Lecture Notes

Statistical Field Theory

Effective Theories of 2nd-Order Phase Transitions and Symmetry Breaking

Ch.G. van Weert
Institute for Theoretical Physics
Valckenierstraat 65
1018 XE Amsterdam

1999

Contents

Chapter 1

Introduction

One of the aims of statistical mechanics is to explain the occurrence of phase transitions. In daily life we are well aware of the existence these phases and the fact that phase transitions are taking place: water turns into ice when cooled, metals can be melted by heating, water and gasoline evaporate etc. Phase transitions are not only central to life on Earth, but also to the understanding of the time-development of the universe. For example, to explain a large cosmological constant in the early universe, some phase transition must have taken place, and also the observed baryon asymmetry, could have been generated by the electro-weak phase transition. The theory of critical phenomena tries to understand this behavior of matter.

1.1 Critical Phenomena

On a phenomenological level, one makes a distinction between *first-order* and *second-order* phase transitions. Common phase transitions, like the transition of water to vapor or ice, or the solidification of molten material, are first-order. This means that the material releases a non-zero quantity of heat, the so-called latent heat, when it goes through a very small temperature range around the transition temperature T_c. This is an indication of a structural change in the material. For example, in the water-ice transition a latent heat of 334 Jg^{-1} is released when the water atoms get ordered into a face-centered cubic lattice, rather than moving around randomly. This is an abrupt change from the disordered fluid to an ordered solid.

In a second-order transition, also called *continuous* phase transition, the properties of the system do not change abruptly. For example, above the critical temperature $T_c = 1043\mathrm{K}$, called the Curie temperature, iron can only be magnetized by applying an magnetic field. Below T_c iron is ferromagnetic, meaning that the material can stay magnetized even in the absence of a magnetic field. The magnitude of the magnetization continuously decreases as the Curie temperature is approached from below, vanishing entirely at T_c and all higher temperatures. In contrast to freezing, there is no abrupt change in the properties of the system, but derivatives may be discontinuous.

Another example of a continuous phase transition is *superconductivity* discovered in

1911 by Heike Kamerlingh Onnes by cooling mercury to about 4.2 K. Since then many other materials have been found to become superconductors at temperatures as high as 120 K. At present this is a very active research area of great technological importance.

Continuous phase transitions are characterized by an so-called *order parameter*. This parameter is generally defined as a quantity that vanishes at one side of the transition (usually the high-temperature side) and increases from zero at the other side. For example, the magnetization $\mathbf{M}$ is a suitable order parameter to describe the ferromagnetic transition. Since the direction of the magnetization is arbitrary, this order parameter is a vector in space. In the case of superconductors the order parameter is a complex quantity Δ defined such that its absolute value is a measure for the density n_s of superconducting electron: $|\Delta|^2 = n_s$. There is no general rule for defining order parameters, and it is a matter of physical intuition and experience to identify the proper order parameter for a given physical system.

In the theory of critical phenomena the appearance of an order parameter is understood as a manifestation of a change of symmetry of the system. Without magnetization a ferromagnetic material is isotropic in all directions. However, when the magnetization appears this defines a preferred direction. One says that the rotational symmetry is broken. The theoretical relation between continuous phase transitions and a change of symmetry was first noted by Lev Landau in 1937. Together with Evgenii Ginzburg he formulated in 1960 a general theory of continuous phase transitions which involve a broken symmetry. This important theory is referred to as the *Ginzburg-Landau model*.

Phase transitions, continuous or not, are characterized by the fact that certain quantities show very large fluctuations as the critical point is approached, and some may even diverge. The heat capacity C, in particular, often diverges in the neighborhood of T_c according to the law

$$C \sim |T_c - T|^{-\alpha}$$

The number α is called a *critical exponent*. Many more of these critical exponents are defined. The surprising fact is that the numerical values found experimentally for these critical exponents for very different systems are often nearly equal to within the experimental error. This very important observation is known as *universality*. One may assign each system to a universality class in such a way that apparently diverse systems in the same universality class have the same critical exponents. The important goal of the theory of critical phenomena is to explain this remarkable congruence in experimental properties.

1.2 Effective Field Theory

The essential tenet of quantum mechanics is the particle-wave duality, that is, the same system can manifest itself under different conditions as either a collection of particles or a collection of waves. This fact is not a paradox, because a system can uniquely behave in either of these two modes only in two extreme classical limits. The actual behavior of a quantum system will always be a mix of the two.

In quantum field theory (QFT), the particle-wave picture is reconciled by canonical field quantization, the particles being the quanta of the fields. This interpretation of QFT finds its natural setting in the formalism of second quantization, where the fields are decomposed into sums of creation and annihilation operators of single-particle states. The rules of canonical quantization have been the traditional approach, since the first papers of Heisenberg and Pauli on general quantum field theory, to introduce the particle picture and to describe the creation and annihilation of particles. The existence of fields is taken for granted relying for justification on the experience with electromagnetism.

However, with Steven Weinberg [Weinberg] we could ask: why should we believe in the rules of canonical quantization? Why should we adopt simple field equations and Lagrangians that are found in the literature ? For that matter, why have fields at all?

This question is even more pressing after the astonishing impact of field theory in the seventies on the understanding of critical phenomena in statistical physics. What have critical phenomena to do with field theory? The fields in these applications are certainly not fundamental in the sense that they describe elementary constituents of matter, but rather they are classical order parameters describing collective phenomena, such as ferromagnetism and superconductivity. The decomposition into normal modes of these fields have an interpretation as basic collective excitations.

