Quantum and classical phase transitions in electronic systems

Habilitationsschrift

zur Erlangung des akademischen Grades
doctor rerum naturalium habilitatus
(Dr. rer. nat. habil.)

von
Dr. Thomas Vojta
geboren am 5. März 1966 in Leipzig

ingereicht am 12. Mai 1999
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.
in Eugene. Particular thanks are given to Dietrich Belitz, Ted Kirkpatrick, Rajesh Narajanan and Andy Millis for the collaboration on the magnetic phase transitions, as well as Michael Schreiber, Frank Epperlein, and Torsten Wappler with whom I worked on the metal-insulator and damage spreading transitions. I greatly appreciated discussions with Alexei Efros, Ferdinand Evers, Roger Haydock, Svetlana Kilina, Bernhard Kramer, Arnulf Möbius, Christian Pfleiderer, Michael Pollak, Rudolf Römer, Achim Rosch, Walter Schirmacher, Jorge Talamantes, John Toner, Matthias Vojta, Dietmar Weinmann, and Isa Zarekeshev. Over the course of this work, many other colleagues have contributed ideas and suggestions for which I am thankful.
## 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
Damage-spreading transitions


In addition to the original publications reproduced here the author has published four printed but unrefereed conference contributions on the topics covered in this thesis:


During his Habilitation time the author has also published five refereed articles which are only loosely connected with the topic of this thesis and have therefore not been included here:


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 hypothetical 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 hypothetic 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 as, 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

\[
\xi \propto t^{-\nu}
\]

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

\[
\tau_c \propto \xi^z \propto t^{-\nu z}
\]

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

\[
H(p_i, q_i) = H_{\text{kin}}(p_i) + H_{\text{pot}}(q_i)
\]

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

\[
Z = \int \prod dp_i e^{-H_{\text{kin}}/k_B T} \int \prod dq_i e^{-H_{\text{pot}}/k_B T} = Z_{\text{kin}}Z_{\text{pot}}
\]

are completely independent from each other. The kinetic contribution to the free energy density \( f = -(k_B T/V) \log Z \) 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 \( m(\mathbf{r}) \) only. All other degrees of freedom have been integrated out in the derivation of the theory starting from a microscopic

\[1\text{ 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.}

\[2\text{ Velocity dependent potentials like in the case of charged particles in an electromagnetic field are excluded.} \]
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,

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

(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)
Analogously, the exponents of the correlation length and correlation function are connected by two so-called hyperscaling relations
\begin{align}
2 - \alpha &= d \nu, \\
\gamma &= (2 - \eta) \nu.
\end{align}

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 $d^+_{uc}$, 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 $d^+_{uc} = 4$). Between $d^+_{uc}$ and a second special dimension, called the lower critical dimension $d^-_{uc}$, a phase transition still exists but the critical behavior is different from mean-field theory. Below $d^-_{uc}$ 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

$$t_x \propto T_c^{1/\nu_z}.$$ \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

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

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
1.3. How important is quantum mechanics?

Law for the free energy density at zero temperature reads

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

(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,

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

(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.
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
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. Obernair (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

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

(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 $k \rightarrow 0$, 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 $T_c = 30$ 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 $d^* = 1$, 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.\(^1\) 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 $x = (\mathbf{x}, \tau)$ and $\int dx = \int dx \int_0^{1/k_B T} d\tau$ the resulting Landau-Ginzburg-Wilson free energy functional reads

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

\(^1\)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 $\Gamma$ 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, $\Gamma g(\epsilon_F) > 1$ (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 diagrammatic 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

$$\chi^{(2)}(q)/\chi^{(2)}(0) = 1 + c_d(|q|/2k_F)^{d-1} + O(|q|^2) \quad (d < 3) \quad (3.2)$$

$$\chi^{(2)}(q)/\chi^{(2)}(0) = 1 + c_3(|q|/2k_F)^2 \ln(2k_F/|q|) + O(|q|^2) \quad (d = 3) \quad . \quad (3.3)$$

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

$$tm - v_dm^d + um^3 = h \quad (d < 3) \quad (3.4)$$

$$tm - v_3m^3 \ln(1/m) + um^3 = h \quad (d = 3) \quad , \quad (3.5)$$
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

$$\omega \propto m^{d-2} q^2 \quad (d < 3) \quad (3.6)$$

$$\omega \propto m \ln(1/m) q^2 \quad (d = 3). \quad (3.7)$$

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
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.

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

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

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
4.2. Hartree-Fock approximation

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

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

(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),

\[
R_p(\varepsilon) = \frac{1}{g(\varepsilon)} \frac{1}{N} \sum_j \lim_{\delta \to 0} \frac{\delta}{\pi} G_{jj}(\varepsilon + i\delta) G_{jj}(\varepsilon - i\delta). \tag{4.3}
\]

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.
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 4.2: Structure of the Hartree-Fock (HF) based diagonalization method.](image-url)
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 $zt$ 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
This chapter summarizes our work on damage spreading. The major part of the research was devoted to gaining an understanding of this non-equilibrium phenomenon on the example of simple kinetic Ising models. We first formulated a master equation for damage spreading and developed mean-field like approximation. The resulting theory was applied to damage spreading in a variety of kinetic Ising models paying particular attention to the influence of details of the dynamical algorithms. This work is summarized in Sec. 5.2. We complemented the mean-field theory by large-scale numerical simulations discussed in Sec. 5.3. In a second line of research also presented in Sec. 5.3 we have started to use damage spreading as a tool to obtain information about the phase space structure and dynamical properties of the random-field Ising model and the Coulomb glass model.

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.\footnote{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.}

In this approximation the probability distribution $P$ by a product of identical single-site distributions $P(\nu_1, \ldots, \nu_N, t) = \prod_{i=1}^{N} P_{\nu_i}(t)$. Using this, the master equation reduces to an equation of motion for the single-site distribution $P_{\nu}$,

$$\frac{d}{dt} P_{\nu} = \sum_{\mu \neq \nu} [-P_{\nu} W(\nu \rightarrow \mu) + P_{\mu} W(\mu \rightarrow \nu)], \tag{5.2}$$

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.
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 flipped if the probability is larger than the random number, in the heat-bath dynamics the spin is 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.

The 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 preceding 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.


Andrews T. (1869), Phil. Trans. R. Soc. 159, 575.


Goldenfeld N. (1992), *Lectures on phase transitions and the renormalization group*, Addison-Wesley (Reading).


Landau L. D. (1937), Phys. Z. Sowjun. 11, 26; *ibid* 545; Zh. Eksp. Teor. Fiz 7, 19; *ibid* 627.


Onsager L. (1944), Phys. Rev. 65, 117.


van der Waals, J. D. (1873), PhD thesis, University of Leiden.


Zhang S.-C. (1997), Science 275, 1089.
Part II

Reprints
Quantum version of a spherical model: Crossover from quantum to classical critical behavior

Thomas Vojta

Department of Physics and Materials Science Institute, University of Oregon, Eugene, Oregon 97403

(Received 16 June 1995; revised manuscript received 21 August 1995)

We investigate a quantum version of the spherical model which is obtained from the classical Berlin-Kac spherical model by a simple canonical quantization scheme. We find a complete solution of the model for short-range as well as for long-range interactions. At finite temperatures the critical behavior is the same as in the classical spherical model whereas at zero temperature we find a quantum phase transition characterized by new critical exponents. Based on a functional-integral representation of the partition function the free energy of the model is shown to be equivalent to that of the nonlinear $\sigma$ model in the limit of infinite order-parameter dimensionality.

I. INTRODUCTION

The classical spherical model introduced by Berlin and Kac\(^1\) is one of the simplest toy models in statistical physics showing nontrivial critical behavior. It appears to be universally applicable to studying a variety of critical phenomena. The classical spherical model can be solved exactly not only for nearest-neighbor interactions\(^1\) but also for long-range power-law interactions,\(^2,3\) random interactions,\(^4,5\) systems in random magnetic fields,\(^6,7\) and disordered electronic systems with localized states.\(^8\) In addition it has been used as a test case for the finite-size scaling hypothesis.\(^9,10\) Reviews on the classical spherical model were given by Joyce\(^3\) and more recently by Khorunzhy et al.\(^11\) for spherical models with disorder.

In recent years there has been a renewed interest in the theory of zero-temperature quantum phase transitions studied by Hertz\(^12\) in 1976 in the context of itinerant ferromagnets. The newer investigations include metal-insulator transitions,\(^13\) the superconductor-insulator transition,\(^14\) as well as order-disorder transitions in quantum antiferromagnets\(^15\) and spin glasses,\(^16\) to name a few. Despite much effort we are far from having a complete picture of the behavior near quantum phase transitions. Thus it would be very useful to have a quantum version of the spherical model which can be used as universally as the classical spherical model.

Actually the idea of a quantum spherical model is not new; it dates back more than 20 years when Obermair\(^17\) suggested a simple canonical quantization scheme for a dynamical spherical model. This was also used later to investigate a quantum spin glass.\(^18\) However, these studies focused on the usual finite-temperature critical behavior and did not deal with the quantum phase transition at zero temperature. Similar models were also studied in the context of structural phase transitions.\(^19,20\) Very recently a quantum version of the spherical model was suggested based on path-integral quantization.\(^21\)

In this paper we consider a quantum version of the spherical model which is obtained by a canonical quantization scheme similar to that of Obermair. Like the classical model, the quantum model is exactly solvable, and we calculate the critical behavior at the finite-temperature classical fixed point as well as at the zero-temperature quantum fixed point. We also derive a functional-integral representation of our model. Based on this representation we investigate the relation to field-theoretic models and find that the free energy is identical to that of an $O(n)$ $\sigma$ model in the limit $n \to \infty$.

II. CANONICAL QUANTIZATION OF THE SPHERICAL MODEL

We consider a classical spherical model\(^1\) of $N = L^D$ ($D$ is the spatial dimensionality) real variables $S_i$, ranging from $-\infty$ to $\infty$ that interact via a pair potential $U_{ij}$ which we assume to be translationally invariant [i.e., $U_{ij} = U(r_i - r_j)$] for simplicity. The Hamiltonian of the model is given by

$$H_c = \frac{1}{2} \sum_{i,j} U_{ij} S_i S_j + h \sum_i S_i,$$

where $h$ is an external “magnetic” field. The values of the $S_i$ are subject to the mean spherical constraint

$$\sum_i (S_i^2) = N/4,$$

where $\langle \cdots \rangle$ denotes the thermodynamic average. In other studies of the spherical model this constraint is often imposed not on the averages but on the values of the variables themselves (strict spherical constraint). Usually both versions of the constraint yield the same results for the thermodynamic quantities\(^22\) although different results have been reported for a spherical spin glass.\(^24\) For a more detailed discussion of the relation between the mean spherical constraint and the strict spherical constraint see, e.g., Ref. 3. In the following we will see, however, that the mean spherical constraint (2) is easier to generalize to the quantum case than the strict constraint.

To define a quantum version of the spherical model (1) we reinterpret the variables $S_i$ as operators and define canonically conjugate “momentum” operators $P_i$ so that the fol-
lowing commutation relations are obeyed (with $\hbar$ set equal to 1):

$$[S_i, S_j] = 0, \quad [P_i, P_j] = 0, \quad [S_i, P_j] = i \delta_{ij}. \quad (3)$$

The quantum spherical model is then obtained from (1) by adding a kinetic energy term. The choice of this term is by no means unique, and depending on the form of the kinetic energy the model shows different dynamical behavior. Here we choose the simplest possible kinetic energy, a sum over the squares of the “momentum” operators. Thus the Hamiltonian is given by

$$H = H_{\text{kin}} + H_{\text{cl}} = \frac{1}{2} \sum_i P_i^2 + \frac{1}{2} \sum_{ij} U_{ij} S_i S_j$$

$$+ \hbar \sum_i S_i + \mu \left( \sum_i S_i^2 - \frac{N}{4} \right), \quad (4)$$

where the coupling constant $g$ determines the importance of quantum fluctuations. Here $g \rightarrow 0$ corresponds to the classical limit. The mean spherical constraint (2) is taken care of by a Lagrange multiplier $\mu$. It is easy to see that an implementation of the strict spherical constraint is more difficult in the quantum case, since here the $S_i$ are not real variables but operators.

We want to emphasize that the commutation relations (3) together with the quadratic kinetic term in the Hamiltonian (4) do not describe quantum Heisenberg-Dirac spins but quantum rotors as will become clearer in Sec. V. The quantum rotors can be seen as a generalization of Ising spins in a transverse field.16 The reader may also be aware of mappings between the low-temperature behavior of quantum Heisenberg antiferromagnets and models of quantum rotors.15,25

The quantum spherical model (4) is equivalent to a system of coupled harmonic oscillators. Therefore it can be solved very easily. A Fourier transformation of the Hamiltonian leads to

$$H = \sum_k \left[ \frac{1}{2} g P(k) P(-k) + \frac{1}{2g} \omega^2(k) S(k) S(-k) \right]$$

$$- \mu \frac{N}{4} \frac{\hbar^2}{4 \mu}, \quad (5)$$

where $P(k)$ and $S(k)$ are the Fourier transforms of the operators and the frequencies $\omega(k)$ are given by

$$\omega^2(k) = 2g \left( \mu + \frac{1}{2} U(k) \right). \quad (6)$$

Here $U(k)$ is the Fourier transform of the interaction matrix $U_{ij}$ and we have fixed our energy scale by assuming that the Fourier component $U(0)$ to $k=0$ is equal to zero. In analogy to a system of harmonic oscillators we can immediately write down the partition function

$$Z = \prod_k \left( 2 \sinh \frac{1}{2} \beta \omega(k) \right)^{-1} \exp \left( \beta \mu \frac{N}{4} + \frac{\beta \hbar^2}{4 \mu} \right). \quad (7)$$

where $\beta$ is the inverse temperature $\beta = 1/k_B T$. Therefore the free energy per site reads

$$f = -\frac{1}{\beta N} \ln Z = -\frac{\mu}{4} + \frac{\hbar^2}{4 \mu} + \frac{1}{\beta N} \sum_k \ln \left( 2 \sinh \frac{1}{2} \beta \omega(k) \right). \quad (8)$$

The spherical constraint which determines $\mu$ is given by

$$0 = \frac{\partial f}{\partial \mu} = -\frac{1}{4} + \frac{\hbar^2}{4 \mu^2} + \frac{1}{N} \sum_k \frac{g}{2 \omega(k)} \coth \frac{1}{2} \beta \omega(k). \quad (9)$$

In the limit $g \rightarrow 0$ this equation approaches the corresponding classical result [note that the frequencies $\omega(k)$ also contain $g$], whereas the free energy (8) contains an extra term proportional to $\ln g$ which is absent in the solution of the classical model (1). This is connected with the pathological thermodynamic behavior of the classical model at low temperatures, which is fixed by the extra term in the quantum case. Similar results were found in Refs. 18 and 22. It is also interesting to look at the limit of vanishing interactions $U(k)=0$ which corresponds to free spherical quantum “rotors.” In this case Eq. (9) yields a finite energy gap (finite $\mu$) even for vanishing field $h$. In contrast, for free Heisenberg-Dirac spins the energy gap vanishes for vanishing field.

III. CRITICAL BEHAVIOR AT FINITE TEMPERATURES

In this section we will discuss the critical behavior of the quantum spherical model at a finite-temperature phase transition. As usual in the spherical model, the critical behavior is determined by the properties of Eq. (9) for the spherical constraint in the limit $g \rightarrow 0$. The system does not show a phase transition if the $k$ sum on the right-hand side of (9) diverges for $N \rightarrow \infty$ and $\mu \rightarrow 0$. If it converges the system has a critical point at $h=0$ and $g=g_c$, with

$$0 = -\frac{1}{4} + \frac{1}{N} \sum_k \frac{g_c}{2 [g_c, U(k)]} \coth \frac{1}{2} \beta [g_c, U(k)] \mu. \quad (10)$$

This integral converges for $D > x$, where $x$ describes the asymptotic behavior of $U_k$: $|U_k| \sim k^{2-x}$ for $k \rightarrow 0$. Consequently, the lower critical dimension is given by $x$. (In the case of short-range interactions we have $x=2$.) In order to calculate the behavior of the system near this critical point we have to investigate (9) for small but finite $\mu$. The main observation is that at any finite temperature (finite $\beta$) we can expand the coth terms in (9) and (10) in the long-wavelength limit $|k| \rightarrow 0$ and for small $\mu$. From this it follows that the leading terms in (9) and (10) are the same as in the classical spherical model. After subtracting (10) from (9) and calculating the remaining $k$ sums we find

$$-t_g \left( \frac{1}{\mu} \right)^2 + \left\{ \begin{array}{ll}
C \mu^{D-x} \mu & (D < 2x) \\
C \mu \ln |\mu| & (D = 2x) \\
C \mu & (D > 2x) \end{array} \right. \quad (11)$$

where $t_g = (g_g - g_c)/g_c$, is the distance from the critical point and the prefactor $C$ is a smooth function of $g$. If we define a "magnetization" $m = \langle \delta \phi(x) \rangle$ we obtain the equation of state
TABLE I. Critical exponents for the quantum spherical model at the zero-temperature quantum fixed point and the finite-temperature classical fixed point as functions of dimensionality.

<table>
<thead>
<tr>
<th>Exponent</th>
<th>Quantum fixed point ((D &lt; D_c = 3\times 2))</th>
<th>Classical fixed point ((D &lt; D_c = 2))</th>
<th>Both fixed points ((D &gt; D_c))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\alpha)</td>
<td>((2D - 3)\sqrt{2})</td>
<td>((D - 2))</td>
<td>0</td>
</tr>
<tr>
<td>(\beta)</td>
<td>(1/2)</td>
<td>(1/2)</td>
<td>(1/2)</td>
</tr>
<tr>
<td>(\gamma)</td>
<td>(2x/(2D - x))</td>
<td>(x/(D - x))</td>
<td>1</td>
</tr>
<tr>
<td>(\delta)</td>
<td>((2D + 3x)/(2D - x))</td>
<td>((D + x)/(D - x))</td>
<td>3</td>
</tr>
<tr>
<td>(\nu)</td>
<td>(2/(2D - x))</td>
<td>(1/(D - x))</td>
<td>(1/\nu)</td>
</tr>
<tr>
<td>(\eta)</td>
<td>(2 - x)</td>
<td>(2 - x)</td>
<td>(2 - x)</td>
</tr>
<tr>
<td>(z)</td>
<td>(x/2)</td>
<td>(x/2)</td>
<td>(x/2)</td>
</tr>
</tbody>
</table>

From this equation we can easily determine the critical exponents of the thermodynamic quantities and the upper critical dimension which is obviously given by \(D_c = 2x\). In order to find the critical exponent of the correlation length we notice that the only relevant length scale near the transition is determined by the long-wavelength behavior of \(\alpha(k)\) which is given by \(\omega^*(k)^{-2g(\mu + k)}\), where we have omitted the prefactor in front of \(k\). Consequently we get \(\xi^{-1/\nu}\) and together with (11) this yields the critical exponent \(\nu\). The exponent \(\xi\) can be calculated from \(\langle S_i S_j \rangle^{-1/2 - k^{-x}}\). The dynamical exponent \(z\) can be obtained from the divergence of the time scale at the phase transition, \(\tau(k)\sim\omega(k)^{-1-k^{-3/2}}\). This yields \(z = x/2\). The critical exponents at the finite-temperature fixed point are summarized in Table I. Except for the dynamical exponent which is not defined in the static classical model (1) all exponents at the finite-temperature critical point of the quantum model agree with those of the classical model. So at any finite temperature the asymptotic critical behavior is controlled by the classical fixed point as is expected from general renormalization-group arguments.\(^{12}\)

IV. CRITICAL BEHAVIOR AT ZERO TEMPERATURE

We again investigate Eq. (9) for the mean spherical constraint, now for zero temperature. In this case the cubic term in (9) is identical to 1 and the equation simplifies to

\[
0 = \frac{\partial f}{\partial \mu} = \frac{h}{4} + \frac{1}{N} \sum \frac{g}{2\omega(k)}.
\]

The \(k\) integral converges for \(D > x/2\) which is therefore the lower critical dimension. The critical coupling strength \(g_f\) is given by

\[
0 = -\frac{1}{4} + \frac{1}{N} \sum \frac{g_f}{[\langle S_i S_j \rangle]^{1/2}}.
\]

In order to calculate the critical exponents we proceed analogously to Sec. III by subtracting (14) from (13). After calculation of the \(k\) sum we obtain

\[
-t_g^{-m^2} + \left\{ \begin{array}{l}
C(h/m)^{D-s-1/2} \\
C(h/m) [\ln(h/m)] \\
C(h/m)
\end{array} \right. \quad (D < 2x) \quad (D = 2x) \quad (D > 2x).
\]

\[
-t_g^{-m^2} + \left\{ \begin{array}{l}
C(h/m)^{2-D-s-1/2} \\
C(h/m) [\ln(h/m)] \\
C(h/m)
\end{array} \right. \quad (D < 3x/2) \quad (D = 3x/2) \quad (D > 3x/2).
\]

The equation of state is given by

\[
-t_g^{-m^2} + \left\{ \begin{array}{l}
C(h/m)^{2-D-s-1/2} \\
C(h/m) [\ln(h/m)] \\
C(h/m)
\end{array} \right. \quad (D < 3x/2) \quad (D = 3x/2) \quad (D > 3x/2).
\]

Obviously the upper critical dimension is \(3x/2\). All critical exponents can be easily calculated from (15) and (16). They are summarized in Table I. As at the classical fixed point the dynamical exponent \(z\) is given by \(x/2\). A comparison with the results of Sec. III shows that the critical exponents at the quantum critical point of the \(D\)-dimensional model are equal to those of a \((D + z)\)-dimensional model at the finite-temperature critical point, as is expected from general renormalization-group arguments.\(^{12}\)

Thus all scaling relations are obeyed if one substitutes \(D\) by \(D + z\).

In order to investigate the crossover from quantum to classical critical behavior arising at small but finite temperatures we first calculate the shift of the critical coupling due to a small but finite temperature. To this end we subtract Eq. (14) from Eq. (10). After calculation of the \(k\) sum we find for all dimensionalities \(D > x\)

\[
g_f - g_{f,0} = -T^{2D-s-1/2}.
\]

Here \(g_f\) is the critical coupling at finite temperature \(T\) and \(g_{f,0}\) is the critical coupling at zero temperature. Therefore the shift exponent is given by \(\phi = (2D - x)/x\). To derive the crossover scaling form of the equation of state,

\[
m = t^P \phi(h^{1/\phi}, T/t_0^P),
\]

we subtract (14) from (9). Here \(t_0\) measures the distance from the critical coupling at zero temperature. This yields
QUANTUM VERSION OF A SPHERICAL MODEL: CROSSOVER... . . .

\[ 0 = \hbar^2 \frac{\Delta}{4m^2} + \frac{1}{N} \sum_i \left\{ \frac{g}{2[2g + \mu + U(k)/2]^{1/2}} \right\}
\times \left( \coth \frac{1}{2} \beta [2g + \mu + U(k)/2]^{1/2} - 1 \right)
\]

\[ + \frac{1}{N} \sum_i \left\{ \frac{g}{2[2g + \mu + U(k)/2]^{1/2}} - \frac{g}{2[U(U(k))]^{1/2}} \right\}
\]

\[ + \frac{1}{N} \sum_i \frac{\sqrt{g} - \sqrt{g,0}}{2[U(U(k))]^{1/2}} \]  

where we have added two terms that are actually zero. Calculating the arising integrals requires some patience. Below the upper critical dimension \( D_u = 3 \) we eventually find

\[ 0 = m^2 + \left[ \frac{h}{m} \right]^{1/2} \left[ \frac{F}{m^{2}} \right]^{1/2} + \frac{h}{m} + t_x, \]  

where we have omitted all prefactors and kept only the leading terms close to the zero-temperature fixed point. The function \( F \) stems from the first of the \( k \) sums in (19). Equation (20) can be easily transformed into a scaling form equivalent to (18):

\[ T = \frac{1}{\beta} \left( 2D - x \right) \left[ \frac{t_x}{m^{2}} \right]^{1/4} \left[ \frac{h}{m} \right]^{1/2} \]  

from which we extract the crossover exponent to be \( \phi = x/(2D - x) \). The crossover exponent is equal to the inverse of the shift exponent and given by \( \phi = z \nu \), as is expected from the analogy between the quantum-to-classical crossover scaling in this model and finite-size scaling.

In dimensions above the upper critical dimension \( D_u \) crossover scaling breaks down. The equation of state cannot be written in a form analogous to (18). This behavior corresponds to the breakdown of finite-size scaling in the spherical model above \( D_u \) (see, e.g., Ref. 10). It can be explained in terms of a dangerous irrelevant variable in the renormalization group.\(^25\) We note that in agreement with the breakdown of crossover scaling the shift of the critical coupling \( g_c \) for \( D > D_u \) is not given by the naive scaling form \( (g_c - g_{c0}) \sim T^{\nu z/y} \) but is much weaker [see Eq. (17)].

V. FUNCTIONAL-INTEGRAL REPRESENTATION OF THE PARTITION FUNCTION

To shed some further light on the properties of the model and its relations to other models for quantum phase transitions we derive a functional-integral representation of the partition function by a method analogous to the Feynman functional integral\(^27\) for the propagator. We start with the Trotter formula\(^28\)

\[ Z = \text{Tr} e^{-\beta H_{\text{int}} + H_{\text{cl}}} = \lim_{n \to \infty} \text{Tr} \left( e^{-\beta H_{\text{int}}/n} e^{-\beta H_{\text{cl}}/n} \right). \]

Inserting appropriate sets of eigenstates of the operators \( S_i \) and \( P_i \) between the exponentials allows us to perform the trace. In the limit \( n \to \infty \) the partition function may now be written as the functional integral

\[ Z = \int D[S(\tau)] \exp \left[ -\beta \int_0^\beta \frac{1}{2g} \sum_i \left( \frac{\partial S_i}{\partial \tau} \right)^2 \right. \]

\[ \left. + H_{\text{cl}}[S(\tau)] \right]. \]  

where we have omitted all prefactors and kept only the leading terms close to the zero-temperature fixed point. The function \( F \) stems from the first of the \( k \) sums in (19). Equation (20) can be easily transformed into a scaling form equivalent to (18):

\[ T = \frac{1}{\beta} \left( 2D - x \right) \left[ \frac{t_x}{m^{2}} \right]^{1/4} \left[ \frac{h}{m} \right]^{1/2} \]  

from which we extract the crossover exponent to be \( \phi = x/(2D - x) \). The crossover exponent is equal to the inverse of the shift exponent and given by \( \phi = z \nu \), as is expected from the analogy between the quantum-to-classical crossover scaling in this model and finite-size scaling.

In dimensions above the upper critical dimension \( D_u \) crossover scaling breaks down. The equation of state cannot be written in a form analogous to (18). This behavior corresponds to the breakdown of finite-size scaling in the spherical model above \( D_u \) (see, e.g., Ref. 10). It can be explained in terms of a dangerous irrelevant variable in the renormalization group.\(^25\) We note that in agreement with the breakdown of crossover scaling the shift of the critical coupling \( g_c \) for \( D > D_u \) is not given by the naive scaling form \( (g_c - g_{c0}) \sim T^{\nu z/y} \) but is much weaker [see Eq. (17)].

V. FUNCTIONAL-INTEGRAL REPRESENTATION OF THE PARTITION FUNCTION

To shed some further light on the properties of the model and its relations to other models for quantum phase transitions we derive a functional-integral representation of the partition function by a method analogous to the Feynman functional integral\(^27\) for the propagator. We start with the Trotter formula\(^28\)

\[ Z = \text{Tr} e^{-\beta H_{\text{int}} + H_{\text{cl}}} = \lim_{n \to \infty} \text{Tr} \left( e^{-\beta H_{\text{int}}/n} e^{-\beta H_{\text{cl}}/n} \right). \]

Inserting appropriate sets of eigenstates of the operators \( S_i \) and \( P_i \) between the exponentials allows us to perform the trace. In the limit \( n \to \infty \) the partition function may now be written as the functional integral

\[ Z = \int D[S(\tau)] \exp \left[ -\beta \int_0^\beta \frac{1}{2g} \sum_i \left( \frac{\partial S_i}{\partial \tau} \right)^2 \right. \]

\[ \left. + H_{\text{cl}}[S(\tau)] \right]. \]  

Here \( D[S(\tau)] \) is, up to a normalization constant, the product of the \( dS_i \) for all sites \( i \) and all infinite imaginary time steps. In this form the partition function is similar to that of a model very recently suggested by Nieuwenhuizen.\(^26\) The kinetic energy of his model, however, contains a first derivative with respect to imaginary time \( \tau \), whereas our model contains a second derivative (after partial integration). As a consequence, his model can be defined only for complex \( S_i \), or by considering the system and its dual at the same time. However, its behavior is closer to the behavior of quantum Heisenberg-Dirac spins. In particular, there is no energy gap for vanishing interactions and vanishing field. Consequently, although both models are similar, the differences in the kinetic energy result in different dynamical behavior. In particular, the models belong to different universality classes at the zero-temperature quantum critical point.

The critical properties of our model are determined only by the long-wavelength behavior of the interaction \( U(k) \); thus we can omit all but the leading term of \( U(k) \) without changing the critical behavior. After a Fourier transformation the partition function then reads

\[ Z = \int D[S(k, \omega)] \exp \left[ -\beta \sum_k \left( \frac{\omega^2}{2g} + c k^c \right) S(k, \omega) S(-k, -\omega) \right]. \]  

where \( c \) is a model-dependent constant. In the case of short-range interactions (\( k = 2 \)) this partition function can be seen as the spherical version of the usual field-theoretic nonlinear \( \sigma \) model.\(^29\) As follows from the arguments given by Stanley\(^30\) for the classical models its free energy is identical to the large-\( n \) limit of the \( O(n) \) nonlinear \( \sigma \) model which describes quantum rotors instead of Heisenberg-Dirac spins. (One major difference between rotors and spins is that the different components of an \( n \)-component rotor commute with each other whereas the components of Heisenberg-Dirac spin operators do not commute.)

VI. CONCLUSIONS

In this paper we have investigated the critical properties of a quantum version of the spherical model. We have obtained a quantum description by reinterpretting the spherical "spins" as operators and defining conjugate "momentum" operators via the canonical commutation relations. The Hamiltonian of the quantum model is given by the sum of a quadratic kinetic energy term and the classical spherical Hamiltonian. Therefore our model describes quantum "rotors" rather than Heisenberg-Dirac spins. Such rotors can be seen as generalization of Ising spins in a transverse field. They arise, e.g., in effective models for the low-temperature behavior of quantum Heisenberg antiferromagnets.\(^17\)\(^25\)
Writing the partition function as a functional integral shows that the free energy of our model with short-range interactions is identical to that of the large-$n$ limit of the field-theoretic $O(n)$ model. Obviously there are many possible choices for the kinetic term (one being that of Ref. 22) different from ours. In general they lead to different universality classes at the quantum critical point whereas the classical finite-temperature critical behavior is determined only by the form of the classical spherical Hamiltonian. It is therefore not influencing by the choice of the kinetic energy.

For our choice of the kinetic energy the critical properties of the $D$-dimensional model at the quantum critical point are identical to those of a $(D + z)$-dimensional model at the finite-temperature critical point. The dynamical exponent $z$ is given by $x/2$ where the exponent $x$ describes the behavior of the interaction $U(k)$ in the limit of small $k$. We consider this model as a starting point for the investigation of more complicated problems which arise, for instance, by adding quenched disorder to the model, which breaks the symmetry between spatial and temporal directions.

ACKNOWLEDGMENTS

The author acknowledges valuable discussions with D. Belitz, T. R. Kirkpatrick, and M. Schreiber. This work was supported in part by the German Academic Exchange Service and by the NSF under Grants No. DMR-92-09879 and No. DMR-95-10185.

Critical behavior of a quantum spherical model in a random field

Thomas Vojta and Michael Schreiber
Institut für Physik, Technische Universität, D-09107 Chemnitz, Germany
(Received 30 November 1995)

We consider the influence of a quenched random field on the critical behavior of a quantum spherical model at the zero-temperature quantum phase transition. We find a complete solution of the model for arbitrary translationally invariant pair interactions. It turns out that the critical behavior for zero as well as finite temperatures is dominated by static random field fluctuations rather than by quantum or thermal fluctuations. Therefore the critical behavior close to the zero-temperature quantum phase transition is identical to that close to a finite-temperature transition. The system does not show a crossover from quantum to classical behavior.

While classical finite-temperature phase transitions are comparatively well understood by now, much less is known about zero-temperature phase transitions which are driven by quantum fluctuations rather than thermal fluctuations. These quantum phase transitions were introduced by Hertz in the context of itinerant ferromagnets. Newer investigations include, e.g., metal-insulator transitions and the superconductor-insulator transition, as well as order-disorder transitions in quantum antiferromagnets and spin glasses. The study of quantum phase transitions in systems with quenched disorder is particularly interesting since the disorder which fluctuates in space but not in time destroys the symmetry between space and time dimensions. Therefore the critical behavior can be expected to be different from that of a classical phase transition in higher spatial dimensions.

Recently, these investigations of quantum phase transitions have stimulated renewed interest in the spherical model introduced as a toy model of a ferromagnet by Berlin and Kac. The classical spherical model is one of the few models in statistical physics that can be solved exactly and shows nontrivial critical behavior. Thus it has been used to investigate a variety of problems since the first studies of phase transitions in ferromagnetic systems. Later it was also used to investigate the influence of disorder on the critical behavior close to classical finite-temperature phase transitions in spin glasses, random field systems, and disordered electronic systems with localized states. In order to study the critical properties close to quantum phase transitions, the classical spherical model has to be quantized. The quantization scheme is, however, not unique. Therefore different quantum versions of the spherical model have been proposed within the last years. While the different models fall into the same universality class at a finite-temperature classical phase transition, the critical behavior at a zero-temperature quantum phase transition differs from model to model. Usually, it also differs from the finite-temperature critical behavior. In this case, for low but finite temperatures the quantum spherical models display a crossover from quantum to classical behavior.

In this paper we study the influence of a quenched random field on the zero-temperature phase transition of a quantum spherical model. Quenched random fields coupling linearly to the order parameter have drastic effects on the critical behavior. At a classical phase transition, they lead to an increase of the lower critical dimension $D_c$ by 1 (Ref. 13) (for the Ising universality class) or 2 (Ref. 11) (for the spherical model). The influence of a random field on quantum critical behavior was first studied by a perturbational renormalization group. It was found that random field fluctuations rather than the quantum fluctuations dominate the critical behavior. However, in some cases perturbational results for the critical behavior of disordered systems have been proven to be wrong since they neglect the very complicated structure of the phase space in disordered systems. Therefore, in this report, we investigate the problem by means of an exact solution of a random field quantum spherical model obtained by a canonical quantization scheme.

In the following we briefly summarize the canonical quantization of the spherical model. In order to define the quantum spherical model we first consider a classical spherical model of $N=L^D$ ($D$ is the spatial dimensionality) real variables $S_i$ ranging from $-\infty$ to $\infty$ that interact via a pair potential $U_{ij}$ which we assume to be translationally invariant [i.e., $U_{ij}=U(r_i-r_j)$] for simplicity. The Hamiltonian of the model is given by

$$H_0=\frac{1}{2}\sum_{i<j} U_{ij} S_i S_j + \sum_i (h + \varphi_i) S_i,$$

where $h$ represents an external "magnetic" field. The random field values $\varphi_i$ are independent random quantities characterized by the first two moments of the probability distribution

$$[\varphi_i]_\mu=0, \quad [\varphi_i \varphi_j]_\nu=\Phi^2 \delta_{ij},$$

where $[\cdots]_\mu$ denotes the average with respect to the random field. The values of the spin variables $S_i$ are subject to the mean spherical constraint

$$\sum_i \langle S_i^2 \rangle=N/4,$$

where $\langle \cdots \rangle$ denotes the thermodynamic average for a particular realization of the random field. In some of the previous studies of the spherical model this constraint was imposed not on the averages, but on the values of the variables themselves (strict spherical constraint). Usually, both versions lead to the same results for thermodynamic quantities. For a detailed discussion of the relation between the mean and
strict spherical constraints see, e.g., Ref. 7. Here we have chosen the mean spherical constraint since it is easier to generalize to the quantum case than the strict constraint.\(^{12}\)

We now reinterpret the variables \(S_i\) as operators and define canonically conjugate “momentum” operators \(P_i\), so that the following commutation relations are obeyed (with \(h\) set equal to 1):

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

(4)
The quantum spherical model is then obtained from (1) by adding a kinetic energy term. As already mentioned, the choice of this term is by no means unique, and depending on the form of the kinetic energy the model displays different dynamical behavior (for comparison, see, e.g., Refs. 11 and 12). Here we choose the simplest possible kinetic energy, a sum over the squares of the momentum operators. Thus the Hamiltonian is given by

\[
H = H_{\text{kin}} + H_{\text{cl}} = \frac{g}{2} \sum_i P_i^2 + \sum_{ij} U_{ij} S_i S_j + \sum_i (h + \varphi_i) S_i + \mu \left( \sum_i S_i^2 - \frac{N}{4} \right),
\]

(5)
where the coupling constant \(g\) determines the importance of quantum fluctuations; \(g \to 0\) corresponds to the classical limit. The mean spherical constraint (3) is taken care of by a Lagrange multiplier \(\mu\). We want to emphasize that the commutation relations (4) together with the quadratic kinetic term in the Hamiltonian (5) do not describe quantum Heisenberg-Dirac spins but quantum rotors. The quantum rotors can be seen as a generalization of Ising spins in a transverse field.\(^{5,6}\) They also describe the low-temperature behavior of quantum antiferromagnets.\(^{4,16}\)

The Hamiltonian of the quantum spherical model (5) is equivalent to that of a system of coupled displaced harmonic oscillators and can therefore be solved easily. A Fourier transformation yields

\[
H = \frac{g}{2} \sum_k \frac{\Phi^2}{2\mu} + 2gh\sum_k \gamma(k) S(k) S(-k) - \frac{\varphi(k)\varphi(-k)}{4\mu + 2U(k)} - \frac{\mu N}{4} + \frac{\mu h^2 + 2N\varphi(k)\varphi(-k)}{4\mu}.
\]

(6)
where \(P(k), S(k),\) and \(\varphi(k)\) are the Fourier transforms of the operators and random field, respectively. The frequencies \(\omega(k)\) are given by

\[
\omega^2(k) = \mu [2\mu + U(k)].
\]

(7)
Here \(U(k)\) is the Fourier transform of the interaction matrix \(U_{ij}\), and we have fixed our energy scale by assuming that the Fourier component \(U(0)\) for \(k=0\) is equal to zero. Now the partition function for a fixed realization of the random field values can be written down easily since it factorizes with respect to \(k\). We obtain

\[
Z[\varphi] = \prod_k \left( 2\sinh \frac{\beta \omega(k)}{2} \right)^{-1} \exp \left( \frac{\beta \mu N}{4} + \frac{\beta N h^2 + 2\sqrt{N} \varphi(k)\varphi(-k)}{4\mu} \right) + \sum_k \frac{\beta \varphi(k)\varphi(-k)}{4\mu + 2U(k)},
\]

(8)
where \(\beta\) is the inverse temperature \(\beta = 1/k_BT\). Thus the free energy per site is given by

\[
f[\varphi] = -\frac{\ln Z[\varphi]}{\beta N} = -\frac{\mu}{4} - \frac{h^2 + 2N\varphi(k)\varphi(-k)}{4\mu} + \frac{1}{\beta N} \sum_k \ln \left( 2\sinh \frac{\beta \omega(k)}{2} \right).
\]

(9)
The Lagrange multiplier \(\mu\) is determined by the equation for the spherical constraint (3):

\[
0 = -\frac{\partial f[\varphi]}{\partial \mu} = -\frac{1}{4} + \frac{h^2 + 2N\varphi(k)\varphi(-k)}{4\mu} + \frac{1}{\beta N} \sum_k \ln \left( 2\sinh \frac{\beta \omega(k)}{2} \right) + \frac{1}{\beta N} \sum_k \frac{g}{2\omega(k)} \coth \frac{\beta \omega(k)}{2}.
\]

(10)
In principle, the value of \(\mu\) could depend on the particular realization of the random field \(\varphi\). A detailed analysis shows, however, that in the thermodynamic limit \(N \to \infty\) \(\mu\) is independent of the realization of the random field.\(^{17}\) Thus the free energy \(f\) and the Lagrange multiplier \(\mu\) are self-averaging quantities. Therefore we can separately average (9) and (10) with respect to the random field to obtain the average free energy.

\[
f = -\frac{\mu}{4} - \frac{h^2}{4\mu} - \frac{1}{\beta N} \sum_k \frac{\Phi^2}{4\mu + 2U(k)} + \frac{1}{\beta N} \sum_k \ln \left( 2\sinh \frac{\beta \omega(k)}{2} \right),
\]

(11)
with

\[
0 = -\frac{1}{4} + \frac{h^2}{4\mu} + \frac{1}{\beta N} \sum_k \frac{\Phi^2}{[2\mu + U(k)]^2} + \frac{1}{N} \sum_k \frac{g}{2\omega(k)} \coth \frac{\beta \omega(k)}{2}.
\]

(12)
In both equations the last term represents quantum and thermal fluctuations, whereas the third term, containing \(\Phi^2\), represents the static random field fluctuations which have exactly the same form as in the classical spherical model.\(^{9,10}\) In particular, the random field terms do not depend on \(g\) or \(\beta\).

As usual in the spherical model, the critical behavior is determined by the solution of Eq. (12) for the spherical constraint close to the critical point. At any finite temperature we can expand the coth terms in (11) and (12) in the long-wavelength limit \(|k| \to 0\) and for small \(\mu\). From this it fol-
lows that the leading terms are the same as in the classical random field spherical model.\textsuperscript{9,10} Consequently, the critical behavior of the quantum spherical model close to a finite-temperature phase transition is identical to that of a classical spherical model as is expected from general renormalization group arguments.\textsuperscript{1}

We now turn to the properties of the quantum phase transition at $T=0$ ($\beta=\infty$). Again, the critical behavior is determined by the solution of the equation for the spherical constraint close to the critical point $g=g_c$. $g_c$ is given by the value of $g$ which separates the regimes where a regular solution of (12) exists (large $g$, disordered phase) or does not exist (small $g$, ordered phase). Thus $g_c$ is the value at which (12) is fulfilled for $\mu=0$ and $h=0$. Since $T=0$ the hyperbel cotangent in (12) is equal to 1 and we obtain

$$0=-\frac{1}{4} \sum_{k} \frac{\Phi^2}{U(k)} + \sum_{k} \frac{g_c}{2 \sqrt{g_c U(k)}},$$

(13)

provided that both of the $k$ sums converge. Otherwise the system does not display a phase transition. Since the random field term in (13) contains the stronger singularity for $k \to 0$ than the term containing the quantum fluctuations, the properties of the random field term are responsible for the existence of a phase transition. Consequently, we find the same behavior as in the classical random field spherical model;\textsuperscript{9} namely, a transition occurs for $D>D_c^*=2x$, where $x$ describes the behavior of $U(k), U(k)-k^4$, close to $k=0$ (short-range interactions yield $x=2$). To determine the equation of state, we expand (12) for small $g$, and small $\mu$. Again, the leading contribution stems from the random field term. Thus, asymptotically close to the transition, we find

$$-t_g^e - \frac{h}{\mu} + \Phi^2 \begin{cases} C\mu^{D-2x} & (D<3x), \\ C\mu \ln |\mu| & (D=3x), \\ C\mu & (D>3x), \end{cases}$$

(14)

where $t_g^e=(g-g_c)g_c$ is the distance from the critical point and the prefactor $C$ is a smooth function of $g$. If we define a

\begin{align*}
& \text{"magnetization" } m = \frac{\partial f}{\partial h} = -h/2\mu \text{ [see Eq. (11)]}, \text{ we obtain the equation of state} \\
& \begin{cases}
C(h/m)^{(D-2x)/x} & (D<3x), \\
C(h/m)\ln(h/m) & (D=3x), \\
C(h/m) & (D>3x).
\end{cases}
\end{align*}

(15)

This equation is identical to the equation of state of a classical random field spherical model close to its finite-temperature phase transition.\textsuperscript{9,10} Consequently, we also find the same critical exponents $\alpha=(D-3x)/(D-2x), \beta=\frac{1}{2}, \gamma=x/(D-2x), \delta=D/(D-2x), \nu=1/(D-2x),$ and $\eta=2-x$ below the upper critical dimension $D_c^*=3x$. Above $D^*$ we get the usual mean-field exponents $\alpha=0, \beta=\frac{1}{2}, \gamma=1, \delta=3, \nu=1/x,$ and $\eta=2-x$.

In conclusion, we have investigated the influence of a quenched random field on the critical behavior of a quantum spherical model at zero temperature. In agreement with perturbational results,\textsuperscript{14} we have found that static random field fluctuations rather than the quantum fluctuations dominate the critical behavior. Therefore the critical behavior at zero temperature is identical to that at finite temperature, and the system does not show a crossover from quantum to classical behavior at low but finite temperatures. We note that these results do not depend on the nature of the particular quantization scheme used to define the quantum spherical model. The reason is that in general random field fluctuations are stronger than thermal fluctuations in the classical spherical model. In addition, at any finite temperature thermal fluctuations are stronger than quantum fluctuations for any model. This corresponds to $T$ being a relevant variable at a quantum phase transition. From this it follows that in general random field fluctuations are stronger than quantum fluctuations in a quantum spherical model and thus they dominate the critical behavior.

One of us (T.V.) acknowledges helpful discussions with D. Belitz and T. R. Kirkpatrick. This work was supported in part by the German Academic Exchange Service and by the NSF under Grant Nos. DMR-92-09879 and DMR-95-10185.

\begin{flushleft}
\textsuperscript{1}J. A. Hertz, Phys. Rev. B 14, 1165 (1976).
\textsuperscript{6}T. H. Berlin and M. Kac, Phys. Rev. 86, 821 (1952).
\textsuperscript{7}For a review of the early work on the spherical model, see G. S. Joyce, in \textit{Phase Transitions and Critical Phenomena} 2, edited by C. Domb and M. S. Green (Academic, New York, 1972), p. 375.
\end{flushleft}
The best known example is the wrong prediction of the lower critical dimension of the classical random field Ising model; for a discussion see D. P. Belanger and A. P. Young, J. Magn. Magn. Mater. 100, 272 (1991).


This was noticed by M. Schwartz, Phys. Lett. 76A, 408 (1980), for a special version of the spherical model; for more details see, e.g., Ref. 10.
Breakdown of Landau-Ginzburg-Wilson theory for certain quantum phase transitions

T. Vojta\textsuperscript{1}, D. Belitz\textsuperscript{1}, R. Narayanan\textsuperscript{1} and T. R. Kirkpatrick\textsuperscript{2}

\textsuperscript{1} Department of Physics and Materials Science Institute, University of Oregon
Eugene, OR 97403, USA
\textsuperscript{2} Institute for Physical Science and Technology, and Department of Physics
University of Maryland - College Park, MD 20742, USA

(received 10 June 1996; accepted in final form 10 September 1996)

PACS. 64.60Ak – Renormalization-group, fractal, and percolation studies of phase transitions.
PACS. 75.10Jm – Quantized spin models.
PACS. 75.40−s – Critical-point effects, specific heats, short-range order.

Abstract. – The quantum ferromagnetic transition of itinerant electrons is considered. It is shown that the Landau-Ginzburg-Wilson theory described by Hertz and others breaks down due to a singular coupling between fluctuations of the conserved order parameter. This coupling induces an effective long-range interaction between the spins of the form $1/r^{d+2-1}$. It leads to unusual scaling behavior at the quantum critical point in $1 < d \leq 3$ dimensions, which is determined exactly.

One of the most obvious examples of a quantum phase transition is the ferromagnetic transition of itinerant electrons at zero temperature $T$ as a function of the exchange coupling between the electron spins. Hertz [1] derived a Landau-Ginzburg-Wilson (LGW) functional for this case in analogy to Wilson’s treatment of classical phase transitions, and analyzed it by means of renormalization group methods. He found that the critical behavior in dimensions $d = 3, 2$ is mean-field like, since the dynamical critical exponent $z$ decreases the upper critical dimension $d_c^+$ compared to the classical case. In a quest for nontrivial critical behavior, Hertz studied a model with a magnetization confined to $d < 3$ dimensions, while the coefficients in the LGW functional are those of a 3-d Fermi gas. For this model he concluded that $d_c^+ = 1$, and performed a $1 - \epsilon$ expansion to calculate critical exponents in $d < 1$. Despite the artificial nature of his model, there is a general belief that the qualitative features of Hertz’s analysis, in particular the fact that there is mean-field–like critical behavior for all $d > 1$, apply to real itinerant quantum ferromagnets as well.

In this letter we show that this belief is mistaken, since the LGW approach breaks down due to the presence of soft modes in addition to the order parameter fluctuations, \textit{viz} spin-triplet particle-hole excitations that are integrated out in the derivation of the LGW functional. These soft modes lead to singular vertices in the LGW functional, invalidating the LGW philosophy.
of deriving an effective local field theory in terms of the order parameter only (1). In Hertz’s original model this does not change the critical behavior in $d > 1$, but it invalidates his $1 - \epsilon$ expansion. More importantly, in a more realistic model the same effect leads to nontrivial critical behavior for $1 < d \leq 3$, which we determine exactly.

Our results for realistic quantum magnets can be summarized as follows. The magnetization, $m$, at $T = 0$ in a magnetic field $H$ is given by the equation of state

$$ tm + v m^d + u m^3 = H, $$

where $t$ is the dimensionless distance from the critical point, and $u$ and $v$ are finite numbers. From (1) one obtains the critical exponents $\beta$ and $\delta$, defined by $m \sim t^\beta$ and $m \sim H^{1/\delta}$, respectively, at $T = 0$. For $\beta$ and $\delta$, and for the correlation length exponent $\nu$, the order parameter susceptibility exponent $\eta$, and the dynamical exponent $z$, we find

$$ \beta = \nu = 1/(d-1), \quad \eta = 3 - d, \quad \delta = z = d \quad (1 < d < 3), $$

and $\beta = \nu = 1/2, \quad \eta = 0, \quad \delta = z = 3$ for $d > 3$. These exponents “lock into” mean-field values at $d = 3$, but have nontrivial values for $d < 3$. In $d = 3$, there are logarithmic corrections to power law scaling. Equation (1) applies to $T = 0$. At finite temperature, we find homogeneity laws for $m$, and for the magnetic susceptibility, $\chi_m$,

$$ m(t, T, H) = b^{-\beta/\nu} m(tb^{1/\nu}, T b^{\delta/\nu}, H b^{\delta/\nu}), $$

$$ \chi_m(t, T, H) = b^{-\gamma/\nu} \chi_m(tb^{1/\nu}, T b^{\delta/\nu}, H b^{\delta/\nu}), $$

where $b$ is an arbitrary scale factor. The exponent $\gamma$, defined by $\chi_m \sim t^{-\gamma}$ at $T = H = 0$, and the crossover exponent $\phi$ that describes the crossover from the quantum to the classical Heisenberg fixed point (FP) are given by

$$ \gamma = \beta(\delta - 1) = 1, \quad \phi = \nu, $$

for all $d > 1$. Notice that the temperature dependence of the magnetization is not given by the dynamical exponent. However, $z$ controls the temperature dependence of the specific-heat coefficient, $\gamma_V = c_V/T$, which has a scale dimension of zero for all $d$, and logarithmic corrections to scaling for all $d < 3$ (2),

$$ \gamma_V(t, T, H) = \Theta(3 - d) \ln b + \gamma_V(tb^{1/\nu}, T b^{2}, H b^{3/\nu}). $$

Equations (1)-(5) represent the exact critical behavior of itinerant quantum Heisenberg ferromagnets for all $d > 1$ with the exception of $d = 3$, where additional logarithmic corrections to scaling appear. We are able to obtain the critical behavior exactly, yet it is not mean-field like. The exactness is due to the fact that we work above the upper critical dimension $d_{uc}^+ = 1$. The nontrivial exponents are due to a singular coupling between the critical modes which leads, e.g., to the unusual term $\sim v$ in (1). Experimentally, we predict that for 3-d magnets with a very low $T_c$ there is a crossover from essentially mean-field quantum behavior to classical Heisenberg behavior. In $d = 2$, where there is no classical transition, we predict that with decreasing $T$, long-range order will develop, and the quantum phase transition at $T = 0$ will display the nontrivial critical behavior shown above.

(1) We use the term “LGW theory” in the narrow sense, in which it is usually used in the literature, of an effective field theory in terms of the order parameter field only.

(2) Wegner [2] has shown how “resonance” conditions between critical exponents lead to logarithmic corrections to scaling. Their appearance for a whole range of dimensionalities in (5) is a consequence of the exact relation $z = d$. 

---

**Footnotes:**

1. We use the term “LGW theory” in the narrow sense, in which it is usually used in the literature, of an effective field theory in terms of the order parameter field only.

2. Wegner [2] has shown how “resonance” conditions between critical exponents lead to logarithmic corrections to scaling. Their appearance for a whole range of dimensionalities in (5) is a consequence of the exact relation $z = d$. 

---

**Page Dimensions:** 595.0x842.0
We now sketch the derivation of these results. A more complete account of the technical details will be given elsewhere [3]. We consider a d-dimensional continuum model of interacting electrons, and pay particular attention to the particle-hole spin-triplet contribution [4] to the interaction term in the action, $S^\text{int}$, whose (repulsive) coupling constant we denote by $J$. Writing only the latter explicitly, and denoting the spin density by $n$, the action reads

$$S = S_0 + S^\text{int} = S_0 + (J/2) \int dx \, n(x) \cdot n(x),$$

where $S_0$ contains all contributions to the action other than $S^\text{int}$. In particular, it contains the particle-hole spin-singlet and particle-particle interactions, which will be important for what follows. \[ \int dx = \int dx \int_0^{1/T} d\tau, \text{ and we use a 4-vector notation } x = (x, \tau), \text{ with } x \text{ a vector in real space, and } \tau \text{ the imaginary time. Following Hertz, we perform a Hubbard-Stratonovich decoupling of } S^\text{int} \text{ by introducing a classical vector field } M(x) \text{ with components } M^i \text{ that couples to } n_i(x) \text{ and whose average is proportional to the magnetization, and we integrate out all fermionic degrees of freedom. We obtain the partition function } Z \text{ in the form}

$$Z = e^{-F_0/T} \int D[M] \exp[-\Phi[M]],$$

where $F_0$ is the noncritical part of the free energy. The Landau-Ginzburg-Wilson (LGW) functional $\Phi$ reads

$$\Phi[M] = \frac{1}{2} \int dx \, dy \, \frac{1}{J} \delta(x - y) M(x) \cdot M(y) + \sum_{n=2}^\infty a_n \int dx_1 \ldots dx_n \chi^{(n)}(x_1, \ldots, x_n) M(x_1) \ldots M(x_n),$$

where $a_n = (-1)^{n+1}/n!$. The coefficients $\chi^{(n)}$ in (7b) are connected n-point spin density correlation functions of a reference system with action $S_0$ [1]. The particle-hole spin-triplet interaction $J$ is missing in the bare reference system, but a nonzero $J$ is generated perturbatively by the particle-particle interaction contained in $S_0$. The reference system then has all of the characteristics of the full action $S$, except that it must not undergo a phase transition lest the separation of modes that is implicit in our singling out $S^\text{int}$ for the decoupling procedure breaks down.

$\chi^{(2)}$ is the spin susceptibility of the reference system. Performing a Fourier transform from $x = (x, \tau)$ to $q = (q, \Omega)$ with wave vector $q$ and Matsubara frequency $\Omega$, we have for small $q$ and $\Omega$ \(^{(3)}\)

$$\chi^{(2)}(q, \Omega) = \chi_0(q)[1 - |\Omega|/|q|],$$

where $q$ and $\Omega$ are measured in suitable units, and $\chi_0(q)$ is the static spin susceptibility of the reference system. We now use the fact that in a Fermi liquid at $T = 0$, $\chi_0$ is a nonanalytic function of $q$ of the form

$$\chi_0(q \to 0) \sim \text{const} - |q|^{d-1} - q^2.$$

Here we have omitted all prefactors, since they are irrelevant for our purposes. This holds

\(^{(3)}\) We are considering $\chi^{(2)}$ in the limit $q \to 0, |\Omega| << |q|$, since for a conserved order parameter, $\Omega$ must be taken to zero before $q$ in order to reach criticality.
for $1 < d < 3$; in $d = 3$ the nonanalyticity is of the form $q^2 \ln |q|$ \( (\dagger) \). Using (8), and with $\int_q = \sum_q T \sum_Q$, the Gaussian part of $\Phi$ can be written

$$\Phi^{(2)}[M] = \int_q M(q) [t_0 + c_n q^{d-1} + c_a q^2 + c_d |Q|/|q|] M(-q). \quad (9)$$

Here $t_0 = 1 - \Gamma_t \chi^{(2)}(q \to 0, \omega_n = 0)$ is the bare distance from the critical point, and $c_n$, $c_a$, and $c_d$ are constants.

For the same physical reasons for which the nonanalyticity occurs in (8b), the coefficients $\chi^{(n)}$ in (7b) are in general not finite at zero frequencies and wave numbers. Let us focus in $\chi^{(4)}$, which will be the most interesting one for our purposes. Again, standard perturbation theory shows that it is given schematically by [3]

$$\chi^{(4)} \sim \text{const} + v \int_k \left[ |k| + |\omega_n| \right]^{-4} \sim u + v|p|^{d-3}. \quad (10)$$

Here we have cut off the singularity by means of a wave number $|p|$, and $u$ and $v$ are finite numbers. More generally, the coefficient of $|M|^n$ in $\Phi$ for $|p| \to 0$ behaves like $\chi^{(n)} = v^{(n)}|p|^{d+1-n}$. This implies that $\Phi$ contains a nonanalyticity which in our expansion takes the form of a power series in $|M|^2/|p|^2$.

The functional $\Phi$ can be analyzed by using standard techniques [5]. We look for a FP where $c_d$ and either $c_n$ (for $1 < d < 3$), or $c_a$ (for $d > 3$) are not renormalized. This fixes the critical exponents $\eta$ and $z$. Choosing the scale dimension of a length $L$ to be $[L] = -1$, standard power counting [5] then yields the scale dimension of $v^{(n)}$ to be $[v^{(n)}] = -(n-2)(d-1)/2$. All non-Gaussian terms are thus irrelevant for $d > 1$, and they all become marginal in $d = 1$ and relevant for $d < 1$. Several features of the critical behavior follow immediately. The critical exponents $\eta$ and $z$ are fixed by the choice of our FP, and $\nu$ and $\gamma$ as given in (2) and (4) are obtained by considering the $q$-dependence of the Gaussian vertex (9). We determine the equation of state by taking the term of order $|M|^4$ in $\Phi$ into account. $\chi^{(4)}$ is dangerously irrelevant with respect to the magnetization. We have shown [3] that for scaling purposes the cut-off $|p|$ in (10) can be replaced by $m$. From this and (9) we obtain the effective equation of state as given in (1).

These results completely specify the critical behavior at $T = 0$. Their most interesting aspect is the nontrivial exponent values found for $1 < d < 3$, which can nevertheless be determined exactly. The reason for this is the $|q|^{d-1}$-term in the Gaussian action (9). It reflects the fact that in an interacting electron system, static correlations between spins do not fall off exponentially with distance, but only algebraically like $r^{-(2d-1)}$. This slow decay leads to a long-range interaction in the effective action which falls off like $1/r^{2d-1}$, see (9). The critical behavior of classical Heisenberg magnets with such a long-range interaction has been studied before [6].

We now turn to the $T$-dependence of the specific heat, $c_V$. We expand the free-energy functional (7b) about the expectation value, $m$, of $M$ to second order, and then perform the Gaussian integral to obtain the partition function. The free energy is obtained as the sum of a mean-field contribution given by $\Phi[m]$, and a fluctuation contribution given by the Gaussian

\(\ast\) The physical origin of this nonanalyticity are mode-coupling effects analogous to those that generate a term $|q|^{d-2}$ in disordered Fermi systems [7]. We have ascertained the presence of the effect in clean systems by calculating $\chi_0$ perturbatively to second order in the interaction. To that order, the sign of the $|q|^{d-2}$-term in eq. (8b) is positive, but higher-order terms will presumably lead to a negative sign for realistic values of the interaction, thus allowing for a ferromagnetic ground state. Here we discuss only the latter case. A more complete discussion, including the physical situation for weak interactions, will be given elsewhere [3].
The latter yields the leading nonanalytic term in the free energy. We find [3] that effectively \( H \) and \( T \) have the same scale dimension, viz. \( d (= z) \), and that at \( t = 0 \) there is a logarithmic \( T \)-dependence of \( \gamma_V \) for all \( 1 < d < 3 \). If we put the \( t \)-dependence back in, we obtain that the scale dependence of \( \gamma_V \) is given by (5).

For the magnetization the leading \( T \)-dependence is given by the mean-field contribution to the free energy. We calculate the temperature corrections to the equation of state (1) and find that for \( m >> T \) (in suitable units) \( m^d \) in (1) will be replaced by \( m^d[1 + \text{const} \times T/m + \ldots] \), while for \( m << T \), \( t \) is replaced by \( t + T^{1/\nu} \). The effective scale dimension of \( T \) in \( m \) is therefore 1 (not \( z \)), and we obtain for \( m \) and \( \chi_m \) the homogeneity laws given by (3). Thus, the relevant operator \( T \) in (3) reflects the crossover from the quantum to the classical FP rather than dynamical scaling. Accordingly, we have written the \( T \)-dependence in (3) in terms of a crossover exponent \( \phi \) which is given by (4).

Next we briefly discuss Hertz's original model, which differs from the one discussed above in two ways. First, the reference ensemble consists of noninteracting electrons. Second, the coefficients \( \chi^{(n)} \) are taken to be the correlation functions of a 3-d fermion system. \( \chi^{(2)} \) is then simply the Lindhard function, so (8) gets replaced by

\[
\chi^{(2)}(q, \Omega) = 1 - q^2 - |\Omega|/|q| + \ldots
\]  

Due to the missing interaction in the reference ensemble, \( \chi^{(2)}(q, 0) \) is now analytic at \( |q| = 0 \). The resulting quadratic term in (7b) allows for a Gaussian FP with mean-field static exponents and a dynamical exponent \( z = 3 \) [1]. Whether this FP is stable depends on the higher \( \chi^{(n)} \).

Hertz considered only the limit \( q = \Omega = 0 \), where all of these terms are finite numbers and irrelevant for \( d > 1 \). The quartic term is marginal in \( d = 1 \) and relevant for \( d < 1 \) [1].

The striking difference between the finite coefficients in Hertz's model and the diverging ones in the realistic model above is due to the latter containing interactions in the reference ensemble. The interactions lead to frequency mixing, and hence to soft particle-hole excitations contributing to the \( \chi^{(n)} \) even in the limit of zero external frequency. A similar effect is achieved for noninteracting electrons by considering correlation functions at nonvanishing external frequency. Therefore we include the higher-order terms in an expansion of the \( \chi^{(n)} \) in powers of \( \Omega \) and analyze the arising LGW functional by the same power counting arguments as above. The details of this calculation will be presented elsewhere [3]. We find that all non-Gaussian terms are still irrelevant for \( d > 2 \) and the critical behavior is mean-field like. In \( d = 1 \), however, the \( \chi^{(n)} \) change their functional form so that an infinite number of operators are relevant (not marginal) with respect to the Gaussian FP in \( d = 1 \) and below. Therefore, the upper critical dimension is not one, but rather the 1-d system is below its upper critical dimension, and will show critical behavior that is substantially different from mean-field behavior.

We conclude with a few remarks. First, the vertices in the LGW functional discussed here are singular only if the order parameter is conserved, and only at zero temperature, which means that the phenomenon is confined to the quantum magnetic transition. Second, our conclusion, although derived for the special example of itinerant quantum ferromagnetism, is rather general: We expect the LGW formalism to break down whenever there are soft modes other than the critical order parameter fluctuations that couple to the order parameter. The general rule is that all of the soft modes should be retained on equal footing in the effective theory. If any of them are integrated out, the resulting penalty are ill-behaved coefficients in the LGW functional. This has been shown recently for disordered electrons [7]. The present results indicate that the underlying principle is very general. Indeed, it also applies to classical phase transitions with additional soft modes. However, there are many modes that are soft at \( T = 0 \) but acquire a mass at finite temperature, making quantum phase transitions more likely candidates. Finally, we mention that Sachdev [8] has noted that something must be wrong
with Hertz’s theory in $d < 1$, since it violates an exact exponent equality for quantum phase transitions with conserved order parameters. He suspected Hertz’s omission of the cubic term in the LGW functional to be at fault. Our analysis provides instead the explanation given above, namely the presence of infinitely many relevant operators due to the soft particle-hole excitations.

