and leads to ferromagnetic order. One of the most remarkable findings about the magnetic phase transition in MnSi is that it changes from continuous to first order with decreasing temperature as is shown in Fig. 3.1. Specifically, in an experiment carried out at low pressure (corresponding to a comparatively high transition temperature) the susceptibility shows a pronounced maximum at the transition, reminiscent of the singularity expected from a continuous phase transition. In contrast, in an experiment at a pressure very close to (but still smaller than) the critical pressure the susceptibility does not show any sign of a divergence at the phase transition. Instead, it displays a finite step suggestive of a first-order phase transition.

A related set of experiments is devoted to a phenomenon called the itinerant electron metamagnetism. Here a high magnetic field is applied to a nearly ferromagnetic material such as Co(Se$_{1-x}$S$_x$)$_2$ (Adachi et al. 1979) or Y(-Co$_{1-x}$Al$_x$)$_2$ (Sakakibara et al. 1990). At a certain field strength the magnetization of the sample shows a pronounced jump. This can easily be explained if we assume that the free energy as a function of the magnetization has the triple-well structure characteristic of the vicinity of a first-order phase transition. In zero field the side minima must have a larger free energy than the center minimum (since the material is paramagnetic in zero field). The magnetic field essentially just ”tilts” the free energy function. If one of the side minima becomes lower than the center (paramagnetic) one, the magnetization jumps.

In the literature the first-order transition in MnSi at low temperatures as well as the itinerant electron metamagnetism have been attributed to sharp structures in the electronic density of states close to the Fermi energy which stem from the band structure of the particular material. These structures in the density of states can lead to a negative quartic coefficient in a magnetic Landau theory and thus to the above mentioned triple-well structure. In the next section it will
be shown, however, that the two phenomena are generic since they are rooted in the universal many-body physics underlying the transition. Therefore, they will occur for all nearly or weakly ferromagnetic materials irrespective of special structures in the density of states.

3.2 Landau-Ginzburg-Wilson theory of the ferromagnetic quantum phase transition

From a theoretical point of view, the ferromagnetic transition of itinerant electrons is one of the most obvious quantum phase transitions. It was also one of the first quantum phase transitions investigated in some detail. Hertz (1976) studied a simple microscopic model of interacting electrons and derived a Landau-Ginzburg-Wilson theory for the ferromagnetic quantum phase transition. Hertz then analyzed this theory by means of renormalization group methods which were a direct generalization of Wilson’s treatment of classical transitions. He found a dynamical exponent of \( z = 3 \). According to the discussion in Sec. 1.3 this effectively increases the dimensionality of the system from \( d \) to \( d + 3 \). Therefore, the upper critical dimension of the quantum phase transition would be \( d_c^+ = 1 \), and Hertz concluded that the critical behavior of the ferromagnetic quantum phase transition is mean-field like in all physical dimensions \( d > 1 \).

Despite the somewhat artificial character of this simplified model there was a general belief that its main qualitative results apply to real itinerant ferromagnets as well.

In a series of papers (reprints 3, 4 and 5) we have shown that this belief is mistaken. The properties of the ferromagnetic quantum phase transition of itinerant electrons have turned out to be much more complicated since the magnetization couples to additional, non-critical soft modes in the electronic system. Mathematically, this renders the conventional Landau-Ginzburg-Wilson approach invalid since an expansion of the free energy in powers of the order parameter does not exist. Physically, the additional soft modes lead to an effective long-range interaction between the order parameter fluctuations. This long-range interaction, in turn, can change the character of the transition from a continuous transition with mean-field exponents to either a continuous transition with non-trivial (non mean-field) critical behavior or even to a first order transition.

The derivation of our theory (reprints 3 and 5) follows Hertz (1976) in spirit, but the technical details are considerably different. We start from a general microscopic model Hamiltonian \( H = H_0 + H_{ex} \) of interacting fermions. \( H_{ex} \) is the exchange interaction which is responsible for the ferromagnetism, \( H_0 \) contains not only the free electron part but also all interactions except for the exchange interaction. Using standard manipulations (see, e.g., Negele and Orland 1988) the partition function is written in terms of a functional integral over fermionic (Grassmann) variables. After introducing the magnetization field \( \mathbf{M}(\mathbf{r}, \tau) \) via a Hubbard-Stratonovich transformation of the exchange interaction, a cumulant expansion is used to integrate out the fermionic degrees of freedom. With the four-vector notation with \( x = (x, \tau) \) and \( \int dx = \int dx \int_0^{1/k_B T} d\tau \) the resulting Landau-Ginzburg-Wilson free energy functional reads

\[
\Phi[\mathbf{M}] = \frac{1}{2} \int dx \, dy \left[ \frac{1}{t} \delta(x - y) - \chi^{(2)}(x - y) \right] \mathbf{M}(x) \cdot \mathbf{M}(y) + \\
+ \sum_{n=3}^{\infty} \frac{(-1)^{n+1}}{n!} \int dx_1 \cdots dx_n \chi^{(n)}_{a_1\ldots a_n}(x_1, \ldots, x_n) M^{a_1}(x_1) \cdots M^{a_n}(x_n), \quad (3.1)
\]

\(^1\)In order to obtain a quantitative description Moriya and Kawabata developed a more sophisticated theory, the so-called self-consistent renormalization theory of spin fluctuations (Moriya 1985). This theory is very successful in describing magnetic materials with strong spin fluctuations outside the critical region. Its results for the critical behavior at the ferromagnetic quantum phase transition are, however, identical to those of Hertz.
where $\Gamma_t$ is the exchange interaction strength. The coefficients in the Landau-Ginzburg-Wilson functional are the connected $n$-point spin density correlation functions $\chi^{(n)}$ of the reference system $H_0$ which is a conventional Fermi liquid. The famous Stoner criterion of ferromagnetism, $\Gamma_t g(\epsilon_F) > 1$ (Stoner 1938) (here $g(\epsilon_F)$ is the density of states at the Fermi energy) can be rediscovered from the stability condition of the Gaussian term of $\Phi[M]$, if one takes the $\chi^{(2)}$ to be that of free electrons.

We have studied the long-wavelength and long-time properties of the spin-density correlation functions of a Fermi liquid (reprint 4) using diagrammatical perturbation theory in the interaction. Somewhat surprisingly, all these correlation functions generically (i.e., away from any critical point) show long-range correlations in real space which correspond to singularities in momentum space in the long-wavelength limit $q \to 0$. Consequently, the Landau-Ginzburg-Wilson functional (3.1) is formally ill defined. However, we have still been able to extract a considerable amount of information.