An answer to these questions lies in the insights of the modern theory of critical phenomena which began with the scaling hypothesis put forward by Ben Widom (1965) and the universality hypothesis of Leo Kadanoff (1966). The intuitive idea is that close to a phase transition the range of correlations between the atoms becomes very long, much longer than the range of the interaction. It seems reasonable, therefore, to suppose that the critical exponents should not depend on the fine details of the interaction, but only on such general features as the dimensionality and symmetry of the interaction.

This basic idea was translated into a recursive mathematical procedure, the so-called *renormalization group* approach, by Kenneth Wilson. He realized that at large distances the correlation functions of a system near a critical point were described by an "effective" theory which can be obtained by a process of renormalization of the fundamental underlying theory. This effective theory manifest itself as a field theory, with the slowly-varying relevant space-dependent physical variables as the essential degrees of freedom. For this fundamental contribution to the theory of critical phenomena Wilson received the Nobel prize for Physics in 1982.

As strongly advocated by Weinberg, this should be the general point of view regarding field theories; successful QFT's, including QED have to be thought of as effective theories, meaning "low energy" or "long distance" approximations to some deeper theory that may not even be a field theory, but something different like a string theory. The reason that QFT's describe physics at accessible energies is that any relativistic quantum theory will look like a quantum field theory at sufficiently low energy. At the level of the elementary particles, QFT is the way it is, simply because it is the only way the reconcile the principles of quantum mechanics with those of special relativity, at least when we insist that the theory be local.

In the same way, at a different energy scale, the theory of critical phenomena is

what it is, because it is an effective theory for the long-wave-length behavior of the system. Since we do not expect the fine details of the interaction, such as the shape of the underlying lattice or the precise form of the short-range interaction, to be crucial for deriving general properties such as critical exponents, we might try to describe the critical behavior by a continuum effective theory. The guiding principle here is the preservation of the general symmetries of the system. This constraint had already been successfully applied by Landau to construct a purely phenomenological theory of phase transitions. The application in the context of effective theories, leads to a particular field theoretic model for the class of second-order phase transition: the Ginzburg-Landau model. This will be one of the central models in these lectures.

Chapter 2

Ising Model

As a first step to a quantitative theory of continuous phase transitions, it is instructive to consider the *Ising model* invented by Lenz in 1920 as a simple model for ferromagnetism. It was first solved by his student Ising in 1925 for $d = 1$. The analytic solution for $d = 2$ was obtained about twenty years later by Onsager in 1944. No analytic solution for $d = 3$ is known, but with the help of modern computational technology numerical solutions are easy to obtain. Despite its simplicity, the Ising model embodies some of the most essential characteristics of the phase transitions:

- It has a broken-symmetry state (space dimension higher than $d = 1$) separated by a second-order phase transition from the normal state
- It possesses an order parameter distinguishing the two states
- close to the phase transition an effective field theory can be constructed for the description of the system

Moreover, it allows us to illustrate some of the tools of statistical field theory.

2.1 Ferromagnetism

A common example of a continuous phase transition is the occurrence of a spontaneous magnetization below the Curie temperature T_c in ferromagnetic materials like iron or zinc. Above T_c the material is paramagnetic, that is, a magnetization $\mathbf{M}$ (magnetic moment per unit volume) is induced by an external magnetic field $\mathbf{B}$. In the ferromagnetic state ($T < T_c$) the material is magnetized $\mathbf{M} \neq 0$ even when no field is applied. The magnetization vanishes as one approaches T_c from below

$$M \sim |T - T_c|^{\beta} \tag{2.1}$$

with the critical exponent $\beta \simeq 0.35$ for iron. The phase transition is continuous which means that the thermodynamic properties of the system do not change abruptly at T_c, but that at least one of the response functions diverges, for example the susceptibility

(for $B = 0$):

$$\chi_T = \left(\frac{\partial M}{\partial B}\right)_T \sim \frac{1}{|T - T_c|^\gamma} \tag{2.2}$$

with $\gamma \simeq 1.3$ for iron. At T_c, the magnetization becomes proportional to a power of the magnetic field

$$M \sim B^{1/\delta}$$

where $\delta \simeq 4.3$ for iron; thus, at T_c the magnetization responds sensitively and highly non-linearly to small fields B.

The magnetization may be identified with some average of atomic magnetic moments

$$\mathbf{M} = \langle \boldsymbol{\mu} \rangle \ . \tag{2.3}$$

This is the order parameter of the ferromagnetic phase: its value is non-zero in the ordered phase and zero in the symmetric one. The occurrence of a spontaneous magnetization is easily understood. Indeed the ground state energy is minimal if all spins are aligned in some arbitrary direction. In this state rotational symmetry is broken. However, the $SO(3)$ symmetry is not broken entirely since rotations around the magnetization axis are still symmetries of the ground state. Therefore, in a ferromagnet the original symmetry is broken down to $SO(2)$, which is isomorphic to the circle group $U(1)$. The broken symmetry corresponds to any rotation changing direction of the magnetization. These rotations are given by the coset $R = SO(3)/U(1) = S^2$, ie the set of rotations represented by the two-sphere. (Note that this set is not a group.)

2.2 Ising Model

The Ising-model represents a system of N magnetic atoms located at the sites $i \in N$ of a cubic lattice. At each site of the lattice there is a spin variable $s_i = \pm 1$. A positive spin is said to be 'up', and a negative spin 'down'. The Hamiltonian describing the system in the presence of a external magnetic field B has the following form:

$$H = -\frac{1}{2}\sum_{i,j} s_i J_{ij} s_j - B\sum_i s_i \tag{2.4}$$

The spins have an exchange interaction $J_{ij} = J$ at neighboring sites. For all other pairs $J_{ij} = 0$. If we set $J > 0$ the neighboring spins try to align parallel to each other and to the direction of B. If on the other hand, the coupling is negative, anti-parallel spins are favored, and the spins are said to have an anti-ferromagnetic coupling. Note that in a more realistic model one should consider *Heisenberg spins* and a vector inner-product interaction $\mathbf{B} \cdot \mathbf{s}_i$.