***

This work was supported by the NSF under grant Nos. DMR-92-17496 and DMR-95-10185, by the DAAD, by the DFG under grant No. Vo 659/1-1, and by the NATO under grant No. CRG-941250. DB would like to thank B. Kramer at the University of Hamburg for hospitality.

REFERENCES

Nonanalytic behavior of the spin susceptibility in clean Fermi systems

D. Belitz
Department of Physics and Materials Science Institute, University of Oregon, Eugene, Oregon 97403

T. R. Kirkpatrick
Institute for Physical Science and Technology and Department of Physics, University of Maryland, College Park, Maryland 20742

Thomas Voja
Department of Physics and Materials Science Institute, University of Oregon, Eugene, Oregon 97403 and Institut für Physik, Technische Universität Chemnitz-Zwickau, D-09107 Chemnitz, Federal Republic of Germany

(Received 12 November 1996)

The wave vector and temperature-dependent static spin susceptibility, $\chi_s(Q, T)$, of clean interacting Fermi systems is considered in dimensions $1 \leq d \leq 3$. We show that at zero temperature $\chi_s$ is a nonanalytic function of $|Q|$, with the leading nonanalyticity being $|Q|^{d-1}$ for $1 < d < 3$, and $Q^2 \ln |Q|$ for $d = 3$. For the homogeneous spin susceptibility we find a nonanalytic temperature dependence $T^{d-1}$ for $1 < d < 3$. We give qualitative mode-mode coupling arguments to that effect, and corroborate arguments by a perturbative calculation to second order in the electron-electron interaction amplitude. The implications of this, in particular for itinerant ferromagnetism, are discussed. We also point out the relation between our results and established perturbative results for one-dimensional systems, as well as for the temperature dependence of $\chi_s(Q=0)$ in $d=3$.

[S0163-1829(97)04216-1]

I. INTRODUCTION

It is well known that in fluids—that is, in interacting many-body systems—there are long-range correlations between the particles. For example, in classical fluids in thermal equilibrium there are dynamical long-range correlations that manifest themselves as long-time tails, or power-law decay of equilibrium time correlation functions at large times. In frequency space, the analogous effects are nonanalyticities at zero frequency. In an intuitive physical picture, these correlations can be understood as memory effects: the particles “remember” previous collisions, and therefore so-called ring collision events, where after a collision the two involved particles move away and later recollide, play a special role for the dynamics of the fluid. Technically, the long-time tails can be described in terms of mode-mode coupling theories. The salient point is that with any quantities whose correlations constitute soft, or gapless, modes (due to conservation laws, or for other reasons), products of these quantities have the same property. In the equations of motion that govern the behavior of time correlation functions this leads to convolutions of soft propagators, which in turn results in nonanalytic frequency dependences. For phase-space reasons, the strength of the effect increases with decreasing dimensionality: while in three-dimensional (3D) classical fluids the long-time tails provide just a correction to the asymptotic hydrodynamic description of the system, in 2D fluids they are strong enough to destroy hydrodynamics.

A natural question to ask is whether such long-range correlations also occur in position space. Indeed, in classical fluids in nonequilibrium steady-state effects occur that may be considered as the spatial analogs of long-time tails, but in thermal equilibrium this is not the case. This changes, however, if we consider quantum fluids. The quantum nature of a system has two major implications as far as statistical mechanics is concerned. First, temperature enters, apart from occupation numbers, through Matsubara frequencies, which means that the system’s behavior as a function of temperature will in general be the same as its behavior as a function of frequency, at least at asymptotically low temperatures. Second, and more importantly, in quantum statistical mechanics statics and dynamics are coupled and need to be considered together. This raises the question of whether in a quantum fluid there might be long-range spatial correlations even in equilibrium.

From studies of systems with quenched disorder, there is evidence that the answer to this question is affirmative. Let us consider interacting fermions in an environment of static scatterers. In dimensions $d>2$, and for a sufficiently small scatterer density, the relevant soft modes in such a system are diffusive, so frequency $\omega$, or temperature $T$, scales like the square of the wave vector $Q$, $\omega \sim T \sim Q^2$. Via mode-mode coupling effects that are analogous to those present in classical fluids, dynamical long-range correlations lead to long-time tails in equilibrium time correlation functions. For instance, the electrical conductivity as a function of frequency behaves like $\omega^{(d-2)/2}$ at small $\omega$ in $d>2$. The dynamical spin susceptibility $\chi_s(Q, \omega)$ shows no analogous long-time tail at $\omega=0$ for reasons related to spin conservation. However, from the above arguments about the coupling of statics and dynamics in quantum statistical mechanics and the scaling of the frequency with wave number, one would expect the static spin susceptibility, $\chi_s(Q, \Omega \to 0)$ at $T=0$, to show a related nonanalyticity at $Q=0$, namely, $\chi_s^{-1}(Q)^{d-2}$. This is indeed the case, as can be seen most easily from perturbative calculations. Schematically, the...
coupintg of two diffusive modes leads to contributions to $\chi$, of the type

$$\int dq \int d\omega \frac{1}{\omega + q^2 - \omega + \Omega + (q + Q)^2},$$

(1.1)

which leads to the above behavior. One can then invoke renormalization-group arguments to show that this is indeed the leading small-$Q$ behavior of $\chi$. Similarly, at finite temperature the homogenous susceptibility behaves as $\chi_s(T=0, \Omega=0) \sim T^{d - 2 - \nu'/2}$. This has interesting consequences for itinerant magnetism in such systems, as has been recently discussed.\textsuperscript{6–8}

Somewhat surprisingly, the situation is much less clear in clean Fermi systems. Here the soft modes are density and spin density fluctuations, as well as more general particle-hole excitations. All of these have a linear dispersion relation, i.e., $\Omega \sim |Q|$. The form of the dispersion relation does not affect the basic physical arguments for nonanalytic frequency and wave-number dependences given above. One might thus expect the spin susceptibility to have mode-mode coupling contributions of a type analogous to those shown in Eq. (1.1), but with ballistic instead of diffusive modes:

$$\int dq \int d\omega \frac{1}{\omega + q^2 - \omega + \Omega + |q + Q|^2},$$

(1.2)

which leads to $\chi_s(Q=0, \Omega=0) \sim \text{const} + |Q|^{d - 1}$ in generic dimensions at $T=0$. In $d=3$, one would expect a $Q^2 \ln|Q|$ behavior, as convolution integrals tend to yield logarithms in special dimensions. Such a behavior of $\chi_s$ would have profound consequences for the critical behavior of itinerant ferromagnets, as has been pointed out recently.\textsuperscript{9} It is therefore of importance to unambiguously determine whether or not the above mode-mode coupling arguments do indeed carry over from disordered to clean systems.

Before we start this task, let us discuss the available information concerning long-range correlations in clean Fermi systems. The specific heat is known to be a nonanalytic function of temperature, viz., $C_V/T \sim T^d \ln T$ in $d=3$. This is a consequence of a nonanalytic correction to the linear dispersion relation of the quasiparticles in Fermi-liquid theory, namely, $\Delta e(p) \sim (p - p_F)^2 \ln|p - p_F|$. Such a nonanalyticity signals the presence of a long-range effective interaction between the quasiparticles, and in general it will lead to nonanalytic behavior of both thermodynamic quantities and time correlation functions. The $T^d \ln T$ term in the specific-heat coefficient is an example of such an effect. In $d=2$ the behavior is $C_V/T \sim T$,\textsuperscript{11} which is consistent with the behavior $C_V/T \sim T^{d - 1}$ in generic dimensions that one would expect from the above arguments. It was natural to look for similar effects in other quantities, in particular in the spin susceptibility. These investigations concentrated on the temperature dependence of $\chi_s$, and several authors indeed reported to have found a $T^d \ln T$ term in the homogeneous static spin susceptibility. However, other investigations did not find such a contribution.\textsuperscript{12} The resulting confusion has been discussed by Carneiro and Pethick.\textsuperscript{13} These authors used Fermi-liquid theory to show that, while $T^d \ln T$ terms do indeed appear in intermediate stages of the calculation of $\chi_s$, as well as of $C_V$, they cancel in the former.

This somewhat surprising result casts some doubt on the general physical picture painted above, which suggests the qualitative equivalence of disordered and clean systems with respect to the presence of long-range correlations, and resulting nonanalyticities in both the statics and the dynamics of quantum systems. On the other hand, a failure of this general picture would be hard to understand from several points of view. For instance, in $d=1$ the instability of the Fermi liquid with respect to the Luttinger liquid is well known to manifest itself in perturbation theory for $\chi_s$ by means of logarithmic singularities.\textsuperscript{14,15} This is precisely what one obtains from the mode-mode coupling integral, Eq. (1.2). By continuity one therefore expects $\chi_s(Q=0, T) \sim T^{d - 1}$, and $\chi_s(Q, T=0) \sim |Q|^{d - 1}$, at least in $d=1 + \epsilon$. Unless the physics changes qualitatively between $d=1 + \epsilon$ and $d=3$, this should still be true in higher dimensions. Also, the corrections to Landau theory we are discussing here can be cast in the language of the renormalization group. In this framework, the Fermi-liquid ground state is described as a stable fixed point,\textsuperscript{16} and the effects we are interested in manifest themselves as an irrelevant operator that leads to corrections to scaling near this fixed point.\textsuperscript{17} In a system where $Q, \Omega, \bar{T}$ all have a scale dimension of unity, this operator should appear as $|Q|^{d-1}, \Omega^{d-1}$, etc., dependences in various correlation functions. From a general scaling point of view it would be hard to understand if this were not the case, except for the possibility that the prefactors of some nonanalyticities might accidentally vanish in certain dimensions.

It is the purpose of the present paper to clarify this confusing point. We will show that the above general physical picture does indeed hold true, and that it is not violated by the previously found absence of a $T^d \ln T$ term in $\chi_s$ in $d=3$, which is accidental. The remainder of this paper is organized as follows. In Sec. II we define our model. In Sec. III we perform an explicit perturbative calculation to second order in the electron-electron interaction. This confirms both our qualitative arguments, and the results of Ref. 13. We explain why there is no contradiction between these results, and we also make contact with established perturbative results in $d=1$. In Sec. IV A we discuss our result in the light of mode-mode coupling arguments that are an elaboration of those given above. In Sec. IV B we make contact with renormalization-group ideas, and argue that the functional forms of the nonanalyticities derived in Sec. III by means of perturbation theory are asymptotically exact. In Sec. IV C we discuss the physical consequences of our results.

II. MODEL, AND THEORETICAL FRAMEWORK

A. The model

Let us consider a system of clean fermions governed by an action\textsuperscript{18}

$$S = -\int d\tau \sum_\sigma \bar{\psi}_\sigma(x) \frac{\partial}{\partial \tau} \psi_\sigma(x) + S_0 + S_{\text{int}}. \quad (2.1a)$$

Here we use a four-vector notation, $x=(x, \tau)$, and $\int d\tau = \int d\tau d\tau$. $x$ denotes position, $\tau$ imaginary time, $\beta = 1/T$, and we choose units such that $\hbar = k_B = 1$. $\sigma$ is the spin label. $S_0$ describes free fermions with chemical potential $\mu$. 
We denote by $$\omega_n=\frac{\pi T}{n+1/2}$$ our Matsubara frequencies, which we denote here. Later we shall also encounter bosonic Matsubara frequencies, which we denote by $$\Omega_m=\frac{\pi T}{m}$$. Using again a four-vector notation, $$k=(\vec{k},\omega_n)$$, $$\int_{\Omega_m} \frac{d\Omega}{(2\pi)^3}$$, we can write

$$S_0=\int dx \sum_{\sigma} \bar{\psi}_\sigma(x)[\Delta(2m+\mu)\psi_\sigma(x)],$$

with $$\Delta$$ the Laplace operator, and $$m$$ the fermion mass. $$S_\text{int}$$ describes a two-particle, spin-independent interaction,

$$S_\text{int}=-\frac{1}{2} \int dx_1 dx_2 \sum_{\sigma_1,\sigma_2} \nu(x_1-x_2) \times \bar{\psi}_{\sigma_1}(x_1) \bar{\psi}_{\sigma_2}(x_2) \psi_{\sigma_1}(x_2) \psi_{\sigma_2}(x_1).$$

The interaction potential $$\nu(x)$$ will be specified in Sec. II B below.

We now Fourier transform to wave vectors $$\vec{k}$$ and fermionic Matsubara frequencies $$\omega_n=\frac{\pi T}{n+1/2}$$. Later we will also encounter bosonic Matsubara frequencies, which we denote by $$\Omega_m=\frac{\pi T}{m}$$. Using again a four-vector notation, $$k=(\vec{k},\omega_n)$$, $$\int_{\Omega_m} \frac{d\Omega}{(2\pi)^3}$$, we can write

$$S_0=\sum_{\sigma} \int \bar{\psi}_\sigma(\vec{k}) [i\omega_n-\vec{k}^2/2m+\mu] \psi_\sigma(\vec{k}),$$

$$S_\text{int}=-\frac{T}{2} \sum_{\sigma_1,\sigma_2} \sum_{k,p} \nu(\vec{k}-\vec{p}) \bar{\psi}_{\sigma_1}(\vec{k}) \bar{\psi}_{\sigma_2}(\vec{p}) \psi_{\sigma_1}(\vec{p}) \psi_{\sigma_2}(\vec{k}).$$

For the long-wavelength, low-frequency processes we will be interested in, only the scattering of particles and holes close to the Fermi surface is important. It is customary and convenient to divide these processes into three classes: \(1\) small-angle scattering, \(2\) large-angle scattering, and \(3\) \(2k_F\) scattering. These classes are also referred to as the particle-hole channel for classes \(1\) and \(2\), and the particle- \(3\) and Cooper channel for class \(3\), respectively. The corresponding scattering processes are schematically depicted in Fig. 1. For our purposes it is convenient to make the phase-space decomposition that is inherent to this classification explicit by writing the interaction part of the action,

$$S_\text{int}=S_\text{int}^{(1)}+S_\text{int}^{(2)}+S_\text{int}^{(3)},$$

where

$$S_\text{int}^{(1)}=-\frac{T}{2} \sum_{\sigma_1,\sigma_2} \sum_{k,p} \nu(\vec{p}+\vec{k}) \bar{\psi}_{\sigma_1}(\vec{p}) \bar{\psi}_{\sigma_2}(\vec{k}) \psi_{\sigma_1}(\vec{k}) \psi_{\sigma_2}(\vec{p}),$$

$$S_\text{int}^{(2)}=-\frac{T}{2} \sum_{\sigma_1,\sigma_2} \sum_{k,p} \nu(\vec{p}-\vec{k}) \bar{\psi}_{\sigma_1}(\vec{k}) \bar{\psi}_{\sigma_2}(\vec{p}) \psi_{\sigma_1}(\vec{p}) \psi_{\sigma_2}(\vec{k}),$$

$$S_\text{int}^{(3)}=-\frac{T}{2} \sum_{\sigma_1,\sigma_2} \sum_{k,p} \nu(\vec{k}+\vec{p}) \bar{\psi}_{\sigma_1}(\vec{k}) \bar{\psi}_{\sigma_2}(\vec{p}) \psi_{\sigma_1}(-\vec{k}) \psi_{\sigma_2}(-\vec{p}).$$

Here the prime on the $$\nu$$ summation indicates that only momenta up to some cutoff momentum $$\Lambda$$ are integrated over. This restriction is necessary to avoid double counting, since each of the three expressions, Eqs. (2.3b)–(2.3d), represents all of $$S_\text{int}$$ if all wave vectors are summed over. The long-wavelength physics we are interested in will not depend on $$\Lambda$$.

The above phase-space decomposition is correct in dimensions $$d\geq 2$$. In $$d=1$$, the Fermi surfaces collapse onto two Fermi points, and the processes we call above large-angle scattering and $$2k_F$$ scattering become indistinguishable. The three independent scattering processes are usually chosen as the ones shown in Fig. 2, and the corresponding coupling interaction potentials are denoted by $$g_1$$, $$g_2$$, and $$g_4$$. Inspection shows that the action written in Eqs. (2.3) counts each of these processes twice. If $$S_\text{int}^{(1)}$$ is dropped, then the $$g_4$$ process is still counted twice. However, it is known that $$g_4$$ does not contribute to the logarithmic terms we are interested in. For our purposes it is therefore sufficient to just drop the particle-particle channel when we are dealing with $$d=1$$. 

**FIG. 1.** Typical small-angle (1), large-angle (2), and $$2k_F$$-scattering processes (3) near the Fermi surface in $$d=2$$.
B. Simplifications of the model

The effective interaction potentials that appear in Eqs. (2.3b)–(2.3d) are all given by the basic potential \( v \), taken at different momenta. \( S^\text{int} \) contains the direct scattering contribution, or \( v(q) \), with \( q \) the restricted momentum. If \( v \) is chosen to be a bare Coulomb interaction, then this leads to singularities in perturbation theory in \( v \) that indicate the need for infinite resummations to incorporate screening. For simplicity, we assume that this procedure has already been carried out, and take \( v \) to be a statically screened Coulomb interaction. For effects that arise from small values of \( |q| \) it is then sufficient to replace \( v(q) \) by the number \( \Gamma' = v(q-0) \).\(^2\) In Eqs. (2.3c) and (2.3d) the moduli of \( k \) and \( p \) are equal to \( k_F \) for the dominant scattering processes, and one usually expands these coupling constants in Legendre polynomials on the Fermi surface. While all of the terms in this expansion contribute to the processes we want to study, we note that the coefficients in the angular momentum expansion are independent coupling constants. In order to establish the existence of a nonanalytic term in \( \chi_s(Q) \), it is therefore sufficient to establish its existence in a particular angular momentum channel. For simplicity we choose the zero angular momentum channel, \( l=0 \). We then have three coupling constants in our theory, namely, \( \Gamma_1 \), \( \Gamma_2 \), and \( \Gamma_3 \), which are \( v(k-p) \) and \( v(k+p) \), respectively, averaged over the Fermi surface. Instead of \( \Gamma_1 \) and \( \Gamma_3 \) one often uses the particle-hole spin singlet and spin triplet interaction amplitudes \( \Gamma_s \) and \( \Gamma_t \) that are linear combinations of \( \Gamma_1 \) and \( \Gamma_2 \). They are related to the Fermi-liquid parameters \( F_0 \) and \( F_0^* \) by

\[
\Gamma_s = \Gamma_1 - \Gamma_2 / 2 = \frac{1}{2N_F} \frac{F_0^*}{1 + F_0^*},
\]

\[
\Gamma_t = \Gamma_1 / 2 = \frac{1}{2N_F} \frac{F_0}{1 + F_0},
\]

where \( N_F \) is the density of states at the Fermi level. Our simplified model is tantamount to taking only \( F_0^* \) and \( F_0 \) into account instead of the complete sets of Landau parameters. As explained above, this is sufficient for our purposes. We also define the Cooper channel amplitude,

\[
\Gamma_c = \Gamma / 2,
\]

and again we keep only the \( l=0 \) channel. The particle-particle channel is neglected in Landau theory.

Our model is now defined as Eqs. (2.2) and (2.3), with \( v(q) \), \( v(p-k) \), and \( v(k+p) \) replaced by \( \Gamma_1 \), \( \Gamma_2 \), and \( \Gamma_3 \), respectively. We thus have three different interaction vertices, which are shown in Fig. 3. In the following section we will calculate \( \chi_s \) in perturbation theory with respect to the interaction amplitudes \( \Gamma_1 \), \( \Gamma_2 \), and \( \Gamma_3 \).

III. PERTURBATION THEORY

A. Contributions to second order in the interaction

We now proceed to calculate the spin susceptibility \( \chi_s \) in perturbation theory with respect to the electron-electron interaction. This can be done by means of standard methods.\(^2\) We will be interested only in contributions that lead to a nonanalytic wave-number dependence. It is easy to see that no nonanalytic behavior can occur at first order in the interaction. At second order, there is also a large number of diagrams for which this is true, and others vanish due to charge neutrality.\(^2\) There remain seven topologically different second-order diagrams, all shown in Fig. 4, that need to be considered. We thus write

\[
\chi_s(Q) = 2\chi_0(Q) + \sum_{i=1}^7 \chi_s^{(i)} + \text{(analytic contributions)},
\]

where \( \chi_0 \) denotes the Lindhard function, and the correction terms are labeled according to the diagrams in Fig. 4. Here

FIG. 3. The three interaction vertices with coupling constants \( \Gamma_1 \), \( \Gamma_2 \), and \( \Gamma_3 \).

FIG. 4. Second order diagrams that contribute to the nonanalytic behavior of \( \chi_s \). The solid vertical line denotes the external spin vertex. 

\[
\chi_s(Q) = 2\chi_0(Q) + \sum_{i=1}^7 \chi_s^{(i)} + \text{(analytic contributions)},
\]
and in the remainder of this section we use again the four-vector notation of Sec. II, so \(Q = (Q_\perp, \Omega)\), etc.

These diagrams can be expressed in terms of integrals over electronic Green’s functions, or bare electron propagators, that can be read off Eq. (2.2a),

\[
G_k = G_k(i\omega_n) = \frac{1}{i\omega_n - k_j^2/2m + \mu}.
\]

In terms of the \(G_k\), we find

\[
\chi^{(1)} = -4\Gamma_1 G_1 \sum_q \sigma_q^1 \sum_q' \langle [J^{(1)}(q, Q)]^2 \rangle,
\]

\[
\chi^{(2)} = -2\Gamma_1 G_1 \sum_q \sigma_q^1 \sum_q' \langle [J^{(1)}(q, Q)]^2 \rangle + J_1^2(q, Q) J_2^2(q),
\]

\[
\chi^{(3)} = -2\Gamma_1 G_1 \sum_q \sigma_q^1 \sum_q' \langle [J^{(3)}(q, Q)]^2 \rangle - q_2 - Q,
\]

\[
\chi^{(4)} = (\Gamma_3)^2 \sum_{\sigma_1, \sigma_2} \sigma_1 \sigma_2 (1 - \delta_{\sigma_1 \sigma_2}) \sum_q \langle I^{(3)}(q, Q) I^{(1)}_2(q, Q) \rangle,
\]

\[
\chi^{(5)} = (\Gamma_3)^2 \sum_{\sigma_1, \sigma_2} \sigma_1 \sigma_2 (1 - \delta_{\sigma_1 \sigma_2}) \sum_q \langle I^{(3)}(q, Q) I^{(2)}(q, Q) \rangle,
\]

\[
\chi^{(6)} = 2 \sum_{\sigma_1, \sigma_2} \sigma_1^1 \sum_q \langle (\Gamma_1)^2 J^{(1)}_1(q, Q) + (\Gamma_2)^2 \rangle \times J_2^2(-q, Q) J_2^2(-q) + 2(\Gamma_3)^2 \times \sum_{\sigma_1, \sigma_2} \sigma_1 \sigma_2 (1 - \delta_{\sigma_1 \sigma_2}) \sum_q \langle I^{(4)}(q, Q) I^{(2)}(q) \rangle,
\]

\[
\chi^{(7)} = \sum_{\sigma_1, \sigma_2} \sigma_1^1 \sum_q \langle (\Gamma_1)^2 J^{(1)}_1(q, Q) J^{(1)}_2(q) + (\Gamma_2)^2 \rangle \times \langle [J^{(3)}(-q, Q)]^2 \rangle - \chi^{(4)}.
\]

Here \(q\) is a bosonic frequency-momentum integration variable. In Eqs. (3.3), the following multiplication factors have been taken into account. In diagram (1) of Fig. 4, either one of the interaction lines can be a \(\Gamma_1\); the other one is then necessarily a \(\Gamma_2\). This leads to a multiplicity factor of 2, and another factor of 2 comes from the existence of an equivalent symmetric diagram. In diagram (2), again either one of the two interaction lines can be a \(\Gamma_1\), with the other line then being a \(\Gamma_2\), but here the two expressions one obtains are not identical. Again, there is an overall symmetry factor of 2. The same holds for diagram (3), but without the overall symmetry factor. Diagrams (4) and (5) can be realized only with \(\Gamma_1\), and they carry no multiplication factors. In diagrams (6) and (7), both interaction lines must be the same, and diagram (6) carries an extra symmetry factor of 2. The spin structures represent the fact that the interaction cannot flip the spin, and that the external vertex carries a factor of \(\sigma\). The functions in the integrands of Eqs. (3.3) are defined as

\[
J^{(1)}(q) = \sum_q G_q G_{q-q'},
\]

\[
J^{(3)}(q, Q) = \sum_q G_q G_{q+q} G_{q-q'},
\]

\[
J^{(4)}(q, Q) = \sum_q (G_q)^2 G_{q+q} G_{q-q'},
\]

\[
J^{(5)}(q, Q) = \sum_q G_q G_{q+q} G_{q+q},
\]

\[
J^{(6)}(q, Q) = \sum_q G_q G_{q+q} G_{q+q} G_{q+q},
\]

The information we are interested in is contained in Eqs. (3.1)–(3.4) in terms of integrals. The remaining task is to perform these integrals. While it is easy to see by power counting that all of the above contributions to \(\chi\) do indeed scale like \(Q^{d-1}\) for \(1 < d < 3\), and like \(O(1)\) and \(O(Q^2)\) with logarithmic corrections in \(d = 1\) and \(d = 3\), respectively, we have found it impossible to analytically perform the integrals in general, i.e., for a finite external wave number in arbitrary dimensions \(d\). However, for a perturbative confirmation of the expected nonanalyticity such a general analysis is not necessary. Rather, it is sufficient to explicitly obtain the prefactors of the logarithmic singularities in \(d = 1\) and \(d = 3\). If they are not zero, then by combining this with power counting and the expected continuity of \(\chi\) as a function of \(d\), it follows that the prefactor of the \(Q^{d-1}\) nonanalyticity does not vanish for generic values of \(d\) either. For the temperature dependence at \(Q = 0\) the integrals can be done in arbitrary \(d\), see Sec. III E below.

In Secs. III B–III D we therefore analyze the above integrals in \(d = 1\) and \(d = 3\). In doing so, we treat the particle-hole and particle-particle channel contributions separately, since they have quite different structures. We also anticipate that we will be interested only in the static spin susceptibility, so \(Q = (0, Q)\). In \(d = 1\), we write \(Q\) for the one-dimensional vector, i.e., a real number that can be either positive or negative.
Let us first consider \( d = 1 \). We do this mainly to make contact with established results in the literature. As explained above, the particle-particle channel must not be taken into account in \( d = 1 \), so we put \( \Gamma_1 = 0 \). Since we are interested in a logarithm that results from an infrared singularity, it suffices to calculate the integrands in the limit of small frequencies and wave numbers. Be performing the integrals in Eqs. (3.4a)–(3.4d) one obtains, with \( Q = (0, \mathbf{Q}) \) and \( q = (\Omega_n, \mathbf{q}) \),

\[
J^{(2)}(q) = -\frac{N_F}{4 + (\Omega_n \mathbf{v}_q)^2},
\]

(3.5a)

\[
J^{(3)}(q, Q) = N_F \left[ \frac{i \Omega_n Q}{\Omega_n^2 + (\mathbf{v}_q)^2} + \frac{i \Omega_n (Q - q) / Q}{\Omega_n^2 + [\mathbf{v}_q(Q - q)]^2} \right],
\]

(3.5b)

\[
J^{(4)}(q, Q) = N_F \left[ \frac{q (\mathbf{v}_q)^2 - \Omega_n^2}{\Omega_n^2 + (\mathbf{v}_q)^2} - \frac{q Q}{\Omega_n^2 + (\mathbf{v}_q)^2} \right]
\]

\[
+ \left[ \frac{q^2 Q^2}{\Omega_n^2 + (\mathbf{v}_q)^2} - \frac{(Q - q)^2 Q^2}{\Omega_n^2 + (\mathbf{v}_q)^2} \right]
\]

\[
+ \left[ \frac{(q + Q)^2 Q^2}{\Omega_n^2 + (\mathbf{v}_q + Q)^2} \right]
\]

(3.5c)

Inserting this into Eqs. (3.3), performing the final integrals, and collecting the results one obtains, apart from analytic terms,

\[
\chi_\lambda(Q) = 2 N_F - 4 N_F (\Gamma N_F)^2 \ln(2k_F/|Q|) .
\]

(3.6)

This result agrees with the well-known one to this order in \( \Gamma_F \). One would expect that the \( \ln|Q| \) gets replaced by a \( \ln \Omega \) or \( \ln \mathbf{T} \) if one works at \( Q = 0 \) and finite \( \Omega \) or \( \mathbf{T} \), respectively. Explicit calculations confirm this. Of course the physical content of this perturbative result is limited, since the ground state is not a Fermi liquid. For later reference we also mention that, to logarithmic accuracy, it is not necessary to keep \( Q \) nonzero in the above calculation. If one works at \( Q = 0 \) and determines the prefactor of the resulting logarithmic divergence, then one obtains the same result as above.

\[ \chi_\lambda(Q) = 2 N_F - 4 N_F (\Gamma N_F)^2 \ln(2k_F/|Q|) . \]

(3.6)
Inspection of the integrand shows that the leading divergence in $I$ is a logarithm squared, in contrast to the particle-hole channel, where the leading term is a simple logarithm. The reason is that $\Sigma_{p}G_{p}G_{p+q}$ contains a term $-\ln |q|$ for $q \to 0$, which is just the usual BCS-type logarithm that is characteristic of the particle-channel function. It also depends on an ultraviolet cutoff, since $\Sigma_{p}G_{p}G_{p+q}$ does not exist in $d=3$ if the integration is extended to infinity. In conjunction with the other factor in the integrand of $I$, which is an algebraic function, this gives the leading behavior:

$$I \sim \int d|q| \int_{0}^{\infty} \frac{q^{2} - 3(\omega_{k}v_{F})^{2}}{|q^{2} + (\omega_{k}v_{F})^{2}|^{2}}.$$  \hspace{1cm} (3.11)

While this diverges like $(\ln |q|)^{2}$ by power counting, the prefactor of the divergence turns out to be zero since the frequency integral in Eq. (3.11) vanishes. This leads to the following conclusion for the particle-particle channel contribution to $\chi_{1}$:

$$\chi_{1}^{p-p} = 2N_{f} + 2N_{s} (\Gamma_{1} N_{b}) \frac{[\ln \frac{2\pi f}{|q|}]}{[\frac{2\pi f}{|q|}]} + O(\ln \frac{2\pi f}{|q|}).$$  \hspace{1cm} (3.12)

Our method of expanding in powers of $Q$, and extracting the prefactor of the ensuing singularity, works only for the leading nonanalytic contribution. With this method, therefore, the result that is expressed in Eq. (3.12) is all we can achieve. In order to determine the prefactor of the next-leading $\ln |Q|$ term, one would have to keep a nonzero external wave number explicitly. As pointed out before in the context of the particle-particle channel, this would be very difficult. However, for our purposes this is not really necessary. We know that the interaction amplitudes in the particle-hole and particle-particle channels, respectively, are independent. Therefore, the particle-particle channel contribution cannot in general cancel the nonzero contribution from the particle-hole channel that we found in Sec. III C. What we have established is that the particle-particle channel is not more singular than the particle-hole channel, and for showing that the leading nonanalyticity in $\chi_{1}$ is $\ln |Q|$ with a nonzero prefactor this is sufficient.

It should be pointed out that low-order perturbation theory probably overestimates the importance of the particle-particle channel. Usually, singularities in the particle-particle channel are logarithmically weaker than those in the particle-hole channel, since a BCS-type ladder resummation changes a $\ln x$ singularity into a $\ln \ln x$, and a $x^{\gamma}$ singularity into a $x^{\gamma}/\ln x$. We expect this mechanism to work in the present problem, so the particle-particle channel singularities are probably in fact asymptotically negligible compared to the particle-hole channel ones. We also note that so far we have not really established that higher-order terms in the perturbation expansion cannot lead to stronger singularities than the ones we found at second order in the interaction amplitudes. This point will be further discussed in Sec. IV below.

E. Temperature dependence of $\chi_{1}(Q=0)$

In the last two subsections we have established that $\chi_{1}$ in $d=3$ at $T=0$ does indeed have a nonanalytic contribution proportional to $Q^{2} \ln |Q|$. As we pointed out in the Introduction, in a Fermi liquid the wave number scales like frequency or temperature, and one would therefore naively expect a $T^{2} \ln T$ contribution to the homogeneous $\chi_{1}$ at $T=0$. This raises the question of whether our results are compatible with those of Carneiro and Pethick,23 who did not find such a contribution. In order to clarify this, let us calculate $\chi_{1}(Q=0,T)$ explicitly within our formalism. For the reasons explained in Sec. III D we restrict ourselves to the particle-hole channel, as did Ref. 13.

To this end, we put $Q=0$ in Eqs. (3.4a)–(3.4d), and consider the temperature dependence of $\chi_{1}(Q=0,T)$, $\chi_{2}(Q=0,T)$, and $\chi_{3}(Q=0,T)$. The relevant integrals are of the structure,

$$\int dqq^{2}T \sum_{\Omega_{n}} f(q,\Omega_{n}) g(q,\Omega_{n}).$$  \hspace{1cm} (3.13)

which are most conveniently done by using the spectral representation for the causal functions $f(q,\Omega_{n})$ and $g(q,\Omega_{n})$. Simple considerations show that there is no $T^{2} \ln T$ term if both $f$ and $g$ are algebraic functions; only if at least one of them possesses a branch cut can such a nonanalyticity arise. This immediately rules out $\chi_{3}(Q=0,T)$, and the first and second contribution to $\chi_{2}(Q=0,T)$, respectively, as sources for a $T^{2} \ln T$. The reason is that an explicit calculation of $J_{1}^{(2)}(q,0,T)$, Eq. (3.4b), in the limit of small $q$ shows that the only singularities in this function are poles. The same is true for $J_{1}^{(4)}(q,0,T)$ and $J_{2}^{(4)}(q,0,T)$, but $J_{2}^{(4)}(q)$, which is minus the Lindhard function, has a branch cut, and so all of the remaining terms potentially go like $T^{2} \ln T$.

Since again we are aiming only at logarithmic accuracy, we can replace $J_{1}^{(4)}(q,0,T)$ and $J_{2}^{(4)}(q,0,T)$ by low-frequency, long-wavelength expressions for which $J_{2}^{(4)}(q,0,T) = -2J_{2}^{(4)}(q,0)$. The contributions from $\chi_{1}(Q=0,T)$ and $\chi_{2}(Q=0,T)$ therefore cancel [remember that diagrams (1) and (2) in Fig. 4 carry multiplication factors 4 and 2, respectively]. The contributions from $\chi_{1}(Q=0)$ and $\chi_{2}(Q=0)$ can both be expressed in terms of an integral

$$J = \int dqq^{2}T \sum_{\Omega_{n}} J_{1}^{(4)}(q,0,T)J_{2}^{(4)}(q).$$  \hspace{1cm} (3.14)

In doing this integral one may encounter individual terms that go like $T^{2} \ln T$, but all of those terms cancel, and the leading $T$ dependence of $J$ is $T^{2}$. There hence is no $T^{2} \ln T$ contribution to $\chi_{1}$ in $d=3$.

This result agrees with the conclusion of Ref. 13, which reached it on the basis of Fermi-liquid theory. We disagree, however, with the assertion of that reference that within the framework of microscopic perturbation theory the absence of the $T^{2} \ln T$ is due to cancellations between vertex corrections and self-energies, and is hence a consequence of gauge invariance. What we find instead is that, for all diagrams in Fig. 4, the $T^{2} \ln T$ terms vanish individually. This is consistent with the result of Ref. 24. These authors calculated $\chi_{1}$ in paramagnon approximation, which in our language corresponds to taking only $\chi_{6}(Q)$ and $\chi_{7}(Q)$ into account, plus infinite resummations that contribute to higher order in the interaction amplitudes. They reported the absence of $T^{2} \ln T$ terms in their calculation, rather than their cancellation between the two diagrams.
This absence of the expected nonanalytic $T$ dependence in $d = 3$ is somewhat accidental. This can be seen from the one-dimensional case, where, as pointed out in Sec. IIIB, there is a $\ln T$ contribution to the homogeneous spin susceptibility. The technical reason is that in $d = 1$, integrands whose only singularities are poles do contribute to the $T^4 \ln T$ terms. Consequently, in $d = 1$ $T$ and $Q$ are interchangeable in the logarithmic terms, while in $d = 3$ they are not. Furthermore, the same types of integrals that lead to a $\ln T$ term in $d = 1$ also contribute to a $T^{d-1}$ nonanalyticity in $1 < d < 3$. In these dimensions we therefore expect to find

$$\chi^{(b)}(Q=0) = 2N_p + 2N_p(\Gamma, N_p)^2 c_d(T/4\epsilon_f)^{d-1},$$

(3.15)

with $c_d$, a $d$-dependent, positive number.

We also mention that the absence of a $T^2 \ln T$ term in the self-energy diagrams in $d = 3$ does not contradict the presence of such a term in the specific-heat coefficient. The relation between the specific heat and the Green’s function is intricate, and the resulting integrals have a different structure from the ones that determine $\chi_i$.

IV. DISCUSSION

A. Our results in a mode-mode coupling theory context

In this section we give a more detailed look at the mode-mode coupling arguments that were presented in the Introduction. We also stress some analogies between classical and quantum fluids, and discuss some important differences between clean and disordered systems.

Let us consider four distinct systems: (1) a classical Lorentz model (i.e., a classical particle moving in a spatially random array of scatterers), (2) a classical fluid, (3) a Fermi liquid with static impurities, and (4) a clean Fermi liquid. These systems represent classical and quantum fluids with and without quenched disorder, respectively. As pointed out in the Introduction, dynamical correlations are ultimately responsible for all of the effects discussed in this paper. However, in classical systems they do not manifest themselves in static equilibrium properties, while in quantum systems they do. In order to discuss the analogies between classical and quantum systems, let us therefore digress and consider an equilibrium time correlation function. A convenient choice is the current-current correlation function, whose Fourier transform determines the frequency-dependent diffusivity $D(\Omega)$. In both of the classical systems, (1) and (2), this correlation function exhibits a long-time tail, so $D(\Omega)$ is nonanalytic at $\Omega = 0$. For $\Omega = 0$ one finds for the classical Lorentz model,

$$D(\Omega)/D(0) = 1 + a i\Omega + b(i\Omega)^{2d/2},$$

(4.1a)

while for the classical real fluid one finds

$$D(\Omega)/D(0) = 1 - b^* (i\Omega)^{d-2/2},$$

(4.1b)

The coefficients $b$ and $b^*$ in Eqs. (4.1) are positive. The long-time tail in the real fluid is stronger than the one in the Lorentz gas because the former has more soft modes. More importantly, the static scatterers in the Lorentz gas lead to a sign of the effect that is different from the one in the real fluid. All of these features can be understood in terms of the number and the nature of the soft modes in these systems. In disordered Fermi liquids one has

$$D(\Omega)/D(0) = 1 + b^* (i\Omega)^{(d-2)/2},$$

(4.1c)

with $b^* > 0$. Here the sign is the same as in the classical Lorentz model, which is due to the quenched disorder in either system. The strength of the long-time tail, however, is equal to that in the classical real fluid. As mentioned in Sec. I, the coupling of statics and dynamics in quantum statistical mechanics leads to a related nonanalyticity in the static spin susceptibility of a disordered Fermi liquid, namely,

$$\chi_i(\mathbf{Q})/\chi_i(0) = 1 - c |\mathbf{Q}|^{d-2},$$

(4.2)

with $c > 0$.

On the basis of these results, it is possible to predict both the strength of the singularity, and the sign of the prefactor, in the $Q$ dependence of $\chi_i$ in a clean Fermi liquid, which is what we are mainly concerned with in this paper. In order to do so, let us recall the origin of the nonanalyticity in the classical fluid, Eq. (4.1b). The density excitation spectrum, i.e., the dynamical structure factor as measured in a light-scattering experiment, in a classical fluid consists of three main features: the Brillouin peaks that describe emission and absorption of sound waves, and the Rayleigh peak that describes heat diffusion. For our purposes, we focus on the former. In the density-density Kubo correlation function, $C(\mathbf{k}, \omega)$ [whose spectrum is in a classical system simply proportional to the structure factor $S(\mathbf{k}, \omega)$], they manifest themselves as simple poles,

$$C(\mathbf{k}, \omega) = \frac{1}{\omega - v k + i y k^2/2} + \frac{1}{\omega + v k - i y k^2/2} = C_s(\mathbf{k}, \omega) + C_\omega(\mathbf{k}, \omega),$$

(4.3)

where $v$ is the speed of sound, and $y$ is the sound attenuation constant. Now let us consider the simplest possible mode-mode coupling process that contributes to Eq. (4.1b), namely, one where a current mode decays into two sound modes that later recombine; see Fig. 5. Consider a process where one of the internal sound propagators is a $C_s$, and the other a $C_\omega$. At zero external wave number, this leads to a convolution integral,
\[ \int d\omega \int dk C_\omega(k,\omega)C_\omega(-k,-\omega+\Omega) \sim \int dk \frac{1}{\Omega+i\gamma k^2} - \Omega^{(d-2)/2}. \] (4.4a)

Note that by this mechanism the long-time tail in a system whose low-lying modes have a linear dispersion becomes as strong as the one in a system with diffusive modes. In contrast, if both of the sound propagators are \( C_+ \) or \( C_- \), one obtains a weaker singularity,

\[ \int d\Omega \int dk C_\omega(k,\omega)C_\omega(-k,-\omega+\Omega) \sim \int dk \frac{1}{\Omega-2vk+i0} - \Omega^{(d-2)/2}. \] (4.4b)

Now let us consider the corresponding quantum system, i.e., the clean Fermi liquid. Again, the low-lying modes (i.e., particle-hole excitations) have a linear dispersion. However, at zero temperature the structure factor and the Kubo function are no longer proportional to one another. Rather, the fluctuation-dissipation theorem shows that they are related by a Bose distribution function that eliminates the pole at \( \omega=ck \) from the structure factor. This is simply a consequence of the fact that at zero temperature there are no excitations that could get destroyed in a scattering process. Consequently, the process described by Eq. (4.4a) is not available in this system, and one is left with the weaker singularity of Eq. (4.4b). Since the diffusion coefficient is infinite at \( T=0 \) in a clean system, we look instead at the spin susceptibility as a function of \( Q \). \( Q \) scales like \( \Omega \), so we expect a singularity of the form \( |Q|^{d-1} \), as opposed to the \( |Q|^{d-2} \) in a disordered Fermi liquid, Eq. (4.2). The sign of the prefactor is determined by whether or not the system contains quenched disorder. It should therefore be opposite to the sign in the dirty case. We thus expect for the wave number dependence of the spin susceptibility in a clean Fermi liquid,

\[ \chi_s(Q)/\chi_s(0) = 1 + c'(Q)|Q|^{d-1}, \] (4.5)

with \( c'>0 \). This is precisely what we found in Sec. III by means of perturbation theory. Notice that the mode-mode coupling arguments suggest that the sign of the prefactor \( c' \) will be positive, regardless of the interaction strength, as is the sign of the long-time tail in a classical fluid. We will come back to this point in Sec. IV C below.

### B. Our results in a renormalization-group context

Another useful way to look at our results is from a renormalization-group point of view. The Fermi-liquid ground state of interacting fermion systems in \( d>1 \) has recently been identified with a stable fixed point in renormalization-group treatments of both a basic fermion theory,\(^2\) and a bosonized version of that theory.\(^2\) The instability of the Fermi liquid in \( d=1 \) is reflected by an infinite number of marginal operators whose scale dimensions are proportional to \( d-1 \), i.e., they all become relevant in \( d<1 \), and are irrelevant in \( d>1 \). In the present context, the Fermi-liquid nature of the ground state in \( d>1 \) is reflected by the fact that the homogeneous spin susceptibility is finite in perturbation theory. The nonanalytic corrections at finite wave number that we are interested in correspond to the leading correction to scaling in the vicinity of the Fermi-liquid fixed point, i.e., to an irrelevant operator with respect to that fixed point. Among the irrelevant operators, there thus must be one whose scale dimension determines the leading wave-number dependence of the spin susceptibility.

An identification of this operator within the framework of a renormalization-group analysis would not only provide another derivation of our result, but would also establish that the behavior we have found in perturbation theory constitutes the leading \( Q \) dependence to all orders in the interaction amplitudes. This program has not been carried out yet, although preliminary results are encouraging.\(^3\) This will provide a connection between the mode-mode coupling arguments presented in the previous subsection and renormalization-group arguments that will be analogous to a corresponding connection in classical fluids that has been known to exist for some time.\(^4\)

In this context it should also be mentioned that there is no universal agreement that the ground state of a weakly interacting Fermi system in \( d>1 \) is a Fermi liquid. It has been proposed that there exists a relevant operator that makes the Fermi-liquid fixed point unstable, and leads to a non-Fermi-liquid ground state.\(^5\) In order to destroy the Fermi liquid in \( d \) dimensions, this would require a long-range effective interaction that falls off more slowly than \( 1/r^{d-1} \) at large distances. While we do find an effective long-range interaction between the spin degrees of freedom, it falls off like \( 1/r^{d-1} \), and hence leaves the Fermi-liquid fixed point intact. The same conclusion was reached in Ref. 11 from studying the specific heat in \( d=2 \).

### C. Summary, and physical consequences of our result

We finally turn to a summary of our results, and to a discussion of their physical consequences. By means of explicit perturbative calculations to second order in the interaction, we have found that the wave-number-dependent spin susceptibility in \( d=3 \) has the form

\[ \chi_s(Q)/\chi_s(Q=0) = 1 + c_s(Q/2k_F)^3 \ln(2k_F/Q) + O(Q^2). \] (4.6a)

We have calculated the particle-hole channel contribution to the constant \( c_s \), and have found it to be positive. More generally, it follows from our analysis that in \( d \)-dimensional systems, the spin susceptibility has a nonanalyticity of the form

\[ \chi_s(Q)/\chi_s(Q=0) = 1 + c_d(Q/2k_F)^{d-1} + O(Q^2). \] (4.6b)

where the particle-hole channel contribution to \( c_d \) is again positive. A very remarkable feature of Eqs. (4.6) is the sign of the leading \( Q \) dependence: For \( d=3 \), \( \chi_s \) increases with increasing \( Q \) like \( |Q|^{d-1} \). For any physical system for which this were the true asymptotic behavior at small \( Q \), this would have remarkable consequences for the zero-temperature phase transition from the paramagnetic to the ferromagnetic state as a function of the exchange coupling. One possibility
is that the ground state of the system will not be ferromagnetic, irrespective of the strength of the spin triplet interaction, since the functional form of \( \chi_s \) leads to the instability of any homogeneously magnetized ground state.\(^5\) Instead, with increasing interaction strength, the system would undergo a transition from a paramagnetic Fermi liquid to some other type of magnetically ordered state, most likely a spin density wave. While there seems to be no observational evidence for this, let us point out that in \( d=3 \) the effect is only logarithmic, and would hence manifest itself only as a phase transition at exponentially small temperatures, and exponentially large length scales, that might well be unobservables. For \( d=2 \), on the other hand, there is no long-range Heisenberg ferromagnetic order at finite temperatures, and the suggestion seems less exotic. Furthermore, any finite concentration of quenched impurities will reverse the sign of the leading nonanalyticity, and thus make a ferromagnetic ground state possible again.

Another possibility is that the zero-temperature paramagnet-to-ferromagnet transition is of first order. It has been shown in Ref. 9 that the nonanalyticity in \( \chi_s(Q) \) leads to a similar nonanalyticity in the magnetic equation of state, which takes the form

\[
 t_m - v_d m^4 + u m^3 = h, \tag{4.7}
\]

with \( m \) the magnetization, \( h \) the external magnetic field, and \( u > 0 \) a positive coefficient. If the soft mode mechanism discussed above is the only mechanism that leads to nonanalyticities, then the sign of the remaining coefficient \( v \) in Eq. (4.7) should be the same as that of \( c_d \) in Eq. (4.6b), i.e., \( v_d > 0 \). This would imply a first-order transition for \( 1 < d < 3 \). In this case the length scale that in the previous paragraph would have been attributed to a spin density wave would instead be related to the critical radius for nucleation at the first-order phase transition. Further work will be necessary to decide between these possibilities.

The conclusion that there is no continuous zero-temperature paramagnet-to-ferromagnet transition is inescapable for any system with a particle-hole channel interaction that is sufficiently weak for our perturbative treatment to be directly applicable. An important question is now whether or not it holds more generally for systems whose interactions are in general not weak. There are four obvious mechanisms by which the sign of the leading \( Q \) dependence of \( \chi_s \) could be switched from positive to negative: (1) higher-order contributions could lead to a sign of \( c_d \) for realistic interaction strengths that is different from the one for weak interactions, or (2) they might lead to a stronger singularity with a negative prefactor that constitutes the true long-wavelength asymptotic behavior, or (3) the particle-particle channel contribution might have a negative sign that overcompensates the positive contribution from the particle-hole channel, or (4) the higher angular momentum channels that we neglected might lead to a different sign. At this point, none of these possibilities can be ruled out mathematically. However, from a physical point of view none is very likely to occur. As we have explained in Sec. IV A, both the functional form and the sign of the nonanalyticity found in perturbation theory are in agreement with what one would expect on the basis of a suggestive analogy with classical fluids. Also, the renormalization-group arguments sketched in Sec. IV B make it appear likely that Eqs. (4.6) constitute the actual asymptotic small-\( Q \) behavior of \( \chi_s \), although an actual renormalization-group proof of this is still missing. This makes the first two possibilities appear unlikely. The third possibility is unappealing for two reasons. First, the effective interaction in the particle-particle channel is typically much weaker than the one in the particle-hole channel. The reason is the characteristic ladder resummation that occurs in the particle-particle channel if one goes to higher orders in perturbation theory. This leads to an effective interaction of the "Coulomb pseudopotential" type that is much weaker (typically by a factor of 5–10) than what low-order perturbation theory seems to suggest.\(^2\) Second, that same resummation weakens any singularity (cf. the discussion at the end of Sec. III D), which probably makes the particle-particle channel singularity subleading. Finally, the higher angular momentum Fermi-liquid parameters are usually substantially smaller than the ones at \( l = 0 \), which makes possibility (4) unlikely, except possibly in particular systems.

If the sign of the nonanalyticity is, for some reason, negative at the coupling strength necessary for a ferromagnetic transition to occur, at least in some systems, then in these systems the quantum phase transition from a paramagnet to a ferromagnet at zero temperature as a function of the interaction strength will be a conventional continuous quantum phase transition with an interesting critical behavior. This is because the nonanalyticity in \( \chi_s \) leads to an effective long-range interaction between spin fluctuations, which in turn leads to critical behavior that is not mean-field-like, yet exactly solvable. This has been discussed recently in some detail.\(^3\)

ACKNOWLEDGMENTS

We would like to thank Roger Haydock, Gilbert Lonzarich, and Andy Millis for stimulating discussions. This work was supported by the NSF under Grants No. DMR-95-10185 and No. DMR-96-32978, by the DAAD, and by the DFG under Grant No. Vo 659/1-1.

---

3 For an elementary discussion, see, e.g., D. Forster, Hydrodynamic Fluctuations, Broken Symmetry, and Correlation Functions (Benjamin, New York, 1975).
We use a field theoretic language in terms of Grassmann valued fields and their expectation values, see, e.g., Ref. 21. Equivalently, one can formulate the same theory in terms of operators and time ordered Green’s functions, see, e.g., Ref. 22.

For charge neutrality, we assume a homogeneous, positively charged background. Therefore \( v(q=0) = 0 \).

One might argue that this conclusion cannot really be drawn, since critical fluctuations near a ferromagnetic phase transition might change the \( Q \) dependence of the two-point vertex function. However, it has been shown in Ref. 9 that any ferromagnetic transition in a system whose spin susceptibility far from criticality is given by Eq. (4.6b) is not driven by fluctuations, but characterized by a Gaussian fixed point. The functional form of the bare two-point vertex therefore is preserved even at criticality.
Quantum critical behavior of clean itinerant ferromagnets

Thomas Vojta1,2, D. Belitz3, R. Narayanan3, T.R. Kirkpatrick4

1 Department of Physics and Materials Science Institute, University of Oregon, Eugene, OR 97403, USA
2 Institut für Physik, TU Chemnitz-Zwickau, D-09107 Chemnitz, Germany
3 Department of Physics and Materials Science Institute, University of Oregon, Eugene, OR 97403, USA
4 Institute for Physical Science and Technology, and Department of Physics, University of Maryland, College Park, MD 20742, USA

Received: 12 December 1996

Abstract. We consider the quantum ferromagnetic transition at zero temperature in clean itinerant electron systems. We find that the Landau-Ginzburg-Wilson order parameter field theory breaks down since the electron-electron interaction leads to singular coupling constants in the Landau-Ginzburg-Wilson functional. These couplings generate an effective long-range interaction between the spin or order parameter fluctuations of the form $1/r^{d-z+1}$, with $d$ the spatial dimension. This leads to unusual scaling behavior at the quantum critical point in $1 < d \leq 3$, which we determine exactly. We also discuss the quantum-to-classical crossover at small but finite temperatures, which is characterized by the appearance of multiple temperature scales. A comparison with recent results on disordered itinerant ferromagnets is given.

PACS: 64.60.Ak; 75.10.Jm; 75.40.Cx; 75.40.Gb

I. Introduction

The physics of quantum phase transitions has been a subject of great interest lately. In contrast to the usual classical or thermal phase transitions, quantum phase transitions occur at zero temperature as a function of some nonthermal control parameter, and the fluctuations that drive the transition are of quantum nature rather than thermal in origin. Among the transitions that have been investigated are various metal-insulator transitions, the superconductor-insulator transition in thin metal films, and a variety of magnetic phase transitions. Early work in this field [1] established that if the quantum phase transition has a classical analog at finite temperature, then the former tends to have a simpler critical behavior in the physical dimensions $d = 3$ or $d = 2$ than the latter. The reason for this tendency is that the coupling between statics and dynamics that is inherent to quantum statistics problems effectively increases the dimensionality of the system from $d$ to $d + z$, with $z$ the dynamical critical exponent. This reduces the upper critical dimension $d^c$, which is the dimension above which mean-field theory yields the exact critical behavior, by $z$ from its value for the classical transition.

One of the most obvious examples of a quantum phase transition, and the first one studied in detail, is the ferromagnetic transition of itinerant electrons that occurs as a function of the exchange coupling between the electron spins. In a pioneering paper, Hertz [1] derived a Landau-Ginzburg-Wilson (LGW) functional for this transition by considering a simple model of itinerant electrons that interact only via the exchange interaction in the particle-hole spin-triplet channel. Hertz analyzed this LGW functional by means of renormalization group (RG) methods that generalize Wilson’s treatment of classical phase transitions. He concluded that the critical behavior in the physical dimensions $d = 3$ and $d = 2$ is mean-field like, since the dynamical critical exponent $z = 3$ decreases the upper critical dimension from $d^c = 4$ for the classical case to $d^c = 1$ in the quantum case. In order to study nontrivial quantum critical behavior, Hertz then considered a model with a magnetization that is defined on a space of arbitrary dimension $d$, while the correlation functions that determine the coefficients in the LGW functional are taken to be those of a $3-d$ Fermi gas. For this model, he calculated non mean-field like critical behavior in $d < 1$ by means of a $1 - \epsilon$ expansion. Despite the somewhat artificial nature of this model, there is a general belief that the qualitative features of Hertz’s analysis, in particular the fact that there is mean-field like critical behavior for all $d > 1$, apply to real itinerant quantum ferromagnets as well.

In this paper we reexamine the ferromagnetic quantum phase transition of itinerant electrons and show that the above belief is qualitatively mistaken. We first consider a model that is more realistic than Hertz’s, viz. with an electron-electron interaction that is not restricted to the particle-hole spin-triplet channel. We find that the LGW approach breaks down due to the presence of soft modes in addition to the critical modes, namely particle-hole excitations that couple to the conserved order parameter. These soft modes are integrated out in the derivation of the LGW functional, and this leads to singular vertices in the order parameter field theory. This is a rather general observation; analogous effects are expected for a large class of quantum phase transitions, and in general they invalidate the applica-

Dedicated to Prof. W. Götze on the occasion of his 60th birthday
The partition function of any fermionic system can be written in the form, \[ Z = \int D\bar{\psi} D\psi \exp \{ S[\bar{\psi}, \psi] \} \] , (2.1a)

where \( \bar{\psi} \) and \( \psi \) are Grassmannian (i.e., anticommuting) fields. \( D\bar{\psi} D\psi \) denotes the Grassmannian functional integration measure, and \( S \) is the action,

\[ S = \int_0^\beta d\tau \int d^d x \bar{\psi}(x, \tau) \frac{\partial}{\partial \tau} \psi(x, \tau) - \int_0^\beta d\tau H(\tau). \] (2.1b)

Here \( x \) denotes position and \( \tau \) imaginary time, \( H(\tau) \) is the Hamiltonian in imaginary time representation, \( \beta = 1/T \) is the inverse temperature, \( i = 1, 2 \) denote spin labels, and summation over repeated covariant and contravariant spin indices is implied. Throughout this paper we use units such that \( k_B = \hbar = c^2 = 1 \). We start with a microscopic model of itinerant, interacting electrons,

\[ H(\tau) = \int d^d x \bar{\psi}_i(x, \tau) \left[ -\frac{1}{2m} \nabla^2 - \mu \right] \psi_i(x, \tau) + \frac{1}{2} \int d^d x d^d y \bar{\psi}_i(x, \tau) \bar{\psi}_j(y, \tau) \psi_j(y, \tau) \psi_i(x, \tau) \] .

(2.2)

Here \( m \) is the electron mass, \( \mu \) is the chemical potential, and \( u(x - y) \) is the electron-electron interaction potential. More realistic models to describe itinerant electron magnetism including, e.g., band structure, can be considered along the same lines. The salient points of the present paper, however, are due to long-wavelength effects and therefore are independent of microscopic details like the band structure.

For our purposes it therefore is sufficient to study the model defined in (2.2).

In order to describe magnetism, it is convenient and standard practice to break the interaction part of the action \( S \), which we denote by \( S_{\text{int}} \), into particle-hole spin-singlet, particle-hole spin-triplet and particle-particle or Cooper channel contributions, which we denote by \( S_{\text{int}}^{(\sigma)} \), \( S_{\text{int}}^{(ij)} \) and \( S_{\text{int}}^{(ii)} \), respectively [7]. For simplicity, we assume that the interactions are short-ranged in all of these channels. In a metallic system this is justified due to screening, and an effective model with a short-ranged interactions can be derived starting from a bare Coulomb interaction [7]. The spin-triplet interaction warrants special attention, since the interactions between spin density fluctuations that are described by \( S_{\text{int}}^{(ij)} \) are what causes ferromagnetism. We therefore consider this part of the action separately, and write

\[ S = S_0 + S_{\text{int}}^{(ij)} , \] (2.3)

with

\[ S_{\text{int}}^{(ij)} = \frac{\Gamma_i}{2} \int d^d x d^d \tau \bar{n}_i(x, \tau) \cdot n_i(x, \tau) \] ,

(2.4a)

where \( n_i \) is the electron spin density vector with components,

\[ n_i^a(x, \tau) = \frac{1}{2} \bar{\psi}^a(x, \tau) \sigma_i^a \psi_i(x, \tau) \] .

(2.4b)

Here the \( \sigma^a \) (\( a = 1, 2, 3 \)) are the Pauli matrices, and \( \Gamma_i \) is the spin-triplet interaction amplitude. \( S_0 \) in (2.3) contains the free electron part and all interaction parts other than the particle-hole spin-triplet contribution to the action. It reads explicitly,
determine the behavior near the critical point. The same ba-
procedure is a LGW theory, i.e. an effective field theory for
all degrees of freedom except for the long wavelength order
parameter relevant for the transition, and by integrating out
proceeds from a microscopic model by identifying the order
ous problem for the former, since at \( t = 0 \) there are more
soft modes are not ‘critical’ in the sense that they change
tion that in general one should worry about both the critical
previous work on itinerant electronic systems, [1] we men-
are now slowly varying in both space and (imaginary) time.
the only principal difference being that the critical modes
wavelength fluctuations of the charge density and the anoma-
\( \Gamma \)
\( n \)
\( S \)
\( Z \)
\( \Phi \)
\( \chi \)
\( M \)
\( \Gamma \)
\( \Omega \)
\( \kappa \)
\( \lambda \)
\( \mu \)
\( \nu \)
\( \sigma \)
\( \tau \)
\( \omega \)
\( \rho \)
\( \theta \)
\( \phi \)
\( \psi \)
\( \xi \)
\( \zeta \)
\( \gamma \)
\( \delta \)
\( \epsilon \)
\( \zeta \)
\( \eta \)
\( \theta \)
\( \vartheta \)
\( \chi \)
\( \psi \)
\( \omega \)
\( \nu \)
\( \kappa \)
\( \lambda \)
\( \mu \)
\( \sigma \)
\( \tau \)
\( \alpha \)
\( \beta \)
\( \gamma \)
\( \delta \)
\( \epsilon \)
\( \zeta \)
\( \eta \)
\( \theta \)
\( \vartheta \)
\( \chi \)
\( \psi \)
\( \omega \)
\( \nu \)
\( \kappa \)
\( \lambda \)
\( \mu \)
\( \sigma \)
\( \tau \)
\( \alpha \)
\( \beta \)
\( \gamma \)
\( \delta \)
\( \epsilon \)
\( \zeta \)
\( \eta \)
\( \theta \)
\( \vartheta \)
\( \chi \)
\( \psi \)
\( \omega \)
\( \nu \)
\( \kappa \)
\( \lambda \)
\( \mu \)
\( \sigma \)
\( \tau \)
\( \alpha \)
\( \beta \)
\( \gamma \)
\( \delta \)
\( \epsilon \)
\( \zeta \)
\( \eta \)
\( \theta \)
\( \vartheta \)
\( \chi \)
\( \psi \)
\( \omega \)
\( \nu \)
\( \kappa \)
\( \lambda \)
\( \mu \)
\( \sigma \)
\( \tau \)
\( \alpha \)
\( \beta \)
\( \gamma \)
\( \delta \)
\( \epsilon \)
\( \zeta \)
\( \eta \)
\( \theta \)
\( \vartheta \)
\( \chi \)
\( \psi \)
\( \omega \)
\( \nu \)
\( \kappa \)
\( \lambda \)
\( \mu \)
\( \sigma \)
\( \tau \)
\( \alpha \)
\( \beta \)
\( \gamma \)
\( \delta \)
\( \epsilon \)
\( \zeta \)
\( \eta \)
\( \theta \)
\( \vartheta \)
\( \chi \)
\( \psi \)
\( \omega \)
\( \nu \)
\( \kappa \)
\( \lambda \)
\( \mu \)
\( \sigma \)
\( \tau \)
\( \alpha \)
\( \beta \)
\( \gamma \)
\( \delta \)
\( \epsilon \)
\( \zeta \)
\( \eta \)
\( \theta \)
\( \vartheta \)
\( \chi \)
\( \psi \)
\( \omega \)
\( \nu \)
\( \kappa \)
\( \lambda \)
\( \mu \)
\( \sigma \)
\( \tau \)
\( \alpha \)
\( \beta \)
\( \gamma \)
\( \delta \)
\( \epsilon \)
\( \zeta \)
\( \eta \)
\( \theta \)
\( \vartheta \)
\( \chi \)
\( \psi \)
\( \omega \)
\( \nu \)
\( \kappa \)
\( \lambda \)
\( \mu \)
\( \sigma \)
\( \tau \)
\( \alpha \)
\( \beta \)
\( \gamma \)
\( \delta \)
\( \epsilon \)
\( \zeta \)
\( \eta \)
\( \theta \)
\( \vartheta \)
\( \chi \)
\( \psi \)
\( \omega \)
\( \nu \)
\( \kappa \)
\( \lambda \)
\( \mu \)
\( \sigma \)
\( \tau \)
\( \alpha \)
\( \beta \)
\( \gamma \)
\( \delta \)
\( \epsilon \)
\( \zeta \)
\( \eta \)
\( \theta \)
\( \vartheta \)
\( \chi \)
\( \psi \)
\( \omega \)
\( \nu \)
\( \kappa \)
\( \lambda \)
\( \mu \)
\( \sigma \)
\( \tau \)
\( \alpha \)
\( \beta \)
\( \gamma \)
\( \delta \)
\( \epsilon \)
\( \zeta \)
\( \eta \)
\( \theta \)
\( \vartheta \)
\( \chi \)
\( \psi \)
\( \omega \)
\( \nu \)
\( \kappa \)
\( \lambda \)
\( \mu \)
\( \sigma \)
\( \tau \)
\( \alpha \)
\( \beta \)
\( \gamma \)
\( \delta \)
\( \epsilon \)
\( \zeta \)
\( \eta \)
\( \theta \)
\( \vartheta \)
\( \chi \)
\( \psi \)
\( \omega \)
\( \nu \)
\( \kappa \)
\( \lambda \)
\( \mu \)
\( \sigma \)
\( \tau \)
\( \alpha \)
\( \beta \)
\( \gamma \)
\( \delta \)
\( \epsilon \)
\( \zeta \)
\( \eta \)
\( \theta \)
\( \vartheta \)
\( \chi \)
\( \psi \)
\( \omega \)
\( \nu \)
\( \kappa \)
\( \lambda \)
\( \mu \)
\( \sigma \)
\( \tau \)
\( \alpha \)
\( \beta \)
\( \gamma \)
\( \delta \)
\( \epsilon \)
\( \zeta \)
\( \eta \)
\( \theta \)
\( \vartheta \)
\( \chi \)
\( \psi \)
\( \omega \)
\( \nu \)
\( \kappa \)
\( \lambda \)
\( \mu \)
\( \sigma \)
\( \tau \)
\( \alpha \)
\( \beta \)
\( \gamma \)
\( \delta \)
\( \epsilon \)
\( \zeta \)
\( \eta \)
\( \theta \)
\( \vartheta \)
In order to study the critical behavior we have to determine $\chi$; we therefore have to calculate the static spin susceptibility. There is a nonanalytic correction to the static spin susceptibility of

$$\chi_{ab} \equiv \frac{1}{2} \chi_{ss},$$

where $\Omega_n = \pi T n$ is a bosonic Matsubara frequency. In order to study the critical behavior we have to determine $\chi^{(2)}$ in the long-wavelength and low-frequency limit. In a system with a conserved order parameter, the frequency must be taken to zero before the wavenumber, otherwise one never reaches criticality [11]. In the critical region we therefore have $|\Omega_n| < q$. In this limit the spin susceptibility has the structure

$$\chi_s(q, \Omega_n) = \int d(x_1 \to x_2) d(\tau_1 \to \tau_2) e^{-i q \cdot (x_1 - x_2)} \chi_s(x_1 - x_2),$$

where $q$ and $\Omega_n$ are being measured in suitable units, and $\chi_s(q)$ is the static spin susceptibility of the reference system.