While analogous generic long-range correlations in time (the so-called long-time tails) are well known from several interacting systems, long-range spatial correlations in classical systems are impossible due to the fluctuation-dissipation theorem. They are known, however, in non-equilibrium steady states (see, e.g., Schmittmann and Zia 1998). The physical reason for the singularities in the coefficients $\chi^{(n)}$ of the Landau-Ginzburg-Wilson functional is that in the process of integrating out the fermionic degrees of freedom the soft particle-hole excitations have been integrated out, too. It is well known from classical dynamical critical phenomena (Hohenberg and Halperin 1977) that integrating out soft modes leads to singularities in the resulting effective theory.

Specifically, in reprint 4 we have found that the static spin susceptibility $\chi^{(2)}(r)$ behaves like $r^{-(2d-1)}$ for large distances $r$. The leading long-wavelength dependence therefore has the form

$$
\begin{align*}
\frac{\chi^{(2)}(q)}{\chi^{(2)}(0)} &= 1 + c_d (|q|/2k_F)^{d-1} + O(|q|^2) \quad (d < 3) \quad (3.2) \\
\frac{\chi^{(2)}(q)}{\chi^{(2)}(0)} &= 1 + c_3 (|q|/2k_F)^2 \ln(2k_F/|q|) + O(|q|^2) \quad (d = 3). \quad (3.3)
\end{align*}
$$

Here $k_F$ is the Fermi momentum and $c_d$ and $c_3$ are dimensionless constants. Remarkably, in second order perturbation theory $c_d$ and $c_3$ turn out to be positive, implying that $\chi^{(2)}$ increases with increasing $q$. If this is the true asymptotic behavior at small $q$ a continuous ferromagnetic quantum phase transition is not possible, since the leading instability of the Gaussian term in (3.1) is at the maximum of $\chi^{(2)}$ with respect to $q$.

In reprint 4 we have discussed several mechanisms that can reverse the signs of $c_d$ and $c_3$. If the sign of the non-analyticity is, for one of these reasons, negative in a particular system, then the ferromagnetic quantum phase transition will be a conventional second order phase transition. We have investigated this phase transition in detail in reprint 5. As a result of the effective long-range interaction between the spin fluctuations the critical behavior is non-mean-field like for all dimensions $d \leq 3$.

The generic case is, however, that $c_d$ and $c_3$ in eqs. (3.2) and (3.3) are positive. In this case two different scenarios are possible. The first possibility is that the zero-temperature ferromagnetic transition is of first order. It has been shown in reprint 5 that the non-analyticity in $\chi^{(2)}$ leads to an analogous non-analyticity in the magnetic equation of state, which takes the form

$$
\begin{align*}
tm - v_dm^d + um^3 &= h \quad (d < 3) \quad (3.4) \\
tm - v_3m^3 \ln(1/m) + um^3 &= h \quad (d = 3), \quad (3.5)
\end{align*}
$$
where \( m = \langle |M(x)| \rangle \) is the thermodynamic magnetization, and \( u, v_d \) and \( v_3 \) are positive constants. This equation of state describes a first-order phase transition since the next-to-leading term for small \( m \) has negative sign. In reprint 7 we have investigated this scenario in some detail. Since the non-analyticities in \( \chi^{(2)} \) and the equation of state are cut off by a finite temperature, the transition will be of first order at very low \( T \) but turn second order at higher temperatures. The two regimes are separated by a tricritical point. The behavior becomes even more interesting with the introduction of quenched disorder into the electron system (see the next Section for a more detailed discussion of the influence of disorder). In this case there are even stronger singularities in \( \chi^{(2)} \) and in the equation of state which are related to the diffusive motion of the electrons. They have, however, the opposite sign. Therefore, sufficiently strong disorder will also suppress the first order transition. The competition between the ballistic and diffusive singularities and the temperature which cuts off both gives rise to a rich phase diagram showing first and second order phase transitions, several multicritical points and even regions with metamagnetic behavior. The theory developed in reprint 7 thus gives a complete qualitative description of the experiments on MnSi with the exception of the spiral ordering (see below).

The second possible scenario arising if \( c_d \) or \( c_3 \) are positive is that the ground state of the system will not be ferromagnetic but instead a spin-density wave at finite \( q \). This scenario has not been studied in much detail so far, but work is in progress. It is tempting to interpret the spiral ordering in MnSi as a signature of this finite-\( q \) instability. This is, however, not very likely since a finite-\( q \) instability caused by our long-range interaction will be strongly temperature dependent due to the temperature cutoff of the singularities. As mentioned above, experimentally the ordering wave vector is essentially temperature independent. Further work will be necessary to decide which of the two possible scenarios, viz. a first-order ferromagnetic transition or a continuous transition to modulated magnetic order, is realized under what conditions. Moreover, let us point out, that in \( d = 3 \) the non-analyticity is only a logarithmic correction and would hence manifest itself only as a phase transition at exponentially small temperatures, and exponentially large length scales. Thus, it may well be unobservable experimentally for some materials.

In addition to the research on the ferromagnetic phase transition summarized above we have also studied the properties of the ordered ferromagnetic phase. In reprint 6 we have investigated the influence of the non-analyticities on the dispersion relation of the ferromagnetic spin waves. Since the non-analyticities are cut off by a finite magnetization it turns out that the dispersion relation remains \( \omega \propto q^2 \) but the prefactor picks up a non-trivial magnetization dependence (different from being proportional to \( m \) as in Stoner theory). For small magnetization \( m \) we find

\[
\omega \propto m^{d-2} q^2 \quad (d < 3) \\
\omega \propto m \ln(1/m) q^2 \quad (d = 3)
\]  

(3.6)  

(3.7)

Until now, the corrections to mean-field theory predicted by (3.6) and (3.7) have not been observed experimentally.