The partition function Z of the model has the following form:

$$\begin{aligned} Z &= \mathrm{Tr} e^{-\beta H} \\ &= \sum_{\{s\}} \exp \beta (B\sum_i s_i + \frac{1}{2}\sum_{ij} s_i J_{ij} s_j) \end{aligned} \tag{2.5}$$

where $\sum_{\{s\}}$ indicates that the sum should be extended over all possible assignments of ± 1 to the lattice sites.

A relevant quantity to calculate is the magnetization m defined as the average value of the spin at each site as a function of the external interaction magnetic field B:

$$\begin{aligned} m(B) &= \frac{1}{N}\sum_i \langle s_i \rangle_B \\ &= \lim_{N\to\infty} \frac{1}{N}\frac{1}{\beta}\frac{\partial \log Z}{\partial B} \ . \end{aligned} \tag{2.6}$$

Below a certain critical temperature T_c we expect to find a non-vanishing magnetization for infinitesimally small B

$$m_0 = \lim_{B\to 0} m(B) \neq 0, \quad T < T_c \ . \tag{2.7}$$

However, this is not at all obvious form the above equation (2.6) for $m(B)$. If one simply inserts $B = 0$, one obtains an average which only contains the bi-linear exchange interaction term $s_i J_{ij} s_j$. This exchange interaction term is symmetric in the spins s_i and s_j, and therefore results in $m_0 = 0$. So there certainly is some subtlety involved in explaining the fact that $m_0 \neq 0$.

The occurrence of symmetry breaking in a magnetic field $B \neq 0$ can be understood as follows. For an arbitrarily weak magnetic field the symmetry between up and down spins along the B-axis is broken by the external field term in the Hamiltonian. The state with magnetization in the direction of B, as compared to the state with opposite magnetization, has the relative probability

$$\frac{P_-}{P_+} = \frac{e^{-\beta BN}}{e^{\beta BN}} = e^{-2\beta BN} \ , \tag{2.8}$$

where N is the number of spins. In the thermodynamic limit $N \to \infty$, we have $P_- \to 0$ for any B. As $B \to 0$, the system is in the state with

$$m_0 = \lim_{B\to 0} \lim_{N\to\infty} \frac{1}{N} < s_i >_B \ . \tag{2.9}$$

Thus, the zero-field state fundamentally depends on the history of preparation. Also the crucial role of the thermodynamic limit is clear; if we keep N finite as $B \to 0$, we would get $P_+ = P_-$ and both states would be equally populated. We conclude that the order of the two limits in (2.9) is crucial and cannot be interchanged.

2.3 Mean-Field Theory

In practice it has proven difficult to start from *ab initio* calculations to describe the physics of phase transitions. Therefore, various simplifying approximations have been introduced which hopefully still contain the relevant aspects of the problem. One of the simplest

is the mean-field approximation (MFA), which was introduced by Weiss in 1907 for the study of the ferromagnetic phase transition. It provides a simple yet useful theory of phase transitions as we will demonstrate by considering the Ising-model.

Consider the case in which the exchange interaction is uniform throughout the lattice. The mean-field approximation in the context of the Ising model means the replacement of the fluctuating values of the exchange field by an average field. Suppose that the expectation value of the magnetization is

$$\langle s_i \rangle_B = m(B,T) \tag{2.10}$$

for all i. The thermal average of a given spin $s_i = \pm$ may be written

$$\begin{aligned} \langle s_i \rangle &= \sum_{\{s\}} \frac{e^{\beta(Js+B)} - e^{-\beta(Js+B)}}{e^{\beta(Js+B)} + e^{-\beta(Js+B)}} \\ &= \langle \tanh \beta(\sum_j J_{ij} s_j + B) \rangle \ . \end{aligned} \tag{2.11}$$

The factor one-half has disappeared; in the partition sum this factor corrects for the fact that each pair of sites is counted twice.

The average in the last member at the right-hand side of (2.11) has to be taken over all configurations. We will handle this complicated problem by the ansatz that s_i may be replaced by its mean value. In this *mean-field* approximation the magnetization satisfies the self-consistent equation:

$$\langle s_i \rangle = \tanh \beta(\sum_j J_{ij} \langle s_j \rangle + B) \ . \tag{2.12}$$

The sum over nearest neighbors can be performed. Setting $J_{ij} = J$ with $J > 0$, we get for the magnetization

$$m = \tanh \beta(zJm + B) \ , \tag{2.13}$$

where z is the coordination number, i.e. the number of nearest neighbors.

To find $m(B,T)$ the self-consistent equation may be solved numerically or graphically. For each $B \neq 0$ there is at least one solution. For $B = 0$ there is always one solution $m_0 = 0$, and if $z\beta J > 1$ a further non-zero solution $m_0 \neq 0$ is found. As $T \to T_c = zJ$, the magnetization $m_0(T)$ decreases and we can obtain its asymptotic dependence by a Taylor expansion

$$m_0 = \beta z J m_0 - \frac{1}{3}(\beta z J)^3 m_0^3 \ , \tag{2.14}$$

or

$$m_0(T) = \sqrt{3} \left(\frac{T}{T_c} \right) \left(1 - \frac{T}{T_c} \right)^{\frac{1}{2}} \ . \tag{2.15}$$

The order parameter vanishes asymptotically with critical exponent $\beta = \frac{1}{2}$. This is called the mean-field value, which is not correct, neither for $d = 2$ nor $d = 3$. Also, MFA underestimates the value of β_c and therefore overestimates T_c, e.g. for $d = 3$ the

numerical result is $\beta_c = 0.222/J$, whereas the MFA value is $\beta_c = 0.133/J$. Nevertheless, MFA is a very useful description of phase transitions. Its validity depends crucially on the dimension d. For d sufficiently large, greater than an upper critical dimension d_c, MFA is very good at all temperatures. It yields the exact critical exponents and is a starting point for systematic corrections. Below d_c, but above a critical dimension d_l, MFA works well except close to the critical point. Below the lower critical dimension, MFA is invalid. We will see that $d = 4$ is the upper critical dimension of the Ising model.

