Lecture Notes

Statistical Field Theory

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

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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

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

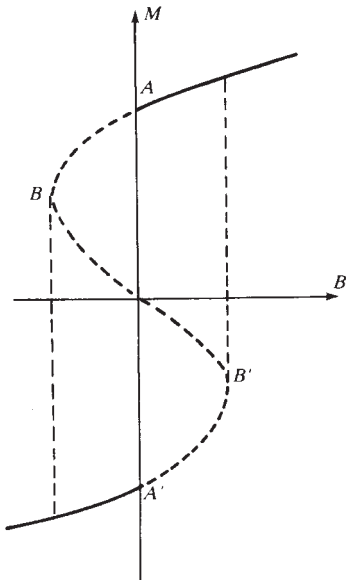


Figure 2.1: The solution of (2.29) for a homogeneous magnetic field. The unphysical region is (A'A)=$[m_-, m_+]$. On the segments (AB) and (A'B') the solution is meta-stable, and unstable on (BB').

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:

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

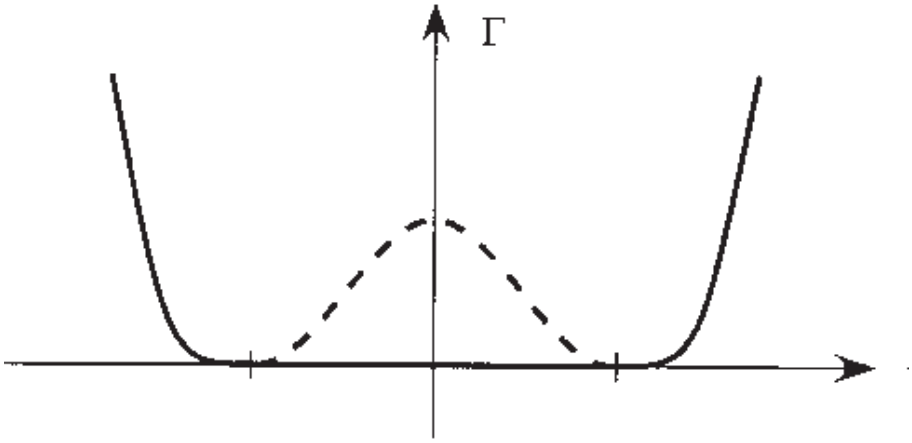


Figure 2.2: The Gibbs free energy (solid line) and the effective action (dashed line).

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

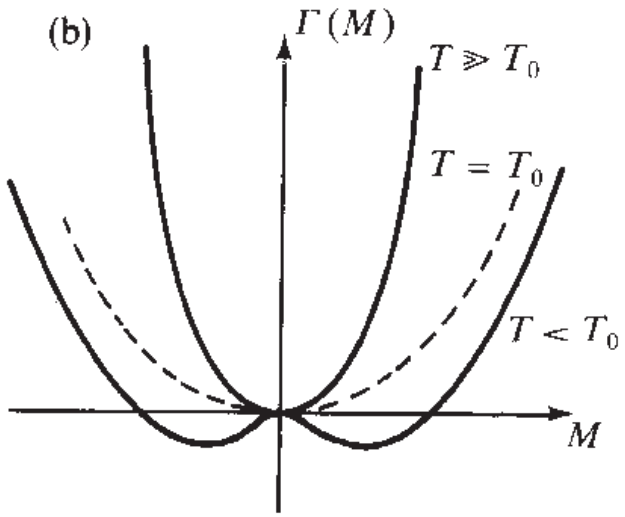


Figure 2.3: Effective action for a second-order phase transition.

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.

2.10 Critical Exponents

Let us consider the asymptotic form of the pair correlation function (2.73) in k-space. Suppose $T > T_c$; since $m = 0$ we have

$$\lim_{\mathbf{k}\to 0} \beta\tilde{G}^{(2)}(\mathbf{k}) \sim \frac{1}{T - T_c + Jk^2a^2} \,. \tag{2.74}$$

From the fluctuation-response theorem (2.63) then follows the susceptibility

$$\lim_{\mathbf{k}\to 0} \beta\tilde{G}^{(2)}(\mathbf{k}) = \chi_+ = (T - T_c)^{-1} \,, \tag{2.75}$$

where $\pm$ distinguishes quantities above and below the phase transition. We conclude that the critical exponent defined by

$$\chi \sim |T - T_c|^{-\gamma} \tag{2.76}$$

has the value $\gamma = 1$.