### 3.3 Influence of disorder and rare regions on magnetic quantum phase transitions

So far we have mostly considered quantum ferromagnetism in clean electronic systems. An interesting question is what happens in the presence of quenched disorder. The general problem of
Chapter 3. Magnetic quantum phase transitions of itinerant electrons

how quenched disorder influences the critical behavior at a continuous phase transition has been investigated for more than 30 years. By comparing the fluctuations of the local critical temperature with the distance from the global critical point Harris (1974) showed that a particular critical behavior is unaffected by quenched disorder if the correlation length exponent $\nu$ obeys the inequality $\nu \geq 2/d$. This is the so-called Harris criterion. In the opposite case, $\nu < 2/d$, the disorder modifies the critical behavior, and three possible scenarios can be distinguished:

- a new conventional critical point that has a correlation length exponent $\nu \geq 2/d$ and is thus stable
- an unconventional critical point where the usual classification in terms of power-law critical exponents loses its meaning
- destruction of the (continuous) phase transition

Independent of the fate of the critical behavior the disorder leads to very interesting phenomena even in the paramagnetic phase. Disorder in general decreases the critical temperature $T_c$ from its value $T_c^0$ for the corresponding clean system. However, in an infinite system one will find, with a small but nonzero probability, arbitrarily large regions that are devoid of impurities. Usually the probability decreases exponentially with the size of the region. In the temperature region $T_c < T < T_c^0$ these regions display local order while the system is still globally disordered. These regions are known as ‘rare regions’, and the order parameter fluctuations induced by them as ‘local moments’ or ‘instantons’. Griffiths (1969) was the first to show that they lead to a non-analytic free energy everywhere in the region $T_c < T < T_c^0$, which is known as the Griffiths phase, or, more appropriately, the Griffiths region. In generic classical systems (with short-range correlated disorder) this is a weak effect, since the singularity in the free energy is only an essential one. In contrast, in quantum systems the singularity is much stronger, leading to a divergence of the susceptibility within the Griffiths region. This is related to the fact that the disorder is static, i.e., completely correlated in the imaginary time dimension.

The Griffiths singularities influence the physics in the disordered phase close to the transition. An interesting question is whether rare regions actually change the critical behavior at the phase transition itself. Recent work (Dotsenko et al. 1995) on a weakly disordered classical Ising model has suggested that the rare regions may actually destroy the conventional critical behavior and lead to activated (i.e., non-power-law) scaling. Fisher (1995) has investigated quantum Ising spin chains in a transverse random field by means of an asymptotically exact real-space renormalization group. He has found activated critical behavior due to rare regions.

In reprints 8 and 9 we have investigated the influence of rare regions on magnetic quantum phase transitions of disordered itinerant electrons and contrasted the cases of itinerant ferromagnets and antiferromagnets. The rare regions or local moments are reflected in the existence of spatially inhomogeneous saddle points of the Landau-Ginzburg-Wilson functional. We have derived an effective theory that takes into account all of these saddle points and small fluctuations around each of them. Thus it contains what would be considered non-perturbative effects in the conventional approach. Technically, the resulting free energy functional for the fluctuations contains a new term in addition to those obtained within the conventional perturbative approach because the inhomogeneous saddle points act as an additional source of disorder. Since the saddle points are static but self-generated by the system (and therefore in equilibrium with the other degrees of freedom) the new disorder term takes the form of static annealed disorder.

\footnote{The following consideration is formulated in the language of a thermal transition. The generalization to a quantum transition is straightforward.}
A renormalization group analysis of the resulting effective theory shows that in the case of antiferromagnets, the previously found critical fixed point is unstable with respect to this new term, and that no stable critical fixed point exists at one-loop order of the perturbation theory. This can be interpreted either as a complete destruction of the antiferromagnetic long-range order in favor of a random singlet phase (Bhatt and Lee 1982) or the existence of a non-conventional critical point (e.g., with activated scaling). The negative result for the antiferromagnets is contrasted with the case of itinerant ferromagnets, where we found that the previously found critical behavior is unaffected by the rare regions due to an effective long-ranged interaction between the order parameter fluctuations.
Chapter 4

Metal-insulator transitions of disordered interacting electrons

4.1 Localization and interactions

If disorder is introduced into a metallic system, e.g., by adding impurity atoms, the nature of the electronic states can change from spatially extended to localized, giving rise to a disorder-driven metal-insulator transition (Anderson 1958). The localization transition of disordered non-interacting electrons, the so-called Anderson transition, is comparatively well understood (for a review see, e.g., Kramer and MacKinnon 1993). The scaling theory of localization (Abrahams et al. 1979) predicts that in the absence of spin-orbit coupling or magnetic fields all states are localized in one and two dimensions for arbitrarily weak disorder. Thus, no true metallic phase exists in these dimensions. In contrast, in three dimensions there is a phase transition from extended states for weak disorder to localized states for strong disorder. These results of the scaling theory are in agreement with large-scale computer simulations of non-interacting disordered electrons.

However, in reality electrons do interact via the Coulomb potential, and the question is, how this changes the above conclusions. The conventional approach to the problem of disordered interacting electrons is based on a perturbative treatment of both disorder and interactions (for a review see, e.g., Altshuler and Aronov 1985). It leads to a scaling theory and a related field-theoretic formulation of the problem (Finkelstein 1983), which was later investigated in great detail within the framework of the renormalization group (for a review see Belitz and Kirkpatrick 1994). One of the main results is that in the absence of external symmetry-breaking (spin-orbit coupling or magnetic impurities, or a magnetic field) a phase transition between a normal metal and an insulator only exists in dimensions larger than two, as was the case for non-interacting electrons. In two dimensions the results of this approach are inconclusive since the renormalization group displays runaway flow to zero disorder but infinite interactions. Furthermore, it has not been investigated so far, whether effects of rare regions analogous to those discussed in Sec. 3.3 for magnetic transitions would change the above conclusions about the metal-insulator transition.

Experimental work on the disorder-driven metal-insulator transition (mostly on doped semiconductors) carried out before 1994 essentially confirmed the existence of a transition in three dimensions while no transition was found in two-dimensional systems. Therefore it came as a surprise when experiments (Kravchenko et al. 1995) on Si-MOSFETs revealed indications of a true metal-insulator transition in 2D (see Fig. 4.1). This discovery induced a burst of
activity, both experimental and theoretical. It soon became clear that the main difference between the new experiments and those carried out earlier was that the electron density in the Si-MOSFETs is very low. Therefore, the Coulomb interaction is particularly strong compared to the Fermi energy, and interaction effects are a likely reason for the metal-insulator transition in the Si-MOSFETs. A complete understanding has, however, not yet been obtained. Different explanations have been suggested based on the perturbative renormalization group, non-perturbative effects, or the transition actually being a superconductor-insulator transition rather than a metal-insulator transition (see reprint 14 for some references).