2.4 Gaussian Transformation

We will seek a general framework of successive approximations in which the leading term embodies MFA. Since the order parameter is singled out as the collective variable representing the essential degrees of freedom, we will cast the partition function in the form of an integral over the order parameter. This is an extremely useful technique that will lead us to the path integral representation of the partition function.

We consider the partition function of the Ising-model, generalized to an inhomogeneous magnetic field that takes different values B_i at different sites

$$Z = \sum_{\{s\}} \exp \beta (B_i s_i + \frac{1}{2} s_i J_{ij} s_j) \; . \tag{2.16}$$

The essential step is to replace the exponent by a product of Gaussian integrals with the help of the identity

$$\exp\left(\tfrac{1}{2} s \cdot L^{-1} \cdot s + \beta B \cdot s\right) \tag{2.17}$$

$$= |\det L|^{\frac{1}{2}} \int \prod_{i=1}^{N} \frac{d\phi_i}{\sqrt{2\pi}} \exp\left(-\tfrac{1}{2}\phi \cdot L \cdot \phi + (\phi + \beta B) \cdot s\right) \tag{2.18}$$

with $L = (\beta J)^{-1} = \beta^{-1} J^{-1}$ and $|\det L|^{\frac{1}{2}} = \beta^{-n/2} |\det J|^{-\frac{1}{2}}$. By this Gaussian trick the quadratic term disappears and the sum over the spin states is now trivial to perform:

$$\sum_{\{s\}} \exp(\phi_i + \beta B_i) s_i = 2 \prod_i \cosh(\phi_i + \beta B_i) \; . \tag{2.19}$$

It is convenient to rescale the auxiliary variable: $\phi \to \beta\phi$. Furthermore, the determinant normalization factor gives an additive contribution to the free energy which is irrelevant and may be deleted. Using these results in the partition function we obtain:

$$Z = \int \prod_i^N \frac{d\phi_i}{\sqrt{2\pi T}} e^{-\beta H(\phi, B)} \; , \tag{2.20}$$

where the effective Hamiltonian for the Ising model is given by

$$H = \tfrac{1}{2} \phi_i J_{ij}^{-1} \phi_j - \frac{1}{\beta} \sum_i \log[2 \cosh \beta(\phi_i + B_i)] \; . \tag{2.21}$$

This demonstrates that the partition function of the Ising-model is identical to the partition function of a model whose configurations can be parameterized by a set of real continuous statistically independent variables ϕ_i, which can take the values $[-\infty, +\infty]$.

There is a loop-hole in this reasoning because the Gaussian trick applies when the matrix J_{ij} is symmetric and positive definite. This is not true for the Ising-model since the diagonal elements of J_{ij} are zero, implying that the sum over the eigenvalues is zero. As a consequence we must expect to encounter divergent integrals. We will discuss this when the problem arises.

The physical interpretation of the variable ϕ_i becomes clear when we calculate the order parameter

$$m_i = \langle s_i \rangle = \frac{1}{\beta} \frac{\partial \log Z}{\partial B_i} \; . \tag{2.22}$$

It is convenient to shift variables and to write the Hamiltonian

$$H = \tfrac{1}{2}(\phi_i - B_i) J_{ij}^{-1} (\phi_i - B_i) - T \sum_i \log[2 \cosh(\beta \phi_i)] \; . \tag{2.23}$$

Differentiation with respect to B_i gives

$$\begin{aligned} \langle s_i \rangle &= \frac{1}{Z} \int \prod_i^N \frac{d\phi_i}{\sqrt{2\pi T}} J_{ij}^{-1} (\phi_i - B_i) e^{-\beta H} \\ &= J_{ij}^{-1} (\langle \phi_j \rangle - B_j) \; . \end{aligned} \tag{2.24}$$

The average at the right-hand side is calculated with respect to the ϕ-variables. In the absence of a field, the order parameter is linearly related to the average of ϕ_i:

$$\langle \phi_i \rangle = J_{ij} \langle s_j \rangle \; . \tag{2.25}$$

This linear combination is also an acceptable order parameter. Since changing the variable of integration by a linear transformation $\chi_i = J_{ij}^{-1} \phi_j$ would not change the physical result, we could use just as well the variable χ_i in which case $\langle \chi_i \rangle = \langle s_i \rangle$. Hence the variable ϕ_i may be considered as a microscopic order parameter in its own right. Its average value has the physical interpretation of a mean molecular field. That is, $\langle \phi_i \rangle$ gives the potential seen at site i as a result of interaction J_{ij} with the mean value $\langle s_j \rangle$ of each of the surrounding spins.