Below T_c the magnetization is given by (2.15). Hence

$$\lim_{\mathbf{k}\to 0} \beta\tilde{G}^{(2)}(\mathbf{k}) = \chi_- = \tfrac{1}{2}\,(T_c - T)^{-1} \tag{2.77}$$

with critical exponent $\gamma = 1$ having the same value as above T_c.

In the appendix it is shown that the asymptotic form (2.73) implies exponential decay in coordinate space

$$G(\mathbf{r}) \sim \frac{e^{-r/\xi}}{r^{\frac{1}{2}(d-1)}} \,, \tag{2.78}$$

with correlation length

$$\xi_+ = \left(\frac{J}{T - T_c}\right)^{\frac{1}{2}} \,, \tag{2.79}$$

which diverges at the critical point according to a power law

$$\xi \sim |T - T_c|^{-\nu} \,. \tag{2.80}$$

The MFA value of the critical exponent is $\nu = \frac{1}{2}$. For $T < T_c$ the correlation length is

$$\xi_- = \left(\frac{J}{2(T - T_c)}\right)^{\frac{1}{2}} \,, \tag{2.81}$$

with the same critical exponent $\nu = \frac{1}{2}$.

At the critical point $T = T_c$ the correlation length diverges. Then the decay of the correlations generally has the power-law behavior

$$\tilde{G}^{(2)}(\mathbf{k}) = k^{-2+\eta} \,, \tag{2.82}$$

which defines the critical exponent η. It is zero in MFA, and usually close to zero in actual experiments.

Chapter 3

Ginzburg-Landau model

Although the Ising model on a lattice has a fundamental microscopic length scale, the lattice spacing a, we have seen that the behavior near the critical point is characterized by fluctuations and a correlation length which becomes arbitrarily large. Thus, for the long-wave-length excitations of the system which dominates the physics, the microscopic length is irrelevant, and the correlation length $\xi \sim |T - T_c|^{-\frac{1}{2}}$ is the physically relevant length scale. At the critical point, where ξ diverges, the system has no characteristic length scale, and is expected to behave as a scale invariant system.

The dominance of the long-wave-length, or infra-red, behavior near the critical point, illustrated here for the Ising model, is completely general and applies both to classical and quantum systems. This leads us to consider the continuum limit, doing away altogether with the microscopic length scale a. This will lead us to the theory of Ginzburg and Landau, which is an effective field theory that replaces the original model in the critical region. The derivation is heuristic, and one may question its validity. However, the model preserves the essential symmetries and yields the Landau theory of phase transitions in the mean-field approximation. This makes it plausible that the Ginzburg-Landau model indeed captures somehow the essence of a phase transition and elucidates how the critical behavior depends on the parameters, such as the dimensionality, of the system.

3.1 Continuum limit

For the Ising model a good starting point is the Hamiltonian (2.21) derived earlier. Without the magnetic field and expanded to fourth-order we have

$$H = \tfrac{1}{2}\phi_i J_{ij}^{-1}\phi_j - \tfrac{1}{2}\beta \sum_i \phi_i^2 + \tfrac{1}{4}\beta^3 \sum_i \phi^4 \ . \tag{3.1}$$

We now derive the continuum form by a simple limiting process. We define a field $\phi(\mathbf{x})$ such that

$$\sqrt{a^d}\phi(\mathbf{x}_i) = \phi_i \ . \tag{3.2}$$

where the position vector takes $\mathbf{x}_i = (i_1, \cdots, i_d)a$. The field has dimension $[length]^{-d/2}$, and may be considered as a "course graining" of the variable ϕ_i over a lattice volume a^d.