We have approached the problem of disordered interacting electrons numerically. The model we have investigated is the quantum Coulomb glass model, a generalization of the classical Coulomb glass model (Efros and Shklovskii 1975) used to study disordered insulators. It is defined on a hypercubic lattice of \( L^d \) sites occupied by \( N = K L^d \) spinless electrons \((0 < K < 1)\). To ensure charge neutrality each lattice site carries a compensating positive charge of \( Ke \). The Hamiltonian is given by

\[
H = -t \sum_{\langle ij \rangle} (c_i^\dagger c_j + c_j^\dagger c_i) + \sum_i \varphi_i n_i + \frac{1}{2} \sum_{i \neq j} (n_i - K)(n_j - K)U_{ij} \tag{4.1}
\]

where \( c_i^\dagger \) and \( c_i \) are the electron creation and annihilation operators at site \( i \), respectively, and \( \langle ij \rangle \) denotes all pairs of nearest neighbor sites. \( t \) gives the strength of the hopping term and \( n_i \) is the occupation number of site \( i \). For a correct description of the insulating phase the Coulomb interaction between the electrons is kept long-ranged, \( U_{ij} = U/r_{ij} \), since screening breaks down in the insulator (the distance \( r_{ij} \) is measured in units of the lattice constant). The
random potential values $\varphi_i$ are chosen independently from a box distribution of width $2W$ and zero average. Two important limiting cases of the quantum Coulomb glass are the Anderson model of localization (for $U_{ij} = 0$) and the classical Coulomb glass (for $t = 0$).

For two reasons the numerical simulation of disordered quantum many-particle systems is one of the most complicated problems in computational condensed matter physics. First, the dimension of the Hilbert space to be considered grows exponentially with the system size. Second, the presence of quenched disorder requires the simulation of many samples with different disorder configurations in order to obtain averages or distribution functions of physical quantities. In the case of disordered interacting electrons the problem is even more challenging due to the long-range character of the Coulomb interaction which has to be retained, at least for a correct description of the insulating phase. We have used two different numerical methods to tackle the problem. First, we have decoupled the Coulomb interaction by means of a Hartree-Fock approximation and numerically solved the remaining self-consistent disordered single-particle problem. This method permits comparatively large system sizes of more than $10^3$ sites. The results of this approach are summarized in Sec. 4.2 together with those of exact diagonalization studies we performed to check the quality of the Hartree-Fock approximation. Since the Hartree-Fock method turned out to be a rather poor approximation for the calculation of transport properties we have then developed an efficient method to calculate the low-energy properties of disordered quantum many-particle systems with high accuracy. This method, the Hartree-Fock based diagonalization, and the results we have obtained this way are summarized in Sec. 4.3.

### 4.2 Hartree-Fock approximation

The Hartree-Fock approximation consists in decoupling the Coulomb interaction by replacing operators by their expectation values:

\[
H_{\text{HF}} = -t \sum_{\langle ij \rangle} (c_i^\dagger c_j + c_j^\dagger c_i) + \sum_i (\varphi_i - \mu)n_i + \sum_{i \neq j} n_i U_{ij} \langle n_j - K \rangle - \sum_{i,j} c_i^\dagger c_j U_{ij} \langle c_i^\dagger c_i \rangle,
\]  

(4.2)

where the first two terms contain the single-particle part of the Hamiltonian, the third is the Hartree energy and the fourth term contains the exchange interaction. $\langle \ldots \rangle$ represents the expectation value with respect to the Hartree-Fock ground state which has to be determined self-consistently. In this way the many-particle problem is reduced to a self-consistent disordered single-particle problem which we solve by means of numerically exact diagonalization.

In reprint 10 we applied this method to investigate the three-dimensional quantum Coulomb glass model. We found that the interaction induces a depletion of the single-particle density of states in the vicinity of the Fermi energy. For small hopping strength $t$ the depletion takes the form of a Coulomb gap known from the classical ($t = 0$) limit. With increasing hopping strength there is a crossover from the nearly parabolic Coulomb gap to a square root singularity characteristic of the Coulomb anomaly in the metallic limit. The depletion of the density of states at the Fermi energy has drastic consequences for the localization properties of the electronic states. Since the degree of localization is essentially determined by the ratio between the hopping amplitude and the level spacing, a reduced density of states directly leads to stronger localization. Specifically, we calculated the inverse participation number and compared the cases of non-interacting and interacting electrons. In the presence of interactions we found a
pronounced maximum at the Fermi energy with values above that of non-interacting electrons. Thus, within the Hartree-Fock approximation electron-electron interactions lead to enhanced localization.

In order to precisely determine how the location of the metal-insulator transition changes as a result of this effect, we used the fact that the spectral statistics on the insulating side is equivalent to that of a Poisson ensemble of random matrices while the spectral statistics on the metallic side is that of a Gaussian orthogonal ensemble of random matrices (Shklovskii et al. 1993, Hofstetter and Schreiber 1993). By analyzing the statistics of the Hartree-Fock levels as a function of the hopping amplitude \( t \) we could thus determine the location of the metal-insulator transition in the phase diagram. In all cases the transition to a metal requires a larger hopping strength for interacting electrons than for non-interacting.

Since the Hartree-Fock method is an uncontrolled approximation it is highly desirable to compare these results to those of exact many-particle calculations. Now the question arises, what quantities are particular suitable for such a comparison. In principle, one should compare the values of physical observables like the conductivity in the case of d.c. transport. However, the Kubo-Greenwood conductivity is a complicated quantity from a numerical point of view since it involves a nontrivial extrapolation to zero frequency. Therefore, it would be nice to apply the simpler localization criteria known from non-interacting systems. This leads, however, to an additional complication. The usual criteria which are based on the (single-particle) participation number or the statistics of (single-particle) energy levels are not even defined for many-particle states. While this does not create any problems at the Hartree-Fock level (the Hartree-Fock states are effective single-particle states) it implies that the criteria cannot directly be applied to true many-particle states. In reprint 11 we discussed how to generalize the participation number to a many-particle state. It turned out that a unique procedure does not exist, and different generalizations have different merits. A promising candidate to replace the inverse participation number is the return probability of single-particle excitations (which for non-interacting systems reduces to the inverse participation number),

\[
R_p(\varepsilon) = \frac{1}{g(\varepsilon)} \frac{1}{N} \sum_j \lim_{\delta \to 0} \frac{\delta}{\pi} G_{jj}(\varepsilon + i\delta) G_{jj}(\varepsilon - i\delta).
\]

(4.3)

Here \( g(\varepsilon) \) is the single-particle density of states and \( G_{jj} \) is the diagonal element of the single-particle Greens function. However, in addition to the desired localization information the return probability also contains information about the decay of the quasi-particles. We have recently found out, how to calculate the quasiparticle weight from our numerical data. In the future we will use this result to disentangle the information about localization and decay contained in the return probability. Clearly, more work on this question is necessary.