2.5 Mean-Field Approximation

We consider the partition function (2.20) of the Ising model with the Hamiltonian (2.23) as given above. We now apply the saddle-point method, often called stationary phase approximation. To leading order this amounts to the replacement of the integral by the value of the integrand for which the exponent is stationary

$$Z = \exp -\beta H(\bar{\phi}, B) \; , \tag{2.26}$$

where the variable $\bar{\phi}$ is the solution of the extremum condition:

$$\left.\frac{\partial H(\phi, B)}{\partial \phi_i}\right|_{\phi=\bar{\phi}} = 0 \; . \tag{2.27}$$

This yields for $\bar{\phi}_i$ the mean-field equation

$$J_{ij}^{-1}\bar{\phi}_j = \tanh\beta(\bar{\phi}_i + B_i) \; . \tag{2.28}$$

The magnetization in this approximation is given by

$$\begin{aligned} m_i &= \frac{1}{\beta}\frac{\partial \log Z}{\partial B_i} = \tanh\beta(\bar{\phi}_i + B_i) \\ &= J_{ij}^{-1}\bar{\phi}_j \; . \end{aligned} \tag{2.29}$$

This is exactly the same self-consistent relation as we obtained earlier by an elementary reasoning.

From (2.28) and (2.29) we immediately determine the magnetic field in terms of the magnetization

$$B_i = \frac{1}{\beta}\tanh^{-1} m_i - J_{ij}m_j \; . \tag{2.30}$$

For small m we may expand

$$\tanh^{-1} x = \tfrac{1}{2}\log\frac{1+x}{1-x} = x + \tfrac{1}{3}x^3 + \cdots \tag{2.31}$$

which yields

$$\beta B = (1 - \beta z J)m + \tfrac{1}{3}m^3 + \cdots \; , \tag{2.32}$$

where we assumed an homogeneous magnetic field. It is easily seen graphically that the equation for zero field $B = 0$ has non-trivial solutions when $\beta z J > 0$, whereas for $\beta z J < 0$ the equation has only the trivial solution $m = 0$. It follows that

$$T_c = zJ \tag{2.33}$$

is the critical temperature separating the ordered low-temperature state with non-zero magnetization, from the high-temperature state where the spontaneous magnetization vanishes.

It is important to note that the magnetic field regarded as a function of the magnetization, is a well defined function, both above and below the phase transition. In the latter case equation (2.30) has three solutions for values of the magnetic field in the range $0 < B < B_0$, where B_0 is the value of the magnetic field where the slope changes sign: $\partial B/\partial m = 0$. The solutions having $m < m_0$ are either metastable or unstable which means

$$\frac{\partial m}{\partial B} = \frac{1}{\beta}\frac{\partial^2 \log Z}{\partial B^2} < 0 \; . \tag{2.34}$$

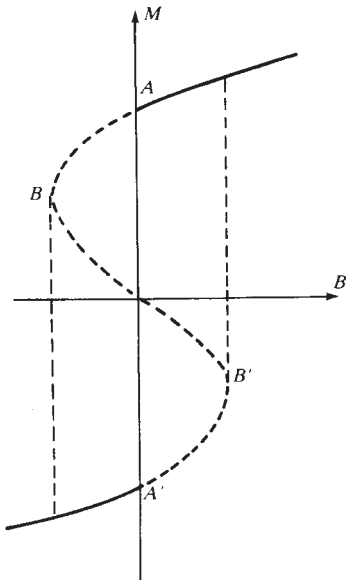

Figure 2.1: The solution of (2.29) for a homogeneous magnetic field. The unphysical region is (A'A)=$[m_-, m_+]$. On the segments (AB) and (A'B') the solution is meta-stable, and unstable on (BB').

The physical solution always has the same direction as the field, and a positive derivative (2.34).

The spontaneous magnetization in zero-field is either m_+ or m_- corresponding to the way in which the magnetic field has been taken to zero. This is the phenomenon of spontaneous symmetry breaking. The range $[m_-, m_+]$ is unphysical, and the relationship (2.30) between magnetic field and magnetization cannot be inverted uniquely.

2.6 Legendre Transform

In MFA the order parameter is obtained by minimizing the effective Hamiltonian (2.23) with respect to the auxiliary field ϕ_i. We can formulate this more generally as a stationarity condition on the order parameter itself. The standard procedure is to define a thermodynamic state function which depends on the magnetization rather than the magnetic field B. This is the Gibbs free energy, or thermodynamic potential, defined through the Legendre transformation

$$\Gamma = -\frac{1}{\beta} \log Z + \sum_i m_i B_i \; . \tag{2.35}$$

Here $B_i = B_i(m)$ is a dependent variable obtained by inverting the defining relation (2.22). It then follows that the function $\Gamma(m)$ so defined satisfies the *reciprocity relation*

$$\frac{\partial \Gamma}{\partial m_i} = B_i \; . \tag{2.36}$$

The inverse transformation is

$$\log Z = -\beta\Gamma + \beta \sum_i m_i B_i \; , \tag{2.37}$$

with now $m_i = m_i(B)$ the dependent variable.

In the broken phase below T_c there is a problem with this construction, because the magnetization in the interval $0 < m < m_+$ is not in one-to-one correspondence with the magnetic field. As a consequence the Legendre transform is only defined outside this interval. Physically this is not a serious problem since the magnetization in the range $[m_-, m_+]$ is not accessible anyway, and for a thermodynamic description of the broken phase it is not necessary to extend the Gibbs free energy in the unphysical region. However, we can chose to do so, for example, by defining Γ to be flat in this region; this would be consistent with (2.36). The function Γ would than have different left and right derivatives at $m = m_\pm$, and be analytic elsewhere.