The static spin susceptibility of non-interacting electrons, i.e. the Lindhard function, as a function of the wavenumber $q$ is analytic at $q = 0$. However, for any electron system with a nonvanishing particle-hole spin-triplet interaction, $\mu_0 \chi_{ss} / \Gamma_s \neq 0$, there is a nonanalytic correction to the static susceptibility [12]. Although our bare reference system $S_0$ does not contain such an interaction term, in a generic reference system a nonvanishing $\mu_0 \chi_{ss} / \Gamma_s$ is generated in perturbation theory. For being generic in this sense, it suffices that the bare system has a nonvanishing Cooper channel interaction amplitude $\mu_0 \neq 0$. This is shown in Appendix A. Effectively, we therefore have to calculate the static spin susceptibility of a paramagnetic Fermi liquid with a nonvanishing $\mu_0$. It has been shown in [12] that the result is

$$\chi_s(q, \Omega_n = 0) = \chi_s(0) \left[ 1 - |\Omega_n| / q + \ldots \right],$$

where $\chi_s(0)$ and $\Omega_n$ are being measured in suitable units, and $\chi_s(q)$ is the static spin susceptibility of the reference system.

In the frequency scales like $T^d$ and in powers of gradients and frequencies. However, for the system under consideration such a gradient expansion does not exist. To illustrate this point, let us first consider the spin susceptibility.

The nonanalytic behavior is confined to zero temperature, at $T = 0$. At finite temperature, where one has to perform a frequency sum rather than a frequency integral to calculate the correlation function, the nonanalytic term is replaced by a term of the schematic structure, [12]

$$q^{d-1} \to (q + T)^{(d-1)}.$$

so for fixed $T > 0$ an analytic expansion about $q = 0$ exists, and the standard local LGW functional is obtained.

We now turn to the higher spin density correlation functions $\chi^{(n)}$. The same physics that causes the nonanalyticity in the spin susceptibility, (2.10a), leads to an even stronger effect in the higher correlation functions, and results in $\chi^{(n)}$ for $d < n - 1$ not being finite in the limit of zero frequencies and wave numbers. One finds that in this limit $\chi^{(n)}$ is schematically given by

$$\chi^{(n)} \sim u_n + v_n (T + m)^{d+1-n},$$

where $u_n$ and $v_n$ are finite numbers and we have cut off the infrared divergence by means of a cut-off momentum $p$. Rotational symmetry in spin space requires $\Omega_{2n+1} = 0$. Again, the nonanalytic behavior is confined to zero temperature, at finite temperature $\chi^{(n)}$ is given by

$$\chi^{(n)} \sim u_n + v_n (T + p)^{d+1-n},$$

which is finite for $p \to 0$. Equations (2.10a) and (2.11a) imply that our LGW functional, (2.7a), contains a nonanalyticity which has the form of a power series in $M / p$. In order to specify the LGW functional, we still need a physical interpretation of the infrared cutoff momentum $p$. This will be given in the next section.

To conclude this section we show that the static correlation functions discussed above provide more important nonanalyticities than higher order terms in a frequency expansion. To see this, we anticipate a result from the next section. We will discuss a fixed point of the renormalization group transformation where the dynamical exponent is $z = d$, i.e. $\Omega_n$ scales like $q^d$. Now let us look at an expansion of $\chi^{(n)}$ in powers of frequency. In our clean system with ballistic modes the term of $m^{th}$ order in $\Omega_n$ carries an additional factor of $q^m$ in the denominator, as can be seen in (2.9) for the spin susceptibility. Thus, if the term of zeroth order in the frequency scales like $q^{d+1-n}$ near criticality, then the $n$th order term scales like $q^{d+1-n + (d-1)}$. For $d > 1$ the static susceptibility therefore has a stronger divergence than the frequency corrections. However, in $d = 1$ the leading divergence is provided by a frequency dependent term, as will be discussed in Sect. V below.
III. The critical behavior at zero temperature

Here we discuss the quantum critical behavior of the Gaussian part of the LGW theory defined in the last section. We do so both by explicitly solving the Gaussian theory, and by studying the renormalization group properties of the Gaussian fixed point. We then analyze the non-Gaussian terms in the field theory, and show that they are irrelevant, in the renormalization group sense, with respect to the Gaussian fixed point for all dimensions \( d > 1 \). This implies that the Gaussian theory yields the exact critical behavior for all of these dimensions, except for logarithmic corrections to scaling in \( d = 3 \) that are discussed in Appendix B. We then construct the equation of state near the critical point. This requires a more detailed discussion of the irrelevant non-Gaussian terms in the field theory, since the equation of state is determined in part by dangerous irrelevant variables.

A. The Gaussian fixed point

According to (2.7), (2.9), and (2.10a), the Gaussian part of the LGW functional \( \Phi[M] \) is,

\[
\Phi_2[M] = \frac{1}{2} \sum_{\mathbf{q}} \sum_{\omega_n} M(\mathbf{q}, \omega_n) \left[ t_0 + a_{d-1} q^{d-1} + a_2 q^2 + \frac{a_\Omega}{|\omega_n|/q} \cdot M(-\mathbf{q}, -\omega_n) \right] (3.1a)
\]

where

\[
t_0 = 1 - \Gamma_t \chi(\mathbf{q} \to 0, \omega_n = 0),
\]

is the bare distance from the critical point, and \( a_{d-1}, a_2, \text{ and } a_\Omega \) are positive constants.

We first analyze the critical behavior implied by (3.1). Later we will show that for \( d > 1 \) fluctuations are irrelevant, and the critical behavior found this way is exact for these dimensions. Four critical exponents can be directly read off (3.1a). These are the correlation length exponent \( \nu \), defined by \( \xi \propto t^{-\nu} \), with \( \xi \) the correlation length and \( t \) the (renormalized) dimensionless distance from the critical point; the exponent \( \eta \) that determines the wavenumber dependence of the magnetic (i.e., order parameter) susceptibility at criticality, \( (\chi_{\nu}(\mathbf{q}, 0) \propto q^{-2\eta}) \); the dynamical scaling exponent \( z \) that characterizes critical slowing down by relating the divergence of the relaxation time, \( \tau_t \), to that of the correlation length, \( \tau_t \sim \xi^z \); and the exponent \( \gamma \) that describes the \( t \)-dependence of the static magnetic susceptibility \( \chi_\nu = \langle M_\nu(0, 0) M_\nu(0, 0) \rangle \sim t^{-\gamma} \). An inspection of (3.1a) yields,

\[
\nu = \begin{cases} 1/(d-1) & \text{for } 1 < d < 3 \\ 1/2 & \text{for } d > 3 \end{cases}, \quad (3.2a)
\]

\[
\eta = \begin{cases} 3 - d & \text{for } 1 < d < 3 \\ 0 & \text{for } d > 3 \end{cases}, \quad (3.2b)
\]

\[
z = \begin{cases} d & \text{for } 1 < d < 3 \\ 3 & \text{for } d > 3 \end{cases}, \quad (3.2c)
\]

\[
\gamma = 1 \quad \text{for all } d > 1. \quad (3.2d)
\]

In \( d = 3 \) there are logarithmic corrections to scaling, see Appendix B.

For later reference, we also discuss the critical behavior given by (3.1) and (3.2) from a renormalization group point of view. Let \( b \) be the renormalization group length rescaling factor. Under renormalization, all quantities change according to \( A \to b^{-\nu A} A \), with \([A]\) the scale dimension of \( A \). The scale dimension of the order parameter is,

\[
[M(q, \omega_n)] = -1 + \eta/2,
\]

or, equivalently,

\[
[M(x, \tau)] = (d + 1)/2.
\]

B. The non-Gaussian terms

We now show that all of the non-Gaussian terms in the field theory are renormalization group irrelevant with respect to the Gaussian fixed point discussed in the last subsection. To do this we determine the scale dimensions of the coefficients \( u_n \) and \( v_n \) of the higher-order terms in the LGW functional which had been defined in (2.11a). Since the latter have been defined in Fourier space, we first take the Fourier transform of the \( n^{\text{th}} \) summand in (2.7a). This yields

\[
\chi^{(n)} = -\frac{1}{2} (n-2)[T/V] - n \left[ M(q_0, \omega_n) \right]
\]

\[
= -\frac{1}{2} (n-2)(d + z) + n(1 - \eta/2), \quad (3.4)
\]

where we have used (3.3a). Next we need to assign a scale dimension to the cutoff momentum \( p \) in (2.11a). The most obvious guess from a scaling point of view is to identify \( p \) with the inverse correlation length \( \xi^{-1} \), which makes \([p] = 1\). We will ascertain in Sect. III.C below that this is indeed the correct choice. It then follows from (2.11a) that of the two parameters \( u_n \) and \( v_n \), \( v_n \) has the larger scale dimension, and hence is more relevant, for \( d < n - 1 \), while \( u_n \) is more relevant for \( d > n - 1 \). For even \( n \) (remember that \( u_{2n+1} = 0 \)) and \( d > n - 1 \) the most relevant parameter thus has a scale dimension

\[
[u_{2n}] = -(d+1)(n-1) + 2, \quad (3.5a)
\]

which is always negative. For odd \( n \), and for \( d < n - 1 \) for even \( n \), we need to consider,

\[
v_n = \begin{cases} -(n-2)(d-1)/2 & \text{for } 1 < d < 3 \\ 2 - n(d-1)/2 & \text{for } d < 3 \end{cases}, \quad (3.5b)
\]

We see that all of the \( v_n \) are irrelevant for \( d > 1 \), while in \( d = 1 \) they all become marginal. We conclude that for \( d > 1 \) the critical Gaussian fixed point is stable, and so the exponents given in (3.2) are exact. In \( d = 1 \) an infinite number of operators seems to become marginal, so naively one would conclude that the upper critical dimension is given by \( d^c = 1 \). However, one has to keep in mind that the functional form of correlation functions in \( d = 1 \) can be qualitatively different.
from that in $d > 1$, so our power counting may be valid only for $d > 1$, and the scale dimension of some operators may change discontinuously from irrelevant in $d > 1$ to relevant in $d = 1$. This actually happens, as will be discussed in Sect. V below.

C. The equation of state

We now determine the equation of state, and calculate the critical behavior of the magnetization and the magnetic susceptibility. Since we have shown in the last subsection that fluctuations are irrelevant for the critical behavior for all $d > 1$, we can determine the equation of state by simply calculating the saddle point contribution to the free energy. However, in order to do so, we have to include the higher order terms in the LGW functional. Although they are irrelevant operators for $d > 1$, they are potentially dangerously irrelevant [16] with respect to the magnetization $m$. We will see below that all of the $v_n$ are indeed dangerously irrelevant, since $m$ is a singular function of the $v_n$ for $v_n \to 0$.

We determine the mean field equation of state by calculating the saddle point contribution to the free energy. To do so, we replace the order parameter field $\Phi$ by the average magnetization $m > 0$ and determine the stationary point of $\Phi$ with respect to $m$. This yields the equation of state in the form

$$t m + u_4 m^3 + v m^d = H,$$

where an external magnetic field $H$ was added. We have only kept the leading terms in each order of $m$, and we have suppressed all numerical prefactors since they are unimportant for our purposes. The equation of states now has the form of a power series in $m/p$. This applies that the cut-off moment $p$ effectively scales like $m$. Thus, all higher order terms effectively have the same power of $m$, viz. $m^d$, and the equation of states now reads

$$t m + u_4 m^3 + v m^d = H,$$

with $u_4$ from (2.11a) and $v$ another finite coefficient. From (3.7) we immediately obtain the exponents $\beta$ and $\delta$, defined by $m(t, H = 0) \sim t^{\beta}$, $m(t = 0, H) \sim H^{1/\delta}$, as

$$\beta = \begin{cases} 1/(d-1) & \text{for } 1 < d < 3 \\ 1/2 & \text{for } d > 3 \end{cases},$$

$$\delta = \begin{cases} d & \text{for } 1 < d < 3 \\ 3 & \text{for } d > 3 \end{cases}.$$ (3.8a, 3.8b)

In $d = 3$ logarithmic corrections to scaling occur, see Appendix B.

We are now in a position to determine the exact scale dimension of the cut-off moment $p$ and to verify the identification of $p$ with $\xi^{-1}$ made in the last subsection. As we have seen after (3.6), the cutoff $p$ scales like $m$, so that $[p] = [m]_{\text{det}}$, where $[m]_{\text{det}} = \beta/\nu$ is the effective scale dimension of $m$, i.e., the scale dimension after the effects of the dangerous irrelevant variables have been taken into account. From (3.8a), (3.2a) we see that $\beta = \nu$, hence $[m]_{\text{det}} = 1$. Consequently, $[p] = 1$ which justifies the identification $p$ with $\xi^{-1}$ for scaling purposes made in Sect. B. These results complete the proof of the statement that the system is above its upper critical dimension for $d > 1$.

IV. Behavior at finite temperatures, and the quantum to classical crossover

In the first part of this section we discuss various sources of temperature dependence in our field theory and the corresponding scaling behavior of the temperature. In the following two subsections we apply the results to a calculation of the equation of state at finite temperatures and of the specific heat, and we discuss the crossover from the quantum Gaussian fixed point to the classical Gaussian fixed point. In the last subsection we discuss the analogous temperature dependence in systems with quenched disorder.

A. Scaling behavior of the temperature

The temperature dependence of the LGW functional, (2.7a), is due to a number of entirely different effects. First, the spin-density correlation functions $\chi^{(n)}$ that determine the coefficients of the LGW functional are temperature dependent as given in (2.10b) and (2.11b). These are correlation functions for the reference ensemble that is far from any critical point. Therefore, the frequency or temperature in $\chi^{(n)}$ scales like the momentum, and consequently we have a temperature scale whose scale dimension is,

$$[T]_{\text{Hall}} = 1.$$ (4.1a)

This we will refer to as the ballistic temperature scale.

A second source of temperature dependence is the usual dynamical scaling. This originates from the fact that the time integration in the LGW functional, (2.7a), extends over the finite interval $[0, 1/T]$. Dynamical scaling is hence equivalent to finite-size scaling in the direction of imaginary time. The scaling behavior of the temperature due to dynamical scaling is described by the dynamical exponent $z$ as given in (3.2c). We therefore have a second temperature scale whose scale dimension is

$$[T]_{\text{det}} = z,$$ (4.1b)

which below we will refer to as the critical temperature scale.

Finally, the distance from the critical point, $t$, is temperature dependent. For the bare $t_0$, this is simply the usual $T^2$ dependence that is familiar from Fermi liquid theory. The scale dimension of this Fermi liquid temperature scale is thus

$$[T]_{FL} = 1/2\nu.$$ (4.1c)

However, upon renormalization $t$ acquires a more intricate temperature dependence. Since the loop or fluctuation corrections involve integrals over critical propagators, the latter depend on the critical temperature scale. However, it also depends on the scale dimensions of the vertices $u_{nn}$ and $v_{nn}$, (2.11a), that are dangerous irrelevant variables with respect to the $T$-dependence of the magnetization and the magnetic susceptibility. Millis [17] and Sachdev [18] have shown that the resulting temperature scale has a scale dimension

$$[T]_{\text{fact}} = z/(1 - \nu \theta).$$ (4.1d)
where $\theta$ is the scale dimension of the appropriate dangerous irrelevant operator, $u_0$ in our case. This we call the fluctuation temperature scale.

Of all the temperature scales that are present in a given quantity, the one with the largest scale dimension will be the dominant one. This means, for instance, that the Fermi liquid scale will be subdominant compared to the ballistic one for all $1 < d < 3$; for $d > 3$ the two scales are indistinguishable. Since $z > 1$ for all $d > 1$ it also means that the critical temperature scale will in general be dominant over both the ballistic scale and the fluctuation scale. There are, however, two possible mechanisms that can invalidate this conclusion. The first possibility is that some quantities with the largest scale dimension will be determined by the equation of state, (3.6), whose coefficients do not depend on the critical temperature scale. For those quantities, the one with the largest scale dimension will be the dominant one. This means, for instance, that the Fermi liquid scale will be subdominant compared to the ballistic temperature scale.

The second possibility is that a subdominant temperature scale is dangerously irrelevant. This possibility cannot be ruled out by general scaling considerations.

### B. Magnetization, and magnetic susceptibility

Since we work above an upper critical dimensionality, the magnetization $m$ and the magnetic susceptibility $\chi_m$ are determined by the equation $q = \Omega_{m} = 0$ Fourier component of the order parameter field, and do not depend on the finite-frequency behavior of the critical modes. Therefore, dynamical scaling does not enter the temperature dependence of $m$ and $\chi_m$ directly. In other words, their behavior is completely determined by the equation of state, (3.6), whose coefficients acquire finite temperature corrections according to (2.10b) and (2.11b). The $m$ term in (3.6) has a correction of the form $m(p+T)^{\delta - 1} \sim m(p+T)^{\delta - 1}$. Similarly, the higher order terms $v_0 p^{d-1} m^{-1}$ have corrections proportional to $(p+T)^{\delta - 1} m^{n-1}$. This is the ballistic temperature scale discussed in Sect. A above. In addition, there is the fluctuation temperature scale that results from the temperature dependence of $t$. By using (3.5a) in (4.1d) we see that $[T]_{\text{ball}} > [T]_{\text{magn}}$, and thus is the dominant temperature scale, for $1 < d < 2$, and for $d > 5$, but that for $2 < d < 5$, $[T]_{\text{magn}}$ is the relevant scale. All of these corrections can be summarized in the following scaling law for the magnetization $m$,

$$m(t, T, H) \sim b^{-3/\nu} m(tb^{1/\nu}, T^{1/\nu}, Hb^{3/\nu})$$

where $b$ is an arbitrary scale factor. The crossover exponent

$$\phi = \begin{cases} 
\nu = 1/d - 1, & \text{for } 1 < d < 2, \\
\nu = 1/2, & \text{for } d = 3, \\
\nu = 1/d + 1, & \text{for } d > 3
\end{cases}$$

(4.2a)

describes the crossover from the quantum critical region to a regime whose behavior is dominated by the classical Gaussian fixed point [17, 19]. Note that, for the reasons explained above, the crossover exponent is not given by $2\nu$ which one would expect from dynamical scaling. Also note the complicated behavior of the crossover exponent $\phi$ as a function of the dimensionality, which is brought about by the competition between the ballistic and the fluctuation temperature scales. The result $\phi = \nu$ that was reported in [5] and [20] was correct only for $1 < d < 2$ and $d > 5$. By differentiating (4.2a) with respect to $H$, we obtain the analogous homogeneity law for the magnetic susceptibility $\chi_m$.

$$\chi_m(t, T, H) \sim b^{\beta/\nu} \chi_m(tb^{1/\nu}, T^{1/\nu}, Hb^{3/\nu})$$

(4.3)

### C. The specific heat

The scaling behavior of the specific heat is determined by the sum of the mean-field and the Gaussian fluctuation contribution to the free energy density $f$. The mean-field contribution follows immediately from (3.7). The Gaussian fluctuation contribution, $f_G$, which gives the leading nonanalyticity for the specific heat at the critical point, can be calculated in complete analogy to the case of classical $\phi^4$-theory in $d > 4$ [21]. Neglecting an uninteresting constant contribution to $f_G$, we obtain,

$$f_G = \frac{T}{2V} \sum_{q_0} \left[ 2 \ln |H/m + q_{d-1} q^{d-1} t + O_{m}/q) + \ln (x_d H/m - (x_d - 1)t + O_{m}/q) \right] + \frac{O_{m}}{q}$$

(4.4)

Here $x_d = d$ for $1 < d < 3$, and $x_d = 3$ for $d > 3$. The specific heat coefficient $\gamma_V$ is conventionally defined by,

$$\gamma_V = \frac{c_V}{T} = -\partial^2 f/\partial T^2$$

(4.5)

Again we are interested only in scaling properties and not in exact coefficients. Keeping this in mind, an adequate representation of (4.4) and (4.5) is given by the integral,

$$\gamma_V = \int_0^\Lambda dq \frac{q^{d-1}}{T + q^2 + q^3 + H/m}$$

(4.6)

with $\Lambda$ an ultraviolet cutoff.

Let us point out two interesting features of this result. First, for all dimensionalities in the range $1 < d < 3$, $\gamma_V$ is logarithmically singular for $T, H \rightarrow 0$. This can be seen most easily from (4.6), and it is also true for the exact result, Eqs. (4.5), (4.4). Such a $d$-independent logarithmic singularity is somewhat unusual. Wegner has discussed how logarithmic corrections to scaling arise if a set of scale dimensions fulfills some resonance condition [22]. In the present case the relevant relation is that the scale dimension of the free energy, $d + z = 2z$ for $1 < d < 3$, is a multiple of the scale dimension of $T$, which is $z = d$ in this region. The fact that the logarithm appears in a range of dimensions, rather than only for a special value of $d$, is due to the dynamical exponent being exactly $d$ in that range. Second, as discussed in Sect. IV A, two different temperature scales appear in (4.6). The first two terms in the denominator indicate that $T \sim \xi^{-1}$, as one would expect from dynamical scaling. However, the last term in (4.6) contains the magnetization, which in turn depends on $[T]_{\text{ball}}$ and $[T]_{\text{magn}}$. These two features imply that the scaling equation for $\gamma_V$ should be written.
\[\gamma_{V}(t, T, H) = \Theta(3 - d) \ln b + F_{\nu}(t^{1/\nu}, T^{1/\nu}, H^{d/3(1/\nu)}, T^{b^{3/\nu}}). \] (4.7)

Note that the scale dimension of \(\gamma_{V}\), ignoring the logarithm, is zero in all dimensions. Since \(z > \phi/\nu\) for all \(d > 1\), one can formally ignore the fourth entry in the scaling function since it is subleading compared to the second entry and its effects can be considered as ‘corrections to scaling’.

We emphasize that in contrast to the magnetization and the magnetic susceptibility, the specific heat does depend on the critical modes, and hence contains the critical temperature scale. As mentioned in Sect. A, the latter is dominant when it is present, and \(\gamma_{V}\) provides an example for that.

D. The disordered case revisited

Let us finally reconsider the case of systems with quenched disorder [4]. We do this partly to point out the remarkable analogy between the clean and dirty cases, and partly to correct a mistake in the results of [4] for dimensions \(d > 3\).

In the presence of disorder, the temperature or frequency far from criticality scales like the wavenumber squared. The ballistic temperature scale of (4.1a) therefore gets replaced by a diffusive one,

\[ [T]_{\text{lat}} = 2. \] (4.8)

The scale dimensions for the other temperature scales, (4.1b)-(4.1d) remain valid, but the values of the exponents \(z, \nu, \) and \(\theta\) change. In the action, the disorder leads to terms in addition to, and structurally different from, those in (2.7a) [4]. In particular, at order \(M^{4}\) a second term appears which coupling constant was denoted by \(v_{d}\) in [4]. This operator, whose scale dimension is \([v_{d}] = -[d - 4]\), is the least irrelevant operator that is dangerous with respect to \(t\), and one therefore has \(\theta = -[d - 4]\) in the fluctuation temperature scale, (4.1d). With \(z, \nu\) as determined in [4], this leads to a crossover exponent

\[ \phi = \begin{cases} 2\nu = 2/(d - 2) & , & 2 < d < \sqrt{5} + 1 \\ \frac{d}{2} & , & \sqrt{5} + 1 < d < 4 \\ \frac{4}{d - 2} & , & 4 < d < 6 \\ 2\nu = 1 & , & d > 6 \end{cases}. \] (4.9)

The result \(\phi = 2\nu\) of [4, 20] was thus not correct for the (unphysical) dimensionality range \(\sqrt{5} + 1 < d < 6\). The scaling behavior of the magnetization and the magnetic susceptibility is given by (4.2a) and (4.3), respectively, with \(\phi\) from (4.9), and all other exponents as given in [4].

V. Hertz’s model revisited

In this section we reexamine Hertz’s original model of the ferromagnetic quantum phase transition [1]. We show that at tree level, the LGW theory for this model breaks down for related, but somewhat different reasons than in the realistic model above. Moreover, starting at one-loop order the renormalization group generates terms that are not in the bare action. As a result, the critical behavior of this model in \(d > 1\) is not mean-field like, but rather the same as that of the more realistic model we have studied so far.

Hertz’s model differs in two respects from the more realistic one given by (2.3) through (2.5). First, the interaction part of the action contains only the particle-hole spin-triplet channel that is decoupled in the derivation of the LGW functional. Consequently, the reference ensemble \(S_{0}\) consists of noninteracting electrons. Second, the coefficients \(\chi^{(n)}\) of the LGW functional are taken to be the correlation functions of a 3-d Fermi gas, irrespective of the dimensionality of the space the magnetization is confined to. For this model the spin susceptibility \(\chi_{s}\) of the reference system is simply the Lindhardt function, so (2.9) gets replaced by

\[ \chi_{s}(q, \Omega_{n}) = c_{0} - c_{2}q^{2} - |\Omega_{n}|/q. \] (5.1)

In comparison to the analogous expression for an interacting Fermi liquid, Eqs. (2.9) and (2.10a), the term proportional to \(q^{d-1}\) is missing, and \(\chi_{s}(q, \Omega_{n} = 0)\) is now analytic at \(q = 0\). The resulting Gaussian part of the bare LGW functional has the form

\[ \Phi[M] = \frac{1}{2} \sum_{q, \Omega_{n}} M(q, \Omega_{n}) \left[ t_{0} + a_{2} q^{2} + a_{1} |\Omega_{n}|/q \right] \times M(-q, -\Omega_{n}). \] (5.2)

This action allows for a Gaussian fixed point with mean-field static exponents and a dynamical exponent \(z = 3\) [1].

Let us now investigate the stability of this Gaussian fixed point. At tree level, we can do this by calculating the scale dimensions of the coefficients of the higher order terms. Hertz considered the higher order correlation functions \(\chi^{(n)}\) only in the limit \(\Omega_{n} = 0, q \rightarrow 0\) where they are finite numbers.

For power counting purposes, i.e. to determine the scale dimensions of the coefficients, it is not necessary to calculate the \(\chi^{(n)}\) completely as functions of \(n - 1\) frequencies and wavevectors. Guided by more complete calculations for the cases \(n = 3, 4, 5\), we have concluded that for power counting purposes it suffices to consider one independent frequency, \(\Omega\), and two directionally independent wavevectors of equal length, \(|q_{1}| = |q_{2}| = |q|\), that form an angle \(\theta\). With these simplifications the leading term of the general coefficient is easily calculated. We find that for odd \(n\) the linear-in-frequency term in the action can symbolically be written

\[ w_{n} \int dx M^{n}(x) \Omega/q^{n-1}, \] (5.3a)

with \(w_{n}\) some coupling constant, while the corresponding terms for even \(n\) are less relevant. The same power counting arguments that we used in Sect. III.B show that the scale dimension of \(w_{n}\) is \([w_{n}] = -(d - 1)(n - 2)/2\), which is negative for all \(d > 1\). The coupling constants \(w_{n}\) are thus irrelevant for all physical dimensions \(d \geq 2\), and seem to become marginal in \(d = 1\). However, (5.3a) holds only if the two independent wavevectors are neither parallel nor
antiparallel, i.e. it holds only if \( d > 1 \). For \( \theta = 0, \pi \) one finds a stronger singularity for the terms with even \( n \),

\[
w_{\omega} \int dx M^n(x) \Omega / q^{2n-3} ,
\]

while the terms with odd \( n \) are less relevant. In dimensions \( d > 1 \) the parallel wavevectors form a set of measure zero and this stronger singularity is of no consequence. In \( d = 1 \), however, (5.3b) represents the generic behavior of the terms of \( O(M^n) \). Power counting yields the scale dimensions to be \( [w_{\omega}] = n - 2 \) in \( d = 1 \), so all of these coefficients are relevant operators. This is sufficient to conclude that the upper critical dimension is not one, but rather that the 1-d system is below its upper critical dimension, and will show nontrivial critical behavior. This provides a technical explanation for Sachdev’s observation [3] that Hertz’s results in \( d < 1 \) cannot be correct.

Moreover, the renormalization of the model beyond the tree level qualitatively changes the form of the Gaussian action, (5.2). Consider, for instance, the one-loop renormalization of \( \Phi_2 \) by the terms of order \( M^4 \) and \( M^2 \). The corresponding diagrams are shown in Fig. 1. It is easy to see that these diagrams are equivalent to those that determine the spin susceptibility of interacting electrons, and have been calculated in [12, 23]. Renormalization therefore leads to a term proportional to \( q^{d-1} \) in the Gaussian action, and hence to a \( \Phi_2 \) as given by (3.1a). We conclude that the critical behavior of Hertz’s model for \( d > 1 \) is not mean-field like, but rather the same as that of the more realistic model discussed in Sects. II–IV.

**VI. Discussion**

In this paper we have shown that clean itinerant quantum ferromagnets at zero temperature do not show, as was previously thought, uninteresting mean-field critical behavior for all dimensionalities \( d > 1 \). Rather, there are two upper critical dimensions. The first one is \( d^c = 1 \), above which the critical behavior is described by a Gaussian field theory but is not mean-field like, and the second one is \( d^{cal} = 3 \), above which one does find mean-field critical behavior. The reason for this unusual behavior is soft modes that lead to an effective long-range interaction between the order parameter fluctuations. As is the case for classical models with long-range interactions, [24] this leads to nontrivial critical behavior that still can be determined exactly. \( d^{cal} \) is the marginal dimension where the soft mode induced long-range interaction coincides with the usual \( r^{-(d-2)} \) behavior. In this final section we discuss a few aspects of these results that have not been covered yet.

First of all, both our approach and our results are remarkably similar to a recent treatment of disordered itinerant quantum ferromagnets [4]. In these papers it was found that the disorder induced diffusive excitations in a Fermi system with quenched disorder lead to similar, but stronger effects, with a long ranged interaction between order parameter fluctuations that falls off like \( r^{-(2d-2)} \), and three ‘upper critical dimensionalities’, viz. 2, 6, and 4. The first two are analogous to \( d^c \) and \( d^{cal} \) above. In addition, the critical exponents \( \nu, \eta, \) and \( z \) take on their mean-field values for \( d > 4 \), while \( \beta \) and \( \delta \) remain anomalous between \( d = 4 \) and \( d = 6 \). In the present case, a different structure of the dangerous irrelevant variables makes the upper two special dimensions coincide. The same difference in the dangerous irrelevant variables leads to a difference in the temperature dependence of the equation of state as a function of dimensionality: In the disordered case, the diffusive temperature scale with \( [T]_{\text{ball}} = 2 \), which is analogous to the ballistic temperature scale \( [T]_{\text{ball}} = 1 \) in the clean case, is dominant in the physical dimension \( d = 3 \). In the clean case, in contrast, the ballistic scale is subdominant compared to the fluctuation temperature scale for \( 2 < d < 5 \).

The present paper shows that the basic concepts of [4] are not restricted to disordered systems. Indeed, an attempt to construct an effective field theory entirely in terms of the order parameter field for any phase transition will break down (in the sense that it is impossible to construct a local effective theory) if there are soft or slow modes other than the order parameter fluctuations that couple to the order parameter. In the present case, the spin-triplet particle-hole excitations that always exist in an interacting Fermi system, and that are distinct from the order parameter mode in that they are soft even in the paramagnetic phase, are such additional soft modes. They lead to the nonanalytic behavior of spin density correlation functions that is displayed in (2.10) and (2.11), and hence to the effective long-ranged interaction between the order parameter modes. In general, the appearance of such additional soft modes would call for the derivation of a different effective theory that does not integrate out as many degrees of freedom, and that keeps all of the soft modes on equal footing. However, as in [4] we have opted here to work with the order parameter effective theory after all, since it turns out that the difficulties introduced by the nonlocal character of the field theory can be overcome. Nevertheless it would be interesting to treat the same problem by means of a local theory that keeps more degrees of freedom explicitly.

It should also be pointed out that our results depend crucially on the fact that the electronic spin density is a conserved quantity. If this feature was lost, e.g. due to some type of spin flip process, then the spin-triplet particle-hole excitations would acquire a mass or energy gap, and at scales larger than this mass the effective interactions between the
order parameter fluctuations would be of short range. The asymptotic critical phenomena would then be described by a local order parameter field theory with mean-field critical behavior in all physical dimensions. At this point one might wonder whether the magnetization in the ordered phase, and magnetic fluctuations in the disordered one, act effectively as magnetic impurities, and why this does not lead to an energy gap that invalidates our conclusions. The answer is that this effect has already been taken into account. In the ordered phase, the magnetization indeed acts as a cutoff, as has been discussed in connection with (3.6), and this leads to the nonanalyticity in the equation of state. In the disordered phase, the cutoff enters only via fluctuations, which are RG irrelevant with respect to the Gaussian fixed point. The effect therefore manifests itself only in the corrections to scaling, not in the leading scaling behavior.

We also mention that all of the qualitative points discussed in [4] and [20] that had to do with the fact that one works above an upper critical dimension, apply here as well. In particular, the presence of dangerous irrelevant variables means that some of Sachdev’s general results [3] are not directly applicable to the transition discussed here. For instance, the Wilson ratio, \( W = (m/H)/(C_V/T) \), diverges at criticality, as it does in the disordered case, rather than being a universal number as would be the case in the presence of hyperscaling. However, due to the different structure of the dangerous irrelevant variables that was already mentioned above in connection with the multiple upper critical dimensionalities, some details are different between the disordered and clean cases. For instance, the scaling function \( F_{\gamma} \), (4.7), is a function of \( T/H \) (if one neglects the subleading ballistic temperature scale) in agreement with the prediction of [3], while in the presence of disorder this is not the case [4].

We add one more remark concerning Hertz’s original model that was discussed in Sect. V. Our conclusion that a proper renormalization of that model leads to a critical behavior that is the same as that of the realistic model solves the following paradox that would otherwise arise: Suppose one divided the interaction term in Hertz’s model into two structurally identical pieces, one carrying some fraction of the interaction amplitude \( \Gamma_t \), and the other the rest. Suppose one then applied the Hubbard-Stratonovich decoupling only to one of these pieces, and lumped the other into the reference ensemble. Then the reference ensemble would contain a nonzero \( \Gamma_t \), and according to [12] the Gaussian action would contain the nonanalytic \( q^{d-1} \) term that leads to non-mean field critical behavior for all \( d < 3 \). If one decouples all of the interaction term, on the other hand, then the reference ensemble has \( \Gamma_t = 0 \), and in the absence of any other interaction amplitudes there is no way to generate a nonzero \( \Gamma_t \) by renormalization. If Hertz’s model had indeed a critical behavior that is different from that of the realistic model, then the inevitable conclusion would be that the result depends on how exactly one performs the decoupling of the interaction term, which would be physically absurd.

Finally, it should be mentioned that an experimental corroboration or refutation of our results is probably harder for the clean case discussed in the present paper than for the disordered case treated in [4]. There are several reasons for this. First of all, the zero-temperature behavior can of course not be observed directly. An experimental study would therefore have to concentrate on the crossover from the quantum critical behavior to the classical one that will occur if the classical transition point is at a sufficiently low temperature for the crossover point to be within the critical region. This requires a ferromagnet with as low a Curie temperature as possible. In addition, the parameter \( t \) that measures the distance from the critical point is, in the quantum case, not the temperature but rather the exchange interaction or some other microscopic parameter that is hard to control. Both of these difficulties can be overcome relatively easily in the disordered case, where a change in the composition of a ferromagnetic alloy changes both the classical transition temperature and \( t \). The quantum critical point is reached in the low-temperature limit in a sample whose composition is such that the Curie temperature just vanishes. As was discussed in [4], this provides a manageable handle on \( t \) that has no obvious analog in the clean case. Furthermore, the differences between the quantum critical exponents in \( d = 3 \) and the classical Heisenberg exponents are more pronounced in the disordered case than in the clean one. As we have seen, the 3-d critical behavior in the latter case is mean-field with logarithmic corrections to scaling. The logarithms would be hard to observe in any case, and the mean-field exponents are much closer to 3-d Heisenberg exponents than those obtained in [4].

This work was supported by the NSF under grant numbers DMR-96-32978 and DMR-95-10185, by the DAAD, by the DFG under grant No. Vo 659/1-1, and by NATO under grant No. CRG-941250. We would like to thank Andy Millis and Subir Sachdev for helpful discussions. DB would like to thank Bernhard Kramer for his hospitality at the University of Hamburg.

Appendix A: renormalization of the particle-hole spin-triplet interaction vertex

In this appendix we show that a nonvanishing particle-particle channel interaction, \( I_\gamma \neq 0 \), generates a particle-hole spin-triplet interaction \( I_t \), even if \( I_t = 0 \) in the bare system.

Fig. 2 shows the three basic types of interaction vertices. Now suppose that \( I_t = 0 \). Then a vertex of this type can be constructed by means of the diagrams shown in Fig. 3, where all of the dashed lines represent Cooper channel interaction amplitudes.

Appendix B: logarithmic corrections to scaling for \( d = 3 \), and for \( 1 < d < 3 \)

There are three distinct mechanisms that produce logarithmic corrections to scaling: (1) Marginal operators, (2) Wegner resonance conditions between a set of scale dimensions, and (3) logarithmic corrections to the scale dimension of a dangerous irrelevant operator. The first two mechanisms are well known [22]. The third is operative only above an upper critical dimension, and is therefore of particular interest for quantum phase transitions.

In the present case, logarithmic corrections to scaling arise due to mechanisms (2) and (3). Mechanism (2) produces corrections to the scaling of the specific heat in all dimensions \( 1 < d \leq 3 \), as was discussed in Sect. IV.C. The
and at the critical point we have

\[ m(t, H = 0) \sim \frac{t^{1/2}}{\sqrt{\ln(1/t)}} \]  

and at the critical point we have

\[ m(t = 0, H) \sim \frac{H^{1/3}}{[\ln(1/H)]^{1/3}} \]  

References

2. We use the term ‘LGW theory’ in the narrow sense, in which it is usually used in the literature, of an effective field theory in terms of the order parameter field only. If one defines it as an effective theory for all soft modes, then it is valid in the present case, too.
8. This becomes clearer in Fourier space, where the sums over wavenumbers that replace the real space integrals in (2.5a) extend over small wavenumbers only. See, e.g., [12] for a more detailed exposition of this point.
9. Our interaction constants \( \Gamma_c \) and \( \Gamma_\omega \) are the zero angular momentum (\( l = 0 \)) components in a multipole expansion of the respective interaction potentials, and hence are related to the \( l = 0 \) Landau parameters. The physics we are interested in is due to hydrodynamic effects, which are strongest in the \( l = 0 \) or density channel. This justifies our neglecting the higher angular momentum \( l \) contributions.
11. This can be seen as follows. Since the magnetization is conserved, ordering on a length scale \( L \) requires some spin density to be transported over that length, which takes a time \( t \sim L/v_F \), with \( v_F \) the Fermi velocity. Now suppose the coherence length is \( \xi \), and we look at the system at a momentum scale \( q \) or a length scale \( L \sim 1/q < \xi \). Because of the time it takes the system to order over that scale, the condition for criticality is \( L < \min(v_F t, \xi) \). In particular, one must have \( L < v_F t \), or \( 1/t < v_F q \).
13. To lowest order in perturbation theory in \( \Gamma_\omega \) one finds \( \varepsilon_{d-1} \sim 0 \), see [12]. In that reference, various mechanisms have been discussed that may lead to \( \varepsilon_{d-1} > 0 \) for realistic values of the interaction strength. In what follows we discuss only systems whose parameter values are such that \( \varepsilon_{d-1} > 0 \), since else the continuous ferromagnetic phase transition we are interested in does not exist.
14. See, e.g., G. Baym and C. Pethick, Landau Fermi Liquid Theory: Concepts and Applications. New York: Wiley 1991. Notice that \( \chi_0(q = 0) \) as a function of temperature in \( d = 3 \) does not show a corresponding nonanalytic \( q \)-dependence. This does not contradict the nonanalytic \( q \)-dependence at zero temperature, see [12].
19. For all dimensions \( d > 2 \), where there is a classical Heisenberg transition, there is still another crossover in the system, namely from the classical Gaussian region to the classical Heisenberg critical region. For \( 1 < d < 2 \), where there is no long-range order at any nonzero temperature, this is not the case. In either case, \( d \) describes the leading low-temperature effect due to the relevance of the temperature with respect to the quantum fixed point.
23. Remember that in writing (5.2) a factor of \( F_\omega \) has been absorbed in the field \( M \), and that the Gaussian vertex is given by \( 1 - F_\omega \). In [12], the spin susceptibility was calculated to second order in \( \Gamma_\omega \), which in the present language also involves some two-loop diagrams.
Nonanalytic magnetization dependence of the magnon effective mass in itinerant quantum ferromagnets

D. Belitz
Department of Physics and Materials Science Institute, University of Oregon, Eugene, Oregon 97403

T. R. Kirkpatrick
Institute for Physical Science and Technology and Department of Physics, University of Maryland, College Park, Maryland 20742

A. J. Millis
Department of Physics and Astronomy, The Johns Hopkins University, 3400 North Charles Street, Baltimore, Maryland 21218

Thomas Vojta
Department of Physics and Materials Science Institute, University of Oregon, Eugene, Oregon 97403
and Institut für Physik, TU Chemnitz-Zwickau, D-09107 Chemnitz, Germany
(Received 26 June 1998)

The spin-wave dispersion relation in both clean and disordered itinerant quantum ferromagnets is calculated. It is found that effects akin to weak-localization physics cause the frequency of the spin waves to be a nonanalytic function of the magnetization $m$. For low frequencies $\Omega$, small wave vectors $k$, and $m\rightarrow 0$, the dispersion relation is found to be of the form $\Omega = \text{const} \times m^{1-\epsilon} |k|^2$, with $\epsilon = (4-d)/2$ ($2 < d < 4$) for disordered systems, and $\epsilon = (3-d)$ ($1 < d < 3$) for clean ones. In $d=4$ (disordered) and $d=3$ (clean), $\Omega \propto m \ln(1/m) k^2$. Experiments to test these predictions are proposed.

One of the best known examples of quantum long-range order is the ferromagnetic (FM) state in itinerant electron systems at zero temperature ($T=0$). An important manifestation of this order is the existence of spin waves.\(^1\) In conventional Heisenberg ferromagnets the damping of the spin wave is negligible, and the dispersion relation has the form\(^2\)

$$\Omega = D(m) k^2 + o(|k|^2), \quad (1)$$

with $o(\epsilon)$ denoting terms that are smaller than $\epsilon$. The coefficient $D$ depends on the dimensionless magnetization $m = (n_{\uparrow} - n_{\downarrow})/n$, with $n_{\uparrow}$ and $n_{\downarrow}$ the densities of spin-up and spin-down electrons, respectively, and $n = n_{\uparrow} + n_{\downarrow}$. In the conventional theory for clean "weak ferromagnets,"\(^2\) $D(m \rightarrow 0) = D_0 m$. $D_0 = v_F/k_F$, with $k_F$ the Fermi wave number and $v_F = k_F/\mu$ the Fermi velocity, is on the order of the inverse of the electron mass $\mu$, and Eq. (1) is valid for $|k| < k_F m \ll k_F$. We will show below that these results do not correctly describe the small-$m$ behavior of metallic ferromagnets.

A crucial assumption in the derivation of Eq. (1) is that the interactions between spin fluctuations are short ranged. This assumption is of doubtful validity in the context of itinerant ferromagnets, since in metals at $T=0$ there exist soft modes that can couple to the spin fluctuations and lead to an effective long-ranged interaction. Indeed, recent work on the $T=0$ FM phase transition in both disordered\(^3\) and clean\(^4\) itinerant electron systems has shown that in spatial dimensions $d=2,3$ the asymptotic critical behavior is largely determined by the coupling of noncritical soft modes to the critical spin fluctuations. In disordered systems, these soft modes are the same "diffusons" that cause the so-called weak-localization effects.\(^5\) In clean systems, they are the usual particle-hole excitations that lead to the well-known nonanalyticities in Fermi liquids\(^6\) that have recently been shown to be the clean analogs of the weak-localization effects.\(^7\) These noncritical soft modes cause the critical spin fluctuations to interact via dimensionality-dependent long-range effective forces. In the paramagnetic phase, the same physics is known to lead to a nonanalyticity in the wave-number-dependent spin susceptibility of the form

$$\chi_s(k) = \text{const} + |k|^\xi, \quad (2)$$

with $\xi = d-2$ (disordered) and $\xi = d-1$ (clean), respectively.\(^8\)

In this paper we consider the FM phase, and show that the long-ranged spin interactions that are mediated by the diffusons, or their clean counterparts, render invalid the standard results for the magnon dispersion. We find that a nonzero magnetization cuts off the long-ranged interaction at a scale $l_m^{-1} m^{-1/2}$ (disordered), which transforms the singular dependence on the wave number into one on the magnetization. The magnon dispersion is then given by Eq. (1), but with a nonanalytic $m$ dependence of $D$. For disordered electronic systems, we find

$$D(m \rightarrow 0) = c_d m [m^{-(4-d)/2} + O(1)] \quad (2 < d < 4), \quad (3a)$$

and $D(m \rightarrow 0) \propto m$ for $d>4$. For clean systems,
\[ D(m=0) = \tilde{c}_d m [m^{-(3-d)} + O(1)] \quad (1 < d < 3), \]
\[ D(m=0) = \tilde{c}_d m [\ln(1/m) + O(1)] \quad (d = 3), \]
and \[ D(m=0) \sim m \text{ for } d > 3. \] In these equations, \( c_d \) and \( \tilde{c}_d \) are positive constants.

In the remainder of this paper we derive and further discuss these results. For simplicity, we consider a \( d \)-dimensional continuum model of interacting clean or disordered electrons,\(^9\) and pay particular attention to the particle-hole spin-triplet contribution to the electron-electron interaction term in the action, whose (repetitive) coupling constant explicitly, and denoting the spin density by \( n_s \), the action reads

\[ S = S_0 + S'_{\text{int}} = S_0 + \frac{\Gamma}{2} \int dx \mathbf{n}_s(x) \cdot \mathbf{n}_s(x), \quad (4) \]

where \( S_0 \) contains all contributions to the action other than \( S'_{\text{int}} \). In particular, it contains the particle-hole spin-singlet and particle-hole spin-triplet interactions, as well as the coupling to the disorder. \( f dx = dx f \int dx f dx \) and we use a \((d+1)\)-vector notation \( x = (x, \tau) \), with \( x \) a vector in real space, and \( \tau \) the imaginary time. We perform a Hubbard-Stratonovich decoupling of \( S'_{\text{int}} \) by introducing a classical vector field \( \mathbf{M}(x) \) with components \( M_i \) \((i = 1, 2, 3)\) that couples to \( \mathbf{n}_s(x) \) and whose average is proportional to the magnetization, and we integrate out all fermionic degrees of freedom.\(^10\) In this way we obtain the partition function in the form

\[ Z = e^{-\mathcal{F}_0/\mathcal{T}} \int D[\mathbf{M}] \exp[-\Phi(\mathbf{M})]. \quad (5a) \]

Here \( \mathcal{F}_0 \) is the part of the free energy that does not depend on the magnetization, and \( \Phi \) is a Landau-Ginzburg-Wilson (LGW) functional,

\[ \Phi(\mathbf{M}) = \frac{\Gamma}{2} \int dx \mathbf{M}(x) \cdot \mathbf{M}(x) - \ln \left\{ \exp \left[ -\Gamma \int dx \mathbf{M}(x) \cdot \mathbf{n}_s(x) \right] \right\} \quad \left( \begin{array}{c} n \end{array} \right)_S, \quad (5b) \]

where \( \left\langle \ldots \right\rangle_S \) denotes an average taken with respect to the reference action \( S_0 \).

Next, we expand in fluctuations about the ordered state. In order to ensure that the \( O(3) \) symmetry is still manifest in the ordered state, we write\(^11\)

\[ \mathbf{M}(x) = \rho(x) \mathbf{\phi}(x), \quad (6a) \]

with \( \rho(x) \) the amplitude of \( \mathbf{M}(x) \) and \( \mathbf{\phi}(x) \) a unit vector,

\[ \mathbf{\phi}^2(x) = 1. \quad (6b) \]

Further, we take the system to be ordered in the 3 direction and parametrize \( \mathbf{\phi} \) and \( \rho \) by

\[ \mathbf{\phi} = (\rho, \mathbf{\sigma}), \quad (7a) \]

with \( \mathbf{\sigma} = (\sigma_1, \sigma_2), \sigma^2 = 1 - \sigma^2, \) and

\[ \rho(x) = m + \delta \rho(x), \quad (7b) \]

with \( m = \langle \rho(x) \rangle \) proportional to the magnetization. According to Goldstone’s theorem, the transverse fluctuations \( \mathbf{\sigma}(x) \) are soft, or of long range. \( \Phi(\mathbf{M}) \) can then be expanded in the fluctuations \( \delta \rho \) and \( \mathbf{\sigma} \) as

\[ \Phi(\mathbf{M}) = \Phi(m \mathbf{\phi}_1) + \delta \mathbf{\Phi}(\mathbf{M}), \quad (8a) \]

with \( \mathbf{\phi}_1 \) a unit vector in 3 direction, and

\[ \delta \mathbf{\Phi}(\mathbf{M}) = \frac{\Gamma}{2} \int dx \left[ \rho^2(x) - m^2 \right] - \ln \left( \left| \mathbf{\sigma}_0 \right| \right) \quad (8b) \]

with \( \mathbf{\sigma}_0 = \mathbf{\sigma}_0(m) = \left\langle \mathbf{\sigma}_1 \right\rangle \). \( \mathbf{\sigma}_0 \) is the transverse part of the spin susceptibility in the reference ensemble with action \( S_0 \).

The correlation functions in Eq. (8b) that one obtains by expanding the exponential determine the coefficients in the LGW functional. They are correlation functions of a reference ensemble whose action is given by Eq. (8c), which describes the reference ensemble \( S_0 \) in an external magnetic field given by \( -\Gamma \mathbf{m} \). Here we are interested in the transverse spin susceptibility, which can be obtained from the imaginary frequency correlation function,

\[ \chi_i(k, \Omega_m) = \left\langle \mathbf{\pi}_i(k, \Omega_m) \right\rangle, \quad (9) \]

with \( \Omega_m \) a bosonic Matsubara frequency. Let us first consider the terms in Eq. (8b) that are bilinear in \( \mathbf{\pi} \), which we denote by \( \delta \mathbf{\Phi}_{\text{eff}} \). We further integrate out \( \rho(x) \) in saddle-point approximation, i.e., we neglect the fluctuations \( \delta \rho \). We will justify this procedure later, and also discuss terms of higher order in \( \mathbf{\pi} \). Taylor expanding Eq. (8b) gives

\[ \delta \mathbf{\Phi}_{\text{eff}} = \frac{\Gamma \mathbf{m}}{2} \int dx dy \sum_{i,j=1}^2 \pi_i(x) K_{ij}(x,y) \pi_j(y), \quad (10a) \]

with

\[ K_{ij}(x,y) = -\Gamma(m(n_{s,i}(x)n_{s,j}(y))_{S_0} - \delta(x-y)\delta_{ij}(n_{s,i}(x))_{S_0}). \quad (10b) \]

In this approximation,

\[ \chi_i(k, \Omega_m) = \frac{K_{i1}(k, \Omega_m)}{\Gamma m} \left[ K_{11}(k, \Omega_m) - K_{12}(k, \Omega_m) \right]^{-1}, \quad (10c) \]

i.e., the kernel \( K_{ij} \) determines the spin-wave spectrum. Note the Goldstone mode structure of this result: Taking the Fourier transform of Eq. (10b), we have \( (i = 1, 2) \)

\[ K_{ij}(k, \Omega_m) = -\Gamma m \chi_j^{(\text{eff})}(k, \Omega_m) - \delta_i(n_{s,3}(k, \Omega_m)_{S_0}). \quad (10d) \]

\[ \chi_j^{(\text{eff})}(k, \Omega_m) = \langle n_{s,i}(k, \Omega_m) n_{s,j}(-k - \Omega_m, j)_{S_0} \rangle \quad (10e) \]

is the transverse part of the spin susceptibility in the reference ensemble with action \( S_0 \). A Ward identity that relates the reference system’s magnetization to its static, homoge-
neous transverse spin susceptibility ensures that \( K_{ij}(0,0) = 0 \), i.e., transverse excitations are soft.

Expanding in powers of the frequency, one finds

\[
\chi_{ij}^{(\text{ref})}(k, \Omega_m) = \delta_{ij}\chi_{ii}^{(\text{ref})}(k) - \frac{i c}{m} [\Omega_m[\delta_{ij}\delta_{2j} + \delta_{ij}\delta_{2j}]],
\]

(11)

with \( c \approx \mu/k_F \) a constant. In the absence of weak-localization effects, one would have \( \chi_{ij}^{(\text{ref})}(k) = \chi_i - c k^2 \), with \( \chi_i \) another constant independent of \( m \). However, due to weak-localization effects in disordered systems, and their analogs in clean ones, \( \chi_{ij}^{(\text{ref})} \) has a singularity at \( k = m = 0 \). For \( m = 0 \) this has been shown using perturbation theory as well as more general renormalization-group (RG) arguments.7,12 It has also been shown that weak-localization effects (their clean counterparts) can be related to corrections to scaling near a disordered (clean) Fermi-liquid fixed point.7 Let us generalize those considerations to include the effects of a small magnetic field. The scale dimension of \( \chi_i \) is zero, so in terms of a scaling function \( F \) we have

\[
\chi_i^{(\text{ref})}(k, l^{-1}, u) = F(b k, k^{-1} u, b^2 u),
\]

(12a)

with \( l^{-1} \) the magnetic length. The latter is determined perturbatively as follows. A nonzero magnetization leads to a mass or frequency cutoff in the soft modes that is given by a cyclotron frequency \( \Omega \). Scaling the wave number with \( l^{-1} \) thus leads to \( l^{-1} = \hbar \) in clean systems, and \( l^{-1} = \hbar \) in disordered ones. \( u \) represents the leading irrelevant variable near the fixed point. Its scale dimension, [\( u \)] is equal to \([u] = -(d-2) \) in disordered systems, and \([u] = -(d-1) \) in clean ones.7,12 \( b \) is a RG length rescaling factor. In the paramagnetic phase, \( l^{-1} = 0 \), and Eq. (12a), with \( b = |k|^{-1} \), yields

\[
\chi_i^{(\text{ref})}(k,0,0) = \chi_i - c |k|^{-2} u,
\]

(12b)

with \( c - u \). This is the nonanalyticity that leads to long-range interactions between the spin fluctuations near the FM phase transition. For \( l^{-1} = 0 \), \( \chi_i^{(\text{ref})} \) is an analytic function of \( k \), and Eqs. (12a) and (12b) give

\[
\chi_i^{(\text{ref})}(k, l^{-1}, u) = \chi_i - c'(m) |k|^2,\]

(12c)

with

\[
c'(m) - m^{-2+\alpha/2} (\text{disordered}) \quad \text{and} \quad m^{-2+\alpha} (\text{clean}).
\]

(12d)

From this, with Eqs. (10) and (11), we immediately obtain our main results, Eqs. (3) [except for the nature of the leading correction terms in Eq. (1), which we will discuss below]. Note that for disordered systems the dimensionless parameter characterizing ‘small’ wave numbers is \( k^2/l^2 \approx 1 \), with \( l \) the diffusive or transport mean free path. The prefactors in Eqs. (3) are hard to estimate, since they depend on the value \( \Gamma_{ij}^{\text{ref}} \) of \( \Gamma_i \) in the fully renormalized reference ensemble.12 For instance, for the clean case in \( d = 3 \) one finds, using the result of Ref. 8, \( \xi = (32 \pi/27)(N_0 \Gamma_{ij}^{\text{ref}})^{1/2} \mu \).

Finally, we note that, at the level of the above scaling argument, the analyticity of \( \chi^{(\text{ref})}(m) \) in powers of \( k^2 \) for \( l^{-1} = 0 \) is an assumption. We have checked this explicitly in perturbation theory, verifying Eqs. (12c) and (12d) using both a \( Q \)-matrix field theory and standard many-body perturbation theory, and will further discuss it from a RG point of view next.

We now show that the corrections to Eqs. (10) that result from taking into account the \( \delta \rho \) fluctuations, as well as terms of higher than Gaussian order in \( \delta \), cannot change the above results. This is most easily done in the framework of the RG. We assign scale dimensions \(-1 \) and \(- \) to lengths and times, respectively, with \( \chi \) the dynamical critical exponent, and scale dimensions \([ \pi(x) ] = (d+z+2 \eta')/2 \) and \([ \rho(x) ] = (d+z+\eta')/2 \) to the fields. Then Eq. (10a) tells us that there is a Gaussian fixed point with exponents

\[
\eta = 2, \quad \eta' = 0, \quad z = 2
\]

(13)

that describes a FM state. To check for relevant operators that would destroy this fixed point, we systematically expand Eq. (8b) in powers of \( \delta \rho \) and \( \delta \), and integrate out \( \delta \rho \) perturbatively to obtain an effective action in terms of \( \delta \). There are several terms that dimensionally could lead to a \( |k|^2 \) correction in the clean case and \( |k|^2 \) in the disordered case in Eq. (12c), rather than a \( k^2 \) with a coefficient that is nonanalytic in \( m \). In RG language, this would be a relevant operator with respect to our Gaussian fixed point. However, it turns out that there are Ward identities that ensure, order by order in the expansion in fluctuations of the order parameter, that all terms of \( O(m^2) \), whether or not they couple to \( \delta \rho \), are multiplied by at least a gradient squared.13 We have also checked this by means of explicit perturbative calculations for selected vertices. Similar arguments show that the second term on the right-hand side of Eq. (11) is the leading frequency dependence. As a result, the Gaussian fixed point identified above is stable by power counting. The leading nonanalytic correction to the \( \Omega - k^2 \) dispersion arises from renormalizations of the Gaussian action due to terms of \( O(m^2) \). The resulting operators potentially have scale dimensions \( 2 - d \) (disordered) and \( d - 1 \) (clean), respectively. This reflects the largest possible corrections due to potentially soft modes; explicit calculations would be necessary to ascertain whether or not terms of this order actually exist.13 We conclude that the Eqs. (12) are asymptotically exact. The exact magnon dispersion relation is thus given by Eq. (1), and the largest possible corrections are of \( O(k^{2+\eta}) \), with \( \xi \) from Eq. (2).

At \( T \approx 0 \), temperature effects will compete with the magnetization in protecting the weak-localization singularities, and their clean counterparts, in the spin-triplet channel. Therefore, for \( m < T \ll T_F \) in appropriate units, the \( m \) in the brackets in Eqs. (3) will be replaced by \( T \), leading to a nonanalytic \( T \) dependence of the coefficient in the dispersion relation. Other consequences of a nonzero temperature are more subtle because of the occurrence of multiple temperature scales1 and will be investigated separately in the future.

We conclude by discussing ways to experimentally verify our predictions. To our knowledge, no systematic studies of the prefactor of the \( k^2 \) term in the dispersion relation have been performed. Such a study should be easier to do for disordered systems than for clean ones, since (1) the pre-
dicted effect is much larger in the disordered case, and (2) in the disordered case it will be easier to find a material near the FM quantum phase transition (e.g., by fine tuning the concentration of the magnetic ingredient in an alloy).

The most convincing experimental evidence would be an explicit measurement of the $m$ dependence of the dispersion relation. This would require measuring different samples with different values of the magnetization $m$, and extracting the $m$ dependence from the measured inverse magnon masses $D(m)$. In a three-dimensional disordered system, $D(m)$ for small $m$ should scale like $m^{1/2}$ (instead of $m$ according to RPA-like theories). Another possibility is to measure a single sample with a small magnetization, and to identify a quantitative difference of the measured magnon mass from that predicted by RPA-like theories. For instance, it has been reported that in Fe and Ni the prefactor is larger than expected by a factor of 2 to 3.\textsuperscript{15} Since the magnetization in these materials is not small, it is unlikely that this discrepancy is related to the predicted effect. However, similar experiments on materials with a small magnetization should suffice to corroborate or refute the present theory.

This work was initiated at the Aspen Center for Physics, and supported by the NSF under Grants No. DMR–95–10185, No. DMR–96–32978, and No. DMR–97–07701 and by the DFG under Grant No. Vo659/1–1.

---

\textsuperscript{1}See, e.g., D. Forster, \textit{Hydrodynamic Fluctuations, Broken Symmetry, and Correlation Functions} (Benjamin, Reading, MA, 1975).


\textsuperscript{5}By “weak localization” we mean the nonanalytic behavior of electronic correlation functions in the limit of zero momentum and/or frequency that is induced by quenched disorder, or by a combination of interactions and disorder. For a review, see, e.g., P. A. Lee and T. V. Ramakrishnan, Rev. Mod. Phys. \textbf{57}, 287 (1985).


\textsuperscript{9}The universal long-wavelength, small-frequency effects we are interested in are independent of the microscopic details of the model used.


\textsuperscript{12}Renormalization effects generate a nonvanishing spin-triplet interaction amplitude $\Gamma^{\text{ref}}_{\text{ss}}$ in the reference ensemble, even though $\Gamma_{\text{ss}}$=0 in the bare reference action. The reference ensemble is thus a fully interacting electron system. The only restriction is that $\Gamma^{\text{ref}}_{\text{ss}}$ must not be large enough to trigger a phase transition in the reference ensemble, lest the separation of scales that is crucial for our approach break down.

\textsuperscript{13}It is important that even the \textit{longitudinal} spin susceptibility of electrons in a magnetic field shows no nonanalytic wave-number dependence of the type found in zero magnetic field, even though the soft-mode structure would in principle allow for one; see D. Belitz and T. R. Kirkpatrick, Rev. Mod. Phys. \textbf{66}, 261 (1994), Sec. V A 2 for the disordered case, and T. Vojta (unpublished) for the clean one. The cancellations governed by these Ward identities reflect the fact that the vertices of the exact effective $\pi$-field theory are still transverse correlation functions in some (complicated) reference system. Rotational invariance of the spins in this reference ensemble then ensures the softness of the transverse modes in the same way as it is ensured in the simple reference system $S_0$ that corresponds to our saddle-point approximation for the $\rho$ fluctuations.