In reprint 12 we compared the Hartree-Fock results to those of numerically exact diagonalizations of the many-particle Hamiltonian. Because the exact calculations require the diagonalization of a matrix whose dimension equals the size of the Hilbert space this comparison was restricted to systems with not more than 16 sites. While we found that the Hartree-Fock approximation yields reasonable results for static quantities like the single-particle density of states, it does a very poor job for localization properties and for time correlation functions such as the conductivity. Thus, we concluded that our Hartree-Fock results for the influence of the electron-electron interaction on transport quantities are highly unreliable. For this reason we decided to develop a new numerical method, the Hartree-Fock based diagonalization which will be discussed in the next section.
do for each disorder configuration
  solve HF approximation
  construct many-particle HF states
  find lowest-in-energy HF states
  transform Hamiltonian to basis of low-energy HF states
  diagonalize Hamiltonian
  transform observables to HF basis and calculate their values
enddo

Figure 4.2: Structure of the Hartree-Fock (HF) based diagonalization method.

4.3 Hartree-Fock based diagonalization

Since numerically exact diagonalizations of the full many-particle Hamiltonian are restricted to very small system sizes and, as we have seen, the Hartree-Fock results for transport properties are unreliable, a different method which gives exact results or at least provides a controlled approximation for comparatively large systems is highly desirable. In reprint 13 we developed such an approximation, the Hartree-Fock based diagonalization. It is related to the configuration interaction (CI) approach used in quantum chemistry (see, e.g., Fulde 1995). The basic idea is to diagonalize the many-particle Hamiltonian not in a real-space or momentum basis but rather in an energetically truncated basis of Hartree-Fock states. The Hartree-Fock states are comparatively close in character to the exact eigenstates in the entire parameter space. Therefore it is sufficient to keep only a very small fraction of the Hilbert space (e.g., 2000 out of \(9 \times 10^9\) states for 18 electrons on 36 lattice sites) to obtain low-energy quantities with an accuracy comparable to that of exact diagonalization. A schematic of the Hartree-Fock based diagonalization method is shown in Fig. 4.2. So far we have carried out test calculations for systems with up to 64 lattice sites (32 electrons) and production runs for up to 36 lattice sites (18 electrons).

As a first application of the Hartree-Fock based diagonalization method we studied the quantum Coulomb glass in two dimensions. The results of this work are presented in reprint 14. In order to determine the influence of the Coulomb interaction on transport we calculated the Kubo-Greenwood conductance. We found that the influence of electron-electron interactions on the d.c. conductance is opposite in the weakly and strongly disordered regimes. The conductance of strongly disordered electrons is considerably enhanced by a weak interactions. With increasing kinetic energy the relative enhancement decreases as does the interaction range where the enhancement occurs. The conductance of weakly disordered electrons is reduced even by weak interactions. In contrast, sufficiently strong interactions always reduce the conductance, and the system approaches a Wigner crystal or Wigner glass state. These results are summarized in Fig. 4.3.

The qualitative difference we found between the weakly and strongly disordered regimes can be explained in terms of two competing effects of the interactions. The dominant effect in the case of strong disorder is the destruction of phase coherence for the single-electron motion. It can be understood from the following simplistic argument: Electron-electron collisions are inelastic
Figure 4.3: d.c. conductance of a 2D system of $5 \times 5$ sites. The disorder strength is $W = 1$. The results represent logarithmic averages over 400 disorder configurations. (from reprint 14)

and thus phase-breaking from the point of view of a single electron. Therefore collisions destroy the quantum interference necessary for Anderson localization.\textsuperscript{1} It is clear that this mechanism to increase the conductance is particularly effective if the localization length is very small to begin with. In the opposite case, i.e., for weak disorder, the dominant effect of the interactions is an increasing pinning of the electrons by the repulsive forces which for strong interactions eventually leads to the formation of a Wigner glass or crystal. This simple arguments also explain, why the Hartree-Fock approximation did not reproduce the enhanced conductance in the localized regime: The Hartree-Fock potential is static and therefore it does not break the phase of the electron – in contrast to real electron-electron collisions.

In reprints 15 and 16 we performed investigations analogous to the above for quantum Coulomb glasses in three and one spatial dimensions, respectively. It turned out that the qualitative disorder and interaction dependencies of the conductance are identical to those in two dimensions. In particular, we always found that weak interactions induce delocalization in the strongly disordered regime. The degree of delocalization seems to be determined essentially by the ratio between disorder strength $W$ and the hopping band width $z t$ where $z$ is the number of nearest neighbor sites.

Our numerical results for the influence of weak interactions on the Kubo-Greenwood conductance can be compared to the results from the perturbative renormalization group (Apel and Rice 1982) which predicts that repulsive interactions always reduce the transport of disordered spinless fermions. Thus, our numerical results agree with those from perturbation theory in the case of weak disorder, while in the strongly disordered regime the perturbative results are qualitatively incorrect.

In addition to the Kubo-Greenwood conductance we have also calculated the above men-

\textsuperscript{1}Of course, this argument is an oversimplification: Taken at face value, it appears to always predict diffusion and thus metallic behavior. In order to obtain a more detailed prediction one has to analyze the phase space for electron-electron collisions in the localized regime. Moreover, what is neglected in the above argument is that the energy and phase of the many-particle state are not changed by a collision.
tioned return probability of single-particle excitations. The return probability at the Fermi energy displays a similar behavior as the Kubo-Greenwood conductance: For weak disorder the return probability increases with the interaction strength. The delocalizing tendency in the strongly localized regime is less pronounced, probably because the Coulomb gap in the single-particle density of states counteracts the delocalization.