However, it more useful to define $\Gamma(m)$ as an analytic extension in the unphysical region. That this is possible, follows from the fact that we can always define $B(m)$ as an analytic function as we have already seen in the preceding section. In fact the mean-field approximation has given us this relation explicitly in (2.30). Typically, any explicit calculation of $\Gamma(m)$ does not give the "true" Gibbs energy, but rather an analytic extension which turns out have the physical interpretation of the probability of the order parameter to take a particular value. This analytic extension $\Gamma(m)$ is called the *effective action* in field theory. This effective action is the Legendre transform of $\log Z$ in the physical region, and its analytic extension inside the unphysical region. Summarizing:

- in general, the effective action $\Gamma(m)$ is not the Legendre transform of $\log Z(B)$
- however, the opposite is true, namely $\log Z(B)$ may be regarded as the Legendre transform of $\Gamma(m)$ in the following sense:

$$-\frac{1}{\beta} \log Z(B) = \min_m \; [\Gamma(m) - m \cdot B] \tag{2.38}$$

  where we wrote $\sum_i m_i B_i = m \cdot B$.

The function $\mathcal{L}(m, B) = \Gamma - m \cdot B$ is called the *Landau function*. Its absolute minima specify the most probable value of m for any given value of B, and T. The Landau function is the basis of the phenomenological Landau theory of phase transitions.

The general reasoning may be illustrated by considering the MFA solution of the Ising model, for which Γ may be constructed explicitly:

$$\Gamma = H(\bar{\phi}, B) + B \cdot m \; . \tag{2.39}$$

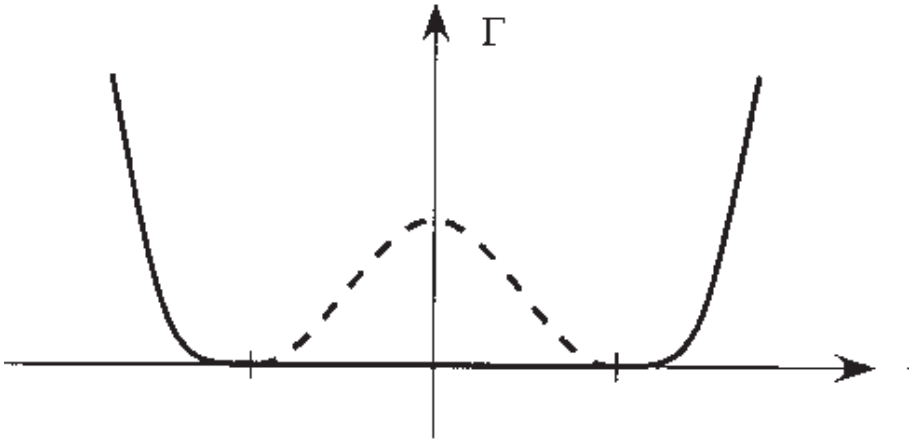

Figure 2.2: The Gibbs free energy (solid line) and the effective action (dashed line).

For small m we may expand and from (2.30) we get to fourth order

$$\beta m \cdot B = -m \cdot J \cdot m + m^2 + \tfrac{1}{3} m^4 \ . \tag{2.40}$$

Using the relation $\cosh(\tanh^{-1} x) = (1 - x^2)^{-\frac{1}{2}}$ we get for the effective action

$$\Gamma = \tfrac{1}{2} m \cdot J \cdot m - \frac{1}{\beta} \sum_i \log\ 2(1 - m_i^2)^{-\frac{1}{2}} + B \cdot m \ . \tag{2.41}$$

Substituting (2.30) we arrive at the result

$$\Gamma = -\tfrac{1}{2} m \cdot J \cdot m + \frac{1}{2\beta} \sum_i \left[(1 + m_i) \log (1 + m_i) + (1 - m_i) \log (1 - m_i) \right] - \frac{N}{\beta} \log 2 \ . \tag{2.42}$$

It is straightforward to verify that the stationarity condition (2.36) reproduces the mean-field equation of state (2.30).

We specialize to a uniform field and expand to fourth order in m. We find

$$\frac{1}{N} \Gamma(m) = -T \log 2 + \tfrac{1}{2} (T - zJ)\ m^2 + \frac{T}{12} m^4 + \mathcal{O}(m^6) \ . \tag{2.43}$$

As it should be the effective action is an extensive quantity. The system has a phase transition when the coefficient of the quadratic term changes sign; this happens when $T = T_c = zJ$. Below the critical temperature T_c, the effective action has the shape of a "sombrero hat" with two minima. The two minima correspond to the positive and

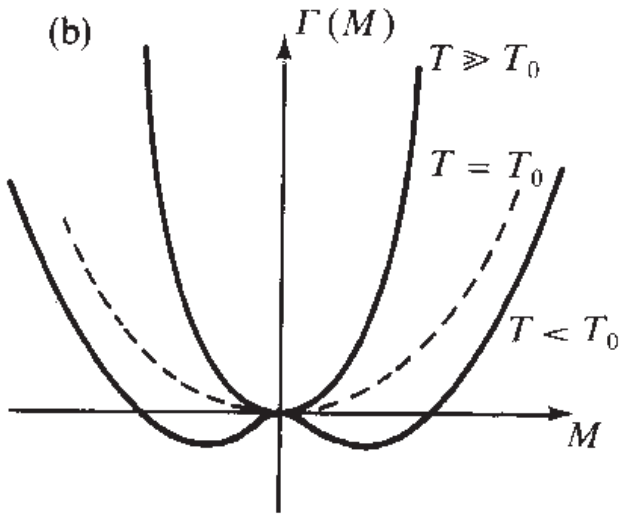

Figure 2.3: Effective action for a second-order phase transition.

negative magnetization phase; in the absence of a magnetic field both have the same free energy. Introduction of a small magnetic field lifts the degeneracy and the Landau function $\Gamma - m \cdot B$ has a unique absolute minimum. In the high-temperature phase the minimum is always $m = 0$.