\textsuperscript{14}For a review, see D. Belitz and T. R. Kirkpatrick, Rev. Mod. Phys. \textbf{66}, 261 (1994).

\textsuperscript{15}T. Moriya, \textit{Spin Fluctuations in Itinerant Electron Magnetism} (Ref. 2), p. 206 and Table 7.1.
First Order Transitions and Multicritical Points in Weak Itinerant Ferromagnets

D. Belitz and T.R. Kirkpatrick

Institute for Theoretical Physics, University of California, Santa Barbara, CA 93106

Thomas Vojta
Institut für Physik, TU Chemnitz, D-09107 Chemnitz, FRG

(April 7, 1999)

It is shown that the phase transition in low-T clean itinerant ferromagnets is generically of first order, due to correlation effects that lead to a nonanalytic term in the free energy. A tricritical point separates the line of first order transitions from Heisenberg critical behavior at higher temperatures. Sufficiently strong quenched disorder suppresses the first order transition via the appearance of a critical endpoint. A semi-quantitative discussion is given in terms of recent experiments on MnSi, and predictions for other experiments are made.

The thermal paramagnet-to-ferromagnet transition at the Curie temperature \( T_C \) is usually regarded as a prime example of a second order phase transition. For materials with high \( T_C \) this is well established both experimentally and theoretically. Recently there has been a considerable interest in the corresponding quantum phase transition of itinerant electrons at zero temperature (\( T = 0 \)), and in the related finite \( T \) properties of weak itinerant ferromagnets, i.e., systems with a very low \( T_C \). Experimentally, the transition in the weak ferromagnet MnSi has been tuned to different \( T_C \) by applying hydrostatic pressure [1]. Interestingly, the transition at low \( T \) was found to be of first order; while at higher transition temperatures it is of second order [2]. The tricritical temperature that separates the two types of transitions was found to roughly coincide with the location of a maximum in the magnetic susceptibility in the paramagnetic phase. Theoretically, it has been shown [3,4] that in a \( T = 0 \) itinerant electron system, soft modes that are unrelated to the critical order parameter (OP) or magnetization fluctuations couple to the latter. This leads to an effective long-range interaction between the OP fluctuations. In disordered systems, the additional soft modes are the same 'diffusons' that cause the so-called weak-localization effects in paramagnetic metals [5]. In clean systems there are analogous, albeit weaker, effects that manifest themselves as corrections to Fermi liquid theory [6]. A Gaussian theory is sufficient to obtain the exact quantum critical behavior in the most interesting dimension, \( d = 3 \), for clean as well as for disordered systems (apart from logarithmic corrections in the clean case) [3,4].

In this Letter we show that at sufficiently low temperatures the phase transition in itinerant ferromagnets is generically of first order. This surprising result is shown to be rooted in fundamental and universal many-body physics underlying the transition, viz. long-wavelength correlation effects, and hence to be independent of the band structure. This suggests that the behavior observed in MnSi is generic, and should also be present in other weak itinerant ferromagnets. We also make detailed predictions about how quenched disorder suppresses the first order transition, which allows for decisive experimental checks of our theory.

Let us start by deriving the functional form of the free energy of a bulk itinerant ferromagnet at finite \( T \), and in the presence of quenched disorder that we parametrize by \( G = 1/\epsilon_F \tau \), with \( \epsilon_F \) the Fermi energy, and \( \tau \) the elastic mean-free time. The general Landau expansion of the free energy \( F \) as a function of the magnetic moment \( m \) in an approximation that neglects OP fluctuations is

\[
F = t m^2 + u_4 m^4 + u_6 m^6 + \ldots . \tag{1a}
\]

The coefficients \( t, u_4, u_6 \), etc. in this expansion can have nontrivial properties and contain important physics. A derivation from a microscopic theory shows that they are given as frequency-momentum integrals over correlation functions in a 'reference system' that depends on the nature of the underlying microscopic model [7]. If the critical magnetization fluctuations are the only soft modes in the system, then they are simply numbers. However, if in the process of deriving the Landau functional some other soft modes have been integrated out, then the coefficients will in general not exist, since they are represented as diverging integrals over the soft modes. In Refs. [3] and [4] it was shown that in an itinerant electron system at \( T = 0 \) there are indeed such soft modes. In the disordered case, these are the 'diffusons' mentioned above, with a dispersion relation \( \omega \sim k^2 \), and they lead to coefficients whose divergent parts have the form

\[
u_{2m} \propto \int_0^\Lambda dk k^2 \int d\omega \frac{1}{(\omega + k^2)^{2m}} . \tag{1b}
\]

Here \( \Lambda \) is a momentum cutoff, and all prefactors in the integrals have been omitted. In the clean case, the relevant soft modes are particle-hole excitations in the spin-triplet channel with a ballistic dispersion relation, \( \omega \sim k \). The resulting integrals are still divergent, although not as strongly as in the disordered case. It was shown in
Ref. [3], [4] that these divergent terms in the Landau expansion can be understood as an illegal expansion of a nonanalytic term in the free energy of the form
\[ f(m) = m^4 \int_0^\Lambda dk k^2 \int_0^\infty d\omega \frac{(-1)^4}{[(\omega + k^2)^2 + m^2]^2}. \]  
Equation (2) yields \( f(m) \propto m^{5/2} \) and \( f(m) \propto m^4 \ln m \) in the disordered and clean cases, respectively. In either case the resulting singularity is protected by the magnetization, which gives the soft modes a mass. The leading effect of \( T \neq 0 \) is adequately represented by replacing \( \omega \rightarrow \omega + T \). In addition, in the presence of disorder the ballistic modes in the clean case obtain a mass proportional to \( 1/T \), so the appropriate generalization of Eq. (2) for the clean case \((x = 1)\) to finite temperature and disorder is obtained by replacing \( \omega \rightarrow \omega + T + 1/T \). Doing the integrals, and adding the usual terms of order \( m^2 \) and \( m^4 \), we obtain a free energy of the form
\[ F = tm^2 + G(N_p \Gamma_1) m^4 \left[ m^2 + (\alpha T)^2 \right]^{-3/4} + v m^4 \ln \left( m^2 + (T + \beta G)^2 \right) + u m^4 + O(m^6), \]  
where \( \Gamma_1 \) is an effective spin-triplet interaction amplitude [3] made dimensionless by means of a density of states at the Fermi level, \( N_p \). If we measure \( F, m, \) and \( T \) in terms of a microscopic energy, e.g. \( \varepsilon \), then \( t, v, \) and \( u \) are all dimensionless. \( v \) is quadratic in \( \Gamma_1 [4], t = 1 - N_p \) \( U \) is the dimensionless distance from the critical point. It depends on the physical spin-triplet interaction amplitude \( U \), with \( N_p U \approx 1 \) in a ferromagnetic or nearly ferromagnetic system, while \( \Gamma_1 \) above is an effective interaction amplitude with \( N_p \Gamma_1 < 1 \). \( \Gamma_1 \) is expected to be relatively larger in strongly correlated systems. Finally, \( \alpha \) and \( \beta \) are parameters that measure the relative strengths of the temperature and the disorder dependence, respectively, in the two nonanalytic terms. They are numbers of order unity, and like \( u \) and \( v \) they are non-universal. Equation (3) provides a functional form of the free energy that correctly describes the leading nonanalytic \( m \)-dependence for both clean and disordered systems, as well as the leading temperature cutoff for either term and the leading disorder cutoff for the clean nonanalyticity.

The sign of \( v \) merits some attention. Perturbation theory to second order in \( \Gamma_1 \) yields \( v > 0 \) [4,8]. Further, \( v > 0 \) indicates a decrease of the effective Stoner coupling constant \( I \) due to correlation effects: \( I \) is a homogeneous spin susceptibility, \( v > 0 \) means that this susceptibility increases as the wavenumber increases from zero [8], and correlation effects decrease with increasing wavenumber. It is well known that correlation effects in general decrease \( I \) [9], and \( v > 0 \) is consistent with that. Ref. [4] has given some possible mechanisms for \( v \) to be negative at least in some materials, and showed that in this case the ferromagnetic transition is always of second order. However, the generic case is \( v > 0 \), which we will now discuss.

We first consider the case \( T = 0 \). The transition in the clean system, \( G = 0 \), is then of first order, since \( m^4 \ln m < 0 \) for small \( m \). Upon disordering the system, \( G > 0 \), the negative term is no longer the leading one at \( t = 0 \). For small values of \( G \), the transition remains first order. However, for \( G > G_c^e \) the first order transition occurs only at \( t < 0 \), and it is pre-empted by a second order transition. Since the negative term is only the third term in an \( m \)-expansion of \( F \), the multi-critical point where the nature of the transition changes is a critical endpoint (CEP) [10]. The phase diagram in the \( G-t \) plane is shown in Fig. 1. For \( G < G_c \), the second order transition at \( t = 0 \) is followed by a second transition, the second one being of first order, to a state with a larger magnetization. The line of first order transitions ends in a critical point (CP) at a disorder value \( G_c \), where the two minima in the free energy merge.

Before we consider \( T > 0 \), let us discuss this result and the validity of our conclusions. To facilitate an analytic discussion, we put \( \beta = 0 \). We then have \( F = tm^2 + G(N_p \Gamma_1) m^3/2 + 2vm^4 \ln m + um^4 \). At \( G = 0 \) there is a first order transition at \( t = v \exp[-(1 + u/v)] \), and the magnetization at the transition has a value \( m = \exp[-(1 + u/v)/2] \). Notice that the nonanalytic term is the leading one in \( F \) after the \( m^2 \) term, and that we know the functional form of \( F \) exactly up to \( O(m^4) \). As long as \( u/v >> 1 \), \( m \) is exponentially small at the transition. For small \( v \), our Landau expansion is therefore controlled in the sense that terms of \( O(m^6) \) and higher would have to have exponentially large coefficients in order to change our results. For \( G > G_c \) \( (4v/3N_p \Gamma_1) \exp[-(1 + 3u/4v)] \), the first order transition is pre-empted by a second order one. At the CEP, the magnetic moment has the value \( m = \exp[-(2/3 + u/2v)] = e^{-1/6} m(G = 0) \). Allowing for \( \beta = O(1) \neq 0 \), and repeating the calculation numerically, leads only to minor quantitative changes of these results.
At $T > 0$, the free energy is an analytic function of $m$, but for small $T$ the coefficients in an $m$-expansion become very large. Our remarks about the validity of our truncated Landau expansion therefore still apply, i.e., at $0 < k_B T < \epsilon_F$, our theory contains the most important terms to every order in an expansion in powers of $m^2$. Let us first consider the clean system, $G = 0$. There is a tricritical point (TCP) at $T_{tc} = \exp(-u/2\nu)$, with a first order transition for $T < T_{tc}$, and a line of Heisenberg critical points for $T > T_{tc}$. To describe the (conventional) tricritical behavior in $d = 3$ our mean-field theory is sufficient (apart from logarithmic corrections) [11], for the critical behavior at $T > T_{tc}$ it is of course not.

For the suppression of the first order transition by disorder at $T > 0$ we find two different possibilities, depending on the value of the parameter $\alpha$. For small $\alpha$ ($\alpha \lesssim 1.5$ with our choice of the remaining parameters, Fig. 2), the TCP is replaced by a CEP for $G$ larger than some $G_{tc} < G_{ce}$. At $G = G_{ce}$, the CEP reaches $T = 0$, and for larger values of $G$ the transition is of second order for all $T$. At small $T$, it is followed by a first order transition. The line of first order transitions ends in a critical point, and disappears only for $G = G_c$. For larger values of $\alpha$ (Fig. 3), the TCP persists for a range of disorder larger than $G_{ce}$. The first order transition first gets preempted in a temperature window between two CEPs. At $G = G_{ce}$, the lower CEP reaches $T = 0$, while the TCP at higher temperature survives. With further increasing disorder, two CPs appear in the ordered phase, and the remaining CEP gets replaced by a TCP. Finally, the two TCPs merge, and the remaining CP reaches $T = 0$, eliminating the last temperature regions with first order transitions. Notice that the interesting features of these phase diagrams do not depend on the logarithm in Eq. (3); similar features are obtained in standard phenomenological Landau expansions with a negative coefficient of the third term [12]. We stress again, however, that in our case the expansion is controlled, and that we have a definite physical mechanism for the appearance of a negative term, in contrast to purely phenomenological theories.

We now turn to a discussion of the available experimental information on this subject. MnSi has a low $T_{ce}$ ($\approx 30$ K) under ambient pressure, and $T_c$ can be driven to zero by a hydrostatic pressure $p_c \approx 15$ kbar. $k_B T / \epsilon_F << 1$ always, and $T$ is low enough to suppress phase breaking processes, so the quantum critical behavior is easily accessible experimentally. This system has been studied in detail by Pfleiderer et al. [1] These authors found from susceptibility measurements that the transition turns first order at a $T_c$ of about 12 K. The line of second order transitions was found to scale with pressure like $T_c \propto (p - p_c)^{3/4}$, while in the first order regime the transition temperature varies like $T_c \propto (p - p_c)^{1/2}$. The scaling of $T_c$ with pressure was explained by a scaling analysis based on the self-consistently renormalized (SCR) theory of Moriya and Kawabata [13], assuming a dynamical exponent $z = 3$. The first order transition at low $T$ was attributed in Ref. [1] to a sharp structure in the density of states at the Fermi level.

Let us look at the experiment in the light of the above discussion. In Ref. [4] it was shown that the quantum phase transition in $d = 3$ is indeed correctly described by SCR theory, apart from logarithmic corrections that would be very difficult to detect experimentally, and that the dynamical critical exponent in $d = 3$ is $z = 3$. The analysis of Ref. [1] was therefore adequate, and in particular the quantum-to-classical crossover exponent $\phi$, which determines the behavior of the critical temperature as a function of $t$ through the relation $T_c \propto t^\phi$, has a value $\phi = 3/4$. If one makes the plausible assumption that $t$ depends linearly on the hydrostatic pressure, at least for small $t$, then this is in agreement with both the experimental finding and the analysis in Ref. [1]. As for the pressure dependence of $T_c$, one of the temperature scales in the problem is the Fermi liquid temperature scale [4], which arises from a quadratic $T$-dependence of $t$. Since the first order transition is determined by the condition $t(T_c) = \text{const.}$, we immediately get $T_c \propto \sqrt{p - p_c}$, where we again assume a linear relation between $p$ and $t$.

We finally discuss the observation [1] that the tricritical temperature roughly coincides with a minimum of the inverse magnetic susceptibility $\chi^{-1}$ in the paramagnetic phase. In $d$ dimensions, the leading $T$-dependence of the paramagnetic susceptibility is of the form [8]

$$\chi/T = 2N_F/1 + 2v_d T^2 T^{-3} - u_d T^2 \, , \quad (4)$$
In $d = 3$, the nonanalyticity is of the form $T^2 \ln T$. A calculation of $\hat{v}_3$ to second order in $\Gamma_2$ revealed [8] that to that order, $\hat{v}_3 = 0$, in agreement with prior results from Fermi liquid theory [15]. Ref. [8] also discussed that there are reasons to believe that the exact value of $\hat{v}_3 = 0$ may be nonzero. If we assume that this is the case, then we obtain a minimum in $\chi^{-1}$ at a temperature $T_{\text{min}} = \exp(-\hat{u}_3/2\hat{v}_3 - 1/2)$. Since the nonanalyticities in $F$ and $\chi$ are manifestations of the same singularity, one expects $\hat{u}_3 \approx u$ and $\hat{v}_3 \approx v$, so that $T_{\text{min}} \approx T_C$. While this provides a possible explanation for the observation, we stress the speculative nature of the above considerations due to the theoretical uncertainty about a nonanalytic $T$ dependence of $\chi$ in $d = 3$.

Our theory thus provides us with a complete explanation for the nature of the transitions observed in MnSi, and in particular for the existence of a first order transition at low $T$, which in Ref. [1] was attributed to a band structure feature characteristic of MnSi. While this feature may well be sufficient to make the transition in MnSi of first order, the present theory leads to the surprising prediction that the first order transition is generic, and thus should be present in other weak itinerant ferromagnets as well. Our theory further predicts in detail how the first order transition will be suppressed by quenched disorder. Observations of such a suppression, or lack thereof, would be very interesting for corroborating or refuting the theory. Semi-quantitatively, the theory predicts that the $T$ region that shows a first order transition will be largest for strongly correlated systems. Conversely, since the dependence of the tricritical temperature on the system parameters is exponential, in some, or even many, systems the first order transition may take place only at very low temperatures. This may explain why in ZrZn$_2$ no first order transition has been observed [1], although the experiment does not seem to rule out a weakly first order transition [14].

We gratefully acknowledge helpful conversations with G. Lonzarich and C. Pfeifer. This work was supported in part by the NSF under grant Nos. PHY94-07194, DMR–98–79597, and DMR–96–32978, and by the DFG under grant No. SFB 393/C2.
Influence of rare regions on magnetic quantum phase transitions

Rajesh Narayanan, Thomas Vojta, D. Belitz, and T.R. Kirkpatrick
1 Department of Physics and Materials Science Institute, University of Oregon, Eugene, OR 97403
2 Institut für Physik, TU Chemnitz, D-09107 Chemnitz, FRG
3 Institute for Physical Science and Technology, and Department of Physics, University of Maryland, College Park, MD 20742
(March 10, 1999)

The effects of quenched disorder on the critical properties of itinerant quantum magnets are considered. Particular attention is paid to locally ordered rare regions that are formed in the presence of quenched disorder even when the bulk system is still in the nonmagnetic phase. It is shown that these local moments or instantons destroy the previously found critical fixed point in the case of antiferromagnets. In the case of itinerant ferromagnets, the critical behavior is unaffected by the rare regions due to an effective long-range interaction between the order parameter fluctuations.

Rare regions and their influence on observables is an important, if intricate, aspect of systems with quenched disorder. An effect that has been known for a long time is the formation of a Griffiths region [1]. To explain this, let us consider a ferromagnet for definiteness. Disorder will decrease the critical temperature from its clean value, \( T_c^0 \), to a value \( T_c < T_c^0 \) in the disordered system. In the temperature region \( T_c < T < T_c^0 \) the system does not display global order, but one will find regions that are devoid of any impurities and hence show local magnetic order. The probability of finding such a 'rare region' in general decreases exponentially with its size. The resulting magnetization fluctuations have very slow dynamics. They are often called 'local moments' or 'instantons', and they lead to a nonanalytic free energy for all temperatures below \( T_c \), even though no long-range order develops until the temperature reaches \( T_c \). For generic classical systems this is a weak effect, the singularity being only an essential one. An important exception is the model studied by McCoy and Wu [2], which is a two-dimensional (2-d) Ising model with random bonds in one direction, but identical bonds in the second direction. The infinite correlation of the disorder in this model leads to much stronger effects, with the average magnetic susceptibility diverging in a finite-width temperature region above \( T_c \). The transition at \( T_c \) is nevertheless sharp. The divergence of the average susceptibility for \( T > T_c \) is caused by atypical fluctuations in the susceptibility distribution, and the averaged order parameter becomes nonzero only for \( T < T_c \). The temperature region \( T_c < T < T_c^0 \) is known as a Griffiths region. Little is known about the influence of rare regions on the critical behavior at \( T_c \), and in the conventional theory of the critical behavior of disordered magnets [3] the rare regions are neglected.

Recent work [4] on a random-\( T_c \) classical Ising model has suggested that the effects of the rare regions go beyond the formation of a Griffiths region, even in this simple model where the conventional theory [3] predicts standard power-law critical behavior. These authors showed that the conventional theory is unstable with respect to perturbations that break the replica symmetry. By approximately taking into account the rare regions, they found a new term in the action that actually induces such perturbations. In some systems replica symmetry breaking is believed to be associated with activated, i.e. non-power law, critical behavior. Although no final conclusion about the fate of the transition could be reached, Ref. [4] thus raised the possibility that the random-\( T_c \) classical Ising model shows activated critical behavior as a result of rare-region effects, as is believed to be the case for the random-field classical Ising model [5].

The problem of rare regions is even less well investigated for the case of quantum phase transitions, i.e. transitions that occur at \( T = 0 \) as a function of some non-thermal control parameter [6]. An important exception to this are certain 1-d systems. Fisher [7] has investigated quantum Ising spin chains in a transverse random field, which is closely related to the classical 2-d McCoy-Wu model (with time playing the role of the dimension along which the disorder is correlated). He found activated critical behavior due to rare regions, which has been confirmed by numerical simulations [8]. Recent simulations [9] suggest that this type of behavior may not be restricted to 1-d systems, raising the possibility that exotic critical behavior dominated by rare regions may be generic in quenched disordered quantum systems.

Apart from their relevance for disordered magnets and their critical properties, rare regions are believed to be a crucial ingredient for understanding other systems with quenched disorder. For instance, it has been proposed that a complete understanding of the properties of doped semiconductors, and of the metal-insulator transitions that are observed in such systems as a function of doping, requires the consideration of local moments [10–12].

In this Letter we study this important problem analytically for quantum phase transitions in \( d > 1 \). We concentrate on magnetic transitions, and contrast the cases of itinerant ferromagnets (FMs) and antiferromagnets (AFMs), respectively. We find that for the latter, the rare regions destroy the critical fixed point (FP) found...
in a previous study [13], and thus have a profound effect on the critical behavior. In contrast, for itinerant FMs we find that, for certain realizations of the disorder, the previously found critical behavior is stable with respect to rare regions, due to an effective long-range interaction between the spin fluctuations. In addition, we find that the ultimate effects of the rare regions depend on how the disorder is realized in a particular system. Therefore, no generally valid conclusions are possible, and the effects of rare regions must be studied carefully and separately for each system under consideration.

Let us first consider the case of itinerant quantum antiferromagnets. Our starting point is the same as in Ref. [13], namely Hertz’s action, which is a φ^4-theory for a p-component order parameter field \( \phi \) whose expectation value is proportional to the staggered magnetization. The action reads

\[
S = \int dx \, dy \, \Gamma(x, y) \phi(y) + u \int dx \, \big( \phi(x) \cdot \phi(x) \big)^2 .
\]  

Here \( x \equiv (x, \tau) \) comprises position \( x \) and imaginary time \( \tau \), and \( \int dx \equiv \int dx \int_0^1 d\tau \). We use units such that \( \hbar = k_B = 1 \). \( \Gamma(x, y) \) is the bare two-point vertex function, whose Fourier transform is

\[
\Gamma(q, \omega_n) = (t + q^2 + |\omega_n|)/2 .
\]

Here \( t \) denotes the distance from the critical point, \( q \) is the wavevector, \( \omega_n \) is a bosonic Matsubara frequency, and we measure both \( q \) and \( \omega_n \) in suitable units.

Disorder is introduced by making \( t \) a random function of position, \( t = t_0 + \delta t(x) \), where \( \delta t(x) \) obeys a Gaussian distribution with zero mean and variance \( \Delta \). The standard procedure is to integrate out the ‘random mass’ \( \delta t(x) \) by means of the replica trick [3], which produces a term of order \( \phi^4 \) with coupling constant \( \Delta \), in addition to the ordinary quantum fluctuation term in Eq. (1a) with coupling constant \( u \). The resulting theory does not easily allow for saddle-point solutions that are inhomogeneous in space, and to incorporate rare regions into it would be very difficult. We therefore follow a different procedure. In analogy to Ref. [4], we consider inhomogeneous saddle-point solutions of the theory for a fixed realization of the disorder. The inhomogeneity comes about since \( \delta t(x) \) has ‘troughs’ that make \( t < 0 \) in some region in space, even though \( t_0 > 0 \). Troughs that are sufficiently deep and wide support locally nonzero saddle-point solutions. These regions we will refer to as ‘islands’. Outside of the islands, the solution is exponentially small. This means that for a system with \( N \) islands, and in the case of an Ising model (\( p = 1 \)), there will be \( 2^N \) almost degenerate saddle-point solutions that can be constructed by considering all possible distributions of the sign of the order parameter on the islands. For \( p > 1 \) there is a whole manifold of almost degenerate saddle points.

Let \( \Phi(x) \) be one of these saddle-point solutions, and let us consider fluctuations about it, \( \phi(x) = \Phi(x) + \varphi(x) \) [14]. The different saddle points are far apart in configuration space and separated by large energy barriers. If we restrict ourselves to small fluctuations about each saddle point, we can therefore write the partition function approximately as the sum of all contributions obtained from the vicinity of each saddle point,

\[
Z \approx \int D[\Phi(x)] P[\Phi(x)] \int D[\varphi(x)] e^{-S[\Phi(x) + \varphi(x)]}. \tag{2}
\]

where \( P[\Phi(x)] \) denotes the distribution of saddle points, and \( \int_\varnothing \) indicates an integration over small fluctuations only. It is clear that this approximation takes into account effects that one would call ‘non-perturbative’ in a standard treatment of quenched disorder. Also, consistent with our approximations, it can be shown that the inhomogeneous saddle-point solutions lead to a lower free energy than the homogeneous saddle point \( \Phi(x) \equiv 0 \).

Performing the integration over the \( \Phi \) in Eq. (2) explicitly is very difficult, and the result will in general depend on the properties of the distribution function \( P \), which in turn depend on the details of the microscopic disorder. However, a very basic observation simplifies our task: The \( \Phi(x) \) represent static randomness, and the average over this randomness is performed for the partition function. That is, we are dealing with static, annealed disorder. This is physically sensible, as the local moments are a self-generated part of the system and therefore in equilibrium with the rest of the degrees of freedom [14].

In addition, of course, there is quenched disorder due to the underlying random mass term. This we handle by means of the replica trick. If we assume that the distribution of the \( \Phi \) is short-range correlated (which will be the case for certain classes of realizations of the disorder, but not for others), we can immediately write down the effective action up to and including terms of \( O(\varphi^4) \):

\[
S_{eff} = \sum_\alpha \int dx \, dy \, \varphi^\alpha(x) \Gamma_\alpha(x, y) \varphi^\alpha(y) + u \sum_\alpha \int dx \, \big( \varphi^\alpha(x) \cdot \varphi^\alpha(x) \big)^2
\]

\[
- \sum_{\alpha, \beta} (\Delta + w \delta_{\alpha\beta}) \int dx \, dy \, (\varphi^\alpha(x))^2 \times (\varphi^\beta(y))^2 \tag{3}
\]

Here \( \Gamma_\alpha \) is the Gaussian vertex, Eq. (1b), with \( t = t_0 \). \( \Delta \) is the variance of the Gaussian random mass distribution, and \( \alpha \) and \( \beta \) are replica indices. \( w \) is the coupling constant of the annealed disorder term. We have also derived Eq. (3) by means of a detailed technical procedure which will be reported elsewhere [15]. The technical derivation shows that \( w \) has the form \( w = w_v \), with \( v \) characteristic of the distribution \( P \), and it also yields
terms of $O(\varphi^6)$ and higher. These turn out to be less relevant for the critical behavior than the quartic terms shown in Eq. (3). Notice that the annealed disorder contribution becomes indistinguishable from the usual $\varphi^4$ or $u$-term in the case of a classical transition. This is the reason why the authors of Ref. [4], who studied classical magnets, considered replica symmetry breaking in order to describe nontrivial effects of the rare regions. In the quantum case we get a nontrivial effect even at the level of a replica symmetric theory, which means that the influence of rare regions on quantum transitions is stronger.

To discuss the properties of the effective action, Eq. (3), we proceed as in Ref. [13]. We consider $d = 4 - \epsilon$ space dimensions and $\epsilon$, time dimensions, and control perturbation theory by means of a double expansion in $\epsilon$ and $\epsilon$, [16]. Defining $\bar{w} = w T^{-\epsilon}$, and putting $T = 0$, we obtain the following renormalization group (RG) flow equations to one-loop order,

\[
\frac{du}{d\tau} = (\epsilon - 2\epsilon)u - 4(p + 8)u^2 + 48u\Delta , \quad (4a)
\]
\[
\frac{d\Delta}{d\tau} = \epsilon\Delta + 32\Delta^2 - 8(p + 2)u\Delta + 8p\Delta \bar{w} , \quad (4b)
\]
\[
\frac{d\bar{w}}{d\tau} = (\epsilon - 2\epsilon)\bar{w} + 4p\bar{w}^2 - 8(p + 2)u\bar{w} + 48\Delta \bar{w} . \quad (4c)
\]

An analysis of Eqs. (4) shows that they possess eight FPs. Four of them have a vanishing FP value of $\bar{w}$, $\bar{w}^* = 0$, and have been discussed before in Ref. [13]. Of particular interest is the nontrivial critical FP $u^* = (\epsilon + \epsilon)/16(p - 1)$, $\Delta^* = [(4 - p) + 4(p + 2)]/64(p - 1)$, $\bar{w}^* = 0$, which on the $\bar{w} = 0$ hypersurface is stable for $p$ smaller than some $p_c$. To one-loop order, and for $\epsilon = \epsilon$, $p_c = 16$. A linear stability analysis reveals that the third eigenvalue, $\lambda_0 = (4 - p)(\epsilon + 4\epsilon)/4(p - 1)$, is positive for $p < 4$. In the most interesting case $p = 3$, $\bar{w}$ is thus a relevant operator with respect to this FP, which means that the rare regions destroy the FP. It is, however, interesting to note that for $p > 4$ the FP is stable and describes power-law critical behavior. There also are four FPs with $\bar{w}^* \neq 0$. They are all unstable except for one with $\bar{w}^* = (p - 4)(\epsilon + 4\epsilon)/8p(10 - p)$, which is negative for $p < 4$. Since the bare value of $\bar{w}$ is positive, and the structure of the flow equations does not allow for $\bar{w}$ to change sign, this FP is unphysical. There is thus no new FP for $p < 4$, and a numerical solution of the flow equations reveals runaway flow in all of physical parameter space.

We conclude that for $p < 4$ the AFM long-range order found in Ref. [13] is unstable against effects induced by rare regions, a result that is consistent with the previous suggestion that AFM long-range order is strongly suppressed by quenched disorder [10]. However, other possibilities exist. For instance, there could be a transition to a long-range ordered state, which is described by the critical behavior which manifests itself as runaway flow in a perturbative RG calculation. The viability of this latter suggestion is underscored by the fact that a calculation of the local moment contribution to the order parameter susceptibility yields $\chi_{LM}(T) \sim 1/T^\gamma$ [15]. This is similar to Fisher’s 1-d result $\chi(T) \sim 1/T^{\gamma'}$ with $\gamma' < 1$ [7]. (Our exponent value of unity is a result of our saddle-point approximation for the local moments.) This shows that we are really describing a Griffiths region, which was shown in Ref. [7] to lead to a transition with activated critical behavior in $d = 1$. A third possibility is that a conventional critical FP exists, but cannot be described with perturbative RG methods. This possibility is consistent with the stability of conventional critical behavior against $\bar{w}$ for $p > 4$, as discussed above.

We now turn to the case of itinerant ferromagnets, which constitute an interesting contrast to the AFM case. In Ref. [17] it was shown that a description of itinerant FMs that neglects rare regions leads to an action that has the same form as Eq. (3) with $w = 0$, except that the bare two-point vertex function reads

\[
\Gamma_0^{FM}(q, \omega_n) = (t_0 + |q|^{d-2} + q^2 + |\omega_n|/q^2)/2 , \quad (5)
\]

and that the field $\varphi(x)$ now describes ferromagnetic fluctuations. There are two crucial, and related, differences between Eq. (5) and its AFM counterpart. The first one is the structure of the frequency dependence, which enters as $|\omega_n|/q^2$ [18] and reflects the diffusive nature of the spins in a disordered environment. In Ref. [17] it was shown that the same diffusive spin dynamics leads to the $q^{d-2}$ term, which dominates the usual gradient squared term as long as $d < 4$. In the original treatment of quantum FMs by Hertz [18], loop corrections would have been required to find this term, while the method of Ref. [17] builds it into the bare theory. Consequently, the correlations between the spin density fluctuations are effectively long-ranged, a feature that is well known to stabilize the Gaussian critical behavior [19]. Indeed, it was shown in Ref. [17] that the Gaussian critical behavior, with $\eta = 4 - d$, $\nu = 1/(d - 2)$, $\gamma = 1$, and $z = d$, is stable for $2 < d < 4$. Here $\eta$, $\nu$, and $\gamma$ are the usual critical exponents, and $z$ is the dynamical critical exponent. They can all be simply read off Eq. (5). The exponents $\beta$ and $\delta$ were also determined in Ref. [17], their values in $d = 3$ are $\beta = 2$, $\delta = 3/2$. The remarkable claim of Ref. [17] was that these exponent values, which in $d = 3$ are very different from both mean-field values and classical Heisenberg values, constitute the exact critical behavior of itinerant quantum FMs.

An obvious question is whether this claim survives the consideration of rare regions. To answer this, we perform an analysis analogous to the one for AFMs above. A simple way to incorporate the rare regions into the action is to write the quenched disorder or $\Delta$-term in the action as a random mass in the Gaussian vertex (i.e., to ‘undo’ the integrating-out of the random mass), to construct inhomogeneous saddle-point solutions and expand about
them, and then to integrate over the manifold of saddle points as in the AFM case. Clearly, this leads to a $u$-term in the action, like in Eq. (3). We have derived the same result starting from a more microscopic formulation. We will report the details of the derivation elsewhere [15], here we mention only one important point: After Eq. (3) we mentioned that $w$ is proportional to $u^2$. Since $u$ in the FM case is wavenumber dependent and diverges in the short-wavelength limit (i.e., its bare scale dimension is negative) [17], this raises the question whether the bare value of $w$ is finite. The answer is affirmative, since the $w$-term arises from field configurations that are nonzero only on islands. The $u$ that contributes to the bare value of $w$ therefore has to be taken at wavenumbers that are on the order of a typical inverse island size, and hence is finite. Once again it is important here that the island size distribution falls off exponentially for large sizes. We can thus treat $w$ as a number.

Now let us perform a power counting analysis to determine the stability properties of the Gaussian FP. Assigning a length $L$ a scale dimension $[L] = −1$, the scale dimension of the imaginary time is $[\tau] = −d = −d$. For the scale dimension of the field we find $[\varphi(x)] = (d+2)/2$. The scale dimensions of both $w$ and $\Delta$ then become $[w] = [\Delta] = 4 − d$, i.e. they are irrelevant with respect to the Gaussian FP for $d < 4$, and marginal in $d = 4$. Terms of higher than quartic order in $\varphi$ that are produced by a technical derivation of the effective action [15] turn out to also be irrelevant. We thus conclude that the FM critical behavior determined previously [17] is stable against rare regions physics, in sharp contrast to the AFM case. The reason for this qualitative difference is the effective long-ranged interaction between the order parameter fluctuations (as expressed in Eq. (5) and in the value of the exponent $\eta$), which is sufficient to suppress all disorder fluctuations, including the ones due to rare regions. By the same arguments, the FM Gaussian FP is also stable against replica symmetry breaking.

We conclude with one additional remark. One might ask why the rare regions or local moments don’t cut off the singular wavenumber denominators $|q|^d−2$ and $|\omega_n|/q^2$ in the Gaussian vertex, Eq. (5). The reason why this does not happen is that both singularities are consequences of spin diffusion, which in turn is a consequence of the spin conservation law. The rare regions ultimately derive from a spin-independent disorder potential, which clearly cannot destroy spin conservation. We note, however, that the above arguments are restricted to a tree-level analysis of our effective field theory. Although the effective theory is a sophisticated one, which at tree level contains many effects that would loop in more standard treatments, we of course cannot exclude the possibility that loop corrections might lead to qualitatively new terms in the action. If such new terms included a RG-generated spin dependent potential, then this might change our conclusions. However, at such a level of analysis one would also have to include effects due to interactions between the rare regions, which we have mostly neglected. Such interactions are known to weaken the effects of the rare region [11], but in general it is not known by how much.

We gratefully acknowledge helpful discussions with Ferdinand Evers and John Toner. This work was supported by the NSF under grant Nos. DMR-98-70597 and DMR-96-32978, and by the DFG under grant No. SFB 393/C2.

---

[14] In general, the saddle-point solutions will depend on imaginary time as well as on position. We concentrate on the zero-frequency component, which one expects to yield the dominant effect.
On the critical behavior of disordered quantum magnets: The relevance of rare regions

Rajesh Narayanan  
Department of Physics and Materials Science Institute, University of Oregon, Eugene, OR 97403

Thomas Vojta  
Department of Physics and Materials Science Institute, University of Oregon, Eugene, OR 97403 and Institut für Physik, TU Chemnitz, D-09107 Chemnitz, FRG

D. Belitz  
Department of Physics and Materials Science Institute, University of Oregon, Eugene, OR 97403

T.R. Kirkpatrick  
Institute for Physical Science and Technology, and Department of Physics, University of Maryland, College Park, MD 20742

(May 5, 1999)

The effects of quenched disorder on the critical properties of itinerant quantum antiferromagnets and ferromagnets are considered. Particular attention is paid to locally ordered spatial regions that are formed in the presence of quenched disorder even when the bulk system is still in the paramagnetic phase. These rare regions or local moments are reflected in the existence of spatially inhomogeneous saddle points of the Landau-Ginzburg-Wilson functional. We derive an effective theory that accounts for small fluctuations around these saddle points. The resulting free energy functional contains a new term in addition to those obtained within the conventional perturbative approach, and it comprises what would be considered non-perturbative effects within the latter. A renormalization group analysis 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. This is contrasted with the case of itinerant ferromagnets, where we find that the previously found critical behavior is unaffected by the rare regions due to an effective long-ranged interaction between the order parameter fluctuations.

1. INTRODUCTION

The influence of static or quenched disorder on the critical properties of a system near a continuous phase transition is a very interesting problem in statistical mechanics. While it was initially suspected that quenched disorder always destroys any critical point, this was soon found to not necessarily be the case. Harris found a convenient criterion for the stability of a given critical behavior with respect to quenched disorder: If the correlation length exponent $\nu$ obeys the inequality $\nu \geq 2/D$, with $D$ the spatial dimensionality of the system, then the critical behavior is unaffected by the disorder. In the opposite case, $\nu < 2/D$, the disorder modifies the critical behavior. This modification may either (i) lead to a new critical point that has a correlation length exponent $\nu \geq 2/D$ and is thus stable, or (ii) lead to an unconventional critical point where the usual classification in terms of power-law critical exponents looses its meaning, or (iii) lead to the destruction of a sharp phase transition. The first possibility is realized in the conventional theory of random-$T_c$ classical ferromagnets, and the second one is probably realized in classical ferromagnets in a random field. The third one has occasionally been attributed to the exactly solved McCoy-Wu model. This is misleading, however, as has recently been emphasized in Ref. 6; there is a sharp, albeit unorthodox, transition in that model, and it thus belongs to category (ii).

Independent of the question of if and how the critical behavior is affected, disorder leads to very interesting phenomena as a phase transition is approached. Disorder in general decreases the critical temperature $T_c$ from its clean value $T_c^0$. In the temperature region $T_c < T < T_c^0$ the system does not display global order, but in an infinite system one will find arbitrarily large regions that are devoid of impurities, and hence show local order, with a small but non-zero probability that usually decreases exponentially with the size of the region. These static disorder fluctuations are known as ‘rare regions’, and the order parameter fluctuations induced by them as ‘local moments’ or ‘instantons’. Since they are weakly coupled, and flipping them requires to change the order parameter fluctuations in a whole region, the local moments have very slow dynamics. Griffiths 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 this is a weak effect, since the singularity in the free energy is only an essential one. An important exception is the McCoy-Wu model, which is a $2-D$ Ising model with bonds that are random along one direction, but identical along the second direction. The
resulting infinite-range correlation of the disorder in one direction leads to very strong effects. As the temperature is lowered through the Griffiths region, the local moments cause the divergence of an increasing number of higher order susceptibilities, $\chi^{(n)} = \partial^n M/\partial B^n \ (n \geq 2)$, with $M$ the order parameter and $B$ the field conjugate to it, starting with large $n$. Even the average susceptibility proper, $\chi^{(1)}$, diverges at a temperature $T_\alpha > T_c$, although the average order parameter does not become non-zero until the temperature reaches $T_c$. This is caused by rare fluctuations in the susceptibility distribution, which dominate the average susceptibility and make it very different from the typical or most probable one.

Surprisingly little is known about the influence of the Griffiths region and related phenomena on the critical behavior. Recent work\(^\text{[5]}\) on a random-$T_c$ classical Ising model has suggested that it can be profound, even in this simple model where the conventional theory predicts standard power-law critical behavior, albeit with critical exponents that are different from the clean case. The authors of Ref. 8 have shown that the conventional theory is unstable with respect to perturbations that break the replica symmetry. By approximately taking into account the rare regions, which are neglected in the conventional theory, they found a new term in the action that actually induces such perturbations. In some systems replica symmetry breaking is believed to be associated with activated, i.e. non-power-law, critical behavior. Reference 8 thus raised the interesting possibility that, as a result of rare-region effects, the random-$T_c$ classical Ising model shows activated critical behavior, as is believed to be the case for the random-field classical Ising model,\(^\text{[6]}\) although in the case of the random-$T_c$ model no final conclusion about the fate of the transition could be reached.

Griffiths regions also occur in the case of quantum phase transitions (QPTs), i.e. transitions that occur at zero temperature as a function of some non-thermal control parameter.\(^\text{[9,10]}\) Their consequences for the critical behavior are even less well investigated than in the classical case, with the remarkable exception of certain 1-D systems. Fisher\(^\text{[6]}\) has investigated quantum Ising spin chains in a transverse random field. These systems are closely related to the classical McCoy-Wu model, with time in the quantum case playing the role of the ‘ordered direction’ in the latter. He has found activated critical behavior due to rare regions. This has been confirmed by numerical simulations.\(^\text{[11]}\) Other recent simulations\(^\text{[12]}\) suggest that this type of behavior may not be restricted to 1-D systems, raising the possibility that exotic critical behavior dominated by rare regions may be generic in quenched disordered quantum systems, independent of the dimensionality and possibly also of the type of disorder.

In this paper we consider this problem analytically for two QPTs in $D > 1$. We first concentrate on a simple model for a quantum antiferromagnet. Previous work,\(^\text{[13]}\) which did not take into account rare regions, had found a transition with some surprising properties. One of our goals is to check whether these results survive taking into account rare regions. We find that they do not; the previously found critical fixed point is unstable with respect to the rare regions, and one finds runaway flow in all of physically accessible parameter space. We will discuss possible interpretations of this result. We then show that the critical behavior of itinerant quantum ferromagnets is not affected by the rare regions, in sharp contrast to the antiferromagnetic case. A brief report of some of our results has been given previously in Ref. 14.

The paper is organized as follows. In Sec. II we derive an effective action for an itinerant antiferromagnet in the presence of rare regions. In Sec. III we perform a one-loop renormalization group analysis of this action, and show that there is no stable critical fixed point to that order. In Sec. IV we perform an analogous analysis for itinerant ferromagnets and show that the previously found critical fixed point is stable with respect to the rare region effects. In Sec. V we discuss our results. Various technical points are relegated to three appendices.

## II. AN EFFECTIVE ACTION FOR DISORDERED ANTIFERROMAGNETS

### A. The model

Our starting point is Hertz’s action\(^\text{[16]}\) for an itinerant quantum antiferromagnet. It is a $\phi^4$-theory with a $p$-component order parameter field $\phi$ whose expectation value is proportional to the staggered magnetization. The bare two-point vertex function is

$$\Gamma_0(\mathbf{q},\omega_n) = t_0 + \mathbf{q}^2 + |\omega_n| \ ,$$

with $t_0$ the mean distance from the mean-field critical point. $\mathbf{q}$ is the wavevector, and $\omega_n$ denotes a bosonic Matsubara frequency. We measure $\mathbf{q}$ and $\omega_n$ in suitable microscopic units to make them dimensionless. As in Ref. 13, we modify this action by adding disorder in the form of a ‘random-mass’ or ‘random-temperature’ term. That is, we add to $t_0$ a random function of position, $\delta t(\mathbf{x})$, which obeys a distribution with zero mean and variance $\Delta$,

$$\langle \delta t(\mathbf{x}) \rangle = 0 \ ,$$

(2.2a)

$$\langle \delta t(\mathbf{x}) \delta t(\mathbf{y}) \rangle = \Delta \delta(\mathbf{x} - \mathbf{y}) \ .$$

(2.2b)

For the sake of simplicity, we have taken the distribution to be delta-correlated. The two-point vertex now reads

$$\Gamma(\mathbf{x} - \mathbf{y}, \tau - \tau') = \Gamma_0(\mathbf{x} - \mathbf{y}, \tau - \tau') + \delta(\mathbf{x} - \mathbf{y}) \delta(\tau - \tau') \delta t(\mathbf{x}) \ .$$

(2.3)

Here $\tau$ denotes imaginary time, and $\Gamma_0(\mathbf{x},\tau)$ is the Fourier transform of $\Gamma_0(\mathbf{q},\omega_n)$ in Eq. (2.1). The action reads
\[ S[\phi] = S_C[\phi] + u \int dx \left( \phi(x) \cdot \phi(x) \right)^2 \] 

with the Gaussian part given by
\[ S_C[\phi] = \frac{1}{2} \int dx dy \left( \phi(x) \Gamma(x-y) \phi(y) \right) . \]

Here we have introduced a four-vector notation, \( x \equiv (\mathbf{x}, \tau) \), \( dx \equiv \int dx / \sqrt{27} \), and we use units such that \( \hbar = k_B = 1 \).

At this point, the conventional procedure would be to integrate out the quenched disorder by means of the replica trick.\(^1\) This would lead to an effective action that does not contain the disorder explicitly any longer, and that therefore does not easily allow for saddle-point solutions that are not spatially homogeneous. While the effective action would still be exact, this latter property would make it hard to incorporate the physics we are concentrating on in this paper. We will therefore take a different approach, and consider saddle-point solutions of the model, Eqs. (2.4), before integrating out the disorder. Our procedure roughly follows the one by Dotsenko et al.\(^8\) for classical magnets. As we will see, however, there are important differences between the classical and quantum cases.

\section*{B. Saddle-point solutions}

Let us consider saddle-point solutions of Eqs. (2.4) that are time independent. For simplicity, we also consider a scalar field, \( p = 1 \), that we denote by \( \phi(x) \). It will be obvious how to generalize the following considerations to the case \( p > 1 \). With these restrictions, the saddle-point equation reads
\[ (t_0 + \delta t(x) - \partial^2_x) \phi_{sp}(x) + 4 u \phi_{sp}^3(x) = 0 . \]

Although \( \phi_{sp}^{(1)}(x) \equiv 0 \) is of course always a solution, inhomogeneous solutions also exist provided that \( \delta t(x) \) has "troughs" that are sufficiently wide and deep.\(^17\) In Appendix A we demonstrate this for a one-dimensional toy problem. We have solved Eq. (2.5) numerically for rotationally invariant potentials \( \delta t(x) = f(|x|) \), and have found behavior that is qualitatively the same as in the one-dimensional model. Thus, if \( \delta t(x) \) has one sufficiently deep and wide trough, there will be a solution of Eq. (2.5) that is exponentially small everywhere except within the trough region, where it shows a single hump. There are actually two equivalent single-hump solutions, one positive, and the other negative. We denote the positive one by \( \phi_{sp}^{(2)}(x) \equiv \psi^{(+)}(x) \). As is intuitively obvious, and demonstrated in Appendix A, it leads to a lower free energy than the homogeneous solution \( \phi_{sp}^{(1)}(x) \equiv 0 \). Although in principle any saddle point can be used as the starting point for a loop expansion, it is therefore reasonable to assume that the inhomogeneous one will already incorporate physics that would be much harder to obtain if we expanded about the homogeneous saddle point.

Next consider a potential \( \delta t(x) \) that contains many troughs that support an essentially non-zero local order parameter field. This will result in a saddle-point solution that contains many regions of local order, which we will refer to as "islands". Of course, for an arbitrary potential \( \delta t(x) \) it is not possible to solve Eq. (2.5) in closed form. However, as long as the concentration of the islands is low, as will always be the case sufficiently deep in the disordered phase (i.e., for sufficiently large \( t_0 \)), the values of \( \phi_{sp} \) outside of the islands will still be exponentially small. If \( \delta t \) has troughs leading to \( N \) islands, which individually would result in positive saddle-point solutions \( \psi^{(+)}(x) \), \( (i = 1, \ldots, N) \), it is therefore a reasonable approximation to write the global saddle-point solution as a linear superposition of the \( \psi^{(+)} \). For independent islands, there are actually \( 2^N \) equivalent saddle points, which we write as
\[ \phi_{sp}^{(a)}(x) \equiv \Phi^{(a)}(x) = \sum_{i=1}^{N} \sigma_i^a \psi^{(+)}(x) \]

where \( a = 1, \ldots, 2^N \) numbers the equivalent saddle points, and the \( \sigma_i^a \) are random numbers whose values are either \( +1 \) or \( -1 \). They thus obey a probability distribution
\[ P[\sigma_i^a] = \prod_i \pi(\sigma_i^a) \] 

with
\[ \pi(\sigma) = \frac{1}{2} \left[ \delta(\sigma-1) + \delta(\sigma+1) \right] . \]

Alternatively, one can consider the \( \psi_i(x) \) random functions that are equal to either plus or minus \( \psi^{(+)}(x) \).

For later reference, let us briefly discuss the effects of a weak interaction between the islands as a result of the exponentially small overlap between the functions \( \psi_i(x) \) centered on different islands. One effect will be that the total amount of the order parameter on each island will not necessarily be equal to plus or minus the amount resulting from that island being ideally ordered, but that small deviations from this amount will be possible. If we still assume that the islands are statistically independent, we can model this effect by using a probability distribution for the \( \sigma_i \) that is given by Eq. (2.7a) with a distribution \( p(\sigma) \) that is a broadened version of the bimodal delta-distribution \( \pi(\sigma) \) given in Eq. (2.7b). We thus generalize Eqs. (2.7a,2.7b) to
\[ P[\sigma_i^a] = \prod_i p(\sigma_i^a) \]
For our purposes we will not need to specify the distribution \( p(\sigma) \) explicitly. It will turn out that an interaction between the islands, no matter how small, leads to new physics compared to a model where these interactions are neglected.

We also note that the islands will have some dynamics, both due to interactions between the islands and due to interactions between an island and its immediate neighborhood. In principle, one could try to build this effect into the saddle-point approximation by looking for time dependent saddle points. However, this dynamics is expected to be very slow due to the inertia of the islands. Moreover, the zero frequency component in a frequency expansion is expected to yield the dominant effect. We therefore restrict ourselves to static saddle points.

We also note that the islands will have some dynamics, both due to interactions between the islands and due to interactions between an island and its immediate neighborhood. In principle, one could try to build this effect into the saddle-point approximation by looking for time dependent saddle points. However, this dynamics is expected to be very slow due to the inertia of the islands. Moreover, the zero frequency component in a frequency expansion is expected to yield the dominant effect. We therefore restrict ourselves to static saddle points.

### C. The partition function for a given disorder realization

Of the \( 2^N \) saddle-point solutions \( \Phi^{(a)}(x) \) discussed in the previous subsection, let us pick one, say \( \Phi^{(1)} \), to expand about:

\[
\phi(x) = \Phi^{(1)}(x) + \varphi(x) \quad .
\]

Then the partition function can be written

\[
Z[\delta t(x)] = \int D[\varphi(x)] e^{-S[\Phi^{(1)}(x) + \varphi(x), \delta t(x)]} \quad ,
\]

where we show \( \delta t(x) \) explicitly as an argument to emphasize that we are still working with a fixed realization of the disorder. Equation (2.8b) is exact as long as the integral extends over all fluctuations \( \varphi(x) \) of the field configuration. However, in practice the integral over \( \varphi(x) \) cannot be performed exactly, and in a perturbative treatment one restricts oneself to small deviations \( \varphi(x) \) from the chosen saddle point. Typical pairs of saddle points picked from the \( 2^N \) \( \Phi^{(a)} \) represent field configurations that are globally very different. They will thus be far apart in configuration space, with large energy barriers between them. (We will justify this statement in Sec. V.A2 below.) Expanding about one of the saddle points, as in Eqs. (2.8), is therefore not expected to yield a good representation of the partition function if one evaluates the functional integral in Eq. (2.8b) perturbatively. On the other hand, the same argument suggests that we can simply sum the contributions to \( Z \) obtained by expanding about all of the \( 2^N \) saddle points, provided that we restrict ourselves to small fluctuations about each saddle point,

\[
Z[\delta t(x)] \approx \sum_{a=1}^{2^N} \int D[\varphi(x)] e^{-S[\Phi^{(a)}(x) + \varphi(x), \delta t(x)]} \quad .
\]

Here \( \int D[\varphi(x)] \) indicates an integration over small fluctuations only. Apart from a normalization factor, this procedure amounts to an arithmetic average over the perturbative contributions coming from the vicinities of all saddle points. This average is our approximate way of taking into account non-perturbative effects.

Since we are interested in the effects of fluctuations about the saddle points, we next subtract the saddle point action from the exponent in Eq. (2.9). That is, we write

\[
Z[\delta t(x)] \approx \sum_{a} \int D[\varphi(x)] e^{-\Delta S[\Phi^{(a)}(x), \varphi(x), \delta t(x)]} \quad ,
\]

where

\[
\Delta S[\Phi^{(a)}, \varphi, \delta t] = S[\Phi^{(a)} + \varphi, \delta t] - S[\Phi^{(a)}, \delta t] = S[\varphi(x)] + 4u \int dx \varphi^2(x) \Phi^{(a)}(x) + 6u \int dx \varphi^2(x) \varphi^{(a)}(x)^2 \quad .
\]

So far we have implicitly assumed that there is no interaction between the islands. In reality, there will be a small interaction, one effect of which will be to replace the bimodal distribution, Eqs. (2.7a,2.7b), by the broadened distribution given in Eq. (2.7c). The sum over \( a \) in Eq. (2.10) is then replaced by an integral over the \( \sigma_i^a \), weighted by the distribution \( p(\sigma) \). The partition function can now be written as

\[
Z[\delta t(x)] \approx \int D[\varphi(x)] e^{-\Delta S[\varphi(x)]} ,
\]

with the correction to the action, \( \delta S \), given by

\[
e^{-\delta S[\varphi(x)]} = \prod_{j=1}^N d\sigma_i \prod_j p(\sigma_j) \times e^{-4u \int dx \varphi^2(x) \sum_i \sigma_i \psi_i^{(a)}(x)} \times e^{-6u \int dx \varphi^2(x) \sum_i \sigma_i \psi_i^{(a)}(x) \psi_j^{(a)}(x)} .
\]

(2.12b)

As mentioned previously, it is crucial to incorporate a small interaction between the islands. Indeed, if we used the distribution function, Eqs. (2.7), for the \( \sigma_i \) that is appropriate for non-interacting islands, then we could do the \( \sigma \)-integral in Eq. (2.12b) exactly. As we will show in Sec. III, the resulting action would not lead to new physical effects compared to Ref. 13. Apart from the broadening of the distribution, there are other, similar effects of the island-island interaction that we will neglect. For instance, in the second exponent on the right-hand-side of Eq. (2.12b), the absence of any overlap between \( \psi_i^{(a)} \) and \( \psi_j^{(a)} \) for \( i \neq j \) makes the spatial integral in that term vanish unless \( i = j \). This is no longer true for interacting islands. However, we will neglect this effect and still take this term to be proportional to \( \delta_{ij} \). Equation (2.12b) can then be written
\[
\delta S[\varphi(x)] = -\sum_i \ln \left( e^{-4u \int dx \varphi^2(x) \psi_i^{(+)}(x) \sigma_i} \right) \\
\times e^{-6u \int dx \varphi^2(x) \left( \psi_i^{(+)}(x) \right)^2 \sigma_i^2} . \tag{2.12c}
\]

Here \( \langle \ldots \rangle \) denotes an average over the \( \sigma \) with respect to the broadened bimodal distribution \( p(\sigma) \). The \( \sigma \)-average is carried out by means of a cumulant expansion in powers of our order parameter fluctuations \( \varphi(x) \). To the order \( \varphi^4 \) we obtain

\[
\delta S[\varphi(x)] = 6u \int dx \varphi^2(x) \sum_i \left( \psi_i^{(+)}(x) \right)^2 (\sigma_i^2) \\
+ 4u \int dx \varphi^3(x) \sum_i \psi_i^{(+)}(x) \langle \sigma_i \rangle \\
-18u^2 \int dx \, dy \, \varphi^2(x) \varphi^2(y) \\
\times \sum_i \left( \psi_i^{(+)}(x) \right)^2 \left( \psi_i^{(+)}(y) \right)^2 (\sigma_i^4 - \langle \sigma_i^2 \rangle^2) . \tag{2.13}
\]

Now \( \langle \sigma_i \rangle = 0 \), \( \langle \sigma_i^2 \rangle > 0 \) and \( \langle \sigma_i^4 \rangle - \langle \sigma_i^2 \rangle^2 \equiv c_i > 0 \). The last relation is only valid for a broadened distribution \( p(\sigma) \) which arises from interactions between the islands. For the original distribution \( p(\sigma) \), \( c_i = 0 \) and so the \( O(\varphi^4) \) term would vanish. If we collect all contributions to the action for one particular disorder configuration, we obtain

\[
S[\varphi(x)] + \delta S[\varphi(x)] \\
= \frac{1}{2} \int dx \, dy \, \varphi(x) \Gamma(x - y) \varphi(y) + u \int dx \, \varphi^{4}(x) \\
+ 18u^2 \int dx \, dy \, \varphi^{2}(x) \varphi^{2}(y) \sum_i c_i \left( \psi_i^{(+)}(x) \psi_i^{(+)}(y) \right)^2 . \tag{2.14}
\]

Here we have used the fact that the first term in (2.13) only renormalizes the random-mass term in the Gaussian action. We will show in Sec. III that truncating the action at \( O(\varphi^4) \) is justified since all higher order terms are irrelevant (in a power-counting sense) with respect to both the Gaussian fixed point and the antiferromagnetic fixed point found in Ref. 13.

### D. The effective action

So far we have considered one particular realization of the disorder. In order to derive an effective action we now need to perform the disorder average. It is important to remember that the Landau functional, Eq. (2.14), depends on the disorder in two different ways: explicitly through the random mass in the Gaussian action, and implicitly through the saddle-point solutions \( \psi_i^{(+)}(x) \) that depend on \( \delta t(x) \).

The quenched disorder average over \( \delta t(x) \) is performed via the replica trick, which is based on the identity

\[
\log Z \{ \delta t \} = \lim_{n \to 0} \frac{1}{n} \langle Z^n \{ \delta t \} \rangle , \tag{2.15}
\]

Here \( \langle \ldots \rangle_{\delta t} \) denotes the disorder average. This results in an effective action \( S_{\text{eff}} \) which is defined by

\[
\{ Z^n \} _{\delta t} = \prod_{\alpha=1}^{n} D[\varphi^{\alpha}(x)] \left\{ e^{-\sum_{\alpha}(\delta S[\varphi^{\alpha}(x)] + \delta S[\varphi^{\alpha}(x)])} \right\}_{\delta t} \\
\equiv \prod_{\alpha=1}^{n} D[\varphi^{\alpha}(x)] e^{-S_{\text{eff}}[\varphi^{\alpha}(x)]} . \tag{2.16}
\]

In the absence of \( \delta S \), carrying out the disorder average yields the usual terms that are familiar from the conventional theory. Up to \( O(\varphi^4) \) they are:

\[
\frac{1}{2} \sum_{\alpha} \int dx \, dy \, \varphi^{\alpha}(x) \Gamma_0(x - y) \varphi^{\alpha}(y) \\
+ u \sum_{\alpha} \int dx \, \varphi^{4}(x) \\
- \Delta \sum_{\alpha,n} \int dx \, d\tau \, d\tau' \left( (\varphi^{\alpha}(x, \tau))^2 (\varphi^{\alpha}(x, \tau'))^2 \right) . \tag{2.17}
\]

Taking into account the additional term, \( \delta S[\varphi^{\alpha}(x)] \), is more subtle since the functions \( \psi_i(x) \) are implicit functions of \( \delta t(x) \). We handle this problem by means of a cumulant expansion. To lowest order, the contribution of \( \delta S \) to the effective action is just the disorder average of \( \delta S \):

\[
\{ \delta S \} _{\delta t} = w \int dx \, dy \, \varphi^{2}(x) \varphi^{2}(y) D_{\text{isl}}^{(2)}(x, y) , \tag{2.18a}
\]

where \( w \propto u^2 \), and the correlation function

\[
D_{\text{isl}}^{(2)}(x, y) = \left\{ \sum_i c_i \left( \psi_i^{(+)}(x) \psi_i^{(+)}(y) \right)^2 \right\}_{\delta t} \tag{2.18b}
\]

essentially describes the probability for \( x \) and \( y \) to belong to the same island. The properties of these correlation functions depend on the precise nature of the disorder. If the microscopic disorder \( \delta t(x) \) is short-range correlated, as we have assumed in our model, then the island size distribution will generically fall off exponentially for large sizes. In this case the correlation function \( D_{\text{isl}}^{(2)} \) is also short-ranged in space. Keeping only the leading term in a gradient expansion, we can then replace it by a spatial \( \delta \)-function. The case of an island size distribution that has a power-law tail (e.g. due to long-range correlations in the microscopic disorder) is discussed in Appendix B.

Collecting all contributions to the effective action \( S_{\text{eff}} \) up to \( O(\varphi^4) \), absorbing a constant into \( w \), and restoring the vector nature of the order parameter field, we finally obtain
\[ S_{\text{eff}}[\varphi^a(x)] = \frac{1}{2} \sum_x \int dx \, dy \, G_0(x-y) \varphi^a(x) \cdot \varphi^a(y) + u \sum_x \int dx \, dy \, (\varphi^a(x, \tau) \cdot \varphi^a(x, \tau_0))^2 - \sum_{\alpha, \beta} \left( \Delta + w \delta_{\alpha \beta} \right) \int dx \, dt \, dt' \times (\varphi^\alpha(x, \tau) \cdot \varphi^\alpha(x, \tau')) (\varphi^\beta(x, \tau') \cdot \varphi^\beta(x, \tau')) . \] (2.19)

The \( w \)-term is generated by taking into account the inhomogeneous saddle points. A perturbative expansion about the homogeneous saddle point, as was performed in Ref. 13, misses this term. It has the time structure of the two-point vertex function \( \Gamma_0 \). To this end, we analyze the effective action, \( S_{\text{eff}} \), Eq. (2.19), at tree level.

Let us denote the scale dimension of any quantity \( Q \) by [\( \hat{Q} \)], and define the scale dimension of a length \( L \) to be [\( \hat{L} = -1 \)]. The scale dimension of the imaginary time is \( \hat{\tau} = -z \), which defines the dynamical critical exponent \( z \). We first analyze the Gaussian fixed point. From the structure of the two-point vertex function \( G_0 \) given in Eq. (2.1), we see that \( \omega_n \) scales like \( q^2 \). This implies \( z = 2 \).

The scale dimension of the field \( \varphi \) is found from the requirement that the action must be dimensionless to be [\( \hat{\varphi} = D/2 \)]. The scale dimensions of the coefficients of the terms of \( O(\varphi^4) \) in Eq. (2.19) are found to be [\( \hat{u} = 2 - D \), and \( \hat{\Delta} = \hat{w} = 4 - D \). Thus, \( u \) is irrelevant with respect to the Gaussian fixed point as long as \( D > 2 \), while \( \Delta \) and \( w \) are relevant for \( D < 4 \). The Gaussian fixed point is therefore unstable, and we will have to perform a loop expansion close to \( D = 4 \) in the next subsection.