Sums are replaced by integrals according to

$$\sum_i = \int d^d i \; \phi_i = \frac{1}{\sqrt{a^d}} \int d^d x \; \phi(\mathbf{x}) \; . \tag{3.3}$$

To rewrite the interaction term we recall the long-wave-length expansion in Fourier space

$$\tilde{J}(\mathbf{k}) \cong 2J(d - \tfrac{1}{2}a^2k^2); . \tag{3.4}$$

Hence

$$\tilde{J}^{-1}(\mathbf{k}) \cong \frac{1}{2dJ}\left(1 + \tfrac{1}{2}\frac{a^2k^2}{d} + \cdots\right) \; . \tag{3.5}$$

which translates into coordinate space as

$$J_{ij}^{-1} \cong \frac{1}{2dJ}\left(1 - \tfrac{1}{2}\frac{a^2}{d}\nabla^2 + \cdots \; .\right) \tag{3.6}$$

It may be shown that higher derivatives are not needed for a description of critical behavior close to the critical point.

Making the substitutions we obtain the result

$$\beta H_{GL} = \int d^d x(-\tfrac{1}{2}\alpha\phi\nabla^2\phi + \tfrac{1}{2}\mu^2\phi^2 + \tfrac{1}{4!}\lambda\phi^4) \; , \tag{3.7}$$

which is the *Ginzburg-Landau* form. The coefficients can be calculated explicitly, but in the Ginzburg-Landau model they are usually treated as phenomenological input.

The partition function now becomes

$$Z = \int \prod_i \frac{d\phi(\mathbf{x}_i)}{\sqrt{2\pi T/a^d}} \; e^{-\beta H_{GL}} \; . \tag{3.8}$$

In the continuum limit this becomes a functional integral or path integral

$$Z = \int \mathcal{D}\phi(\mathbf{x}) \; e^{-\beta H_{GL}[\phi(\mathbf{x})]} \; , \tag{3.9}$$

where for the measure we have written

$$\lim_{a\to 0} \int \prod_i \frac{d\phi(\mathbf{x}_i)}{\sqrt{2\pi T/a^d}} =: \int \mathcal{D}\phi(\mathbf{x}) \; . \tag{3.10}$$

This notation means that the integral has to be summed over all admissible values of the field variable $\phi(\mathbf{x})$. The exponential factor with the Ginzburg-Landau Hamiltonian is proportional to the probability for finding the configuration $[\phi(\mathbf{x})]$.

In practice, the only tractable functional integrals in physics are Gaussian. Unfortunately this usually corresponds to a system without interactions. Interactions can only dealt with by a perturbation expansion in Gaussian functional integrals or by sticking to the lattice formulation and doing the integration as a numerical summation.

3.2 Landau Theory

The GL-Hamiltonian can be generalized to include a external field. The partition function for this model is

$$Z = \int \mathcal{D}\phi(\mathbf{x})\; e^{-\beta H[\phi(\mathbf{X})]+j\cdot\phi}\;, \tag{3.11}$$

where omitted the subscript GL and used the inner product notation:

$$j\cdot\phi = \int d^dx\; j(\mathbf{x})\phi(\mathbf{x})\;. \tag{3.12}$$

The external source $j(\mathbf{x}) := \beta B(\mathbf{x})$ plays a dual role. It allows us to study the influence of an external field and also enables us to calculate correlation functions by functional differentiation.

Let us calculate the extremum of the exponent

$$\left.\frac{\delta H}{\delta\phi(\mathbf{x})}\right|_{\bar\phi} = B(\mathbf{x}) \tag{3.13}$$

and apply the mean field approximation. This approximation yields the partition function in the form

$$\frac{1}{\beta}\log Z = -H[\bar\phi] + B\cdot\bar\phi\;, \tag{3.14}$$

and the magnetization

$$m(\mathbf{x}) = \frac{\delta\log Z}{\delta j(\mathbf{x})} = \bar\phi(\mathbf{x})\;. \tag{3.15}$$

In the Landau approximation the average of the random field is the order parameter. By doing the Legendre transformation we find the effective action functional in the Landau approximation

$$\Gamma[m] = \int d^dx\,(\tfrac{1}{2}\alpha(\nabla m)^2 + \tfrac{1}{2}\mu^2m^2 + \tfrac{1}{4!}\lambda m^4)\;. \tag{3.16}$$

We could have derived this also by taking the continuum limit of the relation (2.42).