The effective action (2.43) has precisely the form of the zero-field Landau function postulated by Landau in his phenomenological description of second-order phase transitions. Hence we conclude that the criterion of validity of the Landau theory is the validity of the mean-field approximation. The equation of state that corresponds to the Landau expansion (2.43) is

$$B = (T - T_c)\, m + \tfrac{1}{3} T m^3 \tag{2.44}$$

When $B = 0$ the solution is $m = 0$ for $T > T_c$, and

$$m = \pm\sqrt{3}\left(\frac{T_c - T}{T}\right)^{\frac{1}{2}} \tag{2.45}$$

for $T < T_c$. Thus, MFA predicts a second-order phase transition

$$m \sim (T_c - T)^{\beta} \tag{2.46}$$

with critical exponent $\beta = \frac{1}{2}$. When critical fluctuations are important, β generally is less than its MFA value, typically $\sim \frac{1}{3}$ in three-dimensional systems. At $T = T_c$ equation (2.43) yields

$$m \sim B^{1/\delta} \tag{2.47}$$

so that in MFA we find the critical exponent $\delta = 3$.

2.7 Correlation Functions

Much of the knowledge of condensed matter systems is derived from experiments

which probe the dynamics with X-rays, laser light neutrons or electrons. In these experiments one directly measures correlation functions such as those of density and magnetization. Scattering of polarized neutrons by a lattice of spins leads rather directly to information about the two-point correlation function of the spins, defined as the expectation value

$$G^{(2)}(i,j) =: \langle s_i s_j \rangle \ , \tag{2.48}$$

where i and j are the position vectors of sites i and j, respectively, and the brackets indicate averaging with the appropriate equilibrium ensemble. In many situations, the system is translationally invariant, either because it forms a crystal lattice or because it is highly disordered. Then $G^{(2)}(i,j)$ only depends on the difference vector $i-j$. If the system is also isotropic, $G^{(2)}(i,j)$ becomes a function of the distance $|i-j|$, only.

Let us consider the Ising model in an external inhomogeneous field B_i. Because the field is different at each site, the thermal average of each spin can be extracted from the partition function (2.16). It is convenient to define the "external source" $j_i = \beta B_i$. Then knowing Z as a function of j_i, allows us to calculate

$$\langle s_i \rangle = \frac{1}{Z}\frac{\partial Z}{\partial j_i} \ , \tag{2.49}$$

and also

$$\langle s_i s_j \rangle = \frac{1}{Z}\frac{\partial^2 Z}{\partial j_i \partial j_j} \ . \tag{2.50}$$

In general N-point correlation functions are defined by

$$\begin{aligned} G^{(N)}(i_1, \cdots, i_N) &= \langle s_{i_1}, \cdots, s_{i_N} \rangle \\ &= \frac{1}{Z}\frac{\partial^N Z}{\partial j_{i_1} \cdots \partial j_{i_N}} \ , \end{aligned} \tag{2.51}$$

and $G^{(N)}$ is a function of the locations $(i_1, \cdots, i_N)$ of the spins being averaged. Since correlation functions of arbitrary order can be obtained by differentiation of the partition function with respect to the external field, $Z(B)$ is called the *generating functional* of the correlation functions.

If the spins are non-interacting the average of products simply factorizes into products of the individual averages

$$\langle s_i s_j \rangle = \langle s_i \rangle \langle s_j \rangle \ . \tag{2.52}$$

However, when the spins interact, correlations become interesting. For example in a ferromagnet we expect that spins which are close together will tend to align in the same directions on average. The correlation will decrease as we consider spins that are further apart. So we expect $G^{(2)}$ to be positive for small site separation and to vanish as the separation becomes large. However, if there is an average magnetization we will find

$$\lim_{|i-j|\to\infty} G^{(2)}(i,j) \to \langle s_i \rangle \langle s_j \rangle \ , \tag{2.53}$$

and the correlation function as defined above will not go to zero.

To ensure that the correlation function only measures the correlations between the spins s_i and s_j due to interactions, we subtract off the contribution from each spin separately. This defines the so-called connected two-point function

$$G_c^{(2)}(i,j) = \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle \ . \tag{2.54}$$

Another way of writing is

$$G_c^{(2)}(i,j) = \langle (s_i - \langle s_i \rangle)(s_j - \langle s_j \rangle) \rangle \ . \tag{2.55}$$

This shows that the connected correlation function describes the correlation between the *fluctuationss*$_i - \langle s_i \rangle$ of the spin from the average value. We expect that the connected correlation function will vanish for large values of the distance $|i-j|$. If this is indeed the case, the state is said to obey the *clustering property*.

The connected correlation function can be obtained by differentiation of $\log Z$

$$G_c^{(2)}(i,j) = \frac{\partial^2 \log Z}{\partial j_i \partial j_j} \ , \tag{2.56}$$

as can be easily checked. The general formula for connected correlation functions is

$$G_c^{(N)}(i_1, \cdots, i_N) = \frac{\partial^N \log Z}{\partial j_{i_1} \cdots \partial j_{i_N}} \ . \tag{2.57}$$

This set of correlation functions carries the same information as the unconnected ones, but are physically more useful, just as $\log Z$ is more useful than Z itself. Like in the two-point case, the connected correlation functions can be obtained by subtracting off redundant information about lower-order correlations. Details can be found in [Bellac]. In the following we shall always use the connected correlation functions without indicating this explicitly by the subscript c.