We now show that all terms of \( O(\varphi^6) \) and higher are irrelevant with respect to the Gaussian fixed point. First of all, there are the conventional terms of the schematic form

\[ u_{2m} \int dx \, \varphi^{2m}(x) , \] (3.1)

with coupling constants \( u_{2m} (n_3 \equiv u) \). These are irrelevant since [\( u_{2m} = 2 - (m-1)D < 0 \). In addition to these terms, the cumulant expansion of (2.12c) generates higher order terms with more time integrations than the conventional terms for a given power of \( \varphi \). For instance, at \( O(\varphi^6) \) we have two terms,

\[ 8u^2 \int dx \, dy \, \varphi^2(x) \varphi^2(y) \sum_i \psi_i^{(1)}(x) \psi_i^{(1)}(y) \langle \sigma_i^2 \rangle , \] (3.2a)

and

\[ -36u^3 \int dx \, dy \, dz \, \varphi^2(x) \varphi^2(y) \varphi^2(z) \sum_i \left( \psi_i^{(1)}(x) \right)^2 \times \left( \psi_i^{(1)}(y) \right)^2 \times \left( \psi_i^{(1)}(z) \right)^2 \times \left( \langle \sigma_i^2 \rangle - 3 \langle \sigma_i^4 \rangle / 8 \right) \] (3.2b)

Upon averaging over the disorder these terms become

\[ v_6 \int dx_1 dx_2 \varphi^2(x_1) \varphi^2(x_2) C^{(2)}_{\text{dd}}(x_1, x_2) , \] (3.3a)

and

\[ w_6 \int dx_1 dx_2 dx_3 \varphi^2(x_1) \varphi^2(x_2) \varphi^2(x_3) \times D^{(3)}_{\text{dd}}(x_1, x_2, x_3) , \] (3.3b)

respectively, with \( v_6 \propto u^2 \), \( w_6 \propto u^3 \). The correlation functions \( C^{(2)}_{\text{dd}}(x, y) \) and \( D^{(3)}_{\text{dd}}(x, y, z) \) are defined analogously to \( D^{(3)}_{\text{dd}}(x, y) \) in Eq. (2.18b), and are related to the probability for \( x, y \) and \( x, y, z \), respectively, to belong to the same island. We again concentrate on the generic case where the island size distribution falls of exponentially for large islands (for a discussion of other cases, see Appendix B). In this case both correlation functions are short-ranged and can be localized for power-counting purposes. This effectively leaves only one spatial integral in Eqs. (3.3a) and (3.3b). Therefore, the scale dimensions of the coefficients are \( [v_6] = 2(2-D) \) and \( [w_6] = 2(3-D) \). Consequently, both terms are irrelevant with respect to the Gaussian fixed point near \( D = 4 \).

More generally, we obtain from Eq. (2.12c) terms that contain powers of \( \varphi^4 \), terms that contain powers of \( \varphi^2 \), and mixed terms that contain both \( \varphi^4 \) and \( \varphi^2 \). For power-counting purposes, the most relevant term for a fixed power of \( \varphi \) is the one with the most time integrations. For even powers of \( \varphi \), these are the terms

\[ w_{2m} \int dx_1 \ldots dx_m \varphi^2(x_1) \ldots \varphi^2(x_m) D^{(m)}_{\text{dd}}(x_1, \ldots, x_m) , \] (3.4)

Localizing the correlation function \( D^{(m)} \) we find for the scale dimension of the coupling constant \( [w_{2m}] = 2m - (m-1)D \). Terms with odd powers of \( \varphi \) are always less relevant than the preceding term of even order. We
conclude that all terms of higher than quartic order are irrelevant with respect to the Gaussian fixed point near $D=4$.

So far we have determined the scale dimensions with respect to the Gaussian fixed point. At the non-trivial critical fixed point discussed in Ref. 13 the anomalous dimension of the field $\varphi$ is $\eta = 0 + O(\epsilon^2)$ since, as in the ordinary $\phi^4$ theory, there is no wavefunction renormalization at 1-loop order. This implies that all results on the irrelevancy of the terms of order $\varphi^6$ and higher carry over from the Gaussian fixed point to the non-trivial critical fixed point found in Ref. 13.

### B. Perturbation theory, and flow equations

In the last subsection we have shown that the Gaussian fixed point is unstable for $D<4$. We must therefore carry out a loop expansion for the effective action, Eq. (2.19). To control the perturbation theory we consider $D = 4 - \epsilon$ spatial dimension and $\epsilon$ time dimensions.\(^{19}\) This leads to the replacement of $\int d\tau$ by $\int d\tau \tau^{\epsilon - 1}$. At the Gaussian fixed point the scale dimension of the field $\varphi$ is now $[\varphi] = (d + 2\epsilon) - 2)/2$. In the same vein the scale dimensions of $u$, $\Delta$, and $w$ are $[u] = \epsilon - z\epsilon$, $[\Delta] = \epsilon$, and $[w] = \epsilon$, respectively. The perturbation theory becomes a double expansion in $\epsilon$ and $\epsilon$.

To obtain the renormalization group flow equations, we perform a frequency-momentum shell RG procedure.\(^{16}\) The diagrams that contribute to the renormalization of the coupling constants $u$, $\Delta$, and $w$ are shown in Fig. 1. To one-loop order, we obtain the following flow equations,

$$\frac{du}{dt} = (\epsilon - 2\epsilon) u - 4 (p + 8) u^2 + 48 u \Delta , \quad (3.5a)$$

$$\frac{d\Delta}{dt} = \epsilon \Delta + 32 \Delta^2 - 8 (p + 2) \Delta + \frac{4p}{4T^{\epsilon s}} (2 \Delta - w) w , \quad (3.5b)$$

$$\frac{dw}{dt} = \epsilon w + \frac{4p}{T^{\epsilon s}} w^2 - 8 (p + 2) w + 24 (2 \Delta - w) w + 8 w^2 . \quad (3.5c)$$

The mass $t$ of the two-point vertex, which describes the distance from the critical point, is of course also renormalized. However, since we are interested in the stability of a critical fixed point, it suffices to consider the flow on the critical surface. The factors of $T^{-\epsilon s}$ in Eqs. (3.5) arise from the fact that some diagrams that contain the $w$-vertex lead to Matsubara frequency sums without an accompanying temperature factor. Since the critical surface for the quantum phase transition is defined by $T=0$ in addition to $t=0$, the natural coupling constant for the $T=0$ flow is $\bar{w} = w T^{-\epsilon s}$. Putting $T=0$,\(^{20}\) the flow equations can then be rewritten in the form

$$\frac{du}{dt} = (\epsilon - 2\epsilon) u - 4 (p + 8) u^2 + 48 u \Delta , \quad (3.6a)$$

$$\frac{d\Delta}{dt} = \epsilon \Delta + 32 \Delta^2 - 8 (p + 2) \Delta + 8 p \Delta \bar{w} , \quad (3.6b)$$

$$\frac{d\bar{w}}{dt} = (\epsilon - 2\epsilon) \bar{w} + 4 p \bar{w}^2 - 8 (p + 2) u \Delta + 48 \Delta \bar{w} . \quad (3.6c)$$

### C. Fixed points and their stability

The flow equations, Eqs. (3.6), possess eight fixed points. The fixed-point values of the coupling constants, and the corresponding eigenvalues of the linearized RG transformation are listed in Table I. Four of the fixed points (Nos. 1–4 in Table I) have a zero fixed-point value of $w$, $\bar{w}^* = 0$. These are the fixed points studied before in Ref. 13. The other four fixed points have $\bar{w}^* \neq 0$.

Let us first consider fixed point No. 4. This is the critical fixed point that was found within the conventional approach.\(^{13}\) We find that the local moments, represented by the $w$-term, render this fixed point unstable for $p<4$, since in this case the third eigenvalue, $\lambda_w$, is positive. However, for $p>4$ the $w$-term is irrelevant with respect to this fixed point, and the fixed point is stable for $4<p<p_c$. To one-loop order, and for $\epsilon = \epsilon_s$, $p_c = 16.\(^{13}\)$

A stability analysis for the new fixed points shows that they are all unstable for $p<4$ with the exception of No. 8. At this fixed point, $w$ has a negative value, while Eq. (2.13), with reasonable assumptions about the distribution $p(w)$, yields a positive value for the bare value of $w$. Since the structure of the flow equations does not allow $w$ to change sign, we conclude that this fixed point is unphysical for generic realizations of the disorder. It is interesting to note, however, that fixed point No. 8 is
stable against replica symmetry breaking (see Appendix C).

For $p < 4$, and to one-loop order in our double expansion in powers of $\epsilon$ and $\epsilon_{\tau}$, there is thus no stable fixed point. Consistent with this, a numerical solution of the flow equations, Eqs. (3.6), shows runaway flow in all of physical parameter space. We will discuss the physical meaning of this result in Sec. V below.

### IV. THE CASE OF ITINERANT FERROMAGNETS

In Ref. 15 a generalized LGW functional for the ferromagnetic transition in a disordered itinerant electron system was derived starting from a fermionic description. The effects of rare regions were not explicitly considered in this work. Here we show that although the rare regions were neglected in the explicit calculations in that paper, the effective field theory derived in Ref. 15 still contains these effects. We will further show that taking them into account does not change the previous conclusions.

We first briefly recall the effective action that was derived in Ref. 15. In the long-wavelength and low-frequency limit, the replicated action is given by

$$S_{\text{eff,1}} = \frac{1}{2} \sum_{\alpha} \int dx_1 dx_2 \left[ \Gamma_0(x_1 - x_2) \mathbf{M}^{\alpha}(x_1) \cdot \mathbf{M}^{\alpha}(x_2) + \sum \int dx_1 dx_2 dx_3 dx_4 u_4(x_1, x_2, x_3, x_4) \right] \times (\mathbf{M}^{\alpha}(x_1) \cdot \mathbf{M}^{\alpha}(x_2)) (\mathbf{M}^{\alpha}(x_3) \cdot \mathbf{M}^{\alpha}(x_4))$$

$$- \Delta \sum_{\alpha, \beta} \int dx \, d\tau \, \tau^* \left[ (\mathbf{M}^{\alpha}(x, \tau))^T (\mathbf{M}^{\beta}(x, \tau'))^T (\mathbf{M}^{\beta}(x, \tau'))^2 + (\mathbf{M}^{\alpha}(x, \tau))^2 \right].$$

Here $\mathbf{M}$ is the order parameter field whose expectation value is the magnetization, and $\alpha$ and $\Delta$ are coupling constants that in general are wavenumber and frequency dependent. An important point is that these coupling constants in general do not exist in the limit of zero frequencies and wavenumbers, i.e. the effective action describes a non-local field theory. This is because in the process of deriving a LGW functional that depends only on the order parameter field, soft (viz., diffusive) fermionic degrees of freedom have been integrated out. In writing Eq. (4.1) we have used that the coupling constant $\Delta$ is finite in the long-wavelength limit, so that it can be treated as a number. $u_4$, on the other hand, is singular in this limit, see Eq. (4.3) below. For small wavenumbers the Fourier transform of the two-point vertex $\Gamma_0$ is given by

$$\Gamma_0(q, \omega_n) = \Gamma_0 + u_2(q) + \omega_n / q^2,$$

with

$$u_2(q) = u_2^{(D-2)} q^{D-2} + u_2^{(0)} q^2.$$

Here $u_2^{(D-2)}$ and $u_2^{(0)}$ are finite numbers. Note that for $D < 4$ (in particular, in the physical dimension $D = 3$), the first term in Eq. (4.2b) dominates the second one as $q \rightarrow 0$. $u_2$, in wavenumber space at zero frequency, is schematically given by

\[
\begin{array}{|c|c|c|c|c|c|c|}
\hline
\text{FP No.} & \text{FP values} & \text{eigenvalues} \\
\hline
1 & 0 & 0 & 0 & \epsilon - 2\epsilon_{\tau} & \epsilon & \epsilon - 2\epsilon_{\tau} \\
2 & \frac{\epsilon - 2\epsilon_{\tau}}{4(p+3)} & 0 & 0 & -\epsilon - 2\epsilon_{\tau})} & \frac{(p+4)\epsilon_{\tau} - (p-4)\epsilon}{p+3} & \frac{(p-4)(\epsilon - 2\epsilon_{\tau})}{p+3} \\
3 & 0 & -\epsilon/32 & 0 & 2\epsilon_{\tau} - \epsilon/2 & -\epsilon & 2\epsilon_{\tau} - \epsilon/2 \\
4 & \frac{\epsilon + \epsilon_{\tau}}{16(p-1)} & \frac{(4-p)(4(p+2)\epsilon_{\tau})}{64(p-1)} & 0 & -A + B & \frac{C - D}{2} & \frac{A - C}{2} \\
5 & 0 & 0 & -\epsilon - 2\epsilon_{\tau}/4p & \epsilon/4 - \epsilon/2 & 4\epsilon_{\tau} & -\epsilon - 2\epsilon_{\tau} \\
6 & \frac{\epsilon - 2\epsilon_{\tau}}{4(p+3)} & 0 & \frac{(p-4)(\epsilon - 2\epsilon_{\tau})}{4p(p+3)} & -\epsilon - 2\epsilon_{\tau})} & \frac{(p-4)(\epsilon - 2\epsilon_{\tau})}{p+3} & \frac{(p-4)(\epsilon - 2\epsilon_{\tau})}{p+3} \\
7 & 0 & (4\epsilon_{\tau} - \epsilon)/64 & -4(\epsilon_{\tau} + \epsilon)/16p & \epsilon_{\tau} + \epsilon/4 & -\epsilon & 2\epsilon_{\tau} - \epsilon/2 \\
8 & \frac{\epsilon + 4\epsilon_{\tau}}{8(10-p)} & \frac{(p-4)(\epsilon + 4\epsilon_{\tau})}{8(10-p)} & \frac{0}{8(p-1)} & -C & \frac{D - C}{2} & \frac{D - C}{2} \\
\hline
\end{array}
\]
Ref. 15 and below, that the last term in Eq. (4.1). To this end we first note, cf. these local moments is implicitly contained already in (4.1). Second, we partially undo the replica trick in Eq. (4.4b). This stabilizes the Gaussian fixed point by the action, explicitly including the effective long-range interaction between the order parameter fluctuations that is described by the $|q|^{D-2}$-term in Eq. (4.2b). This stabilizes the Gaussian fixed point by suppressing all fluctuations, including the static disorder fluctuations responsible for the local moments.

V. DISCUSSION AND CONCLUSION

In this section, we conclude by discussing the results obtained in the previous sections.

\[
u_4(q \to 0) = u_4^{(D-6)}|q|^{D-6} + O(|q|^{D-4}) , \quad (4.3)\]
i.e., $u_4$ diverges for $D < 6$. The singularities in the wavefunction deformations of $u_2$ and $u_4$ mean that the field theory is non-local. As mentioned above, their physical origin are diffusive fermionic particle-hole excitations that were integrated out in deriving Eq. (4.1).

Next we argue that in at least one well-defined physical situation, it is easy to uncover the effects of rare regions that are implicit in Eq. (4.1). The basic argument is that on length scales small compared to the elastic mean free path, the field theory is effectively local. This implies that as long as the local moments or instantons decay on a scale $\lambda < \ell$, the techniques discussed in Sec. II can be used to include the effects of these inhomogeneous saddle points on the final long-wavelength theory. Further we will show that the quenched randomness that leads to the non-locality in Eq. (4.6) is irrelevant when spatial scales shorter than a mean free path are considered. For $\lambda_F \ll \lambda \ll \ell$ we then have,

\[
u_2(q) \approx u_2^{(0)} \left( \frac{q}{k_F} \right)^2 . \quad (4.7)\]
Note that for this argument to be valid we need $\lambda_F/\ell \approx 1/k_F \ell \ll 1$, i.e., weak disorder is required. Similarly, $u_4$ in Eq. (4.3) can be replaced by a constant when $\lambda_F \ll \lambda \ll \ell$. The net result is that when the local moments vary on a length scale smaller than $\ell$, they can be described by a local field theory analogous to the one discussed in Sec. II even though the long-wavelength theory is non-local. If we assume, as we did in the antiferromagnetic case in the previous section, that the island distribution falls off exponentially for large island sizes, this will always be true for sufficiently small disorder.

With the above ideas and the techniques developed in Sec. II, the final long wavelength theory to describe the ferromagnetic phase transition, explicitly including the effects of rare regions, is determined by the action,

\[
S_{\text{eff}} = S_{\text{eff,1}} + \delta S_{\text{eff}}, \quad (4.8a)\]
with $S_{\text{eff,1}}$ given by Eq. (4.1) and

\[
\delta S_{\text{eff}} = -w \sum \int dx \, d\tau \, (\mathcal{M}^a(x, \tau) \cdot \mathcal{M}^a(x, \tau))
\times (\mathcal{M}^a(x, \tau') \cdot \mathcal{M}^a(x, \tau')) , \quad (4.8b)\]

where $w$ is a finite constant. Power counting immediately reveals that the coupling constant $w$, just like $\Delta$, is an irrelevant operator with respect to the Gaussian fixed point discussed in Ref. 15. The rare regions therefore do not change the critical behavior in this case. The physical reason for this is the effective long-range interaction between the order parameter fluctuations that is described by the $|q|^{D-2}$-term in Eq. (4.2b).
A. General considerations

We begin our discussion by considering the physical underpinnings of some general aspects of our technical procedure.

1. Local moments and annealed disorder

Let us first of all give a simple physical interpretation of the \( w \)-term in the effective action, Eq. (2.19), which is the most important of the contributions that reflect the existence of rare regions and local moments. Since the local moments are self-generated by the electronic system, in response to the potential created by the quenched disorder, they are an integral part of the system and in equilibrium with all other degrees of freedom. In our approximation, which takes into account only the static local moment fluctuations, the effect of the rare regions therefore amounts to the existence of static, annealed disorder. Indeed, a straightforward generalization of Eq. (2.10) is to integrate over a manifold of saddle points \( \Phi(x) \), weighted with an appropriate distribution \( P[\Phi(x)] \),

\[
Z \approx \int D[\Phi(x)] P[\Phi(x)] \int_D \varphi(x) \ e^{-\Delta S[\Phi(x),\varphi(x),\delta(x)]},
\]

which makes obvious the annealed-disorder character of the average over the saddle points. The detailed result of the integration over the saddle points will of course depend on the distribution \( P \), which in turn depends on the microscopic details of the disorder realization in the system. However, any physically reasonable distribution will lead in particular to a term in the effective action that has the structure of the \( w \)-term in Eq. (2.19). Since the saddle points are separated by large energy barriers in configuration space (see Sec. V A 2 below), this term clearly cannot be obtained by perturbatively expanding about the trivial homogeneous saddle point as is done in the conventional theory. Thus, our method approximately takes into account what one would call ‘non-perturbative’ effects in the usual approach.

It is important to note that the new term in the action, Eq. (2.19), differs from the usual quantum fluctuation or \( u \)-term only in its time structure. In the classical limit, therefore, \( u \) just renormalizes \( u \), decreasing its bare value. This is indeed well known to be the only effect of static annealed disorder in classical systems. In their analysis of classical magnets, the authors of Ref. 8 therefore considered a more elaborate scheme for doing the sum over saddle points in Eq. (2.10), or the integral in Eq. (5.1), that leads to a term that breaks the replica symmetry. Our way of approximating that integral can be considered as a zeroth order step in the approximation scheme of Ref. 8. In the quantum case, the time structure results in this zeroth step already giving a non-trivial result, and in this sense quantum systems are more sensitive to rare region effects than classical ones. The physical meaning of replica symmetry breaking in this context is not quite clear. However, in the quantum case it is not necessary to enter into this discussion. The AFM fixed point is unstable already under the effects considered above, and no new fixed point exists. Considering replica symmetry breaking in addition to our effect would not change this conclusion. In the FM case, it turns out that the previously found Gaussian fixed point is stable against replica symmetry breaking as well as against the quantum effect, as we will discuss in more detail below.

2. Energy barriers between saddle points

A question that arises in connection with Eq. (2.9) or (5.1) is whether it is really true that there are large energy barriers between the various saddle-point configurations, as our approximation for the partition crucially depends on this assumption. Let us first consider the case of the Ising model \((p = 1)\), for which we performed the explicit derivation in Sec. II. Suppose we have two saddle points that differ only by the sign of the order parameter on one particular island. In order to turn one of these spin configurations into the other, we need to flip all of the spins on that island. (For simplicity, we refer to the order parameter field as ‘spins’.) In order to do so, one must go through an intermediate state with a domain wall across the island. The energy of that domain wall can be estimated from the squared gradient term in the free energy, integrated over the island, \( J \int \varphi(x)(\nabla\varphi(x))^2 \), with \( J \) the coupling between the spins. The thickness of the domain wall is a microscopic length \( a \), and hence the energy of the domain wall, or the energy barrier between the two saddle points, is proportional to \( J L^{D-1} a/a^2 = J L^{D-1} \), with \( L \) the linear size of the island. In the case of a continuous spin model \((p > 1)\) an analogous argument holds, except that now all length scales are of order \( L^1 \). This leads to \( J L^{D-2} \) for the energy of a domain wall. For \( D > 2 \), there is thus only a quantitative difference between the Ising case and the continuous spin case.

In either model, the domain wall energy will have to be multiplied by the number of islands by which two typical saddle points differ. For the Ising case, let us consider \( N \) islands, with \( 2^N \) saddle points and \( 2^{N-1}(2^N-1) \) pairs of saddle points. The probability distribution \( \{p_N(n)\} \), for a pair of saddle points to have \( n \) islands that are different is easily found to be

\[
p_N(n) = \frac{1}{2^N-1} \binom{N}{n}.
\]

For large \( N \), this becomes a Gaussian distribution with mean \( N/2 \) and variance \( \sqrt{N}/2 \),

\[
p_{\infty}(n) = \frac{2}{\sqrt{2\pi N}} e^{-2(n-N/2)^2/N}.
\]
One expects this to be true for the continuous spin case as well, although the statistical analysis becomes much more involved in that case. The microscopic energy of a domain wall thus gets multiplied by a macroscopic number, leading to energy barriers between almost all pairs of saddle points that go to infinity in the thermodynamic limit. This justifies our approximation.

Finally, we note that our considerations maximize, and probably overestimate, the effects of local moments or disorder induced instantons. The discussion above seems to imply an exponential number of saddle point solutions that are unrelated by symmetries, with barriers between them that approach infinity in the bulk limit. This in turn implies an exponential number of thermodynamic states, or a finite complexity. Such a proposition is controversial in other contexts, e.g. for spin glasses. However, in our considerations we have effectively neglected the interactions between the local moments. One anticipates these interactions to correlate and weaken the rare regions. Indeed, in Ref. 23 it was argued that long-range interactions that arise from the itinerant nature of the electrons quench most of the local moments. If this happens in the systems we consider, then we likely overestimate the number of distinct thermodynamic states. It is also possible that our theory is valid only in an intermediate time region, and that the interactions between the local moments must be taken into account in the limit of asymptotically long times.

3. Nature of the local-moment phase

Another point we have not yet addressed is the physical nature of the phase that is induced by the presence of the local moments. In order to show that we are dealing with a Griffiths phase, let us consider the local moment contribution to the order parameter susceptibility, \( \chi_{LM} \). Let us adopt a ferromagnetic language for simplicity, and denote the magnetic moment on the island number \( i \) by \( M_i \). Then we have

\[
\chi_{LM} = \left\{ \frac{1}{\sum_i V_i} \int_0^T dt \sum_{ij} \left( \langle M_i(t) M_j(0) \rangle - \langle M_i \rangle \langle M_j \rangle \right) \right\}_d, \tag{3.3}
\]

where \( \langle \ldots \rangle \) denotes a thermodynamic average. Since there is no overall magnetization, \( \sum_i \langle M_i \rangle = 0 \), and in our saddle-point approximation the island magnetization is static. This yields

\[
\chi_{LM} = \left\{ \frac{1}{\sum_i V_i} T \sum_{ij} \langle M_i M_j \rangle \right\}_d = \frac{\text{const}}{T}, \tag{3.4}
\]

where the constant is given by \( \langle \sum_i (M_i^2) \rangle / \sum_i V_i \). We see that the order parameter susceptibility diverges for \( T \to 0 \) whenever there are islands, and in our simple saddle-point approximation the divergence takes the form of a Curie law. Our saddle point thus really describes a Griffiths phase.

4. Finiteness of the free energy

As a final general point, let us again consider the effective action, Eq. (2.19), which determines the free energy. Since the \( w \)-term and the \( w \)-term have the same structure except for an extra time integral in the former, it seems as if the \( w \)-term contributes a term to the free energy that diverges as the temperature goes to zero. One has to keep in mind, however, that Eq. (2.19) represents a Landau expansion that has been truncated at \( O(\varphi^4) \). It is easy to see that higher order terms in the Landau expansion lead to even more strongly divergent contributions to the free energy, see Eq. (3.4). This simply means that the loop expansion for the free energy of a quantum system with static annealed disorder is singular, and a resummation to all orders would be necessary to obtain a finite result. From a RG point of view, which holds that the higher order terms in the Landau expansion are irrelevant, the solution of this paradox lies in the fact that, if a fixed point existed, it would be \( \bar{w} \) that has a finite fixed-point value, not \( w \). Since \( w = \bar{w} T \) (for the physical case \( \epsilon_0 = 1 \)), this ensures that the fixed-point Hamiltonian has a finite free energy.

B. Results for the AFM case

As we have shown in Sec. III, and reiterated above, taking into account the rare regions in the AFM case destroys the stability of the fixed point found in Ref. 13, and one finds runaway flow in all of the physically accessible parameter space. Three possible interpretations of this result are, (i) there is no transition to a state with long-range order, (ii) there is a transition, but the corresponding fixed point is inaccessible by perturbative RG techniques, or (iii) there is a fluctuation-induced first order transition (which causes the runaway flow). The last conjecture can be checked by calculating the free energy to one-loop order and then explicitly verifying whether it has a double minimum structure as a function of the order parameter. We have performed such a calculation, and found that this is not the case. This rules out scenario (iii).

On the basis of our results, we cannot decide between scenarios (i) and (ii). Scenario (i) would imply that arbitrarily weak disorder necessarily destroys quantum AFM long-range order. This is an unlikely proposition, but it cannot be ruled out at present. The alternative is scenario (ii), i.e. the existence of a non-perturbative fixed point. The nature of such a fixed point, if it exists, is
a priori unclear. The analogies with 1-D systems mentioned in the Introduction, as well as Ref. 12, suggest that an unconventional infinite disorder fixed point with activated scaling is a possible interpretation of the run-away flow. However, there also could be a conventional fixed point that is not accessible by our methods. In this context it is interesting to note that the case $p > 4$ discussed in Sec. III C provides an example of a stable conventional fixed point that describes a transition with power-law critical behavior in the presence of rare regions.

Let us also come back to the fact that in Sec. III we found a stable fixed point (No. 8 in Table I) with $w^* \neq 0$. As was pointed out in Sec. III C, for generic realizations of the disorder, which lead to a positive bare value of $w$, this fixed point is unphysical even if it has $w^* < 0$. However, mathematically one can have $w < 0$ for certain choices of the distribution $P(\sigma_i)$ in Sec. II that are more general than Eq. (2.7c). This leaves open the possibility that at least in some systems there is a stable, conventional critical fixed point that is accessible with our method. We note that this fixed point is stable against replica symmetry breaking, see Appendix C. This is in contrast to the case of classical magnets, where all fixed points are unstable against replica symmetry breaking, and reminiscent of the result of Read et al. on quantum spin glasses, where the quantum model was also found to be more stable against replica symmetry breaking than its classical counterpart. The technical reason for this enhanced stability is very similar to the point discussed at the end of Sec. V A, namely that the parameter that would induce replica symmetry breaking appears as $T$ times a finite fixed point value, and hence vanishes at the quantum critical point.

C. Results for the FM case

For itinerant quantum ferromagnets, we have found that the rare regions do not affect our previous results. The physical reason for this is the long-range interactions between the spin fluctuations in these systems. They are induced by soft modes in the itinerant electron system and stabilize the Gaussian critical behavior against fluctuations, including the static disorder fluctuations that lead to local-moment formation. A crucial point for our conclusion is the survival of these long-range interactions in the presence of local moments, so it is worth discussing this in some detail.

The derivation of the long-range interaction shows that its origin is soft spin-triplet particle-hole excitations in the electron system. An obvious question is whether local moments act effectively as magnetic impurities that give these soft modes a mass. If this were the case, then the singular wavenumber dependences $|q|^3$ and $|\omega_q|/q^2$ in the Gaussian vertex, Eq. (4.2a), would be cut off and the ferromagnetic effective action would have the same structure as the antiferromagnetic one. The answer to this question is not obvious since the local moments are self-generated, and thinking about them as analogous to externally introduced magnetic moments can be misleading. This is underscored by the fact that the rare regions/local-moment physics enters the theory in the form of annealed disorder, as we have seen in Sec. V A above. In our derivation of the effective action, Sec. IV, the wavenumber singularities are not cut off. The physics behind this is that both singularities are consequences of spin diffusion, which in turn is a consequence of the spin conservation law. The rare regions ultimately derive from a spin-independent disorder potential, which clearly cannot destroy spin conservation. The long-range interactions between the spin fluctuations are therefore still present in the bare effective action, and hence the Gaussian fixed point is stable in our tree-level analysis. We note, however, that at present we cannot rule out the possibility that loop corrections might lead to qualitatively new terms in the action. If such new terms included a RG-generated spin dependent potential, then this might change our conclusions. This would not necessarily violate the spin conservation argument given above, since an effective spin-dependent potential acting only on the itinerant electrons, which are not taking part in the local moment formation, could change the critical behavior while preserving spin conservation for the system as a whole.

A more detailed investigation of this point is not feasible within the existing framework of the ferromagnetic theory. This is because in the existing theory all degrees of freedom other than the order parameter, including various soft modes, have been integrated out. This leads to a non-local field theory which is unsuitable for an explicit loop expansion. A remedy would be to derive an effective theory that keeps all soft modes explicitly and treats them on equal footing, leading to well-behaved vertices that allow for explicit calculations. This project is left for future work. We also note that at such a level of the analysis one should also include effects due to interactions between the rare regions, which we have mostly neglected. Such interactions are known to weaken the effects of the rare region, but in general it is not known by how much.

D. Summary, and Outlook

In summary, we have studied the effects of rare disorder fluctuations, and the resulting local moments, on itinerant ferromagnets and antiferromagnets. Technically, this has been achieved by considering non-trivial saddle-point solutions before performing the disorder average. A perturbative RG analysis of the resulting effective field theory incorporates effects that would require non-perturbative methods within a more standard procedure. In the ferromagnetic case we have found that,
at least within our level of analysis, the previously found quantum critical behavior\textsuperscript{13} is stable with respect to local moment physics. The reason is an effective long-range interaction between the spin fluctuations that strongly suppresses fluctuations, stabilizing a Gaussian critical fixed point. In the antiferromagnetic case, however, we have found that the local moments destroy the previously found critical fixed point.\textsuperscript{13} To one-loop order, and for order parameter dimensionalities less than 4, no new fixed point exists and one finds runaway flow in all of physical parameter space. This may indicate either the absence of long-range order, or a transition that is not perturbatively accessible within our theory.

An important technical conclusion is that for quantum phase transitions, and within the framework of a replicated theory, rare regions can have a qualitative effect already at the level of a replica-symmetric theory, in contrast to the case of classical magnets.\textsuperscript{8} The ferromagnetic fixed point, which was found to be stable against the replica-symmetric quantum effects induced by the rare regions, is also stable against replica-symmetry breaking.

We have concentrated on the role of fluctuations about a non-trivial, but fairly crudely constructed, saddle-point solution of the field theory. It would also be interesting to study a somewhat more sophisticated saddle-point theory in more detail, and to determine the detailed properties of the Griffiths phase in such an approximation.

Finally, we mention that our methods are not specific to magnets, and can be applied to other quantum phase transitions as well. For instance, it is believed that for a complete understanding of the properties of doped semiconductors, and of the metal-insulator transitions observed in such systems, it is necessary to consider the effects of local moments.\textsuperscript{24,23,25} This can be studied with the methods developed in this paper.

ACKNOWLEDGMENTS

We are indebted to Ferdinand Evers for a collaboration in the early stages of this work. We also gratefully acknowledge helpful discussions with John Toner. This work was supported by the NSF under grant Nos. DMR-95-10185, DMR-96-32978, and DMR-98-70597, and by the DFG under grant No. SFB 393/C2.

APPENDIX A: A ONE-DIMENSIONAL SADDLE-POINT EQUATION

In this Appendix we discuss the saddle-point equation, Eq. (2.5), for a particular realization of the disorder potential $\delta t(x)$. In particular, we aim to show that the existence of a non-zero solution requires the width and depth of the potential well to be above a threshold, and that the non-zero solution lowers the free energy with respect to the zero one.

We first consider the one-dimensional counterpart of Eq. (2.5),
\begin{equation}
(t_0 + \delta t(x) - \partial_x^2) \phi(x) + g\phi^3(x) = 0 \ , \quad (A1)
\end{equation}
with a simple square well potential,
\begin{equation}
\delta t(x) = \begin{cases}
-V_0 & \text{for } 0 \leq x < a \\
0 & \text{elsewhere}
\end{cases} \ . \quad (A2)
\end{equation}

Standard methods lead to a solution inside the well ($0 \leq x < a$)
\begin{equation}
\phi_{\text{in}}(x) = \frac{\sqrt{v_1}}{g} \frac{\cn{\sqrt{v_2} x/2}}{\dn{\sqrt{v_2} x/2}} \ , \quad (A3a)
\end{equation}
where $\cn$ and $\dn$ are elliptic functions, and a solution outside of the well,
\begin{equation}
\phi_{\text{out}}(x) = \frac{\sqrt{v_0}}{g} \frac{2\sqrt{2} e^{-\sqrt{\pi} x} c}{c^2 e^{-2\sqrt{\pi} x} - 1} \ . \quad (A3b)
\end{equation}
Here
\begin{equation}
v_{2,1} = \alpha \pm \frac{\sqrt{\alpha^2 - 4\beta}}{2} \ , \quad (A4a)
\end{equation}
with
\begin{equation}
\alpha = 2(t_0 - V_0) \ . \quad (A4b)
\end{equation}
$c$ and $\beta$ are constants of integration that are determined by the requirement that the solution and its derivative be continuous at $x = a$. Other solutions exist, but the one given is the only one that satisfies physical boundary conditions. Furthermore, the physical solution exists only for
\begin{equation}
0 < \beta < \alpha^2/4 \ . \quad (A5)
\end{equation}

To demonstrate the existence of a threshold, we expand the above solution for small values of $v_{2,a}$. To leading order in this small parameter, we obtain for the constants of integration
\begin{equation}
c = \frac{1}{4} \sqrt{\frac{\pi}{t_0}} \sqrt{t_0} e^{\sqrt{\pi} v a} \ , \quad (A6a)
\end{equation}
and
\begin{equation}
\beta = \frac{\alpha^2}{4} - \frac{t_0}{2a^2} \ . \quad (A6b)
\end{equation}

From the condition for the existence of the physical solution, Eq. (A5), we see that $\alpha^2 v > 2t_0$ is a necessary and sufficient condition for the solution to exist, which is the desired threshold property.

The free energy in saddle-point approximation is simply given by the saddle-point action. It is physically plausible that the non-homogeneous solution constructed above leads to a negative free energy, and is thus energetically favorable compared to the zero solution. We have
ascertained this numerically for a large variety of well parameter values, and have found the inhomogeneous solution to lead to a negative free energy whenever it exists.

To solve the three-dimensional saddle-point equation, Eq. (2.5), is much harder. For spherically symmetric wells, $t_0 + \delta t(x) = t(r)$, with $r = |x|$, analytic solutions can still be found in closed form for special forms of the potential. By scaling $\phi$ and $t$, the equation can be written

$$\nabla^2 t(r) \phi(r) + \phi^3(r) = 0$$

(A7)

It is easy to show that for

$$t(r) = \frac{-2b}{(1 + br^3)^{1/3}} + \frac{4bc}{(1 + cr^2)^{1/2}} - \frac{2c}{(1 + cr^2)^{3/2}} - \frac{2b}{(1 + cr^2)^{1/2}} - \frac{8c^2}{(1 + cr^2)^2} - \frac{2b}{(1 + cr^2)^{1/2}}$$

(A8a)

the physical solution is given by

$$\phi(r) = \frac{a(1 + br^3) \exp(-br)}{(1 + cr^2)}$$

(A8b)

Here $a$, $b$, and $c$ are parameters that determine the shape of the well. In this case, the physical solution exists for all real values of the three parameters, but the form of the potential is such that the volume of the well cannot be smaller than some minimum value. This is the three-dimensional analog of the threshold behavior demonstrated above for the one-dimensional case. We have also solved the ODE, Eq. (A7), numerically for more general potential wells, and have found the same type of threshold behavior.

As in the 1-D case, physical arguments suggest, and numerical integration confirms, that the inhomogeneous solution leads to a lower free energy than the homogeneous one whenever the former exists. In Fig. 2 we show the solution and the corresponding potential well, Eqs. (A8), as a representative example of a locally ordered region in a 3-D system.

APPENDIX B: ISLAND SIZE DISTRIBUTIONS WITH A POWER-LAW TAIL

In Secs. III and IV we have assumed that the island correlation functions $D_{(m)}$ and $C_{(m)}$ are short-range correlated, i.e. have a scale dimension of $(m - 1)D$. Here we briefly discuss the extent to which one can relax this condition without changing our results.

Suppose that the island-size distribution is power-law correlated, leading to scale dimensions of the above correlation functions that are given by $(m - 1)(D - \alpha)$ with $\alpha > 0$. Let us consider the FM case first. The least irrelevant term, viz. Eq. (4.8b), remains irrelevant with respect to the Gaussian fixed point of Ref. 15 as long as $\alpha < D - 3\sqrt{2}$ (for $2 < D < 4$). The $D$-dependence of this result reflects the fact that for $D > 4$ the effective interaction ceases to be long-ranged, and an ordinary mean-field fixed point is stable. All higher order terms in the action are less relevant than the $w$-term.

In the AFM case, the $w$-term is relevant with respect to the conventional fixed point even for $\alpha = 0$. By power counting, we find the condition that none of the higher order terms become relevant as well, viz. $\alpha < D - 3$ for $D$ close to 4. Here the $D$-dependence reflects the fact that the coupling constant $w_0$ is marginal in $D = 3$ even for $\alpha = 0$, see Sec. III A.
APPENDIX C: STABILITY UNDER REPLICA SYMMETRY BREAKING

In this Appendix we briefly consider the effects of replica symmetry breaking (RSB). A generalization of our action, Eq. (2.19), analogous to Ref. 8 that allows for RSB is

\[ S_{\text{R}}[\phi^\alpha(x)] = \frac{1}{2} \sum_{\alpha} \int dx \, dy \, \phi^\alpha(x) \cdot \Gamma_0(x - y) \phi^\alpha(y) + u \sum_{\alpha} \int dx \, d\tau \, (\phi^\alpha(x, \tau) \cdot (\phi^\alpha(x, \tau)))^2 - \sum_{\alpha} \int dx \, d\tau \, d\tau' \times (\phi^\alpha(x, \tau) \cdot \phi^\alpha(x, \tau')) \cdot (\phi^\alpha(x, \tau') \cdot (\phi^\alpha(x, \tau))'). \]

(C1)

In Sec. II we had \( w_{\alpha\beta} \equiv w \), which resulted in a replica symmetric theory. Now we allow for 1-step RSB in Parisi’s hierarchical scheme, where \( w_{\alpha\beta} \) in the replica limit is parameterized by means of a step function with a parameter \( x_0 \),

\[ w(x) = \begin{cases} w & \text{for } 0 \leq x \leq 1 \\ w_1 & \text{for } x_0 < x \leq 1 \end{cases}. \]

(C2)

Defining \( \tilde{w} = w^{T^*} \) as before, and \( \tilde{w} = w_1, T^{\circ} \), we obtain the 1-loop flow equations

\[ \frac{du}{dt} = (\epsilon - 2\epsilon_\tau) u - 4(p + 8) u^2 + 48 u \Delta \tau, \]

\[ \frac{d\Delta}{dt} = \epsilon \Delta + 32 \Delta^2 - 8(p + 2) \Delta^2 + 8p \Delta \tilde{w} - 8p x_0 \Delta \tilde{w} + 8p \Delta \tilde{w}, \]

\[ \frac{d\tilde{w}}{dt} = (\epsilon - 2\epsilon_\tau) \tilde{w} + 4p \tilde{w}^2 - 8(p + 2) u \tilde{w} + 48 \Delta \tilde{w} - 4p(1 - x_0) \tilde{w}^2, \]

\[ \frac{d\tilde{w}}{dt} = (\epsilon - 2\epsilon_\tau) \tilde{w} + 48 \Delta \tilde{w} - 8(p + 2) u \tilde{w} + 8p \tilde{w}^2 + 8p(1 - x_0) \tilde{w}^2. \]

(C3a)

(C3b)

(C3c)

(C3d)

The replica symmetric case is recovered by putting \( x_0 = 1 \). We now perform a linear stability analysis of fixed point No. 8, with fixed-point values of \( u, \Delta \) and \( \tilde{w} \) as given in Table I, and \( \tilde{w} = 0 \). The first three eigenvalues are as shown in Table I, and the fourth one is \( \lambda_4 = \lambda_\tau = \lambda_\tau = (p - 4)(\epsilon_\tau + 4\epsilon_\tau)/2(10 - p) \). Fixed point No. 8 is therefore stable against 1-step RSB. Although the fixed point is unphysical for generic realizations of the disorder, as discussed in Sec. III, this is an interesting contrast to the classical case,\(^8\) where all fixed points are unstable against successive terms in the hierarchical RSB scheme.

---


11. J. Kisker and A.P. Young, cond-mat/9807025.


17. We will concentrate on rare fluctuations that lead to isolated regions of order within the disordered phase. Therefore, we take \( t_0 \) to be positive, and consider potentials with regions where \( t_0 + a(x) < 0 \).

18. This procedure is not necessary, but it is convenient. We have derived the same final results without using the subtraction of the saddle-point action.


20. Notice that the limit \( T \rightarrow 0 \) does not commute with the classical limit \( \epsilon \rightarrow 0 \). Therefore, the flow equations for the classical model can be recovered from Eqs. (3.5), but not

---

15
from Eqs. (3.6).
Quantum Coulomb glass within a Hartree-Fock approximation

Frank Epperlein, Michael Schreiber, and Thomas Vojta
Institut für Physik, Technische Universität, D-09107 Chemnitz, Germany
(Received 8 April 1997)

We study the influence of electron-electron interactions on the electronic properties of disordered materials. In particular, we consider the insulating side of a metal-insulator transition where screening breaks down and the electron-electron interaction remains long ranged. The investigations are based on the quantum Coulomb glass, a generalization of the classical Coulomb glass model of disordered insulators. The quantum Coulomb glass is studied by decoupling the Coulomb interaction by means of a Hartree-Fock approximation and exactly diagonalizing the remaining localization problem. We investigate the behavior of the Coulomb gap in the density of states when approaching the metal-insulator transition and study the influence of the interaction on the localization of the electrons. We find that the interaction leads to an enhancement of localization at the Fermi level. [S0163-1829(97)03634-5]

I. INTRODUCTION

The influence of electron-electron interactions on the electronic properties of disordered systems has reattracted a lot of attention recently. Already disorder alone can lead to a metal-insulator transition (MIT) by means of spatial localization of the electronic states at the Fermi energy. This MIT, called the Anderson transition, has been investigated extensively within the last two decades. While the qualitative features of the Anderson transition are well understood by now, the description remains inconsistent at a quantitative level. In particular, the critical behavior is not completely understood and the results of several methods do not agree.

Moreover, today it is generally assumed that the MIT in most experimental systems cannot be described by a model of noninteracting electrons since the Coulomb interaction between the electrons plays a crucial role. The metallic regime of the disordered interacting electron system is comparatively well understood, at least qualitatively. Altschuler and Aronov showed that the single-particle density of states (DOS) displays a nonanalyticity at the Fermi energy which was called the Coulomb anomaly. Later the perturbative treatment was extended into the whole metallic phase by means of a field-theoretic renormalization group method, which permits a qualitative discussion of the MIT including the identification of the different universality classes. However, quantitative results are very difficult to obtain from these methods. This is in particular so since the $e$ expansion which has to be used to extrapolate to the physical dimension $d = 3$ is highly singular.

Whereas investigations in the metallic phase can be carried out by means of established diagrammatic methods analogous studies of the insulating phase are not possible. That is because the natural reference system for a perturbation theory, viz. a system having disorder and interactions but no overlap between the states at different sites, is an interacting system and diagrammatic methods cannot be applied since Wick’s theorem does not hold. Instead, the insulating limit itself represents a challenging many-body problem. Almost three decades ago Pollak predicted an interaction-induced reduction of the single-particle DOS at the Fermi energy in disordered insulators. Later Efros and Shklovskii defined the prototype model of disordered electronic systems in the insulating limit, the classical Coulomb glass model. They showed that the zero-temperature single-particle DOS has a power-law gap at the Fermi energy which is called the Coulomb gap. This suggests the question whether Coulomb anomaly and Coulomb gap are manifestations of the same physical phenomenon on the metallic and insulating sides of the MIT, respectively. We will come back to this question in Sec. III. The physics of the classical Coulomb glass model has been investigated in much detail by several analytical and numerical methods and its static properties are comparatively well understood by now. In contrast, the nature of the transport mechanism is still controversially discussed.

Since experiments deep in the insulating regime are difficult to carry out most results on disordered insulators have been obtained from samples not too far away from the MIT. Here the (single-particle) localization length is still much larger than the typical distance between two sites and the description of the electrons in terms of classical point charges becomes questionable. Attempts to include the overlap between different states into the Coulomb glass model have been made earlier by mapping the problem onto a noninteracting model and applying the coherent-potential approximation. However, in this method neither disorder nor interactions are treated completely and different results obtained this way contradict each other. Recently, localization in an interacting disordered system was investigated by the numerical analysis of the many-body spectrum of small clusters from which the authors inferred a delocalizing influence of the interactions.

We note, that in addition to these works which deal with the ground-state properties of many-body systems possessing a finite particle density there has been a very active line of research concerning the behavior of just two interacting particles in a random environment. This type of work concentrates on special highly excited states of the two-electron system which will, in general, behave differently from the ground state at finite particle density.

In this paper we investigate the physics of the disordered
interacting electron problem (having finite particle density) on the insulating side of the MIT. In order to account for a finite overlap between the states we generalize the classical Coulomb glass model to a quantum model by including transfer matrix elements between different sites. We then study two main questions: (i) How does the single-particle DOS and, in particular, the Coulomb gap depend on the overlap between the states at different sites? (ii) How does the Coulomb interaction influence the localization of the electrons?

The paper is organized as follows: In Sec. II we define the quantum Coulomb glass model and explain our calculational method. In Sec. III we present the results for the single-particle DOS and discuss the behavior of the Coulomb gap. The localization properties and the resulting phase diagram of the MIT are considered in Sec. IV and Sec. V is devoted to some discussions and conclusions.

II. THE QUANTUM COULOMB GLASS MODEL

In the insulating limit the overlap between the electronic states at different sites can be neglected and the electrons behave like classical point charges. The generic model for this regime is the classical Coulomb glass model\(^7\) which consists of classical point charges in a random potential which interact via Coulomb interactions. The model is defined on a regular hypercubic lattice with \(N \equiv L^d\) (\(d\) is the spatial dimensionality) sites occupied by \(KN\) (spinless) electrons \((0 < K < 1)\). To ensure charge neutrality each lattice site carries a compensating positive charge of \(Ke\). The Hamiltonian of the classical Coulomb glass reads

\[
H_{cl} = \sum_i (\psi_i - \mu) n_i + \frac{1}{2} \sum_{ij} (n_j - K)(n_j - K)U_{ij}.
\]

Here \(n_i\) is the occupation number of site \(i\) and \(\mu\) is the chemical potential. The Coulomb interaction \(U_{ij} = e^2/\epsilon r_{ij}\) remains long ranged since screening breaks down in the insulating phase. We set the interaction strength of nearest-neighbor sites to 1 which fixes the energy scale. The random potential values \(\psi_i\) are chosen independently from a box distribution of width \(2W_o\) and zero mean.

Our goal is to describe the regime where the overlap between the states at different sites cannot be neglected but the system is still insulating. Therefore, we generalize the Coulomb glass model to a quantum Coulomb glass model by adding hopping matrix elements between nearest neighbors. The Hamiltonian of the quantum Coulomb glass is given by

\[
H = -t \sum_{\langle ij \rangle} (c_i^\dagger c_j + c_j^\dagger c_i) + H_{cl}.
\]

where \(c_i^\dagger\) and \(c_i\) are the electron creation and annihilation operators at site \(i\), respectively, and the sum runs over all pairs of nearest-neighbor sites. In the limit \(t \rightarrow 0\) the model (2) reduces to the classical Coulomb glass, for vanishing Coulomb interaction but finite overlap it reduces to the usual Anderson model of localization.

In order to calculate the electronic properties we decouple the Coulomb interaction by means of a Hartree-Fock approximation giving

\[
H_{HF} = -t \sum_{\langle ij \rangle} (c_i^\dagger c_j + c_j^\dagger c_i) + \sum_i (\psi_i - \mu)n_i + \frac{1}{2} \sum_{ij} n_i U_{ij} (n_j - K) - \sum_{ij} c_i^\dagger c_j U_{ij} c_j^\dagger c_i.
\]

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. [Note that in Eq. (3) several constant terms have been dropped.\(^{15}\)\(^{15}\) represents the expectation value with respect to the Hartree-Fock ground state which has to be determined self-consistently. In this way the quantum Coulomb glass is reduced to a self-consistent disordered single-particle problem which we solve by means of numerically exact diagonalization giving the single-particle energies \(\epsilon_n\) and states \(|\psi_n\rangle\).\(^{15}\)\(^{15}\) We note that the Hartree-Fock approximation is exact for both of the limiting cases mentioned above, viz. the classical Coulomb glass and the Anderson model of localization.

In this study we investigate three-dimensional (3D) quantum Coulomb glass systems with up to \(N = 10^3\) sites and band fillings \(K\) between 1/2 and 15/16. Due to the particle-hole symmetry of the Hamiltonian (2) this also covers the band fillings between 1/16 and 1/2. The disorder strength is fixed at \(W_o = 1\), and the overlap parameter \(t\) varies from zero (classical limit) up to \(t = 0.5\) which is above the MIT. In order to reduce the statistical error we average the results over 100 different configurations of the random potential \(\psi\).

III. SINGLE-PARTICLE DENSITY OF STATES

For several reasons, the single-particle DOS plays a special role in the investigation of the quantum Coulomb glass. First, it is the quantity investigated best for the classical Coulomb glass where it shows the well-known power-law Coulomb gap.\(^{13}\)\(^{13}\) One question we want to address in this section is whether the Coulomb gap remains intact in the presence of a small overlap. This question is of central importance for the justification of the classical model in experiments comparatively close to the MIT where the overlap between different impurity states cannot be neglected. Second, from field-theoretic studies on the metallic side of the MIT it was inferred\(^{17}\) that the single-particle DOS at the Fermi energy is the order parameter of the disorder-driven MIT in interacting systems. Thus it should remain zero in the whole insulating phase and start to increase when crossing the MIT point. Third, in the metallic phase the DOS should display the aforementioned Coulomb anomaly, a square-root nonanalyticity on top of a finite background.

In the context of the Hartree-Fock approximation the single-particle energies are simply given by the eigenvalues \(\epsilon_n\) of the self-consistent Hartree-Fock Hamiltonian (3). Thus, the single-particle DOS is defined by

\[
g(\epsilon) = \frac{1}{N} \sum_n \delta (\epsilon - \epsilon_n).
\]

Our numerical results for the single-particle DOS of the quantum Coulomb glass are comprised in Figs. 1 and 2. Note that the Hamiltonian is particle-hole symmetric for \(K = 0.5\).\(^{15}\)\(^{15}\)
Quantum Coulomb glass within the Hartree-Fock approximation

(Fig. 1). Thus the Fermi energy does not depend on $t$. For $K = 0.75$, in contrast, the Fermi energy increases with $t$, and the shift of the gap position in Fig. 2 exactly matches the shift of the Fermi energy.

In order to address the questions raised at the beginning of this section we study the behavior of the DOS close to the Fermi energy. Let us first discuss our expectations: In the insulating phase the electrons are localized and cannot screen the Coulomb interaction. Consequently, the Hartree part of the DOS becomes small and short ranged. In the insulating phase we can therefore apply a generalization of the Efros-Shklovskii argument to discuss the behavior of the leading terms of the DOS: The original argument\textsuperscript{7,8} shows that an empty state $i$ with an energetic distance smaller than $\delta$ must have a spatial distance larger than $e^\delta/\delta$ since the change $\Delta = e_i - e_j - e^\delta r_{ij}$ of the system energy when moving the electron from $i$ to $j$ must be positive in the many-body ground state. If finite overlaps between different sites are included the electrons become somewhat delocalized and therefore the interaction is screened on short length scales of the order of the localization length. In contrast, the long-range part of the interaction remains unchanged. Since the DOS close to the Fermi energy is determined by the long-range tail of the interaction we expect it to remain unchanged as long as the electrons are localized. However, the region of small and short ranged. In the insulating phase we can therefore apply a generalization of the Efros-Shklovskii argument to discuss the behavior of the leading terms of the DOS: The original argument\textsuperscript{7,8} shows that an empty state $i$ with an energetic distance smaller than $\delta$ must have a spatial distance larger than $e^\delta/\delta$ since the change $\Delta = e_i - e_j - e^\delta r_{ij}$ of the system energy when moving the electron from $i$ to $j$ must be positive in the many-body ground state. If finite overlaps between different sites are included the electrons become somewhat delocalized and therefore the interaction is screened on short length scales of the order of the localization length. In contrast, the long-range part of the interaction remains unchanged. Since the DOS close to the Fermi energy is determined by the long-range tail of the interaction we expect it to remain unchanged as long as the electrons are localized. However, the region of

validity of the classical result shrinks to zero with increasing delocalization and vanishes when the electronic states become extended. Thus the Coulomb gap should become narrower with increasing $t$ and vanish at the MIT.

On the other hand, with increasing delocalization of the electrons the exchange interaction becomes larger and longer ranged. Since the exchange interaction is responsible for the Coulomb anomaly\textsuperscript{17} we expect the DOS to show a crossover from the Coulomb gap behavior to a Coulomb anomaly behavior. To be precise, if the system is close to the MIT but still insulating the DOS should show Coulomb-gap-like behavior in a narrow interval around the Fermi energy and Coulomb-anomaly-like behavior for energies a bit away from the Fermi level.

In Fig. 3 we present a log-log plot of the single-particle DOS in the Coulomb gap region for the system with band filling $K = 0.5$. The data presented are compatible with the above expectations. For small $t$ we find a power-law behavior with an exponent close to 2 as expected for the Coulomb gap in 3D. With increasing $t$ the exponent becomes smaller and approaches 0.5 as expected for the Coulomb anomaly (if the constant background is small). We are, however, not able to explicitly demonstrate the crossover from the Coulomb gap to the Coulomb anomaly at fixed $t$ as a function of energy. The main reason is that the investigation of the DOS very close to the Fermi energy is hampered by strong finite-size effects. The usual problem, viz. that a finite system always possesses a discrete spectrum, is made worse by the long-range character of the interaction. Since the maximum system size considered here is $L = 10$ the Coulomb interaction is effectively cut off at distances $r_{ij} \sim 10$ which corresponds to $U_{ij} \sim 0.1$. Thus the results for energies smaller than $\epsilon \sim 0.1$ are not reliable.

IV. LOCALIZATION PROPERTIES

The usual criteria for localization are defined for noninteracting electrons only, and their generalization to many-body systems is not straightforward. Within the Hartree-Fock approximation, however, we do obtain effective single-
A. Participation number

One of the simplest measures to study the localization properties is the participation number $P$ which describes how many sites are effectively occupied by a single-particle state $|\psi_i\rangle$. Thus the inverse participation number measures the degree of localization. It is defined as the second moment of the spatial probability distribution of the state

$$P^{-1}_v = \frac{1}{N} \sum_i |\langle \psi | i \rangle|^4,$$

where the sum runs over all sites $i$. In practice it is often averaged over all states with a certain energy $e$

$$P^{-1}(e) = \frac{1}{g(e)} \frac{1}{N} \sum_{\epsilon} P^{-1}_v \delta(e - \epsilon_v).$$

In Figs. 4 and 5 we show the results for the inverse participation numbers of systems with $N=8^3$ sites and band filling factors of $K=0.5$ and 0.75, respectively. The most remarkable feature of these results is the strong enhancement of $P^{-1}$ close to the Fermi energy which can be as large as one order of magnitude (note the logarithmic scale in the figures). This enhancement of $P^{-1}$ corresponds to a much stronger localization at the Fermi level compared to the rest of the band. It is a direct consequence of the Coulomb gap in the DOS which means a reduction of the number of states that can be hybridized by a certain overlap $t$. Based on this argument it is also easy to understand how the enhancement depends on the overlap $t$: For very small $t$ all states remain strongly localized so that there is no room for a large enhancement. The largest enhancement is obtained for moderate values of $t$ which are still smaller than the width of the Coulomb gap. In this case the states away from the Fermi level are considerably delocalized while the hybridization at the Fermi energy is still hampered. For overlaps $t$ larger than the width of the Coulomb gap hybridization becomes easier also at the Fermi level and thus the enhancement of $P^{-1}$ is diminished. Note that in contrast to noninteracting electrons the participation numbers depend on the band filling since the electronic states are influenced by the interaction with the other electrons.

A comparison (see Fig. 6) of the inverse participation numbers of the quantum Coulomb glass and of noninteracting electrons shows that close to the Fermi energy the electrons of the interacting system are more strongly localized than noninteracting electrons.

Although the inverse participation number is a useful quantity to study qualitative features of localization it is not well suited to quantitatively determine the MIT and its properties. The reason is that determining the MIT from the participation numbers amounts to detecting changes in the size dependence of $P^{-1}$ which is much harder than detecting changes of $P^{-1}$ itself. ($P$ should remain finite for $N \rightarrow \infty$ for localized states but scale with $N$ for extended states.) We therefore use a different method based on the properties of the eigenvalue spectrum of the Hamiltonian which is explained in the following subsection.

B. Level statistics

The mobility edge, i.e., the energy that separates extended from localized states, can be found by using the statistical properties of the energy levels as was done for the Anderson model of localization. In this method the distribution $P$ of nearest-neighbor level spacings $s$ of the (unfolded) spec-
trum of eigenvalues \( \varepsilon_i \) is considered. In accordance with the
literature we use the notation \( P(s) \) for this distribution, it
should not be confused with the participation number \( P \) dis-
cussed in Sec. IV A. At the MIT the level spacing distribution
function displays a sharp transition from the Poisson
ensemble to GOE has to be described quantitatively. Following
Ref. 19 we fit the numerically obtained distributions
\( s \) to the phenomenological formula

\[
P_{\text{ph}}(s) = A s^\beta (1 + C s^\beta)^{1/\beta} \exp \left[ -\frac{\pi^2}{16} \beta s^2 - \frac{\pi}{4} (2 - \beta)s \right]
\]

with \( f(\beta) = 2^\beta (1 - \beta/2)/\beta - 0.16874 \). This formula interpo-
lates smoothly between PE and GOE. It contains only a
single free parameter since the first two moments of the level
spacing distribution \( P(s) \) are normalized:

\[
\int ds P(s) = \int ds s P(s) = 1.
\]

We then study the dependence of the fit parameters \( A, C, \)
and \( \beta \) on the single-particle energy \( s \) and overlap strength \( t \).
The parameter \( \beta \) shows a particular strong dependence close
to the mobility edge. From Ref. 19 it is known that the criti-
cal ensemble corresponds to \( \beta = 0.875 \) which we use as a
criterion to determine the transition point. The resulting de-
pendence of the mobility edge on energy and overlap is pre-
sented in Figs. 8 and 9. Close to the Fermi energy the mo-
bility edge is shifted to larger overlaps (or, equivalently,
smaller disorder), so the location of the mobility edge also
reflects the enhancement of localization at the Fermi energy.

C. Metal-insulator transition

In a system of noninteracting electrons the states and en-
ergy levels do not depend on the filling of the band. Chang-
ing the filling factor simply leads to a shift of the Fermi
energy within the otherwise unchanged band. When the
Fermi energy crosses the (fixed) mobility edge the system
undergoes a MIT. In a system of interacting electrons, how-
ever, the mobility edge changes with filling factor \( K \). There-
fore, separate calculations have to be done for different fill-
ing factors to determine the phase diagram. The MIT occurs
when the states at the Fermi energy delocalize (or localize).
This means that Figs. 8 and 9 yield only one data point each
for the phase boundary. We have carried out the correspon-
ding calculations for filling factors \( K = 7/8 \) and 15/16, too. The
resulting phase diagram of the MIT is displayed in Fig. 10
and compared to the analogous phase diagram for the Anderson
model of localization.\(^{21}\) We find that the phase boundary
of the quantum Coulomb glass is shifted to significantly
larger values of the overlap \( t \) compared to noninteracting
electrons if the Fermi energy is well within the band. As
discussed above this is a direct consequence of the Coulomb
gap in the single-particle DOS. For band fillings almost up to
FIG. 10. Phase diagram of the MIT of the quantum Coulomb glass and the Anderson model for $W_{0} = 1$. The lines are guides to the eyes only.

$K = 1$ the critical $t$ of the quantum Coulomb glass remains nearly unchanged since the form of the Coulomb gap does not depend on its position in the band whereas the critical $t$ of the Anderson model is reduced because the DOS of the Anderson model decreases near the band edges.

V. CONCLUSIONS

To summarize, we have investigated the combined influence of disorder and interactions on the properties of electronic systems on the insulating side of the MIT. Our work is based on the quantum Coulomb glass model. We have decoupled the interaction by means of the Hartree-Fock approximation and numerically diagonalized the remaining disordered single-particle problem. The resulting single-particle DOS shows a Coulomb gap in the whole insulating phase which becomes narrower when approaching the MIT. The reduced DOS at the Fermi energy leads to an enhancement of localization compared to the rest of the band and also compared to noninteracting electrons.

In this concluding section we will discuss some aspects of the results that have not yet been covered. First, we want to discuss the justification of the Hartree-Fock approximation. On a qualitative level, there are several possible influences of the Coulomb interaction on Anderson localization with competing effects. On the one hand, the Coulomb interaction leads to a reduction of the density of states at the Fermi energy which enhances localization. This process is contained in the Hartree-Fock approximation as is discussed in Sec. III and as we have demonstrated in this paper. On the other hand, one may argue that any interaction leads to transitions between the states of the noninteracting system thus giving the electrons additional hopping possibilities and reducing localization. This second point is not well described within the Hartree-Fock approximation. We have therefore started to compare the results of this paper to that of exact diagonalizations of small lattices. Preliminary results show that the large enhancement of localization at the Fermi level is also found by the exact diagonalizations while the average degree of localization in the band is overestimated by the Hartree-Fock approximation in some parameter regions. Further studies along these lines are in progress. We also note that, as is well known, the Hartree-Fock approximation of the 3D homogeneous interacting electron system produces an artificial soft gap at the Fermi energy since screening is not treated properly. Although this artificial gap is much narrower ($g = 1/\ln(\epsilon - \epsilon_{F})$) than the Coulomb anomaly, and thus difficult to observe, the results for the DOS on the metallic side of the MIT may be influenced and more sophisticated investigations will have to be carried out.

Second, we want to comment on the relation between Coulomb gap in the insulating phase and Coulomb anomaly in the metallic phase. It has been suggested that both are different manifestations of the same physical phenomenon. However, the Coulomb gap is a result of the Hartree part of the interaction and its existence is tied to the long-range nature of the Coulomb interaction. In contrast, the Coulomb anomaly is produced by the exchange interaction and arises independently of the range even for pointlike interactions. Therefore a system with a short-range model interaction will display a Coulomb anomaly but not a Coulomb gap. Further work is necessary to clarify how the Coulomb anomaly changes to the Coulomb gap at the MIT (in the case of long-range interactions) or how it vanishes on the insulating side for short-range interactions.

Note added in proof. The idea that the electron-electron interaction may cause an additional localization of the states with energies far enough from the Fermi level was discussed by I. L. Aleiner and B. I. Shklovskii, J. Mod. Phys. B 8, 801 (1994).

ACKNOWLEDGMENTS

This work was supported in part by the DFG under Grant Nos. SFB 393, Schr231/13-1, and Vo659/1-1.

12G. Vignale, Y. Shinozuka, and W. Hanke, Phys. Rev. B 34, 3003
Quantum Coulomb glass within the Hartree-Fock approximation


15 Similar approaches have been used earlier to study the formation of local moments; M. Milovanovic, S. Sachdev, and R. N. Bhatt, Phys. Rev. Lett. 63, 82 (1989); and the properties of persistent currents, G. Bouzerar and D. Poilblanc, Phys. Rev. B 52, 10 772 (1995); J. Phys. I 7, 877 (1997).