The simple form (3.16) is the basis of the Landau theory of phase transitions. It predicts all the same results as the mean field approximation of the Ising model. Consider for example the correlation function

$$\begin{aligned} G^{-1}(\mathbf{x},\mathbf{x}') &= \frac{\delta^2\Gamma[m]}{\delta m(\mathbf{x})\delta m(\mathbf{x})} && (3.17)\\ &= (\mu^2 + \tfrac{1}{2}\lambda m^2 - \alpha\nabla^2)\delta(\mathbf{x}-\mathbf{x}')\;. && (3.18)\end{aligned}$$

If the magnetic field is uniform, the Fourier transform to momentum-space takes the simple form

$$\begin{aligned}\tilde G(\mathbf{k}) &= \frac{1}{\mu^2 + \frac{1}{2}\lambda m^2 + \alpha k^2}\\ &= \frac{1}{\alpha}\frac{\xi^2}{1+(k\xi)^2}\;,\end{aligned} \tag{3.19}$$

where the correlation length is

$$\xi = \sqrt{\alpha}(\mu^2 + \tfrac{1}{2}\lambda m^2)^{-\frac{1}{2}} \sim |T - T_c|^{-\nu} \ . \tag{3.20}$$

Like for the Ising model in MFA, the critical exponent $\nu = \frac{1}{2}$. This is called the classical value of the critical exponent; these are the values given by MFA or by the Landau approximation which is its generalization.

Let us end by calculating the correlation function in coordinate space in the Landau approximation for $d = 3$. It is customary to rescale so that $\alpha = 1$. We then have

$$G(\mathbf{x}) = \int \frac{d^3k}{(2\pi)^3} \frac{\exp -i\mathbf{k}\cdot\mathbf{x}}{k^2 + \xi^{-1}} \tag{3.21}$$

$$= \frac{\exp -r/\xi}{4\pi r} \ . \tag{3.22}$$

As we expected the critical exponent η vanishes.

3.3 Correlation Functions

Let us consider a single classical field $\phi(x)$ with x a point in d-dimensional Euclidian space. The probability density

$$P[\phi] = e^{-H_{\rm GL}} \tag{3.23}$$

is given by a Hamiltonian of the Ginzburg-Landau type

$$H_{\rm GL} = \int d^dx [\tfrac{1}{2}(\nabla\phi)^2 + \tfrac{1}{2}m^2\phi^2 + \tfrac{1}{4!}\lambda\phi^4] \ , \tag{3.24}$$

where m is a mass and λ a coupling constant. Since the Hamiltonian as defined here is dimensionless, $[H_{\rm GL}] = 0$, the field, mass and coupling constant have the dimensions:

$$[\phi] = \tfrac{1}{2}d - 1 \ , \tag{3.25}$$

$$[m] = 2 \ , \tag{3.26}$$

$$[\lambda] = 4 - d \ , \tag{3.27}$$

with scale -1 attributed to the length scale L.

The essential aim of perturbation theory is to provide a systematic algorithm for calculating arbitrary N-point correlations functions $\langle\phi(x_1)\phi(x_2)\cdots\phi(x_N)\rangle$, where the statistical average is defined by the probability density (3.23). To obtain compact expressions it is convenient to introduce a generating functional

$$Z[j] = \int \mathcal{D}\phi(x)\, P[\phi]\, e^{j\phi} \ , \tag{3.28}$$

where $j(x)$ is some arbitrary function, called the external source, linearly coupled to the field ϕ:

$$j\phi =: \int d^dx\ j(x)\phi(x) \ . \tag{3.29}$$

From the generating functional one obtains the N-point correlation functions by repeated functional differentiation with respect to the source:

$$\langle\phi(x_1)\phi(x_2)\cdots\phi(x_N)\rangle = \frac{1}{Z[0]}\frac{\delta^N Z[j]}{\delta j(x_1)\cdots\delta j(x_N)}\bigg|_{j=0} , \tag{3.30}$$

or by simply expanding out the exponential:

$$\frac{Z[j]}{Z[0]} = \sum_{N=0}^{\infty}\frac{1}{N!}\int d^dx_1\cdots d^dx_N\langle\phi(x_1)\cdots\phi(x_N)\rangle j(x_1)\cdots j(x_N) . \tag{3.31}$$