2.8 Fluctuation-Response relation

For a homogeneous external field, the lowest-order correlation functions directly provide two important thermodynamic quantities. The first one is the average magnetization per site

$$m(B) = \frac{1}{\beta N} \frac{\partial \log Z}{\partial B} = \frac{1}{N} \sum_i \langle s_i \ . \rangle \tag{2.58}$$

This is the order parameter. The second one is the (static) magnetic susceptibility defined as

$$\chi = \frac{\partial m}{\partial B} = \frac{1}{\beta N} \frac{\partial^2 \log Z}{\partial B^2} \ . \tag{2.59}$$

In terms of the two-point correlation function we may write

$$\chi = \frac{\beta}{N} \sum_{i,j} \left(\langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle \right) \ . \tag{2.60}$$

The last result implies that the susceptibility is given by the fluctuations in the system. This is one example of a *fluctuation-response* formula, which can also be derived for other thermodynamic response functions. One can also show from (2.60) that the succeptibility is always positive.

The susceptibility measures how easily the magnetization can be changed by varying the field. This will be easier the larger, or the more probable, the spontaneous fluctuations from the average values are. This is a very general result of statistical mechanics, known as the fluctuation-response theorem.

When the field is uniform, we may assume that the system is translationally invariant. Then the connected correlation function depends only on the relative distance. Let $\mathbf{r}_i$ be the position vector of site i; the Fourier transform of the connected correlation function may then be defined as

$$\tilde{G}(\mathbf{k}) = \sum_j e^{-i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)} G(\mathbf{r}_i - \mathbf{r}_j) \ . \tag{2.61}$$

In the long-wave-length limit we have

$$\lim_{\mathbf{k}\to 0} \tilde{G}(\mathbf{k}) = \frac{\beta}{N} \sum_{i,j} G(\mathbf{r}_i - \mathbf{r}_j) \ . \tag{2.62}$$

Making the connection with the succeptibility (2.60) through the fluctuation-response formula, we conclude that the thermodynamic susceptibility is given by the pair correlation

$$\lim_{\mathbf{k}\to 0} \beta \tilde{G}(\mathbf{k}) = \chi \tag{2.63}$$

in the low-$\mathbf{k}$ limit.

2.9 MFA Pair Correlation

We shall now calculate the pair-correlation function for the Ising-model in MFA. As a matter of fact, rather we will calculate its inverse for which we introduce the notation:

$$[\beta G(i,j)]^{-1} =: \Gamma^{(2)}(i,j) \ . \tag{2.64}$$

Let us first show that this so-called *vertex function* $\Gamma^{(2)}$ is nothing but the second derivative of the effective action:

$$\Gamma^{(2)}(i,j) = \frac{\partial^2 \Gamma}{\partial m_i \partial m_j} \ . \tag{2.65}$$

For the proof we start from the trivial identity

$$\delta_{ij} = \frac{\partial m_i}{\partial m_j} = \sum_k \frac{\partial m_i}{\partial B_k}\frac{\partial B_k}{\partial m_j} \ . \tag{2.66}$$

We know the relations

$$\begin{aligned} \frac{\partial m_i}{\partial B_k} &= \frac{1}{\beta}\frac{\log Z}{\partial B_i \partial B_k} = \beta G^{(2)}(i,j) \ , \\ \frac{\partial B_k}{\partial m_i} &= \frac{\partial^2 \Gamma}{\partial m_i \partial m_k} \ . \end{aligned} \tag{2.67}$$

Hence, with the above identification we obtain

$$\beta G^{(2)}(i,k)\ \Gamma^{(2)}(k,j) = \delta_{ij} \ . \tag{2.68}$$

This is a very useful relationship since it is in general more convenient to calculate $\Gamma^{(2)}$ than the correlation function itself. The effective action may be regarded as the generating functional of this inverse function, and all higher-order vertex functions. By the Legendre transform to the effective action we have in principle constructed the tool for calculating these vertex functions.

As a case in point we consider the Ising-model. We have already calculated the effective action Γ in MFA. Differentiation of (2.42) gives

$$\Gamma^{(2)}(i,j) = -J_{ij} + T\ \delta_{ij}(1 + m_i^2) + \mathcal{O}(m^4) \ . \tag{2.69}$$

Let us consider a d-dimensional lattice with sites given by $\mathbf{r}_l = \mathbf{l}a$, where a is the lattice spacing. The vector $\mathbf{l} = (l_1, \cdots, l_d)$ has integer components $0 \le l_\alpha \le L-1$. The discrete Fourier transform of the interaction function $J_{ij} = J(\mathbf{r}_i - \mathbf{r}_j)$ is defined as

$$\tilde{J}(\mathbf{k}) = \sum_j e^{-i\mathbf{k}\cdot(\mathbf{r}_l - \mathbf{r}_j)} J(\mathbf{r}_i - \mathbf{r}_j) \ . \tag{2.70}$$

Since the interaction function vanishes except for nearest neighbor sites, where it has the value J, the components of the vector $\mathbf{r}_i - \mathbf{r}_j$ can only take the values $\pm a$:

$$\begin{aligned} \tilde{J}(\mathbf{k}) &= 2J \sum_{\alpha=1}^{d} \cos k_\alpha a \\ &= 2J\left[d - \tfrac{1}{2}a^2\mathbf{k}^2 + \mathcal{O}(a^4\mathbf{k}^4)\right] \ . \end{aligned} \tag{2.71}$$

For the Fourier transform we obtain in this way

$$\tilde{\Gamma}^{(2)}(\mathbf{k}) = T - 2J\sum_{\alpha=1}^{d} \cos k_\alpha a + Tm^2 \ . \tag{2.72}$$

This yields the low-k behavior of the correlation function near the critical point as

$$\lim_{\mathbf{k}\to 0} \beta\tilde{G}^{(2)}(\mathbf{k}) \sim \frac{1}{T - T_c + Jk^2a^2 + Tm^2} \ . \tag{2.73}$$

In the next section we extract from this formula some critical exponents.