Quantum Coulomb Glass: Anderson Localization in an Interacting System

T. Vojta\(^1\) (a, b), F. Epperlein (b), and M. Schreiber (b)

\(^1\) Materials Science Institute, University of Oregon, Eugene, OR 97403, USA
(b) Institut für Physik, Technische Universität, D-09107 Chemnitz, Germany

(Received August 19, 1997)

The quantum Coulomb glass model describes disordered interacting electrons on the insulating side of a metal–insulator transition. By taking quantum fluctuations into account it can describe not only the localized limit but also the weakly localized regime. We discuss several possibilities to generalize the concept of Anderson localization to interacting electron systems such as the quantum Coulomb glass and define criteria for localization. The corresponding physical quantities are calculated by numerically exact diagonalization. The results indicate that single-particle excitations close to the Fermi energy become more strongly localized under the influence of interaction.

**Introduction.** Disordered interacting electronic systems such as semiconductor impurity bands or granular metals have attracted a large amount of theoretical and experimental interest [1]. Even the presence of disorder or interaction alone leads to interesting phenomena, and the competition between the two gives rise to a very rich behavior. The single-electron states in non-interacting systems become localized in space for strong enough disorder. This phenomenon is called Anderson localization [2]; it is responsible for the metal–insulator transition in non-interacting systems. The generalization of this concept to interacting systems is not straightforward since many-particle physical properties cannot in general be derived from single-particle properties. Consequently, a definition of localization in many-particle systems will not be unique. In this paper we therefore consider several possibilities to generalize the concept of Anderson localization to interacting systems and discuss their relative merits. As an example we then apply the resulting localization criteria to the quantum Coulomb glass model of disordered insulators and calculate the corresponding physical quantities by numerically exact diagonalization.

The paper is organized as follows: In the second section we motivate and define the quantum Coulomb glass model. The third section is devoted to a discussion of Anderson localization in interacting systems and the presentation of our results. The fourth section contains some discussions and conclusions.

**From Classical to Quantum Coulomb Glass.** Almost the entire current understanding of disordered insulators has been obtained from studying the insulating limit where the electrons are completely localized and can thus be described as classical point

\(^1\) Corresponding author: Phone: +49.371.15313147; Fax: +49.371.15313143; e-mail: vojta@physik.tu-chemnitz.de
charges (we will denote this regime as the classical insulating regime from now on). Although it is not a quantum mechanical system, the classical disordered insulator is a complicated many-body problem. Pollak [3] predicted an interaction-induced reduction of the single-particle DOS at the Fermi energy in disordered insulators. Later Efros and Shklovskii [4] defined the generic model of the classical insulating regime, the classical Coulomb glass model which consists of point charges in a random potential which interact via Coulomb interactions. The model is defined on a regular hypercubic lattice with $N = L^d$ ($d$ is the spatial dimensionality) sites occupied by $KN$ (spinless) electrons ($0 < K < 1$). To ensure charge neutrality each lattice site carries a compensating positive charge of $Ke$. The Hamiltonian of the classical Coulomb glass reads

$$H_d = \sum_i (\varphi_i - \mu) n_i + \frac{1}{2} \sum_{i \neq j} (n_i - K)(n_j - K) U_{ij}.$$  

Here $n_i$ is the occupation number of site $i$ and $\mu$ is the chemical potential. The Coulomb interaction $U_{ij} = e^2/\varepsilon r_{ij}$ remains long-ranged since screening breaks down in the insulating phase. We set the interaction strength of nearest neighbor sites to 1 which fixes the energy scale. The random potential values $\varphi_i$ are chosen independently from a box distribution of width $2W_0$ and zero mean. The physics of the classical Coulomb glass model has been investigated by several analytical and numerical methods and its properties are comparatively well understood by now [6] although the nature of the transport mechanism is still controversially discussed [7]. One of the remarkable features is the power-law gap in the zero-temperature single-particle density of states (DOS) which is called the Coulomb gap [4, 5].

Since experiments deep in the insulating regime are difficult to carry out most results on disordered insulators have been obtained from samples not too far away from the metal–insulator transition [8]. Here the (single-particle) localization length is still much larger than the typical distance between two sites and the description of the electrons in terms of classical point charges becomes questionable. In order to investigate the influence of finite overlaps between the states on the properties of the insulating phase we have defined [9] the quantum Coulomb glass model, the minimal model of the “quantum insulating regime” which accounts for disorder, long-range interactions and the quantum nature of the electrons. It is obtained from the classical Coulomb glass by adding hopping matrix elements of strength $t$ between nearest neighbors. The Hamiltonian of the quantum Coulomb glass reads

$$H = -t \sum_{\langle ij \rangle} (c_i^\dagger c_j + c_j^\dagger c_i) + H_d,$$

where $c_i^\dagger$ and $c_i$ are the electron creation and annihilation operators at site $i$, respectively, and the sum runs over all pairs of nearest neighbor sites. In the limit $t \to 0$ the model (2) reduces to the classical Coulomb glass, for vanishing Coulomb interaction but finite overlap it reduces to the usual Anderson model of localization.

**Localization in an Interacting System.** It has been known for a long time [10] that disorder leads to spatial localization of single-particle states in a non-interacting system. This phenomenon is called Anderson localization [2]. Since a system with localized states at the Fermi level is insulating, the transition between delocalized and localized states corresponds to a metal–insulator transition. There is, however, much experimental and
theoretical evidence that a description of disordered electronic systems in terms of non-interacting particles is inadequate. For this reason one would like to apply the concept of localization to interacting systems. Unfortunately, a direct generalization of the non-interacting case is not possible since single-particle states are not defined in an interacting system while the many-particle states always correspond to extended charge distributions. The deeper reason for these difficulties is, of course, that in a non-interacting system the many-particle properties are completely determined by the single-particle properties whereas the same is not true for interacting systems. Therefore, in a many-particle system one can consider several types of “localization” (for single-particle or different many-particle excitations) which are all unrelated a priori. In this section we discuss some of these ideas and we also present results for the corresponding physical quantities of a two-dimensional quantum Coulomb glass.

From an experimental point of view the most natural quantity to consider is probably the conductance since it is easily measurable and its behavior determines whether the system is metallic or insulating. However, since the conductance is given by a two-particle Green’s function and involves complicated zero-temperature and zero-frequency limits it is difficult to calculate numerically.\(^{2}\)

In the following we concentrate on single-particle localization which is the most direct generalization of Anderson localization to many-body systems. Experimentally, single-particle localization should be reflected in the tunneling response of the system rather than in transport coefficients.

The simplest measure of Anderson localization for a single-particle state \(|n\rangle\) is the participation number \(P\), defined as the inverse second moment of the spatial probability distribution,

\[
P_n^{-1} = \sum_j |\langle n | j \rangle|^4,
\]

where the sum runs over all sites \(j\). In practice it is often averaged over all states with a certain energy \(\varepsilon\),

\[
P^{-1}(\varepsilon) = \frac{1}{g(\varepsilon)} \frac{1}{N} \sum_n P_n^{-1}\delta(\varepsilon - \varepsilon_n).
\]

A consistent generalization of this quantity to interacting systems should fulfill at least the following conditions: (i) it should be well defined for any many-particle state and (ii) it should reduce to (4) for non-interacting electrons. Moreover, the desired quantity should (iii) capture the physical idea of spatial localization and (iv) it should be easy to calculate.

It has been suggested to define localization in a many-particle system via the spatial distribution of the charge difference between the states of the same many-particle system with \(N\) and \(N + 1\) particles, respectively. While this quantity fulfills the above conditions (i), (ii), and (iv) it turns out that it is not a useful measure of localization in a disordered interacting system. The reason is that adding an extra electron to a disordered interacting system will very often not only add some charge at a couple of sites

\(^{2}\) There is a relation between the conductance and the sensitivity of the ground state energy to twisted boundary conditions, see [11], which can be used to calculate the conductance numerically. In dimensions larger than one, however, this method comes with problems of its own.
but completely rearrange the distribution of all electrons due to the frustration introduced by the competition between disorder and interaction. Thus simply calculating the participation number of the extra charge leads to an overestimation of delocalization. This can already be seen at the example of the classical Coulomb glass where we know that the electrons are completely localized. Nevertheless the ground states of systems with \( N \) and \( N + 1 \) particles can be drastically different so that the charge difference between the two is distributed on more than one site, effectively giving a participation number larger than one. In general, the method will always fail, if adding an extra electron leads to a decrease of the charge at some particular site since then the charge density difference is not a proper probability distribution anymore (see Fig. 1).

There is, however, another quantity which fulfills conditions (i), (ii), and (iii) for a generalization of the inverse participation number. In particular, it nicely captures the physical idea of localization. This quantity is the probability \( R_p \) for an electron to return to its starting site in infinite time. The energy-dependent return probability can be expressed in terms of single-particle Greens functions,

\[
R_p(\epsilon) = \frac{1}{N} \sum_{\mathbf{r}} \lim_{\delta \to 0} \frac{\delta}{\pi} G_{\mathbf{r}}(\epsilon + i \delta) G_{\mathbf{r}}(\epsilon - i \delta) .
\]

(5)

For non-interacting electrons \( P^{-1}(\epsilon) = R_p(\epsilon) \). We note, however, that calculating \( R_p \) requires the knowledge of all eigenstates of the Hamiltonian which makes this quantity numerically expensive. In Fig. 2 we show the numerically determined return probabilities of the quantum Coulomb glass and the Anderson model. The two systems behave very differently. For the Anderson model we obtain the well-known behavior of \( P^{-1}(\epsilon) \), viz. a minimum in the band center and higher values in the tails. In the quantum Coulomb glass the return probability has a maximum at the Fermi energy and decreases quickly with increasing distance from the Fermi energy. Thus we conclude that in the quantum Coulomb glass single-particle excitations away from the Fermi energy tend to delocalize while the excitations close to the Fermi energy which dominate the low-temperature

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{6_7_particles}
\caption{Comparison of the ground states of quantum Coulomb glasses with 6 and 7 particles. The size of the circles is proportional to the charge density at the site. Note that adding an extra electron reduces the charge density at the site marked by an arrow.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{return_probability}
\caption{Return probability for a quasiparticle in the quantum Coulomb glass (\( \square \)) and the Anderson model (\( \bullet \)) on a \( 3 \times 4 \) lattice, \( t = 0.3 \), \( W_0 = 1 \), \( K = 0.5 \).}
\end{figure}
Quantum Coulomb Glass: Anderson Localization in an Interacting System

physics tend to localize (note that the opposite was suggested in [13]). We have investigated the value of $R_p$ close to the Fermi level for different values of the overlap $t$. In Fig. 3 we show the resulting dependence and the corresponding data for the Anderson model. The figure shows that for $t > 0.1$ the interactions lead to stronger localization in agreement with the results of our Hartree-Fock calculation [9]. For $t = 0.1$, quantum Coulomb glass and Anderson model show identical behavior. Therefore, we cannot exclude that for very small $t$, the behavior may turn around, i.e., the interactions may favor delocalization, see [12] and the discussion of Fock space localization below.

The return probability discussed above deals with the localization of a single quasiparticle. As already mentioned, in an interacting system many-particle properties cannot in general be derived from single-particle ones. Therefore, to get a complete understanding of the localization properties one has to investigate many-particle quantities, too.\footnote{There has been a very active line of research considering the localization of just two interacting electrons. While this is not a many-particle problem, it tries to capture essential aspects of the interplay of localization and interactions [14].} One approach which is in some sense complementary to the study of the return probability is to analyze the localization properties of the many-particle states with respect to a Fock-space basis set $\{|\alpha\rangle\}$. Here the central quantity is the Fock-space participation number $P_F$ of a many-body state $|\psi\rangle$ which is given by

$$P_F^{-1}(\psi) = \sum_a |\langle \alpha | \psi \rangle|^2.$$  

If we chose the Fock-space basis to consist of Slater determinants of site basis functions, $|\alpha\rangle = c_1^\dagger \cdots c_j^\dagger |0\rangle$, then $P_F = 1$ for completely localized electrons and $P_F > 1$ if the electrons can move. A measure like this has already been used to characterize the influence of long-range interactions on Anderson localization [12]. In Fig. 4 we present our results for the Fock-space participation numbers of the quantum Coulomb glass and the Anderson model. The data show the same tendency as the return probabilities at the Fermi level (Fig. 3): For larger overlap $t$ the interactions lead to stronger localization while for small $t$ we cannot find a statistically significant difference between the quantum Coulomb glass and the Anderson model. Thus, a change in the behavior at very small $t$ cannot be excluded. This would resolve the seeming disagreement with [12], where Fock-space localization in a related model was investigated for very small overlaps, and the authors found a delocalizing influence of the interactions. We note that, in principle, the concept of localization in Fock space can be applied to any problem in which the Hamiltonian can be decomposed into a reference part and a perturbation. Delocalization in Fock space then describes how the perturbation mixes the original eigenstates. In a recent letter [15] this concept has been applied to explain the transition in the width of excited states measured in tunneling conductance experiments in quantum dots [16].

Let us further mention that the localization transitions discussed above also lead to transitions of the statistics of the corresponding energy levels [9, 12, 17, 18]. Analyzing the transitions of the level statistics is often numerically easier than dealing with the electron states themselves.

\textbf{Conclusions.} In this paper we have discussed the generalization of Anderson localization to interacting systems. We first have considered the localization of single-particle
Quantum Coulomb Glass: Anderson Localization in an Interacting System

physics tend to localize (note that the opposite was suggested in [13]). We have investigated the value of $R_p$ close to the Fermi level for different values of the overlap $t$. In Fig. 3 we show the resulting dependence and the corresponding data for the Anderson model. The figure shows that for $t > 0.1$ the interactions lead to stronger localization in agreement with the results of our Hartree-Fock calculation [9]. For $t = 0.1$, quantum Coulomb glass and Anderson model show identical behavior. Therefore, we cannot exclude that for very small $t$, the behavior may turn around, i.e., the interactions may favor delocalization, see [12] and the discussion of Fock space localization below.

The return probability discussed above deals with the localization of a single quasiparticle. As already mentioned, in an interacting system many-particle properties cannot in general be derived from single-particle ones. Therefore, to get a complete understanding of the localization properties one has to investigate many-particle quantities, too.\[^3\] A complementary approach which is in some sense complementary to the study of the return probability is to analyze the localization properties of the many-particle states with respect to a Fock-space basis set \$\{ |\alpha\rangle \}$. Here the central quantity is the Fock-space participation number $P_F$ of a many-body state $|\psi\rangle$ which is given by

$$P_F^{-1}(\psi) = \sum_a |\langle \alpha | \psi \rangle|^4.$$  

(6)

If we chose the Fock-space basis to consist of Slater determinants of site basis functions, $|\alpha\rangle = c_i^\dagger \ldots c_j^\dagger |0\rangle$, then $P_F = 1$ for completely localized electrons and $P_F > 1$ if the electrons can move. A measure like this has already been used to characterize the influence of long-range interactions on Anderson localization [12]. In Fig. 4 we present our results for the Fock-space participation numbers of the quantum Coulomb glass and the Anderson model. The data show the same tendency as the return probabilities at the Fermi level (Fig. 3): For larger overlap $t$ the interactions lead to stronger localization while for small $t$ we cannot find a statistically significant difference between the quantum Coulomb glass and the Anderson model. Thus, a change in the behavior at very small $t$ cannot be excluded. This would resolve the seeming disagreement with [12], where Fock-space localization in a related model was investigated for very small overlaps, and the authors found a delocalizing influence of the interactions. We note that, in principle, the concept of localization in Fock space can be applied to any problem in which the Hamiltonian can be decomposed into a reference part and a perturbation. Delocalization in Fock space then describes how the perturbation mixes the original eigenstates. In a recent letter [15] this concept has been applied to explain the transition in the width of excited states measured in tunneling conductance experiments in quantum dots [16].

Let us further mention that the localization transitions discussed above also lead to transitions of the statistics of the corresponding energy levels [9, 12, 17, 18]. Analyzing the transitions of the level statistics is often numerically easier than dealing with the electron states themselves.

**Conclusions.** In this paper we have discussed the generalization of Anderson localization to interacting systems. We first have considered the localization of single-particle

\[^3\] There has been a very active line of research considering the localization of just two interacting electrons. While this is not a many-particle problem, it tries to capture essential aspects of the interplay of localization and interactions [14].
excitations which can be described in terms of the return probability $R_{\gamma}$. Experimentally, this quantity should be reflected in the tunneling response of the system. We have also discussed the concept of Fock-space localization for disordered interacting electron systems. As an example we have presented some numerical results for the quantum Coulomb glass model of disordered insulators. In this concluding section we will discuss some aspects that have not yet been covered. First, the quantum Coulomb glass is a model of spinless particles. In one-dimensional systems there is, however, some evidence that the electron spin plays an important role in determining the behavior of interacting disordered electrons [19]. Therefore, in order to describe real electrons, including the spin into the quantum Coulomb glass will be necessary in the future. Second, our numerical examples were for very small lattice sizes. In order to quantitatively analyze the behavior of disordered interacting electrons we have to extend the calculations to larger lattices. This can either be done by making approximations such as Hartree-Fock [9] or by developing better numerical algorithms. Third, one of the main tasks of the future will be to establish relations, if any, between the different types of localization and between the different quantities discussed here.

Acknowledgement. This work was supported in part by the DFG under grant Nos. Schr231/13-1, Vo659/1-1 and SFB393 and by the NSF under grant No. DMR-95-10185.

References
Quantum Coulomb Glass: Anderson Localization in an Interacting System


Quantum Coulomb Glass – Hartree-Fock Approximation versus Exact Diagonalization

F. Epperlein (a), M. Schreiber (a), and Th. Vojta1) (a, b)

(a) Institut für Physik, Technische Universität, D-09107 Chemnitz, Germany
(b) Materials Science Institute, University of Oregon, Eugene, OR 97403, USA

(Received August 19, 1997)

We investigate the behavior of disordered interacting electrons in the insulating regime. Our study is based on the quantum Coulomb glass model which is obtained from the classical Coulomb glass by adding hopping matrix elements between neighboring sites. We use two different numerical methods, viz. a Hartree-Fock approximation and an exact diagonalization and compare the results for the tunneling density of states and the localization properties in order to determine the range of validity of the Hartree-Fock method. We find that the Hartree-Fock method gives a good approximation for the density of states for all energies but represents the localization properties correctly close to the Fermi level only. Some consequences for the localization of disordered interacting electrons are discussed.

The physics of disordered interacting electrons has been a subject of great interest within the last two decades. Most work, both experimental and theoretical has concentrated on the metallic regime where experiments are easier to carry out and theoretical studies can be based on established perturbative methods, for a review, see e.g. [1]. In comparison, the insulating regime has seen much less activities. Experimentally, this is due to the fact that transport properties vanish in an insulator at zero temperature. On the theoretical side, the main reason is that perturbative methods cannot be applied since the insulating (classical) limit [2, 3] itself is a complicated many-particle problem. The prototype model in the classical insulating regime is the Coulomb glass model (for reviews, see, e.g. [4]) which describes the electrons as classical point charges.

Recently, the attention has focused on the quantum insulating regime closer to the metal–insulator transition (MIT) where the description in terms of classical point charges becomes questionable. These new studies try to address two main problems: (i) one wants to gain an understanding of the MIT itself by approaching it from the insulating side which is complementary to the usual approach based on perturbation theory around the metallic system; (ii) one wants to know whether the key properties of the insulating limit as, e.g., the Coulomb gap in the single-particle density of states (DOS) [3], carry over to the regime close to the MIT where most of the experiments on insulators are performed.

The prototype model for the quantum insulating regime is the quantum Coulomb glass model [5, 6] (a related model has been investigated by Talmantes et al. [7]). It is defined on a regular hypercubic lattice with \( N = L^d \) (\( d \) is the spatial dimensionality).

1) Contact information: Phone: +493715313147; Fax: +493715313143; e-mail: vojta@physik.tu-chemnitz.de
sites occupied by $KN$ (spinless) electrons ($0 < K < 1$). To ensure charge neutrality each lattice site carries a compensating positive charge of $Ke$. The Hamiltonian of the quantum Coulomb glass is obtained from the classical Coulomb glass by adding hopping terms of strength $t$ between nearest neighbor sites. It reads

$$H = -t \sum_{\langle ij \rangle} (c_j^\dagger c_i + c_i^\dagger c_j) + \sum_i (q_i - \mu) n_i + \frac{1}{2} \sum_{i \neq j} (n_i - K) (n_j - K) U_{ij},$$

(1)

where $c_j^\dagger$ 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. $n_i$ is the occupation number of site $i$ and $\mu$ is the chemical potential. The Coulomb interaction $U_{ij} = e^2/r_{ij}$ remains long-ranged since screening breaks down in the insulating phase. The random potential values $q_i$ are chosen independently from a box distribution of width $2W_0$ and zero mean.

In a previous paper [5] we have investigated the quantum Coulomb glass by means of a Hartree-Fock (HF) approximation. Within this method the interaction was treated at HF level and the arising self-consistent disordered single-particle problem was diagonalized numerically. This method enabled us to study comparatively large systems of up to $10^5$ sites and a large number of different disorder configurations. We found that the Coulomb gap persists in the entire insulating phase but becomes narrower when approaching the MIT. The depletion of the DOS in turn leads to an enhancement of localization close to the Fermi level. This enhancement seems to be in contradiction to the results of Talamantes et al. [7] who inferred an interaction-induced delocalization from an investigation of the many-particle spectrum. Since the HF method is a severe approximation it is not clear whether the seeming disagreement is an artificial result of the HF approximation or whether it can be attributed to the use of different criteria [6] for localization in a many-particle system or being in a different part of parameter space.

In this paper we therefore investigate the range of validity of the HF approximation by comparing it to the results of numerically exact diagonalization of small lattices with up to 16 sites.

We first discuss the single-particle (i.e. tunneling) DOS $g(\epsilon)$. In a many-particle system in general the DOS is defined via the single-particle Greens function

$$g(\epsilon) = -\frac{1}{\pi} \text{Im tr} G^R(\epsilon).$$

(2)

Within the HF approximation the single-particle energies are simply given by the eigenvalues of the HF Hamiltonian. A comparison of the single-particle DOS resulting from the HF and exact calculations for one particular set of parameters in Fig. 1 shows good agreement. We have performed analogous calculations for different values of the overlap ($t = 0$ to 0.8) and filling factors ($K = 0.5$ and 0.25). For all parameter sets investigated we found that the results of both methods agree within the statistical errors. Thus, we conclude that the single-particle DOS of the quantum Coulomb glass is well described within the HF approximation. We note, however, that we cannot make a statement about the validity of the HF approximation asymptotically close to the Fermi energy since the small systems which we can study by exact diagonalization always possess a sizeable hard gap which obscures the Coulomb gap.

We now turn to the localization properties. The simplest measure of localization for a single-particle state $|\psi_\epsilon\rangle$ in a non-interacting system is the inverse participation
Quantum Coulomb Glass

Fig. 1. Comparison of the exact and Hartree-Fock results for the single-particle DOS of a quantum Coulomb glass with $3 \times 4$ sites for $W_0 = 1$, $K = 0.5$ and $t = 0.1$. The data represent averages over 100 different disorder configurations.

number

$$P^{-1}_v = \sum_j |\langle \psi_v | j \rangle|^4,$$

where the sum runs over all sites $j$. In practice it is often averaged over all states with a certain energy $\epsilon$,

$$P^{-1}(\epsilon) = \frac{1}{g(\epsilon)} \frac{1}{N} \sum_v P^{-1}_v \delta(\epsilon - \epsilon_v).$$

The generalization of the participation number to many-particle systems is not straightforward, for a discussion see e.g. [6]. A consistent generalization of $P^{-1}$ is the probability $R_0$ for a particle to return to its starting site in infinite time, which can be expressed in terms of single-particle Greens functions

$$R_0(\epsilon) = \frac{1}{N} \sum_j \lim_{\delta \to 0} \frac{\delta}{\pi} G_{ij}(\epsilon + i\delta) G_{ji}(\epsilon - i\delta).$$

For non-interacting electrons $P^{-1}(\epsilon) = R_0(\epsilon)$. In Fig. 2 we compare the return probability obtained by Hartree-Fock and exact calculations. Close to the Fermi energy the HF and exact results agree reasonably well. Away from the Fermi energy the return probability obtained by exact diagonalization decreases drastically which is not correctly described by HF (note, that the opposite was suggested by Aleiner and Shklovskii [8]). We have carried out analogous calculations for different values of overlap ($t = 0$ to 0.8) and filling factors ($K = 0.5$ and 0.25). For all parameter sets we found the same behavior, viz. the HF method overestimates the return probability away from the Fermi energy whereas both methods agree close to the Fermi level.

To summarize, we have compared the results of a HF approximation and of an exact diagonalization of the quantum Coulomb glass. We found that the results of the two methods for the DOS agree reasonably well for all energies. The localization properties are correctly described by HF close to the Fermi energy only. In particular, the interaction-induced enhancement of localization which we found [5] within the HF approxima-
tion is also present in the exact calculation. Consequently, it appears that the seeming contradiction between the HF calculation [5] and [7] is not an artefact of the HF approximation but either due to the use of different quantities to characterize localization in a many-body system or due to being in different parts of parameter space. Thus a detailed investigation of the different localization criteria seems to be necessary [6]. The results of the present paper not only justify the application of the HF method to analyze at least some properties of the quantum Coulomb glass (taking into account the fact that the relevant physics at low temperatures is dominated by excitations close to the Fermi energy), they also suggest an improved calculational scheme. It consists of two steps: (i) solving the model within HF approximation and (ii) expanding the many-particle states in an energetically cutoff HF basis and diagonalizing this reduced problem. Such a scheme will enable us to treat comparatively large lattices and still obtain almost exact results for energies close to the Fermi energy. Work along these lines is in progress.

This work was supported in part by the DFG under grant Nos. Schr231/13-1, Vo659/1-1 and SFB393 and by the NSF under grant No. DMR-95-10185.

References

Hartree-Fock based diagonalization: an efficient method for simulating disordered interacting electrons

Thomas Vojta, Frank Epperlein and Michael Schreiber
Institut für Physik, Technische Universität, D-09107 Chemnitz, Germany

version October 12, compiled March 17, 1999

Abstract

We present an efficient numerical method for simulating the low-energy properties of disordered many-particle systems. The method which is based on the quantum-chemical configuration interaction approach consists in diagonalizing the Hamiltonian in an energetically truncated basis built of the low-energy states of the corresponding Hartree-Fock Hamiltonian. As an example we investigate the quantum Coulomb glass, a model of spinless electrons in a random potential interacting via long-range Coulomb interaction. We find that the Coulomb interaction increases the conductance of strongly disordered systems but reduces the conductance of weakly disordered systems.

The numerical simulation of disordered many-particle systems is one of the most complicated problems in computational condensed matter physics. First, the size of the Hilbert space to be considered grows exponentially with the system size. Second, the presence of 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 made worse by the long-range character of the Coulomb interaction which has to be retained, at least for a correct description of the insulating phase.

The simulation methods applied to disordered many-particle systems can be roughly divided into two classes. On the one hand, methods like Hartree-Fock [1, 2] have been used to reduce the system to an effective single-particle system. This overcomes the problem of the Hilbert space growing exponentially with system size. The resulting methods permit the simulation of rather large systems (> 10^3 sites) but the approximations involved are uncontrolled and can usually not be improved systematically.

On the other hand, there are several methods which give numerically exact results or which can be taken, at least in principle, to arbitrary accuracy.
However, most of these methods are severely restricted when simulating disordered interacting electrons. Exact diagonalization [3, 4] works only for very small systems (with up to about $4 \times 4$ lattice sites). For one-dimensional systems the density-matrix renormalization group method [5] is a very efficient tool to obtain the low-energy properties. It is, however, less effective in higher dimensions; and it is also not capable of handling the long-range Coulomb interaction which is important in the insulating phase. Quantum Monte-Carlo [6] methods are another means of simulating disordered many-particle systems. They are very effective for bosons at finite temperatures. Very low temperatures are, however, hard to reach. Moreover, simulations of fermions suffer from the notorious sign problem (although this turned out to be less severe in the presence of disorder).

In this paper we present an alternative method for simulating disordered interacting electrons which we call the Hartree-Fock based diagonalization (HFD). It is based on the quantum chemical configuration interaction [7] approach adapted for disordered lattice models. The main idea is to diagonalize the Hamiltonian in a subspace of the Hilbert space spanned by the low-energy eigenstates of the Hartree-Fock approximation of the Hamiltonian. The HFD method consists of 3 steps: (i) solve the Hartree-Fock approximation of the Hamiltonian which is still a non-trivial disordered single-particle problem, (ii) use a Monte-Carlo algorithm to find the low-energy many-particle Hartree-Fock states, and (iii) diagonalize the Hamiltonian in the basis formed by these states and calculate the observables. The efficiency of the HFD method is due to the fact that the Hartree-Fock states are comparatively close in character to the exact eigenstates in the entire parameter space. Thus it works well for all parameters while related methods based on non-interacting or classical eigenstates [9, 10] instead of Hartree-Fock states are restricted to small parameter regions.

In the following we will illustrate the application of the HFD method on the example of the quantum Coulomb glass, a model of interacting spinless electrons in a random potential. It is defined on a regular hypercubic lattice with $M = L^d$ ($d$ is the spatial dimensionality) sites occupied by $N = KM$ electrons ($0 < K < 1$). To ensure charge neutrality each lattice site carries a compensating positive charge of $K e$. The Hamiltonian is given by

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

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. $t$ is the strength of the hopping term, i.e., the kinetic energy, and $n_i$ is the occupation number of site $i$. We parametrize the Coulomb interaction $U_{ij} = e^2/r_{ij}$ by its value $U$ between nearest neighbor sites. For a correct description of the insulating phase the Coulomb interaction has to be kept long-ranged, since
screening breaks down in the insulator. The random potential values \( \varphi_i \) are chosen independently from a box distribution of width \( 2W_0 \) and zero mean. For \( U_{ij} = 0 \) the quantum Coulomb glass becomes identical to the Anderson model of localization and for \( t = 0 \) it turns into the classical Coulomb glass.

We now give a more detailed description of the HFD method for the quantum Coulomb glass. For each disorder configuration the first step consists in numerically diagonalizing the Hartree-Fock approximation

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

of the Hamiltonian as described in Ref. [2]. Here \( \langle \ldots \rangle \) represents the expectation value with respect to the Hartree-Fock ground state which has to be determined self-consistently. This calculation results in an orthonormal set of single-particle Hartree-Fock states \( |\psi_\nu\rangle = b_\nu^\dagger |0\rangle \) which defines a unitary transformation \( b_\nu^\dagger = \sum_i S_{\nu i} c_i^\dagger \).

In the second step of the HFD method we construct many-particle states, i.e., Slater determinants,

\[
|\{\nu\} \rangle = b_{\nu_1}^\dagger \ldots b_{\nu_N}^\dagger |0\rangle . \tag{3}
\]

Note that for the two limiting cases mentioned above, i.e for the Anderson model of localization and for the classical Coulomb glass, these states are also eigenstates of the full Hamiltonian (1). We then determine those of the many-particle states (3) which have the lowest expectation values \( \langle \{\nu\}|H_{HF}|\{\nu\} \rangle \) of the energy. Since the total number of states is too high for a complete enumeration we employ a Monte-Carlo method. It is based on the thermal cycling method [8] in which the system is repeatedly heated and cooled. In addition, at the end of each cycle a systematic local search around the current configuration is performed. The low-energy many-particle states found in this way span the sub-space of the Hilbert space relevant for the low-energy properties. Its dimension \( B \) determines the accuracy of the results.

The third HFD step consists in transforming the Hamiltonian from the original site representation to the Hartree-Fock-representation and calculating the matrix elements \( \langle \{\nu\}|H|\{\mu\} \rangle \). The resulting Hamiltonian matrix \( H_{\{\nu\};\{\mu\}} \) of size \( B \times B \) is then diagonalized using standard library routines. Note that \( H_{\{\nu\};\{\mu\}} \) is usually not very sparse: if \( |\{\nu\} \rangle \) and \( |\{\mu\} \rangle \) differ in the occupation of at most 4 single-particle states, the matrix element is non-zero. Moreover, number and position of the non-zero matrix elements differ between different disorder configurations. Thus, specialized codes for sparse matrices will not increase the performance significantly.
In order to investigate physical observables we transform their operators to the Hartree-Fock representation. This is usually faster than transforming the states back to site or momentum representation.

In order to test the method and to check the dependence of the results on the size $B$ of the basis we carried out extensive simulations for systems with $4 \times 4$ sites and compared the results to those of exact diagonalizations which are not too time-consuming for spinless electrons at this size. We first investigated the dependence of the ground state energy $E_0^B$ on $B$ and compared it to the exact result $E_0$. A typical example is presented in Fig. 1. As usual the ground state energy is not very sensitive to the accuracy of the approximation. Already the relative energy error of Hartree-Fock (cp. $B = 1$ in Fig. 1) is as low as $10^{-4}$. Keeping a basis size of 300 within the HFD method reduces the error by a factor of 10. Further increasing the basis size to 1000 (which is still less than 10% of the total Hilbert space) gives a relative error of less than $10^{-6}$. Knowing that the energy is not sufficient to judge the quality of the ground state we also studied the overlap between approximate and exact ground state as well as several ground state expectation values. Fig. 2 shows the convergence of the occupation numbers as a function of basis size $B$ for the same system as in Fig. 1. While some of the occupation numbers have significant errors within Hartree-Fock approximation, the HFD method with a basis size of 100 gives all occupation numbers with a satisfactory accuracy of better than $10^{-2}$. 

Figure 1: Dependence of the ground state energy $E_0^B$ and its relative error $(E_0^B - E_0)/E_0$ on the size $B$ of the basis used for a system of 8 electrons on 16 sites, $W_0 = 1, t = 0.1, U = 1$. The solid line in the inset is a fit to an exponential law. For comparison, the energy of the first excited state is $E_1 = -24.73$.
After having established the method we now show calculations of the transport properties. We consider the question whether the electron-electron interactions lead to an enhancement or to a reduction of the conductance in a system of disordered electrons. This question has attracted a lot of attention after experiments revealed indications of an unexpected metal-insulator transition in two dimensions [11].

The conductance is calculated from the Kubo-Greenwood formula [12] which relates it to the current-current correlation function in the ground state. Using the spectral representation of the correlation function the real (dissipative) part of the conductance (in units of the quantum conductance $e^2/h$) is obtained as

$$\Re G^{xx}(\omega) = \frac{2\pi^2}{\omega} L^{d-2} \sum_\alpha |\langle 0|j^x|\alpha\rangle|^2 \delta(\omega + E_0 - E_\alpha)$$

where $j^x$ is the $x$ component of the current operator and $\alpha$ denotes the eigenstates of the Hamiltonian. The finite life time $\tau$ of the eigenstates in a real d.c. transport experiment results in an inhomogeneous broadening $\gamma = 1/\tau$ of the $\delta$ functions in the Kubo-Greenwood formula. Here we have chosen $\gamma = 0.05$ which is of the order of the single-particle level spacing. According to eq. (4) the accuracy of the conductance depends not only on the accuracy of the ground state but also on that of the excited states. Therefore we also carried out convergence tests on the conductance itself, following the lines discussed above.

We now discuss the main results for the d.c. conductance of two-dimensional systems. In Fig. 3 we show the extrapolated d.c. conductances for systems of $5 \times 5$ lattice sites containing 12 electrons for different values of kinetic energy and interaction strength. The data show that weak electron-electron interactions enhance the conductance for the case of very small kinetic energy (i.e., large disorder). In this regime the dominant effect of the
interactions is that electron-electron scattering destroys the phase coherence responsible for Anderson localization. In contrast, for higher kinetic energy or sufficiently strong interactions the dominant effects of the interactions are a reduction of the charge fluctuations and an increase in the effective random potential both of which lead to a reduction of the conductance. Analogous simulations with different system size and filling factor show the same qualitative dependence of the conductance on the interaction strength.

To summarize, we have presented an effective method, the Hartree-Fock based diagonalization (HFD), for the numerical simulation of disordered many-particle systems. As an example we have applied it to the calculation of transport properties in the quantum Coulomb glass model of interacting electrons in a random potential. Further results obtained by the HFD method on the transport properties of the quantum Coulomb glass in one, two and three dimensions can be found in Refs. [13, 14, 15].

This work was supported in part by the German Research Foundation.

References


Do Interactions Increase or Reduce the Conductance of Disordered Electrons? It Depends!

Thomas Vojta, Frank Epperlein, and Michael Schreiber
Institut für Physik, Technische Universität, D-09107 Chemnitz, Germany
(Received 16 June 1998)

We investigate the influence of electron-electron interactions on the conductance of two-dimensional disordered spinless electrons. We present an efficient numerical method based on diagonalization in a truncated basis of Hartree-Fock states to determine with high accuracy the low-energy properties in the entire parameter space. We find that weak interactions increase the dc conductance in the strongly localized regime while they decrease the dc conductance for weak disorder. Strong interactions always decrease the conductance. We also study the localization of single-particle excitations at the Fermi energy which turns out to be only weakly influenced by the interactions.

PACS numbers: 72.15.Rn, 71.30.+h, 71.55.Jv

The influence of electron-electron interactions on the transport in disordered electronic systems has been investigated intensively within the past two decades [1,2]. Recently, the problem has attracted a lot of attention after experimental [3] and theoretical [4] results challenged established opinions.

It is well accepted [5] that noninteracting electrons in three dimensions (3D) undergo a localization-delocalization transition at finite disorder. In contrast, all states are localized in 2D and 1D even for infinitesimal weak disorder [6]. However, today it is believed that the metal-insulator transition (MIT) in most experimental systems cannot be explained based on noninteracting electrons. The metallic phase of disordered interacting electrons has been studied intensively within the perturbative renormalization group (RG) [2], leading to a qualitative analysis of the MIT and the identification of different universality classes. One of the results is that the lower critical dimension of the MIT is $d_c = 2$ as it is for noninteracting electrons. Therefore it came as a surprise when experiments [3] on Si-MOSFETs revealed indications of a MIT in 2D. Since these experiments are performed at low electron density where the Coulomb interaction is particularly strong compared to the Fermi energy, interaction effects are a likely reason for this MIT. A complete understanding has, however, not yet been obtained. Explanations were suggested based on the perturbative RG [7], nonperturbative effects [8], or the transition being a superconductor-insulator transition rather than a MIT [9].

Theoretically, surprising results have been obtained for just two interacting particles in the insulating regime [4]. It was found that two particles can form a pair whose localization length is much larger than that of a single particle. Later an even larger delocalization was suggested for clusters of three or more particles [10]. In the case of a repulsive electron-electron, these delocalized states have rather high energy; thus their relevance for the low-energy properties of a degenerate system is not clear. It has been argued that the many-particle problem can be reduced to a few interacting quasiparticles above the Fermi surface [11]. This is, however, only possible if the interactions do not change the nature of the ground state. All in all, not even the qualitative influence of interactions is understood in the insulating regime.

We have numerically studied disordered 2D spinless electrons. Our calculations are summarized in Fig. 1 which is the main result of this Letter. It shows that the influence of repulsive electron-electron interactions on the dc conductance is opposite for high and low kinetic energies (i.e., weak vs strong disorder). The conductance of strongly localized samples ($t = 0.01$ to $0.03$) is considerably enhanced by a weak interaction. With increasing kinetic energy the relative enhancement decreases as does the interaction range where the enhancement occurs. The conductance of samples with the highest kinetic energies ($t = 0.3$ and 0.5) is reduced even by weak interactions. In contrast, sufficiently strong interactions always reduce the conductance. This is not surprising since, for large enough interaction strength, the system will form a Wigner glass.

These findings shed some light on seemingly contradicting numerical results on the transport of disordered spinless electrons in the literature. Studies [12] of a 2D...
model in the diffusive regime yielded that interactions decrease the conductance. The same conclusion was drawn from density-matrix RG studies [13] and exact diagonalizations [14] in 1D. In contrast, for 2D models in the localized regime [15,16], it was found that interactions lead to a delocalization. Up to now, it has been unclear whether these inconsistent results are due to being in different parameter regions (weak vs strong disorder), different quantities studied (conductance, many-particle level statistics, or charge stiffness), or long-range vs short-range interactions. The results of this Letter suggest that being in different parameter regions is the most likely reason for the differences between the results cited above. A result similar to ours was obtained recently [17] in a study of the ground state phase sensitivity in 1D. It was found that, for small disorder, repulsive (nearest-neighbor) interactions reduce the phase sensitivity while, for large disorder, the phase sensitivity shows pronounced peaks at certain values of the interaction.

In the remainder of the Letter we explain the model and the calculational method and further discuss the results. We consider a 2D quantum Coulomb glass model [15,16,18,19]. It is defined on a square lattice with $M = L^2$ sites occupied by $N = KM$ spinless electrons ($0 < K < 1$). To ensure charge neutrality each site carries a compensating charge of $e$. The Hamiltonian reads

$$H = -t \sum_{\langle ij \rangle} (c_i^\dagger c_j + c_j^\dagger c_i) + \sum_i \phi_i n_i + \frac{1}{2} \sum_{i \neq j} (n_i - K)(n_j - K) U_{ij},$$

where $c_i$ and $c_i^\dagger$ are the creation and annihilation operators at site $i$, $n_i = c_i^\dagger c_i$, and $\langle ij \rangle$ denotes all pairs of nearest neighbors. $U_{ij} = e^2/r_{ij}$ represents the Coulomb interaction which is parametrized by its nearest-neighbor value $U$ and $t$ is the kinetic energy. The random potential values $\phi_i$ are chosen from a box distribution of width $2W$ and zero mean. (We always set $W = 1$.) Two important limiting cases of the quantum Coulomb glass are the Anderson model of localization (for $U = 0$) and the classical Coulomb glass (for $t = 0$).

The numerical simulation of disordered many-particle systems is one of the most complicated problems in computational physics. First, the size of the Hilbert space grows exponentially with the system size, making exact diagonalizations of the Hamiltonian impossible already for very small systems. Second, the presence of disorder requires the simulation of many different samples to obtain averages or distributions of physical quantities. For disordered interacting electrons the problem is made worse by the long range of the Coulomb interaction which has to be retained for a correct description of the insulating phase where screening breaks down.

In this Letter we suggest an efficient numerical method to simulate disordered interacting electrons. It is based on the idea of configuration interaction [20] adapted to disordered lattice models. The method, which we call the Hartree-Fock-based diagonalization (HFD), consists of three steps: (i) Solve the Hartree-Fock (HF) approximation of the Hamiltonian as in Ref. [18], (ii) use a Monte Carlo algorithm to find the low-energy many-particle HF states (Slater determinants), and (iii) diagonalize the Hamiltonian in the basis formed by these states [21]. The HF basis states are comparatively close in character to the exact eigenstates in the entire parameter space. Thus it is sufficient to keep only a small fraction of the Hilbert space to obtain low-energy quantities with an accuracy comparable to that of exact diagonalization. The HFD method is very flexible, it works well in any spatial dimension, and is capable of handling long-range and short-range interactions. A detailed description will be given elsewhere. Most of our calculations have been performed for lattices with $5^2$ sites and 12 electrons keeping 500 basis states. We used periodic boundary conditions and the minimum image convention. We also studied $4^2$ and $6^2$ systems with $K = 0.25$ and 0.5 keeping up to 2000 out of $9 \times 10^6$ basis states.

We now turn to the conductance which we compute from linear response theory. The real (dissipative) part of the conductance (in units of $e^2/h$) is given by the Kubo-Greenwood formula [22],

$$\text{Re}G^{\text{xx}}(\omega) = \frac{2\pi\delta}{\omega} \sum_{\nu} |\langle 0 | j^x | \nu \rangle|^2 \delta(\omega + E_{\nu} - E_0),$$

where $\omega$ denotes the frequency. $j^x$ is the $x$ component of the current operator and $\nu$ denotes the eigenstates of the Hamiltonian. Equation (2) describes an isolated system while in a real dc transport experiment the sample is connected to contacts and leads. This results in a finite lifetime $\tau$ of the eigenstates leading to an inhomogeneous broadening $\gamma = \tau^{-1}$ of the $\delta$ functions in (2) [23]. To suppress the discreteness of the spectrum of a finite system, $\gamma$ should be at least of the order of the single-particle level spacing. For our systems this requires a comparatively large $\gamma \gtrsim 0.05$. We tested different $\gamma$ and found that the conductance values depend on $\gamma$ but the qualitative results do not [24].

In a random system, different samples will have different conductance values. Figure 2 shows the probability distribution $P[\log(G(0))]$ for systems in the localized regime with and without interactions. Both distributions show the same qualitative behavior; they are close to normal distributions corresponding to very broad distributions of the conductances themselves. The arithmetic average of the conductance is therefore not a good measure of the typical behavior. We use instead the logarithmic (i.e., geometrical) average $G_{\text{av}} = \exp[\log(G)]$ [25], usually over 400 disorder configurations.

In Figs. 3 and 4 we present results on the dependence of the conductance on the interaction for two sets of
parameters. In Fig. 3 the kinetic energy is very small \( t = 0.03 \). Thus the system is in the strongly localized regime, as we also estimated from the single-particle participation number \( P_{sp} = 2 \). Here a weak Coulomb interaction \( (U = 0.5) \) leads to an increase of the conductance at low frequencies. If the interaction becomes stronger the conductance decreases and finally \( (U = 2) \) falls below the value of noninteracting electrons. We emphasize that the increase of the conductance for weak interactions is a true correlation effect: Within the HF approximation [18], interactions always lead to a decrease of the conductance. The behavior is qualitatively different at higher kinetic energy \((t = 0.3)\) as shown in Fig. 4. Here the system is approaching the diffusive regime \( (P_{sp} > 10) \). Already, a weak interaction \( (U = 0.5) \) leads to a reduction of the low-frequency conductance compared to noninteracting electrons. If the interaction becomes stronger the conductance is decreased further. We have performed analogous calculations for kinetic energies \( t = 0.01–0.5 \) and interaction strengths \( U = 0–2 \). The resulting dc conductances are those presented in Fig. 1.

We also checked for system size and filling factor dependences by simulating systems with \( 4^2 \) and \( 6^2 \) sites, and filling factor \( K = 0.25 \) in addition to 0.5. We found that the increase of the conductance for weak interactions, if the interaction becomes stronger, the conductance is decreased further. We have performed analogous calculations for kinetic energies \( t = 0.01–0.5 \) and interaction strengths \( U = 0–2 \). The resulting dc conductances are those presented in Fig. 1.

In order to find out to what extent the behavior of the conductance is reflected in single-particle localization properties, we also computed the single-particle return probability

\[
R_p(e) = \frac{1}{N} \sum_{ij} \lim_{\delta \to 0} \frac{\delta}{\pi} G_{ij}(e + i\delta)G_{ij}(e - i\delta).
\]

Here \( G_{ij}(e) \) is the single-particle Greens function. \( R_p(e) \) is the generalization of the single-electron state to a many-particle system. Figure 6 shows a typical result for \( R_p(e) \). We performed analogous calculations for \( t = 0.01–0.5 \) and \( U = 0–2 \). For all cases, we obtain the same qualitative behavior: Close to the Fermi energy the return probability falls below the qualitative picture (as presented in Fig. 1) to the same in all cases. As an example, Fig. 5 shows the interaction dependence of \( G(0) \) for \( t = 0.01 \) for the different systems studied. Clearly, the interaction-induced enhancement of the conductance exists in all cases. Moreover, the relative enhancement seems to increase from the \( 4^2 \) system to the \( 6^2 \) system. (A comparison of even and odd linear system sizes is problematic since at half filling a regular array of charges is impossible for odd sizes. Moreover, any quantitative comparison of different sizes would require a more realistic description of the broadening.)
is only weakly influenced by the interaction. Directly at the Fermi energy, which is not accessible in our simulations because of our still too small system sizes, there may develop a slight enhancement of the return probability as a result of the Coulomb gap in the single-particle density of states. Such an enhancement has already been observed within the HF approximation [18]. Within the results obtained in this Letter, the effect, if any, is weaker than within HF. For energies away from the Fermi energy the single-particle excitations in the interacting system become strongly delocalized compared to the noninteracting case. The interaction dependence of the conductance discussed above is, however, not reflected in the single-particle return probability.

In summary, we have used the Hartree-Fock-based diagonalization method to investigate the transport properties of disordered interacting spinless electrons. We have found that a weak Coulomb interaction can enhance the conductivity of localized samples considerably while it reduces the conductance of weakly disordered or noninteracting samples considerably. If the interaction becomes stronger it eventually reduces the conductance also in the localized regime. Let us finally mention that, although we show that interations can enhance the conductivity in certain parameter regions, this does not directly provide an explanation for the MIT in 2D [3] since the importance of the spin degrees of freedom for this transition is established experimentally [26]. We emphasize, however, that our method is very easy to generalize to electrons with spin. Work in this direction is in progress.

We acknowledge financial support by the Deutsche Forschungsgemeinschaft.


[6] Except for the spin-orbit coupling universality class which allows for a MIT in 2D and quantizing magnetic fields in 2D, where extended states can appear in the band center.


[20] A related method based on the low-energy states of the classical Coulomb gas was used previously [15,16]. While a method based on the classical states is restricted to very small values of the kinetic energy, our method works in the entire parameter space.


[23] In order to compare the conductance values for different kinetic energies, $\gamma$ should be $t$ dependent. In the diffusive regime a simple estimate [23] suggests $\gamma \approx t$. Since this would lead to unacceptable large broadenings for our systems we used a $t$-independent $\gamma$ in our calculations.

[24] For noninteracting electrons, it is known that $\log(G)$ is a statistically well-behaved quantity (see, e.g., Ref. [5]).

Electronic transport in disordered interacting systems

Thomas Vojta and Frank Epperlein

Institut für Physik, Technische Universität, D-09107 Chemnitz, Germany

Received 6 October 1998, accepted 8 October 1998 by B. Kramer

Abstract. We numerically investigate the transport properties of disordered interacting electrons in three dimensions in the metallic as well as in the insulating phases. The disordered many-particle problem is modeled by the quantum Coulomb glass which contains a random potential, long-range unscreened Coulomb interactions and quantum hopping between different sites. We have recently developed the Hartree-Fock based diagonalization (HFD) method which amounts to diagonalizing the Hamiltonian in a suitably chosen energetically truncated basis. This method allows us to investigate comparatively large systems. Here we calculate the combined effect of disorder and interactions on the dissipative conductance. We find that the qualitative influence of the interactions on the conductance depends on the relative disorder strength. For strong disorder interactions can significantly enhance the transport while they suppress the conductance for weak disorder.

Keywords: Disorder; Anderson localization; Interactions; Correlated electrons

1 Introduction

After four decades of research the transport properties of systems in which both disorder and strong interactions are equally important are still not even qualitatively understood. Based on Andersons seminal paper [1] investigations of non-interacting disordered electrons led to the development of the scaling theory of localization [2, 3]. In the absence of external symmetry breaking it predicts that all states are localized in one and two dimensions. In contrast, in three dimensions states are extended for weak disorder while they are localized for sufficiently strong disorder. This gives rise to a disorder-driven metal-insulator transition (MIT) at a certain value of disorder strength.

Later also the influence of electron-electron interactions on the transport properties of disordered electrons was investigated intensively by means of many-body perturbation theory, field theory, and the renormalization group [4, 5, 6]. This led to a qualitative analysis of the MIT and the identification of the different universality classes. The topic has reattracted a lot of attention after unexpected experimental [7] and theoretical [8] findings. In order to investigate the localized phase and to check the validity of the perturbative results it seems to be important to investigate the problem of interacting disordered electrons non-perturbatively. One possible way in this direction is numerical simulations although they are very costly for disordered many-body
systems. Recently, we have developed the Hartree-Fock based diagonalization (HFD) method [9, 10] for the simulation of disordered quantum many-particle systems. We have already applied this very efficient method for calculating the transport properties of one-dimensional [12] and two-dimensional [9] disordered interacting electrons. In this paper we extend the investigation to three spatial dimensions.

2 Model and calculations

The model, called the quantum Coulomb glass model [13, 14, 15, 16], is defined on a cubic lattice of $L^3$ sites occupied by $N = KL^3$ electrons ($0 < K < 1$). To ensure charge neutrality each lattice site carries a compensating positive charge of $Ke$. The Hamiltonian is given by

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

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, $U_{ij} = U/r_{ij}$ ($r_{ij}$ is measured in units of the lattice constant), since screening breaks down in the insulator. The random potential values $\varphi_i$ are chosen independently from a box distribution of width $2W$ and zero mean. (In the following we always set $W = 1$.) 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 the present study we have simulated systems with $3^3$ sites and 13 electrons using periodic boundary conditions.

The calculations are carried out by means of the HFD method [9]. This method which is based on the idea of the configuration interaction approach [11] adapted to disordered lattice models is very efficient in calculating low-energy properties in any spatial dimension and for short-range as well as long-range interactions. It consists of 3 steps: (i) solve the Hartree-Fock (HF) approximation of the Hamiltonian, (ii) use a Monte-Carlo algorithm to find the low-energy many-particle HF states, (iii) diagonalize the Hamiltonian in the basis formed by these states. The efficiency of the HFD method is due to the fact that the HF basis states are comparatively close in character to the exact eigenstates in the entire parameter space. Thus it is sufficient to keep only a small fraction of the Hilbert space in order to obtain low-energy quantities with an accuracy comparable to that of exact diagonalization. For the present systems of 13 electrons on 27 sites we found it sufficient to keep 500 to 1000 (out of $2 \times 10^8$) basis states.

In order to calculate the conductance we employ the Kubo-Greenwood formula [17] which connects the conductance with the current-current correlation function in the ground state. Using the spectral representation of the correlation function the real (dissipative) part of the conductance (in units of the conductance quantum $e^2/h$) is obtained as

$$ \text{Re} \, G^{xx}(\omega) = \frac{2\pi^2L}{\omega} \sum_\nu |\langle 0 | j^x | \nu \rangle|^2 \delta(\omega + E_0 - E_\nu) \quad (2) $$
where $j^x$ is the $x$ component of the current operator and $\nu$ denotes the eigenstates of the Hamiltonian. The finite life time $\tau$ of the eigenstates in a real d.c. transport experiment (where the system is not isolated but connected to contacts and leads) results in an inhomogeneous broadening $\gamma = 1/\tau$ of the $\delta$ functions in the Kubo-Greenwood formula [18]. Here we use $\gamma = 0.05$ which is of the order of the single-particle level spacing. Since the resulting conductances vary strongly from sample to sample we logarithmically average all results over several disorder configurations.

![Graph showing conductance $G$ as a function of frequency $\omega$, $W = 1, \gamma = 0.05$ and two different values of the kinetic energy $t$. The truncation of the Hilbert space to 500 basis states restricts the validity of these data to frequencies $\omega < 0.75$.](image)

**Fig. 1** Conductance $G$ as a function of frequency $\omega$, $W = 1, \gamma = 0.05$ and two different values of the kinetic energy $t$. The truncation of the Hilbert space to 500 basis states restricts the validity of these data to frequencies $\omega < 0.75$.

### 3 Results

We now present results on the dependence of the conductance on the interaction strength. In Fig. 1 we show the conductance as a function of frequency for two sets of
parameters. The data represent logarithmic averages over 400 disorder configurations. In the lower diagram the kinetic energy is very small \((t = 0.03)\), i.e., the system is in the highly localized regime. Here not too strong Coulomb interactions \((U = 0.5, 1.0)\) lead to an increase of the conductance at low frequencies. If the interaction becomes stronger \((U = 2)\) the conductance finally decreases again. The behavior is qualitatively different at higher kinetic energy \((t = 0.3)\) as shown in the upper diagram. Here already a weak interaction \((U = 0.5)\) leads to a reduction of the low-frequency conductance compared to non-interacting electrons. If the interaction becomes stronger \((U = 2)\) the conductance decreases further. We have carried out analogous calculations for kinetic energies \(t = 0.01, ..., 0.5\) and interaction strengths \(U = 0, ..., 2\). The resulting d.c. conductances are presented in Fig. 2 which is the main result of this paper. In Fig. 2 we now present results on the dependence of the d.c. conductance \(G(0)\) on the interaction strength for kinetic energies \(t = 0.01, ..., 0.5\) and interaction strength \(U = 0, ..., 2\). The data show that the influence of weak repulsive electron-electron interactions on the d.c. conductance depends on the ratio between disorder and kinetic energy. The conductance of strongly localized samples \((t = 0.01, ..., 0.03)\) becomes considerably enhanced by a weak Coulomb interaction which can be understood from the suppression of localizing interferences by electron-electron scattering. With increasing kinetic energy the relative enhancement decreases as does the interaction range where the enhancement occurs. The conductance of samples with high kinetic energies \((t \geq 0.1)\) is not enhanced by weak interactions. Sufficiently strong interactions always reduce the conductance. In this regime the main effect of the interactions is the reduction of charge fluctuations which reduces the conductance. In the limit of infinite interaction strength the system approaches a Wigner crystal/glass which is insulating for any disorder. Overall, this is the same

**Fig. 2** d.c. conductance \(G(0)\) as a function of interaction strength \(U\) for different kinetic energies \(t\).
qualitative behavior as in the cases of one [12] and two [9] spatial dimensions although
the disorder induced enhancement of the conductance seems to be weaker in three
dimensions. Up to now it is not clear whether this is a true dimensionality effect or
due to the different linear system sizes studied. A systematic investigation of the size
dependence is in progress.

To summarize, we have used the Hartree-Fock based diagonalization (HFD) method
to investigate the conductance and localization properties of disordered interacting
spinless electrons in three dimensions. We have found that a weak Coulomb interac-
tion can enhance the conductivity of strongly localized samples by almost one order
of magnitude, while it reduces the conductance of weakly disordered samples. If the
interaction becomes stronger it eventually reduces the conductance also in the stron-
gly localized regime.

We acknowledge financial support by the Deutsche Forschungsgemeinschaft.

References
Lett. 42 (1979) 637
[5] A. L. Efros, M. Pollak (Eds.), Electron-electron interactions in disordered systems,
North-Holland, Amsterdam, 1985
cond-mat/9806194
cond-mat/9809171
mot/9807385
71 (1958) 585
[18] For a pedagogical discussion see, e.g., S. Datta, Electronic transport in mesoscopic
Transport in disordered interacting systems: Numerical results for one-dimensional spinless electrons

Michael Schreiber, Frank Epperlein, and Thomas Vojta

Institut für Physik, Technische Universität, D-09107 Chemnitz, Germany

Abstract

The combined influence of disorder and interactions on the transport properties of electrons in one dimension is investigated. The numerical simulations are carried out by means of the Hartree-Fock-based diagonalization (HFD), a very efficient method to determine the low-energy properties of a disordered many-particle system. We find that the conductance of a strongly localized system can become considerably enhanced by the interactions. The enhancement for long-range interactions is significantly larger than for short-range interactions. In contrast, the conductance of weakly localized systems becomes suppressed by the interactions.

The transport properties of disordered electrons have been a subject of continuous interest within the last 4 decades. In 1958 Anderson pointed out [1] that the electronic (single-particle) wave function may become localized in space for sufficiently strong disorder. For one-dimensional systems it was later proved rigorously that all states are exponentially localized for arbitrary finite disorder [2–4]. Further investigations of non-interacting disordered electrons led to the development of the scaling theory of localization [5,6]. It predicts that in the absence of a magnetic field or spin-orbit coupling all states are localized not only in one but also in two dimensions. Thus a metallic state does not exist in these dimensions. In contrast, in three dimensions states are extended for weak disorder while they are localized for sufficiently strong disorder. This gives rise to a disorder-driven metal-insulator transition (MIT) at a certain value of disorder strength.

Later also the influence of electron-electron interactions on the transport properties of disordered electrons was investigated intensively by means of many-body perturbation theory [7], scaling theory [8], and the renormalization group (for reviews see, e.g. [9–11]). This led to a qualitative analysis of the MIT and the identification of the different universality classes. One of the main results is that the lower critical dimension of the MIT is $d_c^- = 2$ as it is for
non-interacting electrons [11]. Therefore it came as a surprise when measurements [12] on Si-MOSFETs revealed indications of a MIT in 2D. Since these experiments are carried out at low electron density where the Coulomb interaction is particularly strong compared to the Fermi energy, interaction effects are the most likely reason for this phenomenon. A complete understanding has, however, not yet been obtained. There have been attempts to explain the experiments based on the perturbative renormalization group [13], non-perturbative effects [14], or the transition being a superconductor-insulator transition rather than a MIT [15].

In view of all this it seems to be important to investigate the problem of interacting disordered electrons not only in the perturbative regime (of weak disorder and interactions) but also for strong disorder or/and interactions. Recently, we investigated [16] the transport properties of two-dimensional disordered interacting electrons. We found that weak interactions enhance the conductance in the strongly localized regime while they reduce the conductance in the case of weaker disorder. In contrast, sufficiently strong interactions always reduce the conductance.

In this paper we extend this study to the case of one dimension. We report numerical results for the conductance of a simple model system of interacting disordered electrons, viz. spinless fermions in a random potential interacting via Coulomb or short-range interactions. Our results cover the entire parameter range from weak disorder and interactions to strong disorder and interactions. The model, a one-dimensional version of the quantum Coulomb glass model [17–20], is defined on a ring (using periodic boundary conditions) of sites occupied by \( N = KL \) electrons (0 < \( K \) < 1). To ensure charge neutrality each lattice site carries a compensating positive charge of \( Ke \). The Hamiltonian is given by

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

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 (\( r_{ij} \) is measured in units of the lattice constant). For comparison we also investigate the case of nearest neighbor interaction of strength \( U \). The random potential values \( \varphi_i \) are chosen independently from a box distribution of width \( 2W \) and zero mean. (In the following we always set \( W = 1 \).) 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 \( t = 0 \).)
The simulation of disordered quantum many-particle systems is numerically very costly since the size of the Hilbert space grows exponentially with system size and since many disorder configurations have to be considered to obtain typical values or distribution functions of observables. We have recently developed the Hartree-Fock based diagonalization (HFD) method [16] for the simulation of disordered quantum many-particle systems. This method which is based on the idea of the configuration interaction approach [21] adapted to disordered lattice models is very efficient in calculating low-energy properties in any spatial dimension and for short-range as well as long-range interactions. It consists of 3 steps: (i) solve the Hartree-Fock (HF) approximation of the Hamiltonian, (ii) use a Monte-Carlo algorithm to find the low-energy many-particle HF states, (iii) diagonalize the Hamiltonian in the basis formed by these states. The efficiency of the HFD method is due to the fact that the HF basis states are comparatively close in character to the exact eigenstates in the entire parameter space [22]. Thus it is sufficient to keep only a small fraction of the Hilbert space in order to obtain low-energy quantities with an accuracy comparable to that of exact diagonalization. For the present study we have simulated rings with 24 sites and 12 electrons. For this size we found it sufficient to keep 500 to 1000 (out of 2704156) basis states.

The conductance is calculated from the Kubo-Greenwood formula [23] which connects the conductance with the current-current correlation function in the ground state. Using the spectral representation of the correlation function the real (dissipative) part of the conductance (in units of the quantum conductance $e^2/h$) is obtained as

$$
\Re G^{xx}(\omega) = \frac{2\pi}{L \omega} \sum_\nu |\langle 0 | j^x | \nu \rangle|^2 \delta(\omega + E_0 - E_\nu)
$$

where $j^x$ is the $x$ component of the current operator and $\nu$ denotes the eigenstates of the Hamiltonian. The finite life time $\tau$ of the eigenstates in a real d.c. transport experiment (where the system is not isolated but connected to contacts and leads) results in an inhomogeneous broadening $\gamma = 1/\tau$ of the $\delta$ functions in the Kubo-Greenwood formula [24]. Here we have chosen $\gamma = 0.05$ which is of the order of the single-particle level spacing.

We now present results on the dependence of the conductance on the interaction strength. In Figs. 1 and 2 we show the conductance as a function of frequency for two sets of parameters. The data represent logarithmic averages over 400 disorder configurations. In Fig. 1 the kinetic energy is very small ($t = 0.03$). Thus the system is in the highly localized regime, as we have also estimated from the single-particle participation number which is smaller than 2. Here not too strong Coulomb interactions ($U = 0.5, 1.0$) lead to an increase of the conductance at low frequencies. If the interaction becomes stronger ($U = 2$) the conductance finally decreases again. The behavior is qualitatively
The truncation of the Hilbert space to 500 basis states restricts the validity of these data to frequencies $\omega < 0.75$.

Fig. 1. Conductance $G$ as a function of frequency $\omega$, $W = 1$, $t = 0.03$, $\gamma = 0.05$.

Fig. 2. Same as Fig. 1 but for $t = 0.5$.

different at higher kinetic energy ($t = 0.5$) as shown in Fig. 2. Here the localization is much weaker (the single-particle participation number is of the order of 10). Already a weak interaction ($U = 0.5$) leads to a reduction of the low-frequency conductance compared to non-interacting electrons. If the
interaction becomes stronger \((U = 2)\) the conductance decreases further.