In summary, the results obtained so far clearly show that interactions can have a delocalizing tendency in certain parameter regions. However, it is not clear whether this is sufficient to explain the metal-insulator transition found in two dimensions. More detailed investigations are presently under way to find the finite-size scaling behavior of the conductance. Moreover, we are currently generalizing the simulations to include spin degrees of freedom which have been shown to be important in the experiments on Si-MOSFETs.
Chapter 5

Damage spreading transitions

5.1 Introduction

The question to what extent the time evolution of a physical system depends on its initial conditions is one of the basic questions in nonlinear dynamics which have lead to the discovery of chaotic behavior (see, e.g., Schuster 1984). A related question is studied in the so-called damage spreading problem: How does a small perturbation in a cooperative system evolve in time? Damage spreading was first studied in theoretical biology. Kauffman (1969) investigated to what extent the results of the genetical evolution would have changed in response to small perturbations in the initial conditions. Later the concept found its way into the physics of cooperative systems (Creutz 1986, Derrida and Pomeau 1986, Stanley et al. 1987). In contrast to the phase transitions investigated in Chapters 2 to 4 damage spreading is a non-equilibrium phenomenon.

In a typical damage spreading problem two identical replicas of a system are evolving in time stochastically under the same noise realization (in a simulation this means that the same random numbers are used for both replicas). The two replicas start from different initial conditions. The difference between the microscopic configurations of the two replicas constitutes the 'damage'. It is measured in terms of the Hamming distance $D$ which is defined as the portion of sites at which the two replicas differ. Depending on the system’s parameters the damage can now either spread or heal with time which defines chaotic and regular regions in a damage spreading phase diagram and corresponding damage spreading transitions between them. Since damage spreading is non-equilibrium phenomenon these regions are not thermodynamic phases and the transitions are true non-equilibrium phase transitions.

Damage spreading falls into the large group of non-equilibrium phenomena with absorbing states whose most prominent example is directed percolation. An absorbing state is a state which – once reached – cannot be left any more. In the damage spreading problem the absorbing state corresponds to the undamaged configuration, i.e., both replicas are identical. In contrast to simpler examples like directed percolation, here the absorbing "state" is not static but possesses non-trivial dynamics. Based on the analogy between damage spreading and directed percolation it has been conjectured (Grassberger 1995) that damage spreading phase transitions generically fall into the directed percolation universality class. While many results supported this conjecture it turned out (Hinrichsen and Domany 1997) that for one of the most studied systems, the Ising model with Glauber dynamics, damage spreading falls into the so-called parity conserving universality class rather than the directed percolation universality class. The reason is an additional global up-down symmetry of the Glauber Ising model which leads to the existence of two equivalent absorbing states, viz. $D = 0$ and $D = 1$, and this changes the
5.2 Mean-field theory

Damage spreading in spin systems with purely relaxational single-site dynamics, i.e., a dynamical algorithm in which each spin variable $S_i$ can change its value independently, can be described by a master equation for the joint probability distribution $P$ of the system pair. It reads

\[
\frac{d}{dt} P(\nu_1, \ldots, \nu_N, t) = - \sum_{i=1}^{N} \sum_{\mu_i \neq \nu_i} P(\nu_1, \ldots, \nu_i, \ldots, \nu_N, t) w(\nu_i \rightarrow \mu_i) + \sum_{i=1}^{N} \sum_{\mu_i \neq \nu_i} P(\nu_1, \ldots, \mu_i, \ldots, \nu_N, t) w(\mu_i \rightarrow \nu_i). \tag{5.1}
\]

Here $\mu_i$ and $\nu_i$ are states of a spin pair $(S_i^{(1)}, S_i^{(2)})$ ($i$ is the site index, and (1) or (2) denotes the replica). Each spin variable can have the values $+\,$or $-\,$. Thus, the $\nu_i$ can have the values $++, --, +-,$ or $-+$. $w(\mu_i \rightarrow \nu_i)$ is the transition probability of the spin-pair $(S_i^{(1)}, S_i^{(2)})$ from state $\mu_i$ to $\nu_i$. Equation (5.1) contains the full difficulties of a dynamic many-particle system, it usually cannot be solved exactly. In reprints 17 and 19 we developed a mean-field like approximation to the master equation (5.1). The central idea is to treat the fluctuations at different sites as statistically independent.\(^1\) This amounts to approximating the probability distribution $P$ by a product of identical single-site distributions

\[
P(\nu_1, \ldots, \nu_N, t) = \prod_{i=1}^{N} P_{\nu_i}(t). \tag{5.2}
\]

Using this, the master equation reduces to an equation of motion for the single-site distribution $P_{\nu}$,

\[
\frac{d}{dt} P_{\nu} = \sum_{\mu \neq \nu} [-P_{\nu} W(\nu \rightarrow \mu) + P_{\mu} W(\mu \rightarrow \nu)], \tag{5.3}
\]

where $W(\mu \rightarrow \nu) = \langle w(\mu \rightarrow \nu) \rangle_P$ is the averaged transition probability. Equation (5.2) is a system of four coupled non-linear equations which is much easier to solve than the original master equation. In this formulation the Hamming distance is given as

\[
D = \frac{1}{2N} \sum_i |S_i^{(1)} - S_i^{(2)}| = P_{++} + P_{--}. \tag{5.3}
\]

In reprint 17 we applied the resulting mean-field theory to a two-dimensional kinetic Ising model on a honeycomb lattice. We contrasted the cases of Glauber and heat-bath dynamics.

\(^1\) Usually a mean-field theory is obtained by completely neglecting the fluctuations. In the case of damage spreading this does not lead to a sensible theory since the damage never spreads without fluctuations.
Both algorithms only differ in the way the random numbers are used in the spin updates, they create the same macroscopic dynamics. (In the Glauber dynamics the spin is \textit{flipped} if the probability is larger than the random number, in the heat-bath dynamics the spin is \textit{set} to, say, ”up” if the corresponding probability is larger than the random number.) For Glauber dynamics we found that a small initial damage heals for all temperatures below a certain spreading temperature $T_s$ which is smaller than the ferromagnetic critical temperature $T_c$. For $T_s < T < T_c$ the damage spreads, but the replicas remain partially correlated. Here the asymptotic damage $D$ is finite but smaller than 0.5. The damage also spreads in the paramagnetic phase above $T_c$ where the asymptotic damage is $D = 0.5$, i.e., the two replicas become completely uncorrelated. In contrast, for heat-bath dynamics a small initial damage always heals completely. The qualitative difference between Glauber and heat-bath dynamics which appears to be surprising at the first glance can be understood from the way the random numbers are used in the spin updates. An analogous difference had earlier been found in numerical simulations (Derrida and Pomeau 1986, Stanley et al. 1987).