When calculating these N-point correlation functions, one finds that in general they consist of various connected pieces, that is, sub-units that have the property

$$\lim_{|x_i-x_j|\to\infty}\langle\phi(x_1)\cdots\phi(x_N)\rangle_{\rm con} = 0 \tag{3.32}$$

for any two arguments x_i, x_j. These connected pieces may be isolated by defining a new generating functional $W[j] = \log Z[j]$. This new quantity generates connected correlation functions, also called the cumulants, according to:

$$W[j] = \log Z[0] + \sum_{N=1}^{\infty}\frac{1}{N!}\int d^dx_1\cdots d^dx_N G^{(N)}(x_1,\cdots,x_N)j(x_1)\cdots j(x_N) . \tag{3.33}$$

By comparison one identifies

$$G^{(1)}(x) = \langle\phi(x)\rangle , \tag{3.34}$$

$$G^{(2)}(x_1,x_2) = \langle\phi(x_1)\phi(x_2)\rangle - \langle\phi(x_1)\rangle\langle\phi(x_2)\rangle . \tag{3.35}$$

Explicit expressions of higher-order connected functions may be found in [Bellac]. The general rule is that all possible products of connected pieces of lower order are subtracted. One can then show that the remaining part has the cluster property (3.32).

For the following it is important to mention another general property, namely that cumulants of a Gaussian distribution vanish for $N \geq 3$.

3.4 Wick's Theorem

The Ginzburg-Landau Hamiltonian may be divided into a quadratic part

$$H_0 = \tfrac{1}{2}\int d^dx\,\phi(x)\Lambda(i\nabla)\phi(x) , \tag{3.36}$$

with the differential operator $\Lambda(i\nabla) = -\nabla^2 + m^2$, and an interaction part

$$V = \frac{\lambda}{4!}\int d^dx\,\phi(x)^4 . \tag{3.37}$$

More generally we could consider any polynomial in ϕ or derivative interactions of the type $\phi^2(\nabla\phi)^2$, etc, but for the moment we confine ourselves to the simple ϕ^4 interaction.

Perturbation theory is obtained by first considering the free generating functional

$$Z_0[j] = \int \mathcal{D}\phi(x)\, e^{-H_0+j\phi} \; . \tag{3.38}$$

The integral over the field is Gaussian and can be performed by transcribing formula (5.83) to the continuum case

$$Z_0[j] = Z_0[0] \exp \tfrac{1}{2} \int d^dx d^dy \; j(x)\Delta(x-y)j(y) \; . \tag{3.39}$$

The *propagator* $\Delta(x-y)$ is defined as the inverse of the differential operator $\Lambda(i\nabla)$ as determined by the quadratic part of the Hamiltonian

$$\Lambda(i\nabla)\Delta(x-y) = \delta(x-y) \; . \tag{3.40}$$

Given appropriate boundary conditions, this inhomogeneous differential equation has a unique solution. We impose standard boundary conditions at infinity and obtain by a Fourier transform

$$\Delta(x) = \int \frac{d^dk}{(2\pi)^d} \frac{e^{-ik\cdot x}}{k^2+m^2} \tag{3.41}$$

$$= \langle \phi(x)\phi(0) \rangle_0 \; . \tag{3.42}$$

Generalizing Wick's theorem as derived in the appendix to the continuum case, we conclude that the Gaussian average of an even number of fields may be reduced to a sum of products of propagators

$$\langle \phi(x_1) \cdots \phi(x_l) \rangle_0 = \sum_{\substack{\text{pairings of} \\ (k_1,\ldots,k_l)}} \Delta(x_{k_1} - x_{k_2}) \cdots \Delta(x_{k_{l-1}} - x_{k_l}) \; . \tag{3.43}$$

The sum runs over all possible ways of choosing coordinate pairs. In field theory this procedure is often referred to as "contracting" the coordinate pairs. Each contraction is represented by a propagator at the right hand side of (3.43).