We have carried out analogous calculations for kinetic energies \(t = 0.01, ..., 0.5\) and interaction strengths \(U = 0, ..., 3\). The resulting d.c. conductances are presented in Fig. 3 which is the main result of this paper. It shows that the influence of weak repulsive electron-electron interactions on the d.c. conductance is opposite in the cases of weak and strong disorder. Sufficiently strong interactions always reduce the conductance. This is not surprising since strong interactions will reduce charge fluctuations and in the limit of infinite interaction strength the system approaches a Wigner crystal. In contrast, the effect of weak (compared to the random potential) interactions depends on the value \(t\) of the kinetic energy. The conductance of strongly localized samples \((t = 0.01, ..., 0.05)\) becomes considerably enhanced by a weak Coulomb interaction. In this regime the dominant effect is the suppression of the localizing interference effects by electron-electron scattering events. With increasing kinetic energy the relative enhancement decreases as does the interaction range where the enhancement occurs. The conductance of samples with high kinetic energies \((t \geq 0.3)\) is reduced even by weak interactions. Here the dominant effect is the suppression of charge fluctuations by the interactions. Overall, only the behavior at high kinetic energies (i.e. weak disorder) is in agreement with analytical results based on the perturbative renormalization group [25] while the behavior for low kinetic energy (strong disorder) is qualitatively different.

For comparison we have also investigated nearest-neighbor interactions instead of long-range Coulomb interactions. In Fig. 4 we compare the d.c. con-
ductances of systems with short- and long-range interactions in the localized regime. The data show that the interaction induced enhancement of the conductance is overall weaker in the case of short range interactions. In particular, the maximum enhancement as a function of interaction strength is significantly smaller (by a factor of about two) than in the Coulomb case. Moreover, the maximum occurs for weaker interaction strength.

In the last part of this paper we want to relate our findings to the two-dimensional case [16] and to results in the literature. The qualitative dependence of the d.c. conductance on kinetic energy and interaction is identical in one and two spatial dimensions. The interaction-induced enhancement in the localized regime is, however, significantly larger in the one-dimensional systems investigated. Up to now it is not clear whether this is a true dimensionality effect or a result of the different linear system sizes studied. In order to resolve this question a systematic investigation of the system size dependence is in progress [26]. The resulting scaling behavior of the conductance with system size will also allow us to check for the existence of an interaction-induced MIT. Note, however, that the recently observed MIT in 2D MOSFETs [12] is not likely to be explained by the enhancement of the conductance we found since the importance of the spin degrees of freedom for this transition is well established experimentally [27]. We emphasize, however, that our numerical method is very easy to generalize to electrons with spin. The fact that we find the strongest enhancement of the conductance for very low kinetic energy also
suggests that the mechanism is different from that giving rise to an increased two-particle localization length in the problem of just two interacting particles [28] (where the strongest delocalization is observed for weak disorder). Let us finally mention that the conclusions drawn in this paper are in qualitative agreement with those of a recent DMRG study [29] of the phase sensitivity of the ground state energy for a disordered one-dimensional model of spinless fermions with nearest-neighbor interactions which showed that for small disorder repulsive interactions reduce the phase sensitivity while for large disorder the phase sensitivity shows pronounced enhancements at certain values of the interaction.

To summarize, we have used the Hartree-Fock based diagonalization (HFD) method to investigate the conductance and localization properties of disordered interacting spinless electrons in one dimension. We have found that a weak Coulomb interaction can enhance the conductivity of strongly localized samples by almost one order of magnitude, while it reduces the conductance of weakly disordered samples. If the interaction becomes stronger it eventually reduces the conductance also in the localized regime. The interaction induced enhancement is larger for long-range interactions than for short-range interactions.

We acknowledge financial support by the Deutsche Forschungsgemeinschaft.

References

[22] Similar methods based on eigenstates of either the non-interacting or the classical problem are efficient only in a small part of the parameter space.
LETTER TO THE EDITOR

Damage spreading and dynamic stability of kinetic Ising models

Thomas Vojta
Department of Physics and Materials Science Institute, University of Oregon, Eugene, OR 97403, USA
and
Institut für Physik, TU Chemnitz-Zwickau, D-09107 Chemnitz, Germany

Received 24 September 1996, in final form 10 November 1996

Abstract. We investigate how the time evolution of different kinetic Ising models depends on the initial conditions of the dynamics. To this end we consider the simultaneous evolution of two identical systems subjected to the same thermal noise. We derive a master equation for the time evolution of a joint probability distribution of the two systems. This equation is then solved within an effective-field approach. By analysing the fixed points of the master equation and their stability we identify regular and chaotic phases.

The question to what extent the time evolution of a physical system depends on its initial conditions is one of the central questions in nonlinear dynamics that have lead to the discovery of chaotic behaviour [1]. In more recent years, analogous concepts have been applied to the stochastic time evolution of interacting systems with a macroscopic number of degrees of freedom. Among the simplest of such many-body systems are kinetic Ising models where the above question has been investigated by means of so-called damage spreading simulations [2, 3]. In these Monte Carlo simulations two identical systems with different initial conditions are subjected to the same thermal noise, i.e. the same random numbers are used in the Monte Carlo procedure. The differences in the microscopic configurations of the two systems are then used to characterize the dynamic stability.

Later the name ‘damage spreading’ has also been applied to a different though related type of investigation in which the two systems are not identical but differ in the fact that one or several spins in one of the copies are permanently fixed in one direction. Therefore, the equilibrium properties of the two systems are different and the microscopic differences between the two copies can be related to certain thermodynamic quantities [4, 5]. Note that in this type of simulation the use of identical noise (i.e. random numbers) for the two systems is not essential but only a convenient method to reduce the statistical error. Whereas this second type of damage spreading is well understood and established as a method to numerically calculate equilibrium correlation functions, much less is known about the original problem of dynamic stability. In particular, there are no rigorous results on the transition between regular and chaotic behaviour (called the ‘spreading transition’). Grassberger [6] conjectured that the spreading transition falls into the universality class of directed percolation if it does not coincide with another phase transition. This was supported by high-precision numerical simulations for the Glauber Ising model [7] where the spreading
Letter to the Editor

Transition temperature is slightly lower than the equilibrium critical temperature [8]. In contrast, in the case of heat-bath dynamics the spreading temperature seems to coincide with the equilibrium critical temperature [9, 10].

In this letter we, therefore, concentrate on the original question of the stability of the stochastic dynamics in kinetic Ising models. To this end we investigate the time evolution of two identical systems with different initial conditions which are subjected to the same thermal noise. We derive a master equation for the joint probability distribution of the two systems and solve it within an effective-field approach. By analysing the fixed points of this equation we identify regular and chaotic phases. We find that the location of these phases in the phase diagram is sensitive to the choice of the dynamic algorithm. In particular, Glauber dynamics and heat-bath dynamics give very different dynamical phase diagrams.

For the Glauber Ising model, we discuss the relation of our results to directed percolation.

We consider two identical kinetic Ising models with \( N \) sites, described by the Hamiltonian

\[
H = -\frac{1}{2} \sum_{ij} J_{ij} S_i S_j - h \sum_i S_i
\]

(1)

where \( S_i \) is an Ising variable with the values \( \pm 1 \). The dynamics is given by one of the two following stochastic maps which describe Glauber dynamics

\[
S_i(t+1) = \text{sign}[v[h_i(t)] - \frac{1}{2} + S_i(t)[\xi_i(t) - \frac{1}{2}]]
\]

(2a)

and heat-bath dynamics

\[
S_i(t+1) = \text{sign}[v[h_i(t)] - \xi_i(t)]
\]

(2b)

with

\[
v(h) = \frac{e^{h/T}}{(e^{h/T} + e^{-h/T})}.
\]

(3)

Here \( h_i(t) = \sum_j J_{ij} S_j(t) + h \) is the local magnetic field at site \( i \) and (discretized) time \( t \), \( \xi_i(t) \in [0,1] \) is a random number which is identical for both systems, and \( T \) denotes the temperature. Note that Glauber and heat-bath algorithm differ only in the way the random numbers are used to update the configuration. The transition probabilities \( v \) are identical for both algorithms.

In order to describe the simultaneous time evolution of two systems \( H^{(1)} \) and \( H^{(2)} \) with Ising spins \( S^{(1)} \) and \( S^{(2)} \) we define a variable \( v_i(t) \) with the values \( v = ++ \) for \( S^{(1)} = S^{(2)} = 1 \), \(+−\) for \( S^{(1)} = S^{(2)} = 1 \), \(−−\) for \( S^{(1)} = S^{(2)} = 1 \), and \(−+\) for \( S^{(1)} = S^{(2)} = 1 \) which describes the state of a spin pair \((S^{(1)}, S^{(2)})\). Since we are interested in the time evolution not for a single sequence of \( \xi_i(t) \) but in \( \xi \)-averaged quantities, we consider a whole ensemble of system pairs \((H^{(1)}, H^{(2)})\) and define a probability distribution

\[
P(v_1, \ldots, v_N, t) = \left(\sum_{v_i(t)} \prod_{i} \delta_{v_i(v_i(t))}\right)
\]

(4)

where \( \langle . \rangle \) denotes the ensemble average. The time evolution of \( P(v_1, \ldots, v_N, t) \) for a single-spin dynamical algorithm as, for example, Glauber or heat-bath dynamics is given by a master equation

\[
\frac{d}{dt} P(v_1, \ldots, v_N, t) = -\sum_{i=1}^{N} \sum_{\mu_i \neq v_i} P(v_1, \ldots, v_i, \ldots, v_N, t) w(v_i \to \mu_i)
\]

\[
+ \sum_{i=1}^{N} \sum_{\mu_i \neq v_i} P(v_1, \ldots, \mu_i, \ldots, v_N, t) w(\mu_i \to v_i).
\]

(5)
Letter to the Editor

Here \( w(\mu \rightarrow \nu) \) is the transition probability of the spin pair \((S_1, S_2)\) from state \(\mu\) to \(\nu\). It is a function of the local magnetic fields \(h_1\) and \(h_2\) and can be calculated from (2a) or (2b) for Glauber and heat-bath dynamics, respectively.

A complete solution of the master equation (5) is, of course, out of the question. Therefore, one has to resort to approximation methods, the most obvious being mean-field approximations. A natural way to construct a mean-field theory is usually to take the range of the interaction \(J\) to infinity at the beginning of the calculation. However, a mean-field theory constructed this way does not show the chaotic behaviour found in the Glauber Ising model at high temperatures. A more detailed analysis [11] shows that the absence of any fluctuations in the infinite-range model is responsible for this discrepancy, since the fluctuations are essential for the chaotic behaviour.

We, therefore, develop a slightly more sophisticated effective-field approximation that retains the fluctuations, although in a quite simplistic manner. The central idea is to treat the fluctuations at different sites as statistically independent. This amounts to approximating the probability distribution \(P(\nu_1, ..., \nu_N, t)\) by a product of identical single-site distributions \(P_\nu\),

\[
P(\nu_1, ..., \nu_N, t) = \prod_{i=1}^{N} P_\nu(t). \tag{6}
\]

Using this, the master equation (5) reduces to an equation of motion for the single-site distribution \(P_\nu\),

\[
\frac{d}{dt} P_\nu = \sum_{\mu \neq \nu} \left[ -P_\nu W(\nu \rightarrow \mu) + P_\mu W(\mu \rightarrow \nu) \right] \tag{7}
\]

where

\[
W(\mu \rightarrow \nu) = \langle w(\mu \rightarrow \nu) \rangle_P \tag{8}
\]

is the transition probability averaged over the states \(\nu_i\) of all sites according to the distribution \(P_\nu\). Note that the average magnetizations \(m^{(1)}\) and \(m^{(2)}\) of the two systems and the Hamming distance (also called the damage)

\[
D = \frac{1}{2N} \sum_{i=1}^{N} |S_1^{(1)} - S_1^{(2)}| \tag{9}
\]

which measures the distance between the two systems in phase space can be easily expressed in terms of \(P\),

\[
m^{(1)} = P_{++} + P_{+-} - P_{-+} - P_{--} \tag{10a}
\]

\[
m^{(2)} = P_{++} - P_{+-} + P_{-+} - P_{--} \tag{10b}
\]

\[
D = P_{+-} + P_{-+}. \tag{10c}
\]

So far the considerations have been rather general; to be specific we will now concentrate on a two-dimensional system on a hexagonal lattice with a nearest-neighbour interaction of strength \(J\). The external magnetic field \(h\) is set to zero. To solve the master equation (7) for the single-site distribution \(P\) we first calculate the transition probabilities \(w(\mu \rightarrow \nu)\) between the states of a spin pair from one of the stochastic maps (2a) or (2b) and then average these probabilities over the states of the three neighbouring sites of a certain reference site with respect to the yet unknown distribution \(P\). This yields the transfer rates \(W(\mu \rightarrow \nu)\) which

\[†\] Damage spreading in the infinite-range heat-bath Ising model gives reasonable results in qualitative agreement with simulations of short-range models, see [12].
Letter to the Editor

enter (7). The calculations involved are quite tedious but straightforward, and they will be presented in some detail elsewhere [11].

The resulting system of nonlinear equations for the variables $P_{++}$, $P_{+-}$, $P_{-+}$, and $P_{--}$ can first be used to calculate the thermodynamics. As expected, Glauber and heat-bath dynamics give the same results. In particular, there is a ferromagnetic phase transition at a temperature $T_{c}$ determined by

$$
\tanh \frac{3J}{T_{c}} + \tanh \frac{J}{T_{c}} = \frac{4}{3}
$$

which gives $T_{c}/J \approx 2.11$. In the ferromagnetic phase the magnetization is given by

$$
m^{2} = \frac{3}{4}(\tanh(3J/T) + \tanh(J/T)) - 1
$$

We now discuss the time evolution of the Hamming distance $D$ between the two systems which characterizes the stability of the dynamics. In contrast to the thermodynamics Glauber and heat-bath algorithms give very different results for the Hamming distance. We first consider the Glauber case.

The equation of motion of the Hamming distance can easily be derived from (7) and (10c). In the paramagnetic phase we obtain, after some algebra,

$$
d \frac{D}{dt} = \frac{1}{2}(D - 3D^{2} + 2D^{3}) \tanh \frac{3J}{T}.
$$

This equation has three stationary solutions, i.e. fixed points, $D^{*}$, viz $D_{1}^{*} = 0$ which corresponds to the two systems being identical, $D_{2}^{*} = 1$ where $S^{(1)} = -S^{(2)}$ for all sites, and $D_{3}^{*} = \frac{3}{4}$ which corresponds to completely uncorrelated configurations. To investigate the stability of these fixed points we linearize (13) in $d = D - D^{*}$. The linearized equation has a solution $d \propto e^{\lambda t}$ with $\lambda_{1} = \lambda_{2} = \frac{1}{4} \tanh(3J/T)$ and $\lambda_{3} = -\frac{1}{2} \tanh(3J/T)$. Consequently, the only stable fixed point is $D_{3}^{*} = \frac{3}{4}$. Thus, in the paramagnetic phase the Glauber dynamics is chaotic, since two systems, starting close together in phase space ($D$ small initially) will become separated exponentially fast with a Lyapunov exponent $\lambda_{1}$, eventually reaching a stationary state with an asymptotic Hamming distance $D = \frac{3}{4}$. Note, that the Lyapunov exponent $\lambda_{1}$ goes to zero for $T \to \infty$. Therefore, the time it takes the systems to reach the stationary state diverges with $T \to \infty$, as has also been found in simulations [13].

We now turn to the ferromagnetic phase. In order to find the fixed points of the master equation (7) we can set the magnetizations of both systems to their equilibrium values (12) from the outset. In doing so we exclude, however, all phenomena connected with the behaviour after a quench from high temperatures to temperatures below $T_{c}$. These phenomena require an investigation of the early time behaviour and will be analysed elsewhere [11]. For $m^{(1)} = m^{(2)} = m$ the equation of motion for the Hamming distance reads

$$
d \frac{D}{dt} = \frac{1}{2}(D - 3D^{2} + 2D^{3}) \tanh \frac{3J}{T} - \frac{3}{4}m^{2}\left(2D \tanh \frac{J}{T} - D^{2} \tanh \frac{J}{T} + D^{2} \tanh \frac{3J}{T}\right).
$$

This equation has two fixed points $D^{*}$ in the interval $[0, 1]$. The first, $D_{1}^{*} = 0$ exists for all temperatures. The second fixed point $D_{2}^{*}$ with $0 < D_{2}^{*} < \frac{1}{2}$ exists only for $T > T_{c}$ where the spreading temperature $T_{s}$ is determined by

$$
3m^{2} \tanh \frac{J}{T_{s}} = \tanh \frac{3J}{T_{s}}.
$$
Letter to the Editor

Figure 1. Magnetization $m$, asymptotic Hamming distance $D$ and Lyapunov exponent $\lambda_1$ as functions of temperature for the Glauber Ising model. Below $T_c$ the curve for $D$ has two branches corresponding to the two systems being in the same or in different free energy valleys.

This gives $T_s \approx 1.74 \approx 0.82 T_c$. The stability analysis shows that $D_1^* = 0$ is stable for $T < T_s$ and unstable for $T > T_s$ with a Lyapunov exponent $\lambda_1 = \frac{1}{2} \tanh(3J/T) - \frac{3}{2} m^2 \tanh(J/T)$. The fixed point $D_3^*$ which exists only for $T > T_s$ is always stable. Consequently, we find that the Glauber dynamics is regular with the asymptotic Hamming distance being zero for temperatures smaller than the spreading temperature $T_s$ but chaotic for $T > T_s$. Close to the spreading temperature the asymptotic Hamming distance increases

Figure 2. Magnetization $m$ and Lyapunov exponent $\lambda_1$ as functions of temperature for the heat-bath Ising model.
Letter to the Editor

linearly with $T - T_c$ which corresponds to the spreading transition being of second order with a critical exponent $\beta = 1$. In contrast to the paramagnetic phase, where the two systems become eventually completely uncorrelated, for $T_c < T < T_s$ the asymptotic Hamming distance $D$ is always smaller than $\frac{1}{2}$ so that the two systems remain partially correlated. Directly at the spreading point the term linear in $D$ in (14) vanishes. For small distances the equation of motion now reads $dD/dt \propto -D^2$ which gives a power-law behaviour $D(t) \propto t^{-\delta}$ with $\delta = 1$. Note that the values of the critical exponents, viz $\beta = \gamma = 1$, are identical to the mean-field values of directed percolation.

Analogously, for $m^{(1)} = -m^{(2)} = m$ we find two fixed points, $D^*_s = 1$ which exists for all temperatures and $D^*_s > 1$ with $\frac{1}{2} < D^*_s < 1$ which exists for $T > T_s$ only. $D^*_s$ is always stable if it exists. The results for damage spreading in the Glauber Ising model within our effective-field approximation are summarized in figure 1.

We now investigate the time evolution of the damage for the Ising model with heat-bath dynamics (2b). After calculating the averaged transition rates $W(\mu \to \nu)$ [11] and inserting them into (7), we obtain the equation of motion for the Hamming distance $D$. In the paramagnetic phase it reads

$$\frac{d}{dt} D = 3D - \frac{3}{4} \left[ \tanh \frac{3J}{T} + \tanh \frac{J}{T} - \frac{4}{3} \right] - 3D^2 \left[ \tanh \frac{3J}{T} + \tanh \frac{J}{T} \right]$$

$$+ \frac{D^3}{4} \left[ \tanh \frac{3J}{T} + 3 \tanh \frac{J}{T} \right].$$

(16)

This equation has only a single fixed point in the physical interval $[0,1]$, viz $D^*_s = 0$. It is stable everywhere in the paramagnetic phase. Consequently, the asymptotic Hamming distance is zero for all initial conditions, and the heat-bath Ising model does not show chaotic behaviour for $T > T_c$. The Lyapunov exponent is given by

$$\lambda_1 = \frac{3}{4} \tanh \frac{3J}{T} - \frac{3}{4} \tanh \frac{J}{T} - 1 < 0.$$  

The Lyapunov exponent goes to zero for $T \to T_c$, and thus at the critical temperature we again find for small Hamming distances $dD/dt \propto -D^2$ which gives $D(t) \propto t^{-1}$. Note that the time decay of the damage is governed not by the exponent $\beta/z\nu$ (here $\beta$, $z$, and $\nu$ are the usual equilibrium critical exponents) with the mean-field value $\frac{1}{2}$ which characterizes the decay of the magnetization. This is in agreement with numerical results [9] where the decay of the damage is found to follow a power law with a new independent exponent $\delta$.

In the ferromagnetic phase for $m^{(1)} = m^{(2)} = m$ the equation of motion is given by

$$\frac{d}{dt} D = 3D - \frac{3}{4} \left[ (1+m^2) \tanh \frac{3J}{T} + (1-3m^2) \tanh \frac{J}{T} - \frac{4}{3} \right]$$

$$- 3D^2 \left[ \tanh \frac{3J}{T} + \tanh \frac{J}{T} \right] + \frac{D^3}{4} \left[ \tanh \frac{3J}{T} + 3 \tanh \frac{J}{T} \right].$$

(17)

Here we also obtain only one fixed point $D^*_s = 0$ which is stable for all temperatures. The Lyapunov exponent is given by

$$\lambda_1 = \frac{3}{4} (1+m^2) \tanh \frac{3J}{T} + \frac{3}{4} (1-3m^2) \tanh \frac{J}{T} - 1 < 0.$$  

† In contrast to the Glauber dynamics, the heat-bath algorithm does not preserve the symmetry with respect to a global flip of all spins. Therefore, $D = 1$ is not a fixed point here.

‡ A direct determination of the dynamical exponent $\nu$ as in [9,10] is not possible in our mean-field theory since it lacks the notion of space. However, the combination $\beta/z\nu$ can, of course, be determined from the decay of the magnetization at the critical point.
Thus, the behaviour is not chaotic and the asymptotic Hamming distance is \( D = 0 \). Analogously, in the ferromagnetic phase for \( m^{(1)} = -m^{(2)} = m \) we obtain a single stable fixed point \( D^*_2 = m \). The results for damage spreading in the heat-bath Ising model within our effective-field approximation are summarized in figure 2.

In conclusion, we studied the simultaneous time evolution of two kinetic Ising models subjected to the same thermal noise by means of an effective field theory. For the heat-bath dynamics we found that two only slightly different equilibrium configurations stay close together in phase space for all times in both the paramagnetic and the ferromagnetic phase, i.e. an equilibrated heat-bath Ising model does not show chaotic behaviour. For the Glauber dynamics we found a richer behaviour. For all temperatures smaller than a spreading temperature \( T_s \) the two equilibrium configurations stay together for all times. For \( T > T_s \), however, their distance increases exponentially which corresponds to chaotic behaviour. In agreement with numerical simulations for Glauber dynamics the spreading temperature \( T_s \) is not identical to the equilibrium critical temperature but slightly smaller. We determined two critical exponents of the spreading transition, viz \( \beta \) which characterizes the dependence of the asymptotic damage on the reduced temperature and \( \delta \) which governs the time decay of the damage at the spreading point. The two exponents were found to be identical to the mean-field values of directed percolation, in agreement with Grassberger’s conjecture [6].

As with any mean-field theory we have, of course, to discuss in which parameter region it correctly describes the physics of our system. Since we treated the fluctuations in a very simplistic way, viz treating fluctuations at different sites as independent, our effective-field theory will be reliable if the fluctuations are small, i.e. away from the critical point. Therefore, our theory correctly describes the high- and low-temperature behaviour, whereas it might misrepresent the details close to the critical point. It is nonetheless able to distinguish the behaviour of heat-bath and Glauber dynamics close to the spreading transition. Open questions are connected with the influence of external magnetic fields, long-range interactions, and disorder. Some investigations along these lines are in progress.

This work was supported in part by the NSF under grant No DMR-95-10185, and by the DFG under grant No Vo 659/1-1.

References

Wang F and Suzuki M 1996 Physica 223A 34
Monte Carlo simulations of the dynamical behavior of the Coulomb glass

Torsten Wappler
Institut für Physik, Technische Universität, D-09107 Chemnitz, Federal Republic of Germany

Thomas Vojta
Institut für Physik, Technische Universität, D-09107 Chemnitz, Federal Republic of Germany
and Materials Science Institute, University of Oregon, Eugene, Oregon 97403

Michael Schreiber
Institut für Physik, Technische Universität, D-09107 Chemnitz, Federal Republic of Germany
(Received 3 September 1996)

We study the dynamical behavior of disordered many-particle systems with long-range Coulomb interactions by means of damage-spreading simulations. In this type of Monte Carlo simulation one investigates the time evolution of the damage, i.e., the difference of the occupation numbers of two systems, subjected to the same thermal noise. We analyze the dependence of the damage on temperature and disorder strength. For zero disorder the spreading transition coincides with the equilibrium phase transition, whereas for finite disorder we find evidence for a dynamical phase transition well below the transition temperature of the pure system.

I. INTRODUCTION

The combined influence of disorder and long-range interactions on the properties of many-particle systems has been a subject of great interest for some time. In electronic systems already disorder or interactions alone can drastically change the physical behavior. Disorder can lead, e.g., to a metal-insulator transition due to Anderson localization. On the other hand, a metal-insulator transition can also be induced by correlations due to electron-electron interactions. If disorder and interactions are both significant then complex physical problems and phenomena arise, many of which are not completely understood.

The behavior of strongly localized correlated electrons in disordered insulators is especially complicated, both experimentally and theoretically. Thus progress has been slow since the first investigations. Many properties of such systems are still poorly understood. In particular there are only few and contradicting results on thermodynamics, phase diagram, phase transitions or critical behavior, and the examination of the dynamical behavior is only at its beginning. Two of the central questions are whether or not the disordered interacting electron system shows glassy behavior and what is the nature of the glassy "state." Two different views can be found in the literature. In the earlier work the formal similarity between disordered localized electrons and spin glasses had lead to speculations about a possible equilibrium phase transition to a spin-glass-like low-temperature phase. More recent investigations show, however, growing experimental and theoretical evidence of the transition being of dynamical nature.

In this paper we study the dynamical behavior of disordered localized electrons by means of the damage-spreading method. In this type of Monte Carlo simulation the microscopic differences of the time evolution between two systems are investigated. In particular, we address the question of a dynamical phase transition from a dynamically active high-temperature phase to a frozen low-temperature phase upon changing characteristic parameters like disorder or temperature. Our paper is organized as follows. In Sec. II we introduce the Coulomb-glass model, the prototype model of disordered localized electrons. In Sec. III we describe the damage-spreading technique, whereas in Sec. IV we present the results for the dynamical behavior of the model. Section V is dedicated to some discussions and conclusions.

II. MODEL

Our investigation is based on the Coulomb-glass model proposed by Efros and Shklovskii to describe compensated doped semiconductors. Later it was also applied to simulate granular metals and conducting polymers. The model consists of a square or cubic lattice of linear size \( L \) with \( N = L^d \) sites (in \( d \) dimensions) and lattice constant \( a \). The sites can be occupied by \( KN \) \((0 < K < 1)\) electrons. These electrons are interacting via an unscreened Coulomb potential. To guarantee charge neutrality every site carries a compensating charge of \( \pm Ke \) (\( e \) is the charge of the electron). The disorder of this system is described by the random potential \( \varphi_i \). The Hamiltonian of the Coulomb glass is given by

\[
H = \sum_i (\varphi_i - \mu) n_i + \frac{1}{2} \sum_{i \neq j} (n_i - K)(n_j - K) U_{ij}, \quad U_{ij} = \frac{e^2}{r_{ij}}
\]

where \( \mu \) is the chemical potential, \( n_i \) (with values 0 or 1) is the occupation number of site \( i \) and \( r_{ij} \) denotes the distance between sites \( i \) and \( j \). In the rest of the paper we set the interaction strength between nearest-neighbor sites \( e^2/a^2 = 1 \), which fixes the energy scale. The random potential energies \( \varphi_i \) are independent from each other and are chosen according to some probability distribution \( W(\varphi) \). We use the box dis-
Monte Carlo simulations of the dynamical... 


55

MONTE CARLO SIMULATIONS OF THE DYNAMICAL...

Fig. 1. Single-electron density of states of the Coulomb glass at $T=0.008$ for different strengths of disorder. $e_m$ indicates the Madelung energy, $e_F$ the Fermi energy.

...tribution with mean 0 and width $W_0$. The parameter $W_0$ measures the strength of the disorder. Specifically, we investigate a half-filled system ($K=\frac{1}{2}$). Then the Coulomb glass model is particle-hole symmetric and the chemical potential vanishes. (Note that the two quantities $K$ and $\mu$ are not independent of each other. We treat $K$ as a free parameter and calculate $\mu$ from it.)

For later reference we briefly mention some properties of the Coulomb-glass model. One of the central quantities is the single-electron density of states

$$g(\varepsilon, T) = \frac{1}{N^2} \sum_{i} \langle \delta(\varepsilon - \varepsilon_i) \rangle$$

at energy $\varepsilon$ and temperature $T$, where $\langle \ldots \rangle$ denotes thermal and disorder averages. $\varepsilon_i$ are the single-electron energies given by

$$\varepsilon_i = \varepsilon_m - \mu + \sum_{j \neq i} U_{ij}(n_j - K).$$

The single-electron density of states of the Coulomb glass shows a pronounced gap, called the Coulomb gap, close to the Fermi energy $e_F$ (see Fig. 1). At zero temperature the density of states actually vanishes at the Fermi energy, close to the Fermi energy it can be described by a power law

$$g(\varepsilon) \propto |\varepsilon - e_F|^\alpha,$$

where $\alpha$ is approximately 1.2 for two-dimensional (2D) and 2.5 for 3D systems.15 At finite temperature the Coulomb gap is filled gradually (for recent simulation results see, e.g., Ref. 14).

The Coulomb-glass model (1) describes a system without internal dynamics. In reality the electrons, though localized, are coupled to additional (vibrational) degrees of freedom, which lead to transitions between the many-electron states. Phenomenologically this can be simulated by a Monte Carlo method. In every Monte Carlo step we change the occupation numbers of one or several sites with a certain probability. Within the Metropolis algorithm this probability is given by

$$P = \begin{cases} 1, & \Delta H < 0 \\ \frac{\exp(-\Delta H/k_B T)}{1 + \exp(-\Delta H/k_B T)}, & \Delta H > 0, \end{cases}$$

where $\Delta H$ is the energy difference between the many-particle states before and after such a change, and $k_B$ is the Boltzmann constant. $N$ such Monte Carlo steps are called a Monte Carlo sweep which is the natural time scale of our calculations.

To simulate the dynamics one can use different “move classes,” which determine how the occupation numbers are changed in every Monte Carlo step to get the new configuration. The simplest move class consists of exchanging a single electron with a reservoir (i.e., the conduction band in the case of doped semiconductors), other classes include hopping of single electrons between the sites, or correlated hopping of several electrons. In this paper we present results obtained by using only single-electron exchanges between the system and a reservoir, but we have also checked more complicated move classes. As long as we do not include distance-dependent “tunneling terms” into the transition probabilities (5), applying different move classes yields data which do not show a qualitatively different behavior. We attribute this result to the fact that single- and multiple-electron hops can be combined from the moves in our implementation of single-electron exchanges with an external reservoir. Thus all many-electron states with $KN$ electrons are available in our simulation. A more detailed investigation of this question including the effects of distance-dependent transition probabilities on the damage-spreading simulations is in progress.

III. DAMAGE SPREADING

The damage-spreading technique15 is a modification of the usual Monte Carlo method. The idea is to look not at the time evolution of a single system but to compare the time evolutions of two systems which are subjected to the same thermal noise (i.e., the same random numbers are used within the Metropolis algorithm). Usually, at the beginning of the simulation the occupation numbers of both systems differ only at a single site (or at a few sites, e.g., a single column in a 2D lattice system).

Since both systems are thermodynamically identical, averages of equilibrium quantities will be the same for both systems. Microscopically, however, the two systems may evolve differently from each other. The central observable in damage-spreading simulations is the Hamming distance $D(t)$, which is the portion of sites for which the occupation numbers differ between the two systems. $D(t)$, which measures the “damage,” is given by

$$D(t) = \frac{1}{N} \sum_{i} |n_i^1(t) - n_i^2(t)|,$$

where $n_i^1(t)$ and $n_i^2(t)$ are the occupation numbers of site $i$ of the original system and the copy at (Monte Carlo) time $t$. 
For $D(0)=0$ the two systems are identical, $D(t) = \frac{1}{t}$ describes completely uncorrelated configurations, and for $D(t) = 1$ the two systems are totally anticorrelated. In the course of the time evolution the two systems evolve towards a steady state, in which $D(t)$ fluctuates around an asymptotic average value

$$D = \lim_{t \to \infty} \lim_{n \to \infty} \frac{1}{n} \int_{t}^{t+n} dt' D(t').$$

(7)

Depending on the values of the external parameters temperature and disorder different regimes can be observed, in principle, if the initial damage $D(0)$ is small: The damage may heal out during the time evolution ($D=0$), the systems may stay partially correlated for infinite time ($D<\frac{1}{2}$), or the systems may become completely uncorrelated so that $D = \frac{1}{2}$ . In contrast to the thermodynamics the detailed behavior of $D(t)$ depends on the choice of the dynamical algorithm. Whereas Metropolis, Glauber, and heat-bath dynamics give the same results for equilibrium quantities of a single system, the damage-spreading results differ. For the Metropolis dynamics which we use (as well as for the Glauber dynamics) the damage tends to heal at low temperatures and tends to spread at high temperatures. In contrast the heat-bath dynamics yields healing at high temperature and frozen configurations at low temperatures. (Note that since $D$ is not a thermodynamic quantity but measures the microscopic differences between two systems, there is no reason to expect that different dynamical algorithms give the same results.)

We apply the damage-spreading technique to the 2D Coulomb-glass model at half filling $K = \frac{1}{2}$ and linear system sizes $L = 20, \ldots, 80$. The simulation proceeds as follows: (i) We create the initial system by choosing random potential values according to the probability distribution $W(\varphi)$ and occupy the sites at random with $KN$ electrons. (ii) We equilibrate this system at temperature $T$ by performing several (at least 300) Monte Carlo sweeps according to the Metropolis algorithm. (iii) A copy of the system is created and modified at a single site (or several sites). This difference in the occupation numbers constitutes the initial damage. (iv) We study the time evolution of the original and the copy using the same random numbers in the Metropolis algorithm for both systems. The damage $D(t)$ is recorded and its asymptotic value $D$ is determined.

Note that there is a modification of the damage-spreading method that can be used to determine equilibrium quantities instead of purely dynamic ones. In that kind of simulation the occupation number of a single site in one of the systems is fixed whereas it is allowed to fluctuate in the other system. Consequently, the two systems are thermodynamically different and the damage can be related to equilibrium correlation functions. Since in this paper we are interested in the properties of the dynamics rather than in equilibrium quantities our data is gained by means of the original damage-spreading method, where the occupation numbers of both systems are allowed to fluctuate.

![FIG. 2. Time dependence of the Hamming distance of the 2D Coulomb glass for different temperatures and $\omega = 0$.](image)

### IV. RESULTS

#### A. Time evolution

In this subsection we present data on the time evolution of the damage $D(t)$ starting with an initial damage consisting of a single site. In analogy to the well studied 2D Ising model we find that for temperatures below a certain temperature $T_s$, called the spreading temperature, the damage $D(t)$ remains small and eventually heals, giving an asymptotic value of $D=0$. For temperatures larger than $T_s$ the damage increases with time until a steady state is reached where $D(t)$ fluctuates around a finite value. Consequently, the asymptotic damage $D$ is finite in this regime. In Fig. 2 the time evolution of $D(t)$ is shown for the Coulomb glass with zero disorder $\omega = 0$. The three curves presented correspond to the three regimes discussed in the last section. At $T=0.5$ the damage increases quickly and then fluctuates around $D = \frac{1}{2}$. This means the two systems become completely uncorrelated very fast. Consequently we are above the spreading temperature $T_s$. At $T=0.1$ the evolution of $D(t)$ is much slower and the asymptotic damage is smaller than $\frac{1}{2}$. This behavior occurs because the system is in the vicinity of the spreading transition at $T_s$. It corresponds to the critical slowing down in ordinary critical phenomena. At $T=0.06$ the damage remains small and eventually heals, thus the system is below the spreading temperature $T_s$. In the case of finite disorder $\omega$ the time evolution of the damage is similar (see Fig. 3). The asymptotic damage $D$ is, however, different from 0 or $\frac{1}{2}$ even far away from the spreading transition. The dependence of the damage on the external parameters temperature and disorder is investigated in more detail in Sec. IV C.

#### B. Influence of the long-range interaction

The character of the interaction has a large influence on the time evolution of the damage. In systems with nearest-neighbor interactions, e.g., the Ising model, the damage can only spread within a single Monte Carlo step from one site of the system to its neighbor. Therefore the clouds of damaged sites can grow only slowly in space and tend to be more...
compact (but not necessarily connected). In contrast, in systems with long-range interactions the occupation number of any site affects all other sites. The damage can spread from one site of the system to any other site within a single Monte Carlo step. Therefore the damage spreads much faster as in systems with short-range interaction and the damage clouds are usually not compact. A comparison of the two cases is presented in Fig. 4.

Note, that since the damage can spread from one site to any other site in the case of long-range interactions, some of the methods developed to analyze the damage-spreading simulations\textsuperscript{15,17} cannot be used for systems with long-range interactions. This applies to all methods that measure the spatial extension of the damage and its evolution, because the spatial extent of the damage cloud is not a well defined quantity for systems with long-range interactions.

### C. Temperature and disorder dependence of the asymptotic damage

We now turn to the main results of this paper. Figure 5 shows an overview of the temperature and disorder dependence of the asymptotic Hamming distance $D$. For disorder strength $W_0=0$ there is a pronounced transition at a spreading temperature of approximately $T_s=0.1$ between a low-temperature regime with $D=0$ and a high-temperature regime with $D=\frac{1}{2}$. Within our numerical accuracy the spreading temperature $T_s$ coincides with the equilibrium critical point $T_c$ of the model without disorder which we determined from the peak in the specific heat $C_v$ of the Coulomb-glass model as a function of temperature (see Fig. 6). For very high temperatures $T\to\infty$ the spreading of the damage is drastically slowed down due to the fact that the probability $P$ in the Metropolis algorithm, Eq. (5), becomes independent of the actual configuration of the two systems (original and copy) and reaches $P=1$. This means that in both systems nearly every exchange of electrons is performed and differences in the occupation numbers occur only rarely. Our investigations of the spreading behavior for very high temperatures show that the Hamming distance $D$ still reaches a plateau if plotted versus time as in Figs. 2 and 3, but the relaxation time diverges as is predicted in a recent mean-field theory.\textsuperscript{21} The damage-spreading transition in the
Monte-Carlo simulations of the dynamical behavior of the Coulomb glass

...around the Fermi energy electron density of states at low temperatures has a hard gap $W$ increases with increasing potential the electrons are trapped for that is easy to understand: In the presence of a random potential the electrons are trapped (repulsed) at sites with small (high) potential values $\phi_i$. These sites are identical in the original system and its copy. Therefore the presence of a random potential tends to reduce the damage. With increasing strength of disorder this trapping effect becomes larger, so that the maximum value of the damage is more and more reduced. On the other hand, increasing temperature makes it easier to overcome the potential differences so that the described reduction of the damage becomes less effective.

The second effect of the disorder concerns the behavior of $D$ at low temperatures and close to the spreading point. This region is shown in more detail in Fig. 7. In the case of finite disorder the asymptotic damage remains finite even at temperatures below the spreading temperature of the model without disorder. This somewhat counterintuitive result, viz. an acceleration of the dynamics by disorder, can be understood by looking at the single-electron density of states of the Coulomb-glass model (see Fig. 1). For $W_0=0$ the single-electron density of states at low temperatures has a hard gap around the Fermi energy $\varepsilon_F=0$ and two peaks at the Madelung energies $\pm e_M/L$. Therefore there are only exponentially few sites that can be excited at low temperatures and thus the Hamming distance vanishes. In contrast, for finite disorder $W_0$, the gap in the density of states is not exponential but the power-law Coulomb gap (4). Therefore more sites can be excited at low temperature and the dynamics does not freeze completely, i.e., the Hamming distance remains finite.

As can be seen in Fig. 7, even for finite disorder strength $W_0$ there is, however, a spreading temperature $T_s(W_0)$ below which the asymptotic damage vanishes. $T_s(W_0)$ decreases with increasing $W_0$, but seems to tend to a finite limiting value for large $W_0$ which we approximately determined to $T_s(\infty) \approx 0.03$. Note that the existence of a spreading transition in the case of finite disorder is a purely dynamical phenomenon, since the system does not undergo an equilibrium phase transition.

In order to determine more detailed properties of the spreading transition a careful analysis of finite-size effects is necessary. In Fig. 8 we show the dependence of the Hamming distance $D$ on the system size. As expected from the analogy with usual critical phenomena, the spreading transition becomes sharper with increasing system size. Figure 8 also shows that a system size of $L=20$ already gives reasonable results for the determination of the spreading temperature of the Coulomb-glass model, provided the disorder strength is comparatively small.

V. CONCLUSIONS AND OUTLOOK

We have used the damage-spreading technique to examine the low-temperature dynamics of disordered electronic systems with localized states based on the Coulomb-glass model. We have found that the dynamics of the system freezes below a spreading temperature $T_s$. For zero disorder this damage spreading transition coincides with the equilibrium phase transition within our accuracy. At finite disorder strength, when there is no equilibrium phase transition, the spreading point $T_s$ is shifted to lower temperatures. However, $T_s$ remains finite even for larger disorder strengths. Consequently, there is a low-temperature "phase" of the Coulomb glass with frozen dynamics and a high-temperature phase where the damage spreads through the system. In the case of finite disorder $W_0$ the spreading transition is a purely dynamical transition which does not possess an equilibrium counterpart. A more detailed investigation of this transition is in progress. It is, however, hampered by finite-size effects since the long-range interaction severely restricts the possible system sizes in our simulations. These limited system sizes are also the reason why the spreading point $T_s$ for high values of disorder could not yet be determined exactly.

For small disorder strengths the spreading point $T_s$ is still close to the (second-order) equilibrium phase transition temperature $T_c$ of the system without disorder. If both transitions coincide for zero disorder we expect the Hamming distance $D$ to obey the homogeneity relation (since physical quanti-
ties in the vicinity of a critical point can usually be described by scaling laws)

\[ D(W_0, T) = t^{\beta}\left(\frac{W_0}{T}\right) , \quad t = |T - T_c| \]  

(8)

with the critical exponents \( \beta \) and \( \gamma \). However, the damage-spreading transition in models with Glauber or Metropolis dynamics does not generically coincide with the equilibrium transition. Therefore the confirmation of this scaling law and the determination of the exponents remain a task for the future.

In order to compare our results to experiments on glassy behavior in disordered insulators a direct relation between the Hamming distance and measurable quantities would be desirable. To this end a relation between the Hamming distance and characteristics (probably more complex) of a single system should be found. Similar relations are known in the theory of chaos where characteristics of chaotic behavior show up in a single system as well as in the time evolution of the phase space distance between two copies. However, such relations have not been found for damage spreading in cooperative systems up to now.

One might also ask, how the results change if more sophisticated dynamical algorithms are used, which represent the physical processes in disordered insulators better than the simple Metropolis algorithm with single-particle exchange with a reservoir. The question is of particular importance, since the properties of damage spreading depend on the type of dynamics used in the simulation more strongly than the thermodynamic quantities. We have begun to study the Coulomb-glass model with distance-dependent tunneling probabilities between the sites. Results of this numerically much more involved investigation will be published elsewhere.

ACKNOWLEDGMENTS

This work was supported in part by the DAAD, by the DFG under Grant No. Vo 659/1-1 and SFB 393 and by the NSF under Grant No. DMR-95-10185.

Chaotic behavior and damage spreading in the Glauber Ising model:
A master equation approach

Thomas Vojta
Institut für Physik, Technische Universität, D-09107 Chemnitz, Germany
and Department of Physics and Materials Science Institute, University of Oregon, Eugene, Oregon 97403
(Received 2 December 1996)

We investigate the sensitivity of the time evolution of a kinetic Ising model with Glauber dynamics against the initial conditions. To do so we apply the ‘‘damage spreading’’ method, i.e., we study the simultaneous evolution of two identical systems subjected to the same thermal noise. We derive a master equation for the joint probability distribution of the two systems. We then solve this master equation within an effective-field approximation which goes beyond the usual mean-field approximation by retaining the fluctuations though in a quite simplistic manner. The resulting effective-field theory is applied to different physical situations. It is used to analyze the fixed points of the master equation and their stability and to identify regular and chaotic phases of the Glauber Ising model. We also discuss the relation of our results to directed percolation.

PACS number(s): 05.40.+j, 64.60.Ht, 75.40.Gb

I. INTRODUCTION

The physics of dynamic phase transitions and dynamic critical phenomena has been a subject of great interest for the last two decades. Whereas the dynamic behavior at and close to usual static phase transitions is well understood [1,2], much less is known about dynamic phase transitions which do not have a static counterpart. Sometimes it is not even known whether or not a particular dynamic transition coincides with an equilibrium phase transition.

One of these dynamic phenomena is the so-called ‘‘damage spreading’’ [3–5]. The central question of this problem is how a small perturbation (called the damage) in a cooperative system changes during the further time evolution. Among the simplest of such cooperative systems are kinetic Ising models where the above question has been investigated by means of Monte Carlo simulations [4,5]. In these simulations two identical Ising models with different initial conditions are subjected to the same thermal noise, i.e., the same random numbers are used in the Monte Carlo procedure. In analogy to the physics of chaotic dynamics [6] the differences in the microscopic configurations of the two systems are then used to characterize the dynamics and distinguish regular and chaotic phases, depending on external parameters (e.g., temperature and magnetic field).

Later the name ‘‘damage spreading’’ has also been applied to a different though related type of investigations in which the two systems are not identical. Instead, one or several spins in one of the copies are permanently fixed in one direction. Therefore the equilibrium properties of the two systems are different, and the microscopic differences between the two copies can be related to static and dynamic correlation functions [7,8]. Note that in this type of simulations it is not essential to use identical noise (i.e., random numbers) for the two systems. Instead it is only a convenient method to reduce the statistical error.

Whereas this second type of damage spreading is well understood and established as a method to calculate equilibrium properties numerically, much less is known about the original problem of damage spreading, viz. how sensitive is the dynamics of the Ising model to different initial conditions. In particular, there are no rigorous results on the transition between regular and chaotic behavior (called the ‘‘spreading transition’’).

There are two different mechanisms by which the damage can spread in a kinetic Ising model. First, the damage can spread within a single ergodic component (i.e., a pure state or free-energy valley) of the system. This is the case for Glauber or Metropolis dynamics. Numerical simulations here consistently give a transition temperature slightly lower than the equilibrium critical temperature [9]. Grassberger [10] conjectured that the spreading transition falls into the universality class of directed percolation if it does not coincide with another phase transition. This was supported by high-precision numerical simulations for the Glauber Ising model [11].

Second, the damage can spread when the system selects one of the free-energy valleys at random after a quench from high temperatures to below the equilibrium critical temperature. This is the only mechanism to produce damage spreading in an Ising model with heat-bath dynamics. In this case the spreading temperature seems to coincide with the equilibrium critical temperature below which both pure states separate [4,12,13]. Thus at the spreading point there are long-range static correlations in the systems, and the transition is expected to fall into a universality class different from directed percolation.

In this paper we investigate the damage spreading in the Glauber Ising model by deriving and solving a master equation for the time evolution of a joint probability distribution for two identical systems with different initial conditions and subjected to the same thermal noise. The paper is organized as follows. In Sec. II A we define the model. Transition probabilities between the states of a spin pair are calculated in Sec. II B, and the master equation for the joint probability distribution is derived in Sec. II C. We discuss how to construct a mean-field approximation for this equation in Sec. II D.
III A. In Secs. III B, III C, and III D we present solutions of the master equation within this approximation for different physical situations. Finally, Sec. IV is dedicated to conclusions and an outlook on future work. A short account of part of this work has already been published [14] together with a comparison to the heat-bath Ising model.

II. MASTER EQUATION FOR DAMAGE SPREADING

A. Glauber Ising model

We consider two identical kinetic Ising models with \( N \) sites described by the Hamiltonians \( H^{(1)} \) and \( H^{(2)} \) given by

\[
H^{(n)} = -\frac{1}{J_n} \sum_{ij} J_{ij} S_i^{(n)} S_j^{(n)} - h \sum_i S_i^{(n)},
\]

where \( S_i^{(n)} \) is an Ising variable with the values \( \pm 1 \) and \( n = 1, 2 \) distinguishes the two copies. \( J_{ij} \) is the exchange interaction between the spins and \( h \) denotes an external magnetic field. The dynamics of the Ising models is given by the Glauber algorithm, i.e., in every time step a lattice site \( i \) is chosen at random (the same site in both copies). The value of the spin at this site is calculated according to

\[
S_i^{(n)}(t+1) = \text{sgn}[v[H_i^{(n)}(t)] - \frac{1}{T} S_i^{(n)}(t)[\xi_i(t) - \frac{1}{2}]],
\]

where the transition probability \( v(x) \) is given by the usual Glauber expression

\[
v(x) = e^{x/T}(e^{x/T} - e^{-x/T}).
\]

Here \( h_i^{(n)}(t) = \sum_{j} J_{ij} S_j^{(n)}(t) + h \) is the local magnetic field at site \( i \) and \( \xi_i(t) \) is a random number taken from a uniform distribution between 0 and 1. \( T \) denotes the temperature. The spins at all sites different from site \( i \) are unchanged within this time step.

The central quantity in any damage spreading process is the distance between the two systems in phase space, called the Hamming distance (or the damage). It is defined by

\[
D(t) = \frac{1}{2N} \sum_{i=1}^{N} |S_i^{(1)}(t) - S_i^{(2)}(t)|,
\]

and is identical to the portion of sites where the spins in the two systems differ.

In order to describe the simultaneous time evolution of the two systems \( H^{(1)} \) and \( H^{(2)} \), we define a variable \( \nu(t) \) at each lattice site which describes the state of a spin pair \( (S_i^{(1)}, S_i^{(2)}) \). It has the values \( \nu = + + \) for \( S_i^{(1)} = S_i^{(2)} = 1 \), \( + - \) for \( S_i^{(1)} = - S_i^{(2)} = 1 \), \( - + \) for \( - S_i^{(1)} = S_i^{(2)} = 1 \), and \( -- \) for \( S_i^{(1)} = S_i^{(2)} = -1 \). A complete configuration of the two Ising models is thus described by the set \( \{\nu_1, \ldots, \nu_N\} \).

Since we are interested in the time evolution not for a single sequence of \( \xi_i(t) \), but in \( \xi \)-averaged quantities we consider a whole ensemble of system pairs \( (H^{(1)}, H^{(2)}) \) and define a probability distribution

\[
P(\nu_1, \ldots, \nu_N, t) = \left( \prod_{i} \delta_{\nu_i, \nu_i(t)} \right)
\]

where \( \langle \cdot \rangle \) denotes the ensemble average.

**Table I. Transition probabilities \( w(\nu \rightarrow \mu) \) between the states of a spin pair.**

<table>
<thead>
<tr>
<th>( \nu \rightarrow \mu )</th>
<th>Transition probability</th>
</tr>
</thead>
<tbody>
<tr>
<td>(+ + \rightarrow + + )</td>
<td>( v\left[\max(h^{(1)}, h^{(2)})\right] )</td>
</tr>
<tr>
<td>(+ + \rightarrow + - )</td>
<td>( v\left[\min(h^{(1)}, h^{(2)})\right] )</td>
</tr>
<tr>
<td>(+ + \rightarrow - + )</td>
<td>( \Theta(h^{(2)} - h^{(1)})[v(h^{(1)}) - v(h^{(2)})] )</td>
</tr>
<tr>
<td>(+ + \rightarrow -- )</td>
<td>( \Theta(h^{(1)} - h^{(2)})[v(h^{(1)}) - v(h^{(2)})] )</td>
</tr>
<tr>
<td>(+ - \rightarrow + + )</td>
<td>( \Theta(-h^{(1)} - h^{(2)})[v(-h^{(1)}) - v(h^{(2)})] )</td>
</tr>
<tr>
<td>(+ - \rightarrow + - )</td>
<td>( \Theta(h^{(1)} + h^{(2)})[v(h^{(2)}) - v(-h^{(1)})] )</td>
</tr>
<tr>
<td>(+ - \rightarrow - + )</td>
<td>( e^{\left{-[\min(h^{(1)}, h^{(2)})] - \xi\right}} )</td>
</tr>
<tr>
<td>(+ - \rightarrow -- )</td>
<td>( e^{\left{-\max(-h^{(1)}, h^{(2)})\right}} )</td>
</tr>
</tbody>
</table>

B. Transition probabilities

In order to formulate a master equation for the probability distribution \( P(\nu_1, \ldots, \nu_N, t) \) we need to know the transition probabilities \( w(\nu \rightarrow \mu) \) between the states \( \nu \) of a spin pair. Since the Glauber dynamics (2) involves only a single lattice site within each time step, we have to consider transitions between the states \( \nu \) of a single site only. Let us look, e.g., at the transition of site \( i \) from state \( -- \) to \(+ + \). This corresponds to both \( S_i^{(1)} \) and \( S_i^{(2)} \) changing from \(-1 \) to \(1 \). According to the Glauber dynamics (2) this requires \( v(h_i^{(1)}) - \xi_i > 0 \) and \( v(h_i^{(2)}) - \xi_i > 0 \). Since \( v(h) \) is a monotonic function of \( h \), both equations are simultaneously fulfilled for \( v(\min(h_i^{(1)}, h_i^{(2)})) - \xi_i > 0 \). Because \( \xi_i \) is a random number taken from a uniform distribution between 0 and 1, the transition probability is given by

\[
w(- - \rightarrow + +) = v(\min(h_i^{(1)}, h_i^{(2)})).
\]

Analogously, for a transition from state \( -- \) to \(+ + \) the two inequalities \( v(h_i^{(1)}) - \xi_i > 0 \) and \( v(h_i^{(2)}) - \xi_i > 0 \) have to be fulfilled. Since \( v(h) \) is a monotonic function of \( h \), this is only possible for \( h_i^{(1)} > h_i^{(2)} \). The transition probability is obviously given by

\[
w(- - \rightarrow + +) = \Theta(h_i^{(1)} - h_i^{(2)})[v(h_i^{(1)}) - v(h_i^{(2)})].
\]

The transition probabilities \( w(\nu \rightarrow \mu) \) fulfill the following symmetry relations:

\[
w(+ + \rightarrow + + ) = w(\nu \rightarrow \mu),
\]

\[
w(\nu \rightarrow + + ) = w(- + \rightarrow + ),
\]

for any state \( \nu \) as can easily be seen by making the substitutions \( S_i^{(n)}(t) \rightarrow - S_i^{(n)}(t) \) and \( \xi_i(t) \rightarrow 1 - \xi_i(t) \) on the right-hand side of Eq. (2).

The remaining transition probabilities can be calculated along the same lines as above. They are summarized in Table I.

C. Master equation

Having calculated the transition probabilities between the states \( \nu \) of a spin pair we are now in the position to write down the equation of motion for the probability distribution \( P(\nu_1, \ldots, \nu_N, t) \). It has the form of a usual master equation
d \frac{d}{dt} P(v_1, \ldots, v_N, t)
\begin{align*}
&= -\sum_{i=1}^{N} \sum_{\mu_i \neq v_i} P(v_1, \ldots, v_i, \ldots, v_N, t) w(v_i \rightarrow \mu_i) \\
&\quad + \sum_{i=1}^{N} \sum_{\mu_i \neq v_i} P(v_1, \ldots, \mu_i, \ldots, v_N, t) w(\mu_i \rightarrow v_i), \quad (9)
\end{align*}

where the term in the second line describes the decrease of $P(v_1, \ldots, v_N, t)$ due to the initial configuration \{v_1, \ldots, v_N\} being changed at one of the sites $i$ from $v_i$ to $\mu_i$. The term in the third line of the master equation describes the increase of $P(v_1, \ldots, v_N, t)$ due to ”scattering” from all the other states into \{v_1, \ldots, v_N\}. Note that we have suppressed the factor $1/N$ in the transition probabilities which corresponds to random selection of one of the lattice sites in every time step. This neglect corresponds to a redefinition of the time scale (which is now independent of the system size) and does not change the dynamic behavior.

This master equation contains, of course, the full difficulty of the dynamic many-body problem. A complete solution is therefore out of question, and one has to resort to approximation methods. In the following section we discuss how to construct a mean-field-like approximation to the master equation (9).

### III. EFFECTIVE-FIELD APPROXIMATION

Usually a mean-field theory of a phase transition can be obtained by taking the range of the interaction to infinity:

$$J_{ij} = J_0/N \quad \text{for all } i,j.$$  

(10)

In the thermodynamic limit $N \to \infty$ this suppresses all fluctuations. In particular, the local magnetic fields $h_i^{(n)}$ of all sites in one system become equal and identical to the mean-field value $J_0 m$. Since the two Ising models $H^{(1)}$ and $H^{(2)}$ are thermodynamically identical, this leads to $h_i^{(1)} = h_i^{(2)}$. However, some of the transition probabilities depend on the existence of fluctuations (see Table I), i.e., $w(v \rightarrow \mu)$ go to zero with $h_i^{(1)} - h_i^{(2)} \to 0$. In particular, this is true for $w(- \to -)$ and $w(- \to +)$, which are responsible for increasing the damage $D$. Consequently, if the thermodynamic limit and the limit of infinite range of the interaction are taken at a too early stage of the calculation, the resulting model does not show any spreading of the damage. To circumvent these problems we develop a slightly more sophisticated effective-field approximation that retains the fluctuations though in a quite simplistic manner. As will be shown in Sec. III C, taking the range of the interaction to infinity within the framework of this approximation yields a sensible limit.

#### A. Effective-field theory for short-range models

The central idea of this effective-field method is to retain the fluctuations but to treat the fluctuations at different sites as statistically independent. This amounts to approximating the probability distribution $P(v_1, \ldots, v_N, t)$ by a product of identical single-site distributions $P_{v_i}$.

Inserting this into the master equation (9) and summing over all states of sites $i = 2, \ldots, N$ gives an equation of motion for the single-site distribution $P_{v_i}$:

$$\frac{d}{dt} P_{v_i} = \sum_{\mu_i \neq v_i} \left[ - P_{v_i} W(\mu_i \rightarrow v_i) + P_{\mu_i} W(\mu_i \rightarrow v_i) \right],$$  

(12)

where

$$W(\mu_i \rightarrow v_i) = \langle w(\mu_i \rightarrow v_i) \rangle_p,$$

(13)

is the transition probability averaged over the states $v_i$ of all sites $i \neq 1$ according to the distribution $P_{v_i}$. Since all sites of the systems are equivalent, the site index $i$ will be suppressed from now on.

Note that the average magnetizations $m^{(1)}$, $m^{(2)}$ of the two systems and the Hamming distance $D$ can be easily expressed in terms of $P_{v_i}$,

$$m^{(1)} = P_{+} + P_{-},$$

$$m^{(2)} = P_{+} - P_{-},$$

(14a)

$$D = P_{+} + P_{-}.$$

(14b)

(14c)

So far the considerations have been rather general. In the following subsections we will apply the general formalism to different physical situations. In Sec. III B we investigate a two-dimensional system with short-range interactions and vanishing external field. We determine not only the location of the spreading transition but also calculate the stationary states of the systems. Section III C deals with the limit of infinite-range interactions, and in Sec. III D we study the influence of an external magnetic field on the spreading transition.

#### B. Solution of a two-dimensional model

In this subsection we investigate the damage spreading for a two-dimensional Glauber Ising model on a hexagonal lattice (with each site having three nearest neighbors). The initial state is taken to be a configuration where all sites have the same state $v$.


<table>
<thead>
<tr>
<th>$h^{(2)}$</th>
<th>$h^{(1)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$3J$</td>
<td>$P^3_{+}$</td>
</tr>
<tr>
<td>$J$</td>
<td>$3P^2_{+}P_{-}$</td>
</tr>
<tr>
<td>$-J$</td>
<td>$3P^2_{-}P_{+}$</td>
</tr>
<tr>
<td>$-3J$</td>
<td>$P^3_{-}$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$h^{(2)}$</th>
<th>$h^{(1)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$3J$</td>
<td>$3P^2_{+}P_{-}$</td>
</tr>
<tr>
<td>$J$</td>
<td>$3P^2_{-}P_{+}$</td>
</tr>
<tr>
<td>$-J$</td>
<td>$3P^2_{+}P_{-}$</td>
</tr>
<tr>
<td>$-3J$</td>
<td>$3P^2_{-}P_{+}$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$h^{(2)}$</th>
<th>$h^{(1)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$3J$</td>
<td>$P^3_{+}$</td>
</tr>
<tr>
<td>$J$</td>
<td>$3P^2_{+}P_{-}$</td>
</tr>
<tr>
<td>$-J$</td>
<td>$3P^2_{-}P_{+}$</td>
</tr>
<tr>
<td>$-3J$</td>
<td>$P^3_{-}$</td>
</tr>
</tbody>
</table>
interaction is taken to be a nearest-neighbor interaction of strength $J$, and the external magnetic field is set to zero.

In order to solve the master equation (12) for the single-site distribution $P_v$, we first determine the effective transition probabilities $W(v \rightarrow \mu)$. Let us calculate the probabilities for a particular site $i$. To this end we have to average the transition probabilities given in Table I with respect to the states of all other sites of the system. However, since the interaction is between nearest neighbors, the transition probabilities depend on the states of these three neighbors of site $i$ only.

$$W(-\rightarrow + +) = \langle w(-\rightarrow + +) \rangle = \langle v \min(h^{11}, h^{12}) \rangle$$

$$= p_1 v_1 + 3p_2^2 - p_{-2} - p_{-1} + 3p_1^2 + p_{3}^2 - v_{-1} + (3p_2^2 + p_{-2} + 3p_3^2 - p_{-3})v_{-3} + (3p_2^2 + p_{-2} + 6p_1 + 6p_{-1} + 6p_{-2} + 6p_{-3})v_{-1}$$

$$= (3p_1^2 + 3p_2^2 + 3p_3^2 + 3p_4^2 + 3p_{-2} + 6p_1 + 6p_{-1} + 6p_{-2} + 6p_{-3})v_{-1}$$

$$+ (3p_2^2 + 3p_3^2 + 3p_4^2 + 3p_{-2} + 6p_1 + 6p_{-1} + 6p_{-2} + 6p_{-3})v_{-3} + (3p_1^2 + 3p_2^2 + 3p_3^2 + 3p_4^2 + 3p_{-2} + 6p_1 + 6p_{-1} + 6p_{-2} + 6p_{-3})v_{-1}$$

$$+ (3p_2^2 + 3p_3^2 + 3p_4^2 + 3p_{-2} + 6p_1 + 6p_{-1} + 6p_{-2} + 6p_{-3})v_{-3}, \quad (15)$$

with

$$v_n = v(nJ). \quad (16)$$

Equations of motion for the magnetizations $m^{(1)}$ and $m^{(2)}$ as well as for the damage $D$ can be derived by inserting definitions (14) into the single-site master equation (12). After some manipulations the equations of motion for the magnetizations read

$$\frac{d}{dt} m^{(n)} = m^{(n)} \left[ -1 + \frac{1}{2} \left( \tanh(3J/T) + \tanh(J/T) \right) \right] + \frac{1}{2} (m^{(n)})^2 \left[ \tanh(3J/T) - 3 \tanh(J/T) \right]. \quad (17)$$

These equations are, of course, identical to the equation of motion of the magnetization derived for a single system within the same framework of statistically independent fluctuations. The point at which the coefficient of the term linear in $m$ on the right-hand side of Eq. (17) changes sign defines the (equilibrium) critical temperature $T_c$ of the Ising model within our approximation. $T_c$ is thus determined by

$$\frac{1}{2} \left[ \tanh(3J/T_c) + \tanh(J/T_c) \right] = 1, \quad (18)$$

which gives $T_c/J \approx 2.104$. The stationary solution of Eq. (17) can be used to determine the magnetization as a function of temperature. For temperatures $T < T_c$, we obtain

$$(m^{(n)})^2 = \frac{1}{2} \left[ \tanh(3J/T) + \tanh(J/T) \right] - 1 \frac{\tanh(J/T) - \frac{1}{2} \tanh(3J/T)}{\tanh(J/T) - \frac{1}{2} \tanh(3J/T)}. \quad (19)$$

We now turn to the discussion of the Hamming distance $D$. After inserting Eq. (14) into (12), the equation of motion of the Hamming distance $D$ can be written as

Each of the neighbors can be in one of four states, thus we have to consider 64 different configurations of the neighboring sites. The probabilities for these configurations and the resulting local magnetic fields are given in Table II.