In reprint 19 we studied the Ising model with Glauber dynamics in more detail. In addition to the two-dimensional model we also considered the limit of infinite dimensions which we found to have qualitatively the same properties. An external magnetic field suppresses the damage spreading, i.e., $T_s$ increases with increasing field. Above a certain critical field the damage always heals. This is not very surprising since a sufficiently strong field pins the spin variables in both replicas in the same preferred direction. We also calculated the critical properties at the spreading transition. Within our mean-field theory the critical behavior is identical to the mean-field limit of both directed percolation and the parity conserving universality class (which have the same mean-field limit). Thus, within the mean-field theory we cannot distinguish the two universality classes.

Reprint 20 is devoted to the influence of a random magnetic field on the damage spreading in the Ising model with Glauber dynamics. We generalized the mean-field approach by allowing the single-site distributions $P_\nu$ to depend on the local random field value. Instead of a single mean-field equation (5.2) we now obtain a finite or infinite set of equations (one equation for each possible value of the random field) which have to be solved simultaneously. In simple cases this can still be done exactly. Specifically, we considered a two-dimensional Ising model on a honeycomb lattice with a bimodal random field. We found that a weak random field supports damage spreading, i.e., $T_s$ first decreases with increasing random field strength. At a certain random field strength, which roughly coincides with the strength which completely suppresses long-range magnetic order, the trend reverses. Stronger random fields hinder the damage spreading, i.e., $T_s$ increases with increasing random field strength. At some critical strength the spreading temperature diverges. This behavior can be understood from the competition of two effects: (i) the random field suppresses long-range order which helps damage spreading and (ii) the random field leads to a preferred orientation of the spins, identical for both replicas, which reduces the damage.

All work described so far was concerned with single-site dynamical algorithms in which only a single spin is updated in each time step. In reprint 21 we generalized the master equation approach and the mean-field approximation to a second important class of dynamical algorithms, in which the spins at two sites exchange their values in each step. If the spin variables are interpreted as occupation numbers this corresponds to single-particle hops from one site to another. Note that the dynamical algorithms in this class are order-parameter conserving (i.e., the total magnetization does not change with time). As an example we investigated the damage spreading in a two-dimensional Ising model with Kawasaki dynamics. We found that in this system the damage spreads for all temperatures, and the configurations of the two repli-
cas become completely uncorrelated in the long-time limit. We further showed that the fact that the damage never heals is not restricted to this model. Instead, it is generic for systems with spin-exchange dynamics. This can be understood as follows: For spin-exchange dynamics damaged sites can only heal in pairs, therefore the damage death rate is proportional to $D^2$ for small $D$. In contrast, the damage birth rate is linear in $D$ since already a single damaged site can induce further damage on the sites it is coupled to by the interactions. Consequently, for small $D$ the birth rate is always larger than the death rate, and the damage never heals.

5.3 Damage spreading simulations

In addition to the mean-field theory we also carried out numerical simulations of damage spreading in kinetic Ising models and in the Coulomb glass model. In reprint 22 we reported results from a large-scale simulation devoted to the influence of details of the update procedure on damage spreading. Specifically, we studied damage spreading in a Glauber Ising model on a cubic lattice and compared the results of different rules for the order in which the lattice sites are updated within a Monte-Carlo sweep. We considered five different site orders: typewriter (regularly going from one site to the next), checkerboard (first regularly going through one sublattice, then through the other), and three different random orders. We found that not only the time evolution of the damage depends on the rule chosen, but also the stationary damage values and hence the temperature of the damage spreading phase transition. Having in mind that damage spreading is a non-equilibrium phenomenon, this is not really surprising. Since a detailed balance condition does not exist for non-equilibrium phenomena the stationary states can well depend on the details of the update scheme (in addition to the single-site transition probabilities which contain the full information about the equilibrium distribution). However, in the damage spreading literature this question has largely been ignored so far, and damage spreading investigations have been performed without specifically paying attention to such details as the site order.

As a byproduct of this work we determined the spreading temperatures for the three-dimensional Glauber Ising model with the different update schemes with a relative precision of $10^{-3}$, and we also studied the critical behavior. In all cases the critical exponents at the spreading transition have the mean-field values of the directed percolation and parity conserving universality classes (which are identical). This is in agreement with the suggestion (Hinrichsen 1997) that the upper critical dimension for these universality classes is below three.

We also carried out large scale simulations for the Ising model with Kawasaki spin exchange dynamics to confirm the mean-field theory of reprint 21. We found that the main mean-field predictions, viz. that the damage spreads for all temperatures, and the two replicas become completely uncorrelated in the long-time limit, are confirmed by the simulations with very high accuracy. These results are published together with the mean-field theory in reprint 21.

All the work described in this chapter so far was concerned with the properties of the damage spreading transition as an example of a non-equilibrium phase transition. In a second line of research we have also started to use damage spreading as a tool to obtain information about the phase space structure and dynamic properties of the underlying system. It is clear that the phase space structure of a system has a strong influence on its damage spreading properties. If the free energy landscape possesses many nearly degenerate minima with large barriers inbetween, both the spreading and the healing of the damage will be hindered. This can be understood as follows: If the number of minima is (exponentially) large already a very small initial damage will put the two replicas into different free energy minima. Due to the diverging barriers they will remain there for all times, giving rise to a small but finite damage in the
steady state even in a parameter region where one would usually expect (e.g., from mean-field theory) the damage to heal completely. Numerically, we have found a clear indication for such a behavior in the random field Ising model. Figure 5.1 shows the stationary damage values for a three dimensional Glauber Ising model with bimodal random field. Here at intermediate random field strength the steady damage remains finite down to very low temperatures while all damage within one free-energy valley is known to heal for zero temperature.