3.5 Perturbation Theory

Wick's theorem allows the systematic calculation of any correlation function derivable from the generating functional (3.28) written as:

$$Z[j] = \int \mathcal{D}\phi(x)\, P_0[\phi]\, e^{-V+j\phi} \; . \tag{3.44}$$

By expanding out the exponent one gets

$$Z[j] = Z_0[0]\{1 + \langle -V + j\phi \rangle_0 + \tfrac{1}{2}\langle (-V+j\phi)^2 \rangle_0 + \cdots\} \tag{3.45}$$

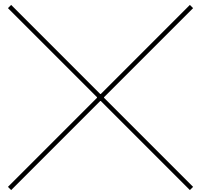
Any two fields are contracted and replaced by the propagator (3.42). It proves to be extremely convenient to introduce a graphical notation:

(i) a contraction is represented by a line joining the two arguments

$$\langle\phi(x)\phi(y)\rangle_0 = \Delta(x-y) = - - - - \tag{3.46}$$

(ii) the four-interaction is represented by a four-point vertex

$$-\lambda\phi(z)^4 = \tag{3.47}$$



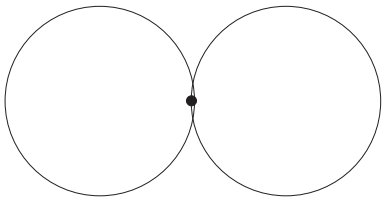
(iii) an external source attached to a field $\phi(x)$ is marked by a cross:

$$j(x) = - - - - \times \tag{3.48}$$

(iv) all vertex- and source coordinates are integrated over: $\int d^dx$

In this manner any term in the Wick expansion of (3.45) can be represented by a unique *Feynman diagram*. For example

$$\begin{aligned}\langle V\rangle_0 &= \frac{\lambda}{4!}\int d^dx\langle\phi(x)^4\rangle = \frac{\lambda}{8}\int d^dx\,[\Delta(0)]^2 \\ &= \end{aligned} \tag{3.49}$$



.

Such a diagram without external point is called a vacuum or bubble diagram. Vacuum graphs are not connected to a source and do not contribute to correlation functions. The sum of all vacuum diagrams equals the partition function:

$$Z[0] = Z_0[0]\sum_{n=0}^{\infty}\frac{1}{n!}\langle V^n\rangle_0\ . \tag{3.50}$$

In the preceding section we already introduced the notion of a cumulant expansion. In the present case cumulants may be formally defined by writing:

$$Z[0] = Z_0[0]\exp\sum_{n=1}^{\infty}\frac{1}{n!}\langle V^n\rangle_{\rm c}\ . \tag{3.51}$$

The cumulants may be identified by expanding out both (3.50) and (3.51) with respect to the coupling constant, and identifying terms of equal power. By working out a few examples it becomes clear that the cumulant construction is such that all disconnected

pieces from any term $\langle V^n \rangle_0$ are subtracted, leaving only terms that are represented by a connected diagram. Hence we may write for the logarithm of the partition function (3.50), which is the quantity of physical interest in statistical mechanics:

$$\log Z[0] = \log Z_0[0] + \langle e^{-V} - 1 \rangle_{\rm c} \ , \tag{3.52}$$

where the last term stands for the sum of all connected vacuum diagrams.

We carry on with the full generating functional. Since the coupling of the external source to the field is just another type of vertex, we may follow the same reasoning and write

$$\log Z[j] = \log Z_0[0] + \langle e^{-V+j\phi} - 1 \rangle_{\rm c} \ , \tag{3.53}$$

where the second term at the right-hand side is the sum of all connected diagrams. For example, for the 2-point correlation function we have the expression:

$$G^{(2)}(x,y) = \langle e^{-V} \phi(x)\phi(y) \rangle_{\rm c} \ . \tag{3.54}$$

Working out the terms with Wick's theorem, we find each term in the perturbative expansion as a product of propagators $\Delta(x_i - x_j)$, represented by a connected Feynman digram. The only factor that is not completely obvious is the multiplicative numerical factor, called the *symmetry factor* that we have to assign to each diagram.

The symmetry factor is obtained in a straightforward