With the help of Tables I and II the averaged transition probabilities (13) can be easily calculated by adding up the contributions of all 64 configurations. The resulting expression are quite lengthy though simple. Therefore we present only the example

$$\frac{d}{dt} D = (1 - D) \left[ W(--\rightarrow +) + W(--\rightarrow +) \right]$$

$$+ D [-1 + W(--\rightarrow +) + W(--\rightarrow +)]. \quad (20)$$

Since in the following we will be mainly interested in the stationary solutions of this equation, we restrict the considerations to cases where both systems are in equilibrium at the beginning of the damage spreading process. In doing so we exclude, however, all phenomena connected with the behavior after a quench from high temperatures to temperatures below $T_c$. These phenomena require an investigation of the early-time behavior and will be analyzed elsewhere [15].

It is now useful to distinguish three cases, (i) damage spreading in the paramagnetic phase ($T > T_c$), (ii) the ferromagnetic phase ($T < T_c$) where both systems are in the same pure state (i.e., free energy valley), $m^{(1)} = m^{(2)} = m$, and (iii) the ferromagnetic phase ($T < T_c$) where the two systems are in different pure states, $m^{(1)} = -m^{(2)} = m$.

1. Paramagnetic phase

In the paramagnetic phase all $P_v$ can be expressed in terms of $D$:

$$P_{++} = P_{--} = \frac{1}{2}(1 - D), \quad (21a)$$

$$P_{+-} = P_{-+} = \frac{1}{2} D. \quad (21b)$$

By inserting this into the transition probabilities $W(v \rightarrow \mu)$ calculated from Eq. (13) and Table II, the equation of motion (20) of the Hamming distance $D$ can be written as

$$\frac{d}{dt} D = \frac{1}{2} (D_p^3 - 2D^3) \tanh(3J/T). \quad (22)$$
FIG. 1. Magnetization $m$, asymptotic Hamming distance $D^*$, and Lyapunov exponent $\lambda_1$ as functions of temperature for the Glauber Ising model. Below $T_c$, the curve for $D^*$ has two branches corresponding to the two systems being in the same or in different free energy valleys.

This equation has three stationary solutions (fixed points), viz. $D^*_1 = 0$ which corresponds to both systems being identical, $D^*_2 = 1$ where $S^{(1)} = -S^{(2)}$ for all sites and $D^*_s = \frac{1}{2}$ which corresponds to the two systems being completely uncorrelated [16]. To determine the stability of the fixed points, we linearize the equation of motion (22) in $d_t = D - D^*_s$. The linearized equation has the solution

$$d_t(t) = d_0 e^{\lambda_1 t},$$

with $\lambda_1 = \lambda_2 = \frac{1}{2} \tanh(3J/T)$ and $\lambda_3 = -\frac{1}{2} \tanh(3J/T)$. Consequently, the only stable fixed point is $D^*_s = \frac{1}{2}$. In the whole paramagnetic phase the damage spreads, and asymptotically reaches the value $D = \frac{1}{2}$. If the two systems start very close together ($D$ small initially) their distance in phase space increases exponentially with a Lyapunov exponent $\lambda_1 = \frac{1}{2} \tanh(3J/T)$. Therefore the Glauber dynamics shows chaotic behavior in the whole paramagnetic phase. Note that for large temperatures the Lyapunov exponent $\lambda_1$ goes to zero as $\lambda_1 \sim -3J/T$. Thus the time it takes the system to reach the stationary state $D = D^*_s = \frac{1}{2}$ diverges for $T \to \infty$. This has recently also been found in simulations [17]. The dependence of the Lyapunov exponent on temperature is presented in Fig. 1.

2. Ferromagnetic phase with $m^{(1)} = m^{(2)} = m$

In this section we study the case where both systems are in the same free energy valley. The single-site probabilities $P_{\pm}$ can be expressed in terms of $D$ and $m$:

$$P_{++} = \frac{1}{2}(1 - D + m),$$

$$P_{--} = \frac{1}{2}(1 - D - m),$$

$$P_{+} = P_{-} = \frac{1}{2} D.$$   

After inserting this into the averaged transition probabilities (13) the equation of motion of the Hamming distance takes the form

$$\frac{d}{dt} D = \frac{1}{2}(D - 3D^2 + 2D^*) \tanh(3J/T) - \frac{1}{2} m^2 [2D \tanh(J/T) - D^2 \tanh(J/T) + D^2 \tanh(3J/T)].$$

This equation has two fixed points $D^*$ in the interval $[0,1]$. The first fixed point is $D^*_1 = 0$. By linearizing Eq. (25) in $D_t = D - D^*_1$ we investigate the stability of this fixed point. We again find that $d_t(t)$ follows the exponential law (23) with $\lambda_1 = \frac{1}{2} \tanh(3J/T) - \frac{1}{2} m^2 \tanh(J/T)$. Using expression (19) for $m^2$, it is easy to discuss the behavior of $\lambda_1$. For temperatures larger than a spreading temperature $T_s$ which is defined by

$$3m^2 \tanh(J/T_s) = \tanh(3J/T_s),$$

the Lyapunov exponent $\lambda_1$ is positive and thus the fixed point $D^*_1$ is unstable. For $T < T_s$, the Lyapunov exponent $\lambda_1$ is negative, and the fixed point $D^*_1$ is stable. Consequently, the Glauber dynamics is chaotic for temperatures above $T_s$ but regular below. Equation (26) gives $T_s \approx 1.739 J \approx 0.826 T_C$.

For temperatures $T > T_s$, the equation of motion (25) possesses another fixed point $D^*_2$ with $0 < D^*_2 < \frac{1}{2}$, which is always stable. Its temperature dependence is presented in Fig. 1. Close to the spreading temperature the asymptotic Hamming distance $D^*_s$ increases linearly with $T - T_s$, which corresponds to the spreading transition being of second order. The order parameter exponent $\beta$, defined by $D^*_s = (T - T_s)^\beta$ is given by $\beta = 1$. In contrast to the paramagnetic phase, where the two systems eventually become completely uncorrelated, for $T_c < T < T_s$ the asymptotic Hamming distance $D$ is always smaller than $\frac{1}{2}$ so that the two systems remain partially correlated (as it must be the case since both systems are in the same free energy valley). Directly at the spreading point the term linear in $D$ in Eq. (25) vanishes. For small Hamming distances the equation of motion now reads $dD/dt \sim -D^2$, which gives a power-law behavior $D(t) \sim t^{-\delta}$. The critical exponent is given by $\delta = 1$.

3. Ferromagnetic phase with $m^{(1)} = -m^{(2)} = m$

We now turn to the case where the two systems are in different free-energy valleys. The single-site probabilities $P_{\pm}$ can be expressed in terms of $D$ and $m$:

$$P_{++} = P_{--} = \frac{1}{2}(1 - D),$$

$$P_{+} = P_{-} = \frac{1}{2} (D + m),$$

$$P_{+-} = P_{-+} = \frac{1}{2} (D - m).$$

With this substitutions the equation of motion (20) of the Hamming distance can be written as
\[
\frac{d}{dt} D = \frac{1}{2}(D - 3D^2 + 2D^3) \tanh(3J/T)
\]
\[
+ \frac{1}{2} m^2 \left[ \tanh(3J/T) + \tanh(J/T) - 2D \tanh(3J/T) \right]
\]
\[
+ D^3 \tanh(3J/T) - D^3 \tanh(J/T) \right].
\]  
\[
(28)
\]

Analogously to Sec. III B 2, this equation possesses two fixed points. The fixed point \(D^*_2 = 1\) exists for all temperatures. It is stable for temperatures below \(T_S\) and unstable above. For \(T > T_S\), Eq. (28) has another fixed point \(D^*_1\), with \(\frac{1}{2} < D^*_1 < 1\), which is always stable. Its temperature dependence is given in Fig. 1.

\textbf{C. Limit of high dimensions}

In this subsection we study damage spreading in the Glauber Ising model in the limit of high dimensions, i.e., in the mean-field limit proper. Within the framework of our effective field approach high dimensions correspond to high coordination numbers, i.e., high numbers of nearest neighbors. We therefore consider a Glauber Ising model on a lattice with \(z\) nearest neighbors, and study the limit \(z \to \infty\).

To obtain a physically sensible limit we scale the interaction strength with \(z\), \(J = J_0/z\).

In the limit \(z \to \infty\) the thermodynamics is described by the usual mean-field theory. The equilibrium critical temperature is given by \(T_c = J_0\), and in the ferromagnetic phase the magnetization is determined by the equation of state

\[
m = \tanh(m J_0/T).
\]  
\[
(29)
\]

In order to determine the spreading temperature \(T_S\) it is sufficient to study the equation of motion (20) of the Hamming distance to linear order in \(D\). To this end we have to determine \(W(- \to + \to -)\) and \(W(- \to + \to +)\) to the limit \(z \to \infty\). In the transition probability is thus given by (see Table I)

\[
W(- \to + \to -) = \Theta(-h'(1) - h'(2)) \exp(-J_0|m|/T),
\]  
\[
(30a)
\]

\[
W(- \to + \to +) = \Theta(-h'(1) - h'(2)) \exp(-J_0|m|/T),
\]  
\[
(30b)
\]

We now calculate \(W(- \to + \to -)\) and \(W(- \to + \to +)\) to linear order in \(D\). These transition probabilities do not have a zeroth-order contribution. In linear order in \(D\) only those configurations of the \(z\) neighboring sites contribute which for the two systems differ in the state of a single site. In this case \(h'(1)\) and \(h'(2)\) differ by \(2J_0/z\). Therefore we obtain

\[
W(- \to + \to -) = \Theta(-h'(1) - h'(2)) \Theta(h'(1) - h'(2)) \exp(-J_0|m|/T + \exp(-J_0|m|/T)
\]
\[
+ A J_0/T
\]
\[
\frac{\exp(-J_0|m|/T) + \exp(-J_0|m|/T)}{\exp(-J_0|m|/T)}.
\]  
\[
(31a)
\]

This can be simplified to

\[
\lambda = -m + (1 - m^2) J_0/T.
\]  
\[
(34)
\]

In the paramagnetic phase \((m = 0)\) the Lyapunov exponent is simply \(\lambda = J_0/T > 0\). Thus the Glauber dynamics is chaotic in the whole paramagnetic phase.

The temperature dependence of the Lyapunov exponent \(\lambda\) in the ferromagnetic phase is presented in Fig. 2. \(\lambda\) changes sign at \(T_s = 0.827 J_0 = 0.827 T_c\). Consequently, the dynamics is chaotic for temperatures larger than \(T_s = 0.827 J_0\) and regular for temperatures smaller than \(T_s\). Note that the value for \(T_s/T_c\) for the two-dimensional model of Sec. III B is very close to but not identical to the value for the case \(z \to \infty\).

\textbf{D. Damage spreading in a field}

In this subsection we generalize the effective-field theory to a finite external magnetic field \(h\). For simplicity, we do...
Chaotic behavior and damage spreading in the Glauber Ising model

The phase boundary between the chaotic and the regular phase can be easily determined by solving the equation \( \lambda = 0 \). The resulting phase diagram is presented in Fig. 4. For comparison we also give simulation results [18] for a three-dimensional Glauber Ising model. An investigation of Eqs. (35) and (36) for large temperatures shows that the spreading temperature \( T_s(h) \) diverges for \( hJ_0 - 1 \) as

\[
T_s(h)/J_0 = 1/(1 - hJ_0) \quad \text{for} \quad hJ_0 - 1.
\]

Consequently, for external fields \( h > J_0 \) the dynamics is always regular.

**IV. CONCLUSIONS**

To summarize, we developed a master equation approach to damage spreading and applied it to the Glauber Ising model. The master equation is an exact description of the damage spreading problem; it does not contain any approximations. We then solved the master equation within an effective-field theory for various physical situations.

In this final section we discuss some aspects which have not yet been covered. First, we compare the results of our effective-field theory with numerical simulations of damage spreading of the Glauber Ising model in two and three dimensions [9,11,18]. In agreement with the simulation results we find a spreading transition below the equilibrium critical temperature of the Ising model. Our mean-field value \( T_c/J_0 \approx 0.827 \) is considerably lower than the latest numerical values [11] of 0.992 for a two-dimensional Glauber Ising model, and 0.922 for a three-dimensional Glauber Ising model. We expect our value to be exact, however, for an infinite-dimensional model or, equivalently, for infinite range of the interaction. Grassberger [10] conjectured that the damage spreading transition in the Glauber Ising model is in the universality class of directed percolation. Our results are compatible with that, since the values of the critical exponents \( \beta \) (which describes the dependence of the stationary damage on the reduced temperature) and \( \delta \) (which describes the time decay of the damage at the spreading temperature) are identical to the mean-field values \( \beta = \delta = 1 \) of directed percolation.

Second, we want to clarify the relation to damage spreading in an Ising model with heat-bath dynamics. As already discussed in Sec. I, the heat-bath Ising model does not show any spreading of damage within a single pure state (free-energy valley). When applying our effective-field theory to the heat-bath Ising model we find [14] only a single fixed point \( D^+_R = 0 \) if both systems are in the same pure state [19]. If the two systems are in different pure states (for \( T < T_c \)) we also find a single fixed point only, viz \( D^+_R = m \). Thus there is no chaotic behavior within one pure state. However, the damage can spread (or, at least, will not heal) in the heat-bath Ising model if the two copies start in different pure states or choose to develop into different pure states after a quench from high temperatures. For this case a mean-field theory similar to ours has been considered before [20].

Finally, we discuss possible extensions of the present theory. In principle, the master equation approach of Sec. II can be applied to any damage spreading problem in which the dynamics of a single system is given by a stochastic map as in Eq. (2) (or a more general map that involves several
Recently some interesting results have also been achieved in particular in the case of random interactions. Such systems have been numerically investigated in some detail, in particular in the case of random interactions [21]. Recently some interesting results have also been achieved for random fields [17]. Some investigations on the application of the master equation approach to disordered systems are in progress.

ACKNOWLEDGMENTS

This work was supported in part by the DFG under Grant No. Vo 659/1-1 and by the NSF under Grant No. DMR-95-10185.

[16] For vanishing external field the Glauber algorithm is invariant under a global flip of all spins. Thus the existence of $D^*_0 = 0$ automatically implies the existence another fixed point $D^*_1 = 1$ with the same stability properties.
[19] In contrast to the Glauber dynamics the heat-bath algorithm does not preserve the symmetry with respect to a global flip of all spins. Therefore $D = 1$ is not a fixed point here.
LETTER TO THE EDITOR

Damage spreading in random field systems

Thomas Vojta
Institut für Physik, Technische Universität, D-09107 Chemnitz, Germany and Materials Science Institute, University of Oregon, Eugene, OR97403, USA

Received 3 June 1997

Abstract. We investigate how a quenched random field influences the damage-spreading transition in kinetic Ising models. To this end we generalize a recent master equation approach and derive an effective field theory for damage spreading in random-field systems. This theory is applied to the Glauber Ising model with a bimodal random-field distribution. We find that the random field influences the spreading transition by two different mechanisms with opposite effects. First, the random field favours the same particular direction of the spin variable at each site in both systems which reduces the damage. Second, the random field suppresses the magnetization which in turn tends to increase the damage. The competition between these two effects leads to a rich behaviour.

The central question of damage spreading (DS) [1–3] is how a small perturbation in a cooperative system changes during the time evolution. This is analogous to the question to what extent the time evolution depends on the initial conditions, one of the main questions in non-linear dynamics that lead to the discovery of chaotic behaviour [4]. In order to study DS the simultaneous time evolution of two replicas of a cooperative system is considered. The two replicas evolve stochastically under the same noise realization (i.e. the same random numbers are used in a Monte Carlo procedure). The differences in the microscopic configurations of the two replicas are then used to characterize the dynamics and to distinguish regular and chaotic phases, depending on external parameters.

Among the simplest cooperative systems are kinetic Ising models where DS has been investigated quite intensively within the last years using different dynamical algorithms such as Glauber [3, 5–8] or heat-bath dynamics [2, 7, 9, 10]. In contrast to the equilibrium critical behaviour the results of DS do depend on the particular choice of the dynamical algorithm although recently an attempt has been made to give a more objective definition of DS [11]. In general, there are two different mechanisms by which damage can spread in a kinetic Ising model. First, the damage can spread within a single ergodic component (i.e. a pure state or free-energy valley) of the system. This is the case for Glauber or Metropolis dynamics. Second, the damage can spread when the system selects one of the free-energy valleys at random after a quench from high temperatures to below the equilibrium critical temperature. This is the only mechanism to produce DS in an Ising model with heat-bath dynamics. This algorithm is thus well suited for exploring the structure of the free-energy landscape.

In the literature the name DS has been applied not only to the studies discussed above but also to a different though related type of investigation in which the two systems are not identical. Instead, one or several spins in one of the copies are permanently fixed.
in one direction. Thus the equilibrium properties of the two replicas deviate from each other and their microscopic differences can be related to equilibrium correlation functions [12, 13]. Note that in these works the use of identical noise (i.e. random numbers) for the two systems is not essential but only a method to reduce the statistical error.

Whereas DS in clean Ising models is comparatively well understood less is known about disordered models. The influence of random fields has been investigated in a two-dimensional Ising-like model with Metropolis dynamics giving a reduction of the damage at high temperatures but an increase at low temperatures [14]. By using the heat-bath algorithm DS has been used to study the phase-space structure of Ising spin glasses [15–17] and the corresponding critical behaviour at the DS transition [18].

In this letter we consider the original DS problem, namely the time evolution of two identical systems and study the influence of a quenched random field on DS in kinetic Ising models. To this end we generalize the master-equation approach [7, 8] to random-field systems. The resulting effective-field theory of DS is then applied to the Glauber Ising model with a bimodal random-field distribution. We study the dependence of the spreading transition on temperature and field and determine the phase diagram.

We consider two identical Ising models with \( N \) sites described by the Hamiltonians \( H^{(1)} \) and \( H^{(2)} \) given by

\[
H^{(n)} = -\frac{1}{2} \sum_{ij} J_{ij} S^{(n)}_i S^{(n)}_j - \sum_i \phi_i S^{(n)}_i
\]

where \( S^{(n)}_i \) is an Ising variable with the values \( \pm 1 \) and \( n = 1, 2 \) distinguishes the two replicas. \( J_{ij} \) is the (non-random) exchange interaction between the spins. The random-field values \( \phi_i \) are chosen independently from a distribution \( \rho (\phi) \). The dynamics of the systems are given by stochastic maps \( S^{(n)}_i (t+1) = F(\{ S^{(n)}_j (t) \}) \), e.g. the Glauber algorithm

\[
S^{(n)}_i (t+1) = \text{sgn}[v[h^{(n)}_i (t)] - \frac{1}{2} + S^{(n)}_i (t)(\xi_i (t) - \frac{1}{2})]
\]

where the transition probability \( v(x) \) is given by the usual Glauber expression

\[
v(x) = e^{x/T} / (e^{x/T} + e^{-x/T}).
\]

Within the master equation approach [7, 8] the simultaneous time evolution of the two replicas is described by the probability distribution

\[
P(v_1, \ldots, v_N, t) = \left\langle \sum_{\delta_{v_i(v)}(t)} \prod_i \delta_{v_i, v_i(t)} \right\rangle
\]

where \( \langle \cdot \rangle \) denotes the average over the noise realizations. The variable \( v_i \) with the values ++, +−, −+, or −− describes the states of the spin pair \( (S^{(1)}_i, S^{(2)}_i) \). The distribution \( P \) fulfills the master equation

\[
\frac{d}{dt} P(v_1, \ldots, v_N, t) = -\sum_{i=1}^N \sum_{\mu_i \neq v_i} P(v_1, \ldots, v_i, \ldots, v_N, t) w(v_i \rightarrow \mu_i)
\]

\[+ \sum_{i=1}^N \sum_{\mu_i \neq v_i} P(v_1, \ldots, \mu_i, \ldots, v_N, t) w(\mu_i \rightarrow v_i).\]  

The transition probabilities \( w(\mu_i \rightarrow v_i) \) have to be calculated from the properties of the stochastic map \( F \) which defines the dynamics.
As in the clean case we derive an effective-field theory by assuming that fluctuations at different sites are statistically independent which amounts to approximating the distribution \( P(\nu_1, \ldots, \nu_N, t) \) by a product of single-site distributions \( P_\nu(i, t) \). However, in a disordered system different sites are not equivalent and thus their \( P_\nu(i, t) \) are not identical. This is the main difference to the clean case \([7, 8]\) where the single-site distributions are all identical.

In the following we further assume that \( P_\nu(i, t) \) is determined by the local value \( \phi_i \) of the random-field only, \( P_\nu(i, t) \equiv P_\nu(\phi_i, t) \). In general, this is an approximation since sites with identical random-field values may well have different environments which should influence the distribution. In the mean-field limit of infinite dimensions over infinite-range interactions, however, the above assumption becomes exact.

Inserting the decomposition
\[
P(\nu_1, \ldots, \nu_N, t) = \prod_{i=1}^{N} P_\nu(\phi_i, t)
\]
into the master equation (5) gives a system of coupled equations of motion for the single-site distributions
\[
\frac{d}{dt} P_\nu(\phi) = \sum_{\mu \neq \nu} \left[ -P_\nu(\phi) W(\nu \rightarrow \mu, \phi) + P_\mu(\phi) W(\mu \rightarrow \nu, \phi) \right]
\]
where \( W(\mu \rightarrow \nu, \phi) \) is the transition probability \( w \) averaged over the states \( \nu_i \) of all sites. We now define the local damage \( d(\phi) \equiv P_{++}(\phi) + P_{--}(\phi) \). The total damage is obtained as the corresponding disorder average
\[
D = \left\langle \frac{1}{N} \sum_{i=1}^{N} S_i^{(1)} \right\rangle = \int d\phi \rho(\phi) D(\phi).
\]
The equation of motion of the local damage can be easily determined from (7). Using some symmetry relations \([8]\) between the transition probabilities \( W \), it reads
\[
\frac{d}{dt} d(\phi) = -|m(\phi)| d(\phi) + J_0 \frac{T}{2} [1 - m^2(\phi)] D.
\]
If we concentrate on DS processes starting in equilibrium conditions the local magnetization
\[
m(\phi) = \tanh[(J_0 m + \phi)/T]
\]
and the average magnetization \( m \) are time-independent. Equation (10) is very similar to the corresponding equation (36) of \([8]\) for DS in a homogeneous field. The main difference is that for random-field systems we have to distinguish between the local damage \( d(\phi) \) which determines the healing probability (first term in (10)) and the average damage \( D \) which determines the damaging probability of a site (second term in (10)). In a homogeneous
L646  Letter to the Editor

![Figure 1. Thermodynamic phase diagram of the mean-field Ising model with bimodal random field. TCP denotes the tricritical point.](image)

system local and average damage are identical. Consequently, replacing \(d(\varphi)\) by \(D\) and \(m(\varphi)\) by \(m\) in (10) exactly gives the corresponding equation for the homogeneous system.

To proceed further we have to specify the random-field distribution \(\rho(\varphi)\). As an example we will discuss the bimodal distribution

\[
\rho(\varphi) = \frac{1}{2} \left[ \delta(\varphi - \varphi_0) + \delta(\varphi + \varphi_0) \right] \quad (\varphi_0 > 0). \tag{12}
\]

The thermodynamics of the mean-field Ising model with a bimodal random field was investigated in detail almost 20 years ago [19]. The equation of state takes the form

\[
m = \frac{1}{2} \left[ \tanh \left( \frac{J_0 m + \varphi_0}{T} \right) + \tanh \left( \frac{J_0 m - \varphi_0}{T} \right) \right]. \tag{13}
\]

The resulting phase diagram is summarized in figure 1. There is a tricritical point at \(T_{TCP} = 2J_0/3\) and \(\varphi_{TCP} \approx 0.439J_0\). For \(T > T_{TCP}\) the ferromagnetic phase transition is of second order, for \(T < T_{TCP}\) it is of first order.

We now turn to our results on DS in this model. Using the notations \(d_\pm = d(\pm \varphi_0)\), \(d = (d_+, d_-)\) and \(m_\pm = m(\pm \varphi_0)\) the equation of motion (10) can be written as

\[
\frac{d}{dt}d = A \cdot d. \tag{14}
\]

The dynamical matrix is given by

\[
A = \begin{bmatrix}
-|m_+| + (1 - m_+^2) \frac{J_0}{2T} & (1 - m_+^2) \frac{J_0}{2T} \\
(1 - m_-^2) \frac{J_0}{2T} & -|m_-| + (1 - m_-^2) \frac{J_0}{2T}
\end{bmatrix}. \tag{15}
\]

The question whether the damage spreads or heals can be answered by means of the eigenvalues of \(A\). If both eigenvalues are negative the damage heals, if at least one of them is positive the damage spreads.

In the paramagnetic phase we have \(|m_+| = |m_-| = \tanh(\varphi_0/T)\). The eigenvalues of \(A\) are given by \(\lambda_1 = -m_+ + (1 - m_+^2)J_0/T\) and \(\lambda_2 = -m_+\). The corresponding eigenmodes are the average damage \(D\) and the damage difference \(d_+ - d_-\), respectively. Consequently,
Figure 2. Lyapunov exponents of the mean-field Glauber Ising model with bimodal random field. The peak in the curve for $\varphi_0 = 0.4$ corresponds to the $T$ where $m_-$ vanishes.

In the paramagnetic phase the Lyapunov exponent which is given by the largest eigenvalue of $A$ reads

$$\lambda = -\tanh(\varphi_0/T) + \left[1 - \tanh^2(\varphi_0/T)\right]J_0/T. \quad (16)$$

Its dependence on temperature and random-field strength is visualized in figure 2. In the paramagnetic phase the Lyapunov exponent decreases with increasing random field $\varphi_0$ and therefore the spreading temperature $T_s$ which is defined by $\lambda = 0$ increases. This can be easily understood from the fact that a random field favours a particular spin direction at each site. Since this direction is the same for the two replicas the corresponding spins in the two replicas tend to be parallel which reduces the damage. For random-field strength $\varphi_0 > J_0$ the Lyapunov exponent remains negative for all temperatures and thus the damage never spreads. Asymptotically for $\varphi_0 \rightarrow J_0$ we obtain

$$T_s^2 = \frac{2}{3} \frac{J_0^2}{1 - \varphi_0/J_0}. \quad (17)$$

We note that the critical $\varphi_0$ which completely suppresses DS has the same value as the corresponding critical homogeneous field [8] although the functional dependence of $T_s$ on the field is different.

In the ferromagnetic phase $|m_+|$ and $|m_-|$ are different. In this case the eigenvalues of $A$ are given by

$$\lambda_{1,2} = \frac{1}{2} \left[-|m_+| - |m_-| + \frac{J_0}{2T} (1 - m_+^2 + 1 - m_-^2) \right] \pm \frac{1}{4} \left(|m_+| - |m_-|)^2 \right.$$

$$\lambda_{1,2} = \frac{J_0^2}{16T^2} (1 - m_+^2 + 1 - m_-^2) + \frac{J_0}{4T} (|m_+| - |m_-|)(m_+^2 - m_-^2) \right]^{1/2}. \quad (18)$$

In order to calculate the Lyapunov exponent we first determine the average magnetization $m$ as a function of $\varphi_0$ and $T$ from the equation of state (13). We then calculate $m_+$ and $m_-$ and insert them into (18). The resulting Lyapunov exponents are presented in figure 2. In contrast to the paramagnetic phase the spreading temperature decreases with increasing random-field strength. At a first glance this seems to contradict the argument given above,
namely that a random field favours a particular spin direction and thus reduces the damage. However, the random field also influences DS via a reduction of the magnetization since the Lyapunov exponent (18) is determined by the local magnetizations. In the ferromagnetic phase this effect is stronger than that of the preferred orientation discussed above and thus $T_s$ is reduced.

By means of (16) and (18) we have determined the spreading temperature as a function of the random-field strength. The resulting phase diagram of DS in the mean-field Glauber Ising model with bimodal random field is shown in figure 3. The minimum spreading temperature $T_{s,\text{min}} \approx 0.438$ is obtained when the spreading transition coincides with the ferromagnetic phase transition which occurs for $\varphi_0 \approx 0.480$ (see figure 2).

To summarize, we investigated the influence of a quenched random field on DS in kinetic Ising models. We generalized the master-equation approach [7, 8] to random-field systems and derived an effective field theory for DS. As an example we studied the mean-field Glauber Ising model with bimodal random field. We found that the random field supports the spreading of damage in the ferromagnetic phase but hinders it in the paramagnetic phase. For strong enough field the damage never spreads.

In the concluding paragraph we discuss other random-field distributions and compare our results with the numerical simulation [14]. The influence of the particular form of the random-field distribution on DS can be discussed qualitatively by means of (10). This equation shows that the healing probability is proportional to the local magnetization. This means that the damage on sites with local magnetization zero cannot heal. Consequently, DS will be qualitatively different in systems with a continuous random-field distribution since even for very strong random fields there will be sites with vanishing local magnetization. Thus damage will spread on a subset of sites with low enough random field. However, with $T \to 0$ the measure of this subset goes to zero. A detailed investigation of this case will be published elsewhere [20]. These results also help to understand the numerical simulation [14] which was carried out for a box distribution. It shows a decrease of the spreading temperature with increasing random field although the stationary value of $D$ is reduced at high temperatures. This is consistent with a reduction of $T_s$ due to a suppression of the

---

**Figure 3.** Damage-spreading phase diagram of the mean-field Glauber Ising model with a bimodal random field.
local magnetization and spreading on a subset of sites at low temperatures. However, a
direct comparison with the mean-field theory is not possible since in the simulations a two-
dimensional system was used which—due to fluctuations—does not have an ordered phase
for any finite random field. Finally, we discuss possible extensions of this work. Besides
a systematic investigation of different random-field distributions the damage equation of
motion should be solved beyond first order in the damage. This will permit the determination
of the stationary damage values and the investigation of the critical behaviour at the
spreading transition. Some studies along these lines are in progress [20].

This work was supported in part by the DFG under grant numbers Vo659/1-1 and SFB393
and by the NSF under grant number DMR-95-10185.

References

[4] See, for example, Schuster H G 1984 Deterministic Chaos (Wienheim: VCH)
  Le Caër G 1989 Physica 159A 329
  Wang F and Suzuki M 1996 Physica 223A 34
  Derrida B and Weisbuch G 1987 Europhys. Lett. 4 657
[20] Vojta T to be published
In an Ising model with spin–exchange dynamics damage always spreads

Thomas Vojta
Institut für Physik, Technische Universität, D-09107 Chemnitz, Germany

Received 5 March 1998, in final form 4 June 1998

Abstract. We investigate the spreading of damage in Ising models with Kawasaki spin–exchange dynamics which conserves the magnetization. We first modify a recent master equation approach to account for dynamic rules involving more than a single site. We then derive an effective-field theory for damage spreading in Ising models with Kawasaki spin–exchange dynamics and solve it for a two-dimensional model on a honeycomb lattice. In contrast to the cases of Glauber or heat-bath dynamics, we find that the damage always spreads and never heals. In the long-time limit the average Hamming distance approaches that of two uncorrelated systems. These results are verified by Monte Carlo simulations.

1. Introduction

Damage spreading (DS) investigates how a small perturbation in a cooperative system changes during the time evolution [1–4] (for a short review see, e.g. [5]). In order to study DS two replicas of the system are considered which evolve stochastically under the same noise realization (i.e. the same random numbers are used in a MC procedure). The difference in the microscopic configurations of the two replicas constitutes the ‘damage’. Depending on the Hamiltonian, the dynamic rules, and the external parameters the damage will either spread or heal with time (or remain in a finite spatial region). This behaviour distinguishes chaotic or regular phases.

Kinetic Ising models are among those systems for which DS has been studied most intensively. The majority of the work has been devoted to single-spin–flip dynamic rules such as Glauber, Metropolis or heat-bath dynamics [3–11] but also the Swendson–Wang cluster algorithm has been investigated [12]. It has been found that the properties of DS (e.g. the question whether the damage spreads or heals for a particular model) depend sensitively on the dynamic rule chosen, i.e. DS is uniquely defined only if one specifies the Hamiltonian and the dynamics. (Note that by considering all possible dynamic rules which are consistent with physics of a single replica an unambiguous definition of DS for a particular model can be obtained [13].)

The Glauber, Metropolis or heat-bath algorithms (as well as all other single-spin–flip algorithms) are examples for a dynamics with non-conserved order parameter. There are, however, many physical systems that can be described by kinetic Ising models with order parameter conservation. A prominent example are, e.g. localized electrons where the Ising variables describe the electronic occupation numbers, and the dynamics consists of thermally assisted hops of an electron from one site to another. The simplest order parameter conserving dynamics in an Ising model is the spin–exchange dynamics of Kawasaki [14]. In
In this paper we want to investigate DS for this dynamics. To this end we first generalize the master equation approach [10, 11] to dynamic rules involving more than one site. We then derive an effective-field theory for DS in an Ising model with spin–exchange dynamics and solve it for a two-dimensional model on a honeycomb lattice. We find that in this model the damage always spreads. The stationary value of the damage is given by

\[ D^* = \left(1 - m^2\right)/2 \]

\( m \) is the magnetization which corresponds to completely uncorrelated configurations. The results of the effective-field theory are confirmed by Monte Carlo (MC) simulations.

2. Master equation approach

We consider two identical Ising models with \( N \) sites described by the Hamiltonians \( H^{(1)} \) and \( H^{(2)} \) given by

\[ H^{(n)} = -\frac{1}{2} \sum_{ij} J_{ij} S^{(n)}_i S^{(n)}_j \]

where \( S^{(n)}_i \) is an Ising variable with the values \( \pm 1 \), and \( n = 1, 2 \) distinguishes the two replicas. \( J_{ij} \) is the exchange interaction between the spins which we take to be \( J \) for nearest neighbour sites and zero otherwise. The dynamics (also called the Kawasaki dynamics [14]) consists of exchanging spins on nearest-neighbour sites if the probability

\[ P = v(\Delta E/2) = \frac{e^{-\Delta E/2T}}{e^{\Delta E/2T} + e^{-\Delta E/2T}} \]

is larger than a random number \( \xi \in [0, 1] \). Here \( \Delta E \) is the energy change due to the exchange of the spins and \( T \) denotes the temperature. With this dynamics the total magnetization does not change with time, i.e. it is a conserved quantity.

Within the master equation approach [10, 11] the simultaneous time evolution of the two replicas is described by the probability distribution

\[ P(v_1, \ldots, v_N, t) = \left\langle \prod_{i=1}^N \delta_{v_i(v_i(t))} \right\rangle \]

where \( \langle \cdot \rangle \) denotes the average over the noise realizations. The variable \( v_i \) with the values ++, +−, −+, or −− describes the states of the spin pair \((S^{(1)}_i, S^{(2)}_i)\). In the case of a spin–exchange dynamics the distribution \( P \) fulfills the master equation

\[ \frac{d}{dt} P(v_1, \ldots, v_N, t) = -\sum_{(ij)} \sum_{\mu_i, \mu_j} P(v_1, \ldots, v_{i-1}, v_i \rightarrow \mu_i, v_j \rightarrow \mu_j) \]

\[ + \sum_{(ij)} \sum_{\mu_i, \mu_j} P(v_1, \ldots, v_{i-1}, v_i \rightarrow \mu_i, v_j \rightarrow v_j) \]

where \( (ij) \) denotes all pairs of nearest neighbours and \( w(v_i, v_j \rightarrow \mu_i, \mu_j) \) is the probability for a transition of the states of the sites \( i \) and \( j \) from \( v_i, v_j \) to \( \mu_i, \mu_j \). These transition probabilities can be obtained from (2). In table 1 we list all processes \((v_i, v_j \rightarrow \mu_i, \mu_j)\) which lead to creation or destruction of damage, the probabilities for these processes will show up in the damage equation of motion later on. An important observation is that damaged sites can be created and destroyed only in pairs. All damage creating processes in table 1 can be transformed into each other by exchanging systems 1 and 2 and sites \( i \) and \( j \). Their transition probabilities are therefore also related by symmetry. The same is true for all damage destroying processes. Thus, it is sufficient to calculate only two independent
In an Ising model with spin–exchange dynamics

Table 1. Damage creating and destructing processes for spin–exchange dynamics, all other processes do not change the damage.

<table>
<thead>
<tr>
<th>Two damaged sites created</th>
<th>+++, -- → +−, ++</th>
</tr>
</thead>
<tbody>
<tr>
<td>--−, ++ → −+, ++</td>
<td></td>
</tr>
<tr>
<td>−−, ++ → −+, ++</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Two damaged sites destroyed</th>
<th>--−, -- → ++, --</th>
</tr>
</thead>
<tbody>
<tr>
<td>++, -- → +−, ++</td>
<td></td>
</tr>
<tr>
<td>--+, -- → ++, --</td>
<td></td>
</tr>
</tbody>
</table>

of the probabilities \( w(v_i, v_j \rightarrow \mu_i, \mu_j) \), e.g.

\[
w(++, -- \rightarrow ++, --) = [v(h_i^{(2)} + h_j^{(1)} - h_i^{(1)} + 2J)]^2 \times \Theta(h_i^{(1)} - h_j^{(1)} - h_i^{(2)} + h_j^{(2)})
\]

\[
w(--, ++ \rightarrow ++, --) = [v(h_i^{(2)} + h_j^{(1)} - h_i^{(1)} + 2J)]^2 \times \Theta(h_i^{(1)} - h_j^{(1)} - h_i^{(2)} + h_j^{(2)})
\]

where \( h_i = \sum J_j S_j \) is the local magnetic field of site \( i \).

As in the case of Glauber or heat-bath dynamics we derive an effective-field theory by assuming that fluctuations at different sites are statistically independent which amounts to approximating the distribution \( P(v_1, \ldots, v_N, t) \) by a product of single-site distributions \( P_{v_i}(t) \). Order parameter conservation in the two systems imposes two conditions: \( P_{++}(t) + P_{−−}(t) = \) constant and \( P_{++}(t) + P_{−−}(t) = \) constant. Inserting the decomposition

\[
P(v_1, \ldots, v_N, t) = \prod_{i=1}^{N} P_{v_i}(t)
\]

into the master equation (4) gives a system of coupled equations of motion for the single-site distributions

\[
\frac{d}{dt} P_{v_i} = \sum_{v_j, \mu_i, \mu_j} [−P_{v_i} P_{v_j} W(v_i, v_j \rightarrow \mu_i, \mu_j) + P_{\mu_i} P_{\mu_j} W(\mu_i, \mu_j \rightarrow v_i, v_j)]
\]

where \( W(v_i, v_j \rightarrow \mu_i, \mu_j) \) is the transition probability \( w \) averaged over the states \( v \) of all sites except for \( i \) and \( j \). The total damage (Hamming distance) \( D \) can be expressed in terms of the single-site distribution \( P_{v_i} \):

\[
D = \left( \frac{1}{2N} \sum_{i=1}^{N} |S_i^{(1)} - S_i^{(2)}| \right) = P_{++} + P_{−−}.
\]

We note, that in contrast to Ising models with a non-conserved order parameter, the effective-field theory (7) is not very useful in describing a single system since the only remaining dynamic variable for a single system, namely \( m \), does not change during the time evolution. The damage is, however, not conserved and (7) constitutes a useful mean-field theory for its time evolution.

From the single-site master equation (7) and table 1 we derive an equation of motion of the damage. Using some symmetry relations [15] between the transition probabilities \( W \), it
In an Ising model with spin-exchange dynamics damage always spreads is introduced. Thus, stability. We restrict ourselves to the case that the system is in equilibrium when the damage is zero for $T > T_c$ (heat-bath dynamics) because already a single damaged site can produce further damage in its neighbourhood. Consequently, for small enough $D$ the birth term will always be larger than the death term and the damage will never heal completely.

We now discuss the stationary solutions of the damage equation of motion (9) and their stability. We restrict ourselves to the case that the system is in equilibrium when the damage is zero for $T > T_c$ (heat-bath dynamics) because already a single damaged site can produce further damage in its neighbourhood. Consequently, for small enough $D$ the birth term will always be larger than the death term and the damage will never heal completely.

We now discuss the stationary solutions of the damage equation of motion (9) and their stability. We restrict ourselves to the case that the system is in equilibrium when the damage is zero for $T > T_c$ (heat-bath dynamics) because already a single damaged site can produce further damage in its neighbourhood. Consequently, for small enough $D$ the birth term will always be larger than the death term and the damage will never heal completely.

We now discuss the stationary solutions of the damage equation of motion (9) and their stability. We restrict ourselves to the case that the system is in equilibrium when the damage is zero for $T > T_c$ (heat-bath dynamics) because already a single damaged site can produce further damage in its neighbourhood. Consequently, for small enough $D$ the birth term will always be larger than the death term and the damage will never heal completely.

We now discuss the stationary solutions of the damage equation of motion (9) and their stability. We restrict ourselves to the case that the system is in equilibrium when the damage is zero for $T > T_c$ (heat-bath dynamics) because already a single damaged site can produce further damage in its neighbourhood. Consequently, for small enough $D$ the birth term will always be larger than the death term and the damage will never heal completely.

We now discuss the stationary solutions of the damage equation of motion (9) and their stability. We restrict ourselves to the case that the system is in equilibrium when the damage is zero for $T > T_c$ (heat-bath dynamics) because already a single damaged site can produce further damage in its neighbourhood. Consequently, for small enough $D$ the birth term will always be larger than the death term and the damage will never heal completely.

We now discuss the stationary solutions of the damage equation of motion (9) and their stability. We restrict ourselves to the case that the system is in equilibrium when the damage is zero for $T > T_c$ (heat-bath dynamics) because already a single damaged site can produce further damage in its neighbourhood. Consequently, for small enough $D$ the birth term will always be larger than the death term and the damage will never heal completely.

We now discuss the stationary solutions of the damage equation of motion (9) and their stability. We restrict ourselves to the case that the system is in equilibrium when the damage is zero for $T > T_c$ (heat-bath dynamics) because already a single damaged site can produce further damage in its neighbourhood. Consequently, for small enough $D$ the birth term will always be larger than the death term and the damage will never heal completely.

We now discuss the stationary solutions of the damage equation of motion (9) and their stability. We restrict ourselves to the case that the system is in equilibrium when the damage is zero for $T > T_c$ (heat-bath dynamics) because already a single damaged site can produce further damage in its neighbourhood. Consequently, for small enough $D$ the birth term will always be larger than the death term and the damage will never heal completely.

We now discuss the stationary solutions of the damage equation of motion (9) and their stability. We restrict ourselves to the case that the system is in equilibrium when the damage is zero for $T > T_c$ (heat-bath dynamics) because already a single damaged site can produce further damage in its neighbourhood. Consequently, for small enough $D$ the birth term will always be larger than the death term and the damage will never heal completely.

We now discuss the stationary solutions of the damage equation of motion (9) and their stability. We restrict ourselves to the case that the system is in equilibrium when the damage is zero for $T > T_c$ (heat-bath dynamics) because already a single damaged site can produce further damage in its neighbourhood. Consequently, for small enough $D$ the birth term will always be larger than the death term and the damage will never heal completely.

We now discuss the stationary solutions of the damage equation of motion (9) and their stability. We restrict ourselves to the case that the system is in equilibrium when the damage is zero for $T > T_c$ (heat-bath dynamics) because already a single damaged site can produce further damage in its neighbourhood. Consequently, for small enough $D$ the birth term will always be larger than the death term and the damage will never heal completely.

We now discuss the stationary solutions of the damage equation of motion (9) and their stability. We restrict ourselves to the case that the system is in equilibrium when the damage is zero for $T > T_c$ (heat-bath dynamics) because already a single damaged site can produce further damage in its neighbourhood. Consequently, for small enough $D$ the birth term will always be larger than the death term and the damage will never heal completely.

We now discuss the stationary solutions of the damage equation of motion (9) and their stability. We restrict ourselves to the case that the system is in equilibrium when the damage is zero for $T > T_c$ (heat-bath dynamics) because already a single damaged site can produce further damage in its neighbourhood. Consequently, for small enough $D$ the birth term will always be larger than the death term and the damage will never heal completely.

We now discuss the stationary solutions of the damage equation of motion (9) and their stability. We restrict ourselves to the case that the system is in equilibrium when the damage is zero for $T > T_c$ (heat-bath dynamics) because already a single damaged site can produce further damage in its neighbourhood. Consequently, for small enough $D$ the birth term will always be larger than the death term and the damage will never heal completely.

We now discuss the stationary solutions of the damage equation of motion (9) and their stability. We restrict ourselves to the case that the system is in equilibrium when the damage is zero for $T > T_c$ (heat-bath dynamics) because already a single damaged site can produce further damage in its neighbourhood. Consequently, for small enough $D$ the birth term will always be larger than the death term and the damage will never heal completely.

We now discuss the stationary solutions of the damage equation of motion (9) and their stability. We restrict ourselves to the case that the system is in equilibrium when the damage is zero for $T > T_c$ (heat-bath dynamics) because already a single damaged site can produce further damage in its neighbourhood. Consequently, for small enough $D$ the birth term will always be larger than the death term and the damage will never heal completely.

We now discuss the stationary solutions of the damage equation of motion (9) and their stability. We restrict ourselves to the case that the system is in equilibrium when the damage is zero for $T > T_c$ (heat-bath dynamics) because already a single damaged site can produce further damage in its neighbourhood. Consequently, for small enough $D$ the birth term will always be larger than the death term and the damage will never heal completely.

We now discuss the stationary solutions of the damage equation of motion (9) and their stability. We restrict ourselves to the case that the system is in equilibrium when the damage is zero for $T > T_c$ (heat-bath dynamics) because already a single damaged site can produce further damage in its neighbourhood. Consequently, for small enough $D$ the birth term will always be larger than the death term and the damage will never heal completely.
In an Ising model with spin–exchange dynamics

Since $\lambda_3$ is always negative the FP $D^*_3 = \frac{1}{2}$ is stable in the entire paramagnetic phase. The temperature dependence of $\lambda_3$ is also shown in figure 1.

In the ferromagnetic phase there are two more stationary solutions of (9) in addition to $D^*_1 = 0$ and $D^*_2 = 1$. If the two systems have the same value of the magnetization, $m^{(1)} = m^{(2)} = m$ we obtain the FP $D^*_3 = (1 - m^2)/2$. If the two systems have opposite magnetization $m^{(1)} = -m^{(2)} = m$ we obtain the FP $D^*_4 = (1 + m^2)/2$. Since $D^*_3$ and $D^*_4$ are related by a global flip of all spins in one of the systems, they have the same stability properties. The corresponding Lyapunov exponents are given by

$$\lambda_3 = \lambda_4 = \left( -\frac{3}{8} m^2 + \frac{m^4}{4} + \frac{m^6}{2} + \frac{m^8}{8} \right) \frac{2J}{T} + \left( -\frac{13}{64} + \frac{5m^2}{16} + \frac{m^4}{32} - \frac{3m^6}{16} + \frac{3m^8}{64} \right) \frac{4J}{T}. \tag{14}$$

They are always smaller than zero, thus $D^*_3$ and $D^*_4$ are stable in the entire ferromagnetic phase. The temperature dependence of $D^*_3$ and $\lambda_3$ is shown in figure 1.

We now show that at the stable FPs the configurations of the two systems are completely uncorrelated. From the definition (8) of the damage we obtain

$$D = \frac{1}{2N} \sum_{i=1}^{N} |S_i^{(1)} - S_i^{(2)}| = \frac{1}{2N} \sum_{i=1}^{N} (1 - |S_i^{(1)} S_i^{(2)}|). \tag{15}$$

For uncorrelated configurations of $S_i^{(1)}$ and $S_i^{(2)}$ we have $\langle S_i^{(1)} S_i^{(2)} \rangle = \langle S_i^{(1)} \rangle \langle S_i^{(2)} \rangle = \pm m^2$ if the two systems have equal or opposite magnetization, respectively. Thus, for uncorrelated configurations we obtain $D = (1 \mp m^2)/2$. These are exactly the values of $D^*_3$ and $D^*_4$.

3. MC simulations

We have verified the main predictions of the mean-field theory by MC simulations of a three-dimensional Ising model with Kawasaki spin–exchange dynamics according to (2). The simulations are carried out on cubic lattices with up to $N = 101^3$ sites with periodic
In an Ising model with spin-exchange dynamics damage always spreads. By comparing different system sizes we verify that any finite-size corrections to the results are smaller than the statistical error of the simulation. This is easily possible since we are away from a spreading transition and thus the damage correlation length is finite.

In this study we are not interested in phase separation processes. We thus prepare the system with the correct equilibrium magnetization value for each temperature simulated. 2000 MC sweeps are carried out to equilibrate the system. Then the initial damage $D_0$ is created by exchanging randomly chosen pairs of nearest-neighbour spins in one of the systems. We use values of $D_0$ between $5 \times 10^{-4}$ and $5 \times 10^{-2}$. After that both systems evolve in parallel using the same random numbers. Examples of the time evolution of the damage are shown in figure 2. Within the first 5 to 10 MC sweeps the damage increases approximately exponentially with time. A fit of the data to an exponential law gives an estimate for the Lyapunov exponent $\lambda_1$. We note that the damage time evolution shows a systematic deviation from an exponential law which manifests in a slight downward curvature in figure 2. This deviation stems from the fact that we are simulating a lattice system. Since with Kawasaki dynamics the damage can spread at most two lattice constants per time step the increase of the damage with time is bounded by a power law, $D(t) \leq D_{\text{max}} \sim (2t)^{3/2} D_0$. Therefore, a pure exponential spreading can only be observed as long as the probability for any site (or pair of sites) to become damaged during a particular time step is small compared to one. (In this case the above bound set by the lattice does not play a role.) For our system this condition is, however, only fulfilled for small temperatures.

In order to determine the long-time limit of the average damage we average its values over 5000 MC sweeps after a plateau has been reached. The results of our simulations are summarized in figure 3. We indeed find that the FP $D_1^*$ is unstable, and that the damage always spreads. The Lyapunov exponent $\lambda_1$ of the FP $D_1^*$ is positive for all temperatures investigated. The asymptotic average damage takes exactly the value of two uncorrelated configurations, namely $D_2^* = (1 - m^2)/2$. (We did not observe the other stable FP $D_4^* = (1 + m^2)/2$ since we always started with the two systems having the same magnetization.)
In an Ising model with spin–exchange dynamics

Figure 3. Asymptotic average damage $D^*_3$ and Lyapunov exponent $\lambda_1$ for the kinetic Ising model with spin–exchange dynamics. The Lyapunov exponents have been obtained from 100 runs of a $27^3$ system. The FP values $D^*_3$ has been calculated from 10 runs of a $101^3$ system. Their statistical errors are smaller than the symbol size.

4. Conclusions

To summarize, we have used an effective-field theory and MC simulations to show that the time evolution of a kinetic Ising model with Kawasaki spin–exchange dynamics is chaotic for all temperatures in the sense that the FP $D^*_1 = 0$ is unstable. Moreover, we have shown that two systems whose initial configurations differ only at a few sites become completely uncorrelated in the long-time limit. This corresponds to an asymptotic average damage of $D = (1 - m^2)/2$.

In this last part of this paper we wish to discuss how general these results are. Since the properties of DS are known to depend on how the random numbers are used in the update process [13] for single-spin–flip dynamics, an analogous comparison for spin–exchange dynamics is desirable. However, the main properties of our solution will be robust against such changes in the update rules. In particular, the fact that the damage death rate (see equation (9)) is of order $D^2$ is a result of the spin–exchange mechanism alone. It is therefore independent of how the random numbers are used in the update rule. This suggests that the main finding of this paper, namely that the spin–exchange dynamics is chaotic for all temperatures is valid not only for the Kawasaki update rule (2) but in general. As a first step of a future systematic investigation of different update rules we have studied a modified version of the Kawasaki dynamics. The modification consists of using the random number $\xi$ if the configuration of the spin pair selected for the exchange is $(+ -)$ but using $1 - \xi$ instead if the configuration is $(- +)$. This modified update rule can be seen as the spin–exchange analogue of the heat-bath dynamics (in the same sense as the Kawasaki dynamics can be seen as the analogue of the Glauber dynamics). In figure 4 we compare the asymptotic average damage of the Kawasaki and the modified spin–exchange dynamics. The modified dynamics gives lower damage values than the Kawasaki dynamics for all temperatures. Nonetheless, the fixed point $D^*_1 = 0$ is unstable for all finite temperatures, and the asymptotic damage is finite. This is in agreement with the above suggestion that a spin–exchange dynamics is always chaotic irrespective of the particular update rule.
Let us finally discuss the relation of the DS process discussed here with other non-equilibrium processes. As already mentioned, a key feature of DS with spin–exchange dynamics is that damaged sites can heal only in pairs while they can diffuse alone and also create further damage. This is different from the contact process and other processes in the directed percolation universality class where a single active site can die locally with finite probability. There is, however, a simple reaction-diffusion process which should show qualitatively the same behaviour as DS with spin–exchange dynamics. Since for small damage $D$ the birth rate is proportional to $D$ (and since damage is created in pairs) while the death rate is proportional to $D^2$ (see equations (9), (10)), such a reaction–diffusion process could be defined by the reactions

$$A \xrightarrow{p_b} 3A$$
$$2A \xrightarrow{p_d} 0$$

and additional diffusion of the substance $A$. For small concentrations of $A$ it should have the same qualitative behaviour as DS with spin–exchange dynamics for small damage.

Acknowledgments

This work was supported in part by the DFG under grant nos Vo659/1-1 and SFB393 and by the NSF under grant no DMR-95-10185.

References

In an Ising model with spin–exchange dynamics

Grassberger P 1995 *Physica* 214A 547
Wang F and Suzuki M 1996 *Physica* 223A 34
Vojta T 1997 *Phys. Rev. E* 55 5157
Hinrichsen H, Domany E and Stauffer D 1998 *Preprint* cond-mat/9802115
[15] Vojta T to be published
Differences between regular and random order of updates in damage-spreading simulations

Thomas Vojta and Michael Schreiber
Institut für Physik, Technische Universität, D-09107 Chemnitz, Germany
(Received 16 July 1998)

We investigate the spreading of damage in the three-dimensional Ising model by means of large-scale Monte Carlo simulations. Within the Glauber dynamics we use different rules for the order in which the sites are updated. We find that the stationary damage values and the spreading temperature are different for different update order. In particular, random update order leads to larger damage and a lower spreading temperature than regular order. Consequently, damage spreading in the Ising model is nonuniversal not only with respect to different update algorithms (e.g., Glauber vs heat-bath dynamics) as already known, but even with respect to the order of sites. [S1063-651X(98)12312-7]

PACS number(s): 05.40.−j, 64.60.Ht, 75.40.Gb

Damage spreading (DS) investigates how a small perturbation in a cooperative system changes during the time evolution. It was first studied in theoretical biology [1] in the context of genetic evolution. Later the DS concept found its way into the physics of cooperative systems [2–4]. In order to study DS two replicas of the system are considered which evolve stochastically under the same noise realization (i.e., the same random numbers are used in a Monte Carlo procedure). The difference in the microscopic configurations of the two replicas constitutes the “damage.” Depending on the Hamiltonian, the dynamic rules, and the external parameters a small initial amount of damage will either spread or heal with time (or remain finite in a finite spatial region). Initially, it was believed that the DS behavior can be used to distinguish chaotic and regular phases of the model. However, it was realized early that the properties of DS depend sensitively on the update rule employed in the Monte Carlo procedure. For instance, in the Ising model with Glauber dynamics [4] the damage heals at low temperatures and spreads at temperatures above a certain spreading temperature $T_s$. In contrast, the Ising model with heat-bath dynamics [3] shows qualitatively different behavior: the damage heals with time e.g., Glauber vs heat-bath dynamics) as already known, but even with respect to the order of sites.

The Hamiltonian is given by

$$H = - \sum_{ij} J_{ij} S_i S_j,$$

where $S_i = \pm 1$ is the Ising variable at site $i$, and $J_{ij}$ is the exchange energy, which we take to be one for nearest-neighbor sites and zero otherwise. The Glauber dynamics is given by the stochastic map

$$S_i(t+1) = \text{sgn}\left[ v[h_i(t)] - \frac{1}{2} S_i(t) \left( \xi_i(t) - \frac{1}{2} \right) \right],$$

with the transition probability

$$v(h) = e^{hT}(e^{+hT} + e^{-hT}).$$

Here $h_i(t) = \sum_j J_{ij} S_j(t)$ is the local magnetic field at site $i$ and (discretized) time $t$. $T$ denotes the temperature, and $\xi_i(t) \in [0,1]$ is a random number which is identical for the two copies of the system considered in a DS simulation. In any DS simulation the central quantity studied is the Hamming distance (damage) $D$ as a function of time $t$

$$D(t) = \frac{1}{2N} \sum_i |S_i^{(1)}(t) - S_i^{(2)}(t)|,$$
where the upper index of the spin variable distinguishes the two replicas.

DS in the Glauber Ising model has been intensively investigated both numerically [4,10–13] and using an effective field theory [7,14]. The most precise estimate of the spreading temperature $T_c$ (above which the Hamming distance remains finite in the long-time limit) in three dimensions was obtained in Ref. [12] for systems with up to $309 \times 309 \times 310$ sites using helical boundary conditions and a checkerboard update scheme. The result was a spreading temperature of $T_c/T_s = 0.9225 \pm 0.0005$ ($T_s = 4.162$) where $T_c = 4.5115$ is the equilibrium critical temperature of the ferromagnetic phase transition (all temperatures are measured in units of the nearest-neighbor interaction).

We have carried out extensive DS simulations for systems with up to $N = 10^4$ sites with periodic and helical boundary conditions giving both the time evolution of the damage and its asymptotic stationary value. Different update sequences have been used: typewriter (regularly going from one site to the next), checkerboard (regularly going from one site to its next nearest neighbor, effectively updating first one sublattice, then the other), and three different types of random sequences. For the first random sequence the site to be updated is chosen independently for each time step. In the second random scheme each site is updated exactly once during each sweep (a sweep consists of $N$ Monte Carlo updates), but the (random) order is different from sweep to sweep. In the third random procedure, we use identical (random) order in all sweeps.

In Fig. 1 we show an example for the time evolution of the damage averaged over $400$ runs with different noise realizations. The temperature $T = 4.25$ is slightly below $T_c = 4.5115$. The figure shows that not only the approach to the stationary state but also the stationary damage itself depend on the order of sites in the update process.

The short-time behavior is comparatively easy to understand: If the sites to be updated are chosen independently some sites will be updated twice or even several times while some will not be updated at all during the first sweep through the lattice. In contrast, for all other update sequences each site is updated exactly once during each Monte Carlo sweep.

Now, in the example in Fig. 1 the initial damage is higher than its stationary value. Thus, the damage has to be reduced during the first few sweeps. However, if some sites are not updated at all, their damage cannot heal and consequently the case of independently chosen sites leads to slower decrease of the damage within the first few sweeps. In accordance with this explanation Fig. 1 shows that after the first sweep the damage is identical for all sequences that update each site exactly once in each sweep.

Let us now turn to the stationary states. Figure 1 indicates that the stationary state of the pair of replicas is indeed different for different site order in contrast to the stationary state of a single replica which is independent of the site order as discussed above. A closer inspection of Fig. 1 shows that the stationary damage for all those schemes for which the order of sites does not change from sweep to sweep (typewriter, checkerboard, and identical random) is the same within the statistical accuracy. A significantly higher stationary damage value is obtained if we use different random sequences but still update each site exactly once in each sweep. Finally, for a completely uncorrelated sequence of sites the stationary damage value is largest. We also note that the mean-field theory [7] cannot explain this new dependence of DS on the update sequence since within the mean-field theory the problem is reduced to a single-site problem.

We have carried out high precision calculations at different temperatures using the various update schemes discussed above in order to obtain the temperature dependence of the average stationary damage values. In these calculations the two replicas are prepared with a small initial amount of damage. The time evolution is monitored and after a stationary regime has been reached the damage is averaged over a large number ($10^4$) of Monte Carlo sweeps. The results for the typewriter and independent random update schemes are shown in Fig. 2. Analogous calculations have been carried out for the other update schemes. In the paramagnetic phase ($T > T_c$) the average stationary damage value is 0.5 for all update sequences investigated. In the ferromagnetic phase, however, the results are different. The three schemes that use the same sequence of sites in all sweeps (typewriter, checkerboard, and identical random) give identical stationary damage values within the statistical accuracy. For these schemes we obtain a spreading temperature of $T_s = 4.1625 \pm 0.0050$, i.e., $T_s/T_c = 0.9225 \pm 0.0010$. This is exactly the result obtained by Grassberger [12] (using the checkerboard update scheme). In contrast, for the independent random sequence the spreading temperature is significantly lower. We obtain $T_s = 4.0950 \pm 0.0050$, i.e., $T_s/T_c = 0.9075 \pm 0.0010$. The results shown in Fig. 2 also indicate that the critical behavior at the spreading transition is the same for the update schemes investigated. Since DS in the Glauber-Ising model has two equivalent absorbing states (corresponding to $D = 0$ and $D = 1$), the critical behavior should be in the parity conserving (PC) universality class [15]. It has been suggested [16] that the model with two absorbing states in three dimensions is already above its upper critical dimension. It should then have a critical exponent $\beta = \beta_{\text{PC}} = 1$, see, e.g., Ref. [7] [ $\beta$ is defined by $D(T) \sim (T - T_c)^{\beta}$]. The data in Fig. 1 indicate this behavior, with $\beta$ being close to 1.
The curves represent averages over ten runs of a system with 10185 sites. In each run the damage is averaged over 10,000 Monte Carlo sweeps after a stationary regime has been reached. The inset shows the spreading transition region. The statistical error is smaller than the symbol size in the main figure and approximately given by the symbol size in the inset.

are roughly consistent with this prediction for both update schemes although the inset seems to suggest a slightly smaller exponent. We plan to publish a systematic investigation of the critical behavior elsewhere [17].

All the results reported so far have been obtained using periodic boundary conditions. For comparison we have also investigated the influence of helical boundary conditions. Within the statistical accuracy the results of both boundary conditions are the same.

Furthermore, we have also checked whether the choice of the random number generator does play any role. Three very different random number generators have been used in the simulations: a combined linear congruential generator (RAN2 from Ref. [18]), a very simple linear feedback shift register generator (R250, see Ref. [19]), and a state-of-the-art combined linear feedback shift register generator (LFSR113 from Ref. [20]). All random number generators lead to the same results in our DS simulations. From this we exclude any errors due to poor random numbers.

To summarize, we have studied the dependence of damage spreading in the three-dimensional Glauber-Ising model on the order of the sites in the Monte Carlo update scheme. By using five different update schemes we have provided numerical evidence that the stationary damage and thus the spreading temperature are different for different site order. For all schemes which use the same site sequences in each sweep (typewriter, checkerboard, identical random) we have obtained a spreading temperature of \( T_s \). For completely uncorrelated random site sequences we have obtained a significantly lower spreading temperature of \( T_s / T_c \approx 0.9075 \pm 0.0010 \). To our knowledge there are no published data for DS in the case of a random site sequence. (In Refs. [10,11] regular site order was used. Moreover, the accuracy would not have been high enough to distinguish the different cases.)

From our results we conclude that the stationary state of DS is very sensitive to changes in the details of the Monte Carlo procedure even if they do not influence the stationary state of a single replica. For the ferromagnetic Glauber-Ising model in three dimensions a change of the site order only leads to a shift of the spreading temperature \( T_s \). For more complicated systems it appears to be possible, however, that changing the site order leads to qualitative changes of DS as was found for the change from sequential to parallel updates [8]. Investigations in this direction are in progress.

This work was supported in part by the DFG under Grant No. SFB393 and by the NSF under Grant No. DMR-95-10185.

---

[6] In the case of Glauber dynamics the random number determines whether the spin is flipped, while in the heat-bath case it determines whether it is set to +1.
[9] Note that the influence of the site order has recently been investigated for certain cellular automata: N. Rajewsky and M. Schreckenberg, Physica A 245, 139 (1997); N. Rajewsky, L. Santen, A. Schadschneider, and M. Schreckenberg, Report No. cond-mat/9703156.
Erklärungen


Chemnitz, 10. Mai 1999