Reprint 18 is devoted to a numerical investigation of damage spreading in the Coulomb glass model. Here the motivation was to find evidence for glassy behavior in the Coulomb glass at low temperatures. We indeed found a dynamic transition from frozen to active dynamics at a temperature well below all other energy scales in the system. However, the relation between this transition in the damage spreading behavior and a glass transition of the Coulomb glass is not fully understood so far. Exploring this relation remains a task for the future.
Chapter 6

Summary and outlook

In this Habilitation thesis we have presented research results on phase transitions in electronic systems. After an introductory chapter on the similarities and differences between classical and quantum as well as equilibrium and non-equilibrium transitions, respectively, we have concentrated on four specific examples: quantum phase transitions in the spherical model, magnetic quantum phase transitions of itinerant electrons, the disorder-driven metal-insulator transition, and damage spreading transitions. In this final chapter we want to summarize the results from a common perspective and discuss the remaining open questions as well as future research directions.

Theoretical description of a particular phase transition occurring in nature usually starts with the identification of the relevant variables, the most important one being the order parameter. To proceed further, analytical investigations often follow the Landau-Ginzburg-Wilson philosophy, i.e., all degrees of freedom other than the order parameter fluctuations are integrated out, resulting in an effective theory in terms of the order parameter only. If a rigorous analytical derivation is complicated, the Landau-Ginzburg-Wilson theory is sometimes guessed based on general symmetry considerations. (This is true in particular when constructing toy models like the quantum spherical model.) However, our work on the ferromagnetic quantum phase transition has shown that great care has to be taken in such an approach. At zero temperature an electronic system usually contains many non-critical soft modes in addition to the critical order parameter fluctuations. If these soft modes couple to the order parameter integrating them out leads to a singular behavior in the Landau-Ginzburg-Wilson theory. This mechanism is not restricted to zero temperature. Any soft mode coupling to the order parameter can – when integrated out – produce singularities in the resulting Landau-Ginzburg-Wilson theory. However, in electronic systems the number of soft modes at zero temperature is much higher than at finite temperatures.

In the case of itinerant ferromagnets we have shown that these singularities result either in unusual non-mean-field scaling behavior at the quantum phase transition or in the quantum phase transition being of first order (as is the case experimentally for the transition in MnSi). Within the singular Landau-Ginzburg-Wilson theory it is very hard to find out what scenario is realized for what microscopic parameters since explicit calculations are next to impossible. A much more promising though technically more challenging approach consists in not integrating out all degrees of freedom other than the order parameter. Instead, the effective field theory should treat all soft modes in the system on the same footing. We will explore the merits of such an approach in the future.

Another potential problem of the standard approach is caused by the fact that it is based on perturbation theory: First, integrating out the microscopic degrees of freedom in the derivation
of the Landau-Ginzburg-Wilson theory can usually be done only perturbatively. Second, the analysis of the effective theory is done by means of the perturbative renormalization group. Now, if the free energy landscape in configuration space contains many, nearly degenerate minima separated by large barriers, as for instance in the presence of random interactions or random fields, a straight-forward perturbative approach may miss part of the physics. We have shown this explicitly for the antiferromagnetic quantum phase transition of weakly disordered itinerant electrons. By approximately taking into account the non-perturbative degrees of freedom connected with the many nearly degenerate free energy minima we have derived a correction to the effective action of the standard perturbative approach. This new term destabilizes the conventional critical behavior. However, within our theory the ultimate fate of the transition could not be determined. Further work will be necessary to decide between the different possibilities, viz., a complete destruction of the antiferromagnetic long-range order or an unconventional transition that may be characterized by an infinite-disorder fixed point and activated scaling.

It should be emphasized here that we have also shown that including the non-perturbative degrees of freedom connected with the many-valley structure of the free energy in the presence of disorder does not always destroy the conventional critical behavior. For itinerant quantum ferromagnets, for instance, the long-range interaction between the order parameter fluctuations stabilizes the conventional critical fixed point.

In principle, the approach we used for the magnetic quantum phase transitions of disordered itinerant electrons can be applied to any quantum phase transition in the presence of quenched disorder. An alternative way to go beyond perturbation theory are numerical simulations. We have chosen this approach for our investigations of the disorder-driven metal-insulator transition. We have developed an efficient numerical method, the Hartree-Fock based diagonalization method which is related to the configuration interaction approach used in quantum chemistry. It allows us to calculate with high accuracy the low-energy properties of disordered interacting electrons for moderately large systems. So far, we have mostly obtained qualitative results concerning the influence of the electron-electron interactions on the transport properties: For systems of spinless fermions the interactions reduce the d.c. conductance for weak disorder (in agreement with perturbative results) while they enhance the d.c. conductance for strong disorder. In future work we plan to extend this work to a systematic finite-size scaling study which will lead to quantitative results about the metal-insulator transition. Moreover, we are working on including the spin degrees of freedom into our numerical scheme. This is of particular importance since the spin degrees of freedom have proven to be crucial for the recently discovered metal-insulator transition in two dimensions.

In contrast to the transitions discussed so far, the damage spreading transitions are non-equilibrium phase transitions rather than thermodynamic transitions. It turned out that even qualitative features of damage spreading like the existence or non-existence of a spreading phase depend on microscopic details of the model and its dynamics. Consequently, the universality classes of damage spreading are much narrower than that of thermodynamic transitions. In the research presented here we have concentrated on models for which the damage spreading transition is distinct from any equilibrium phase transition. For these cases the critical behavior at the spreading transition has been predicted to fall into the directed percolation universality class (if an additional symmetry does not exist) or into the parity conserving universality class (if there are two equivalent absorbing states). Our results are consistent with these predictions. However, all the systems we investigated so far were above their upper critical dimension and displayed mean-field exponents. Since the mean-field universality classes are usually much wider than the regular ones, definite conclusions require the simulation of lower-dimensional systems to get below the upper critical dimension. Another open question is concerned with the influence
of disorder on the critical behavior at the spreading transition. Within our mean-field theory
the critical behavior is unchanged by disorder. We are presently carrying out simulations to
study this question beyond mean-field theory. In addition, we plan to derive an effective field
theory which would allow to study the damage spreading transition by standard renormalization
group methods.
Bibliography

The literature on the topics discussed in the preceeding chapters is vast. In accordance with the introductory and pedagogical character of the first part of this Habilitation thesis mostly review articles have been included in the following list. In addition, reference is given to a few influential original publications. For a more comprehensive coverage of the literature the reader is referred to the references in the original publications collected in part II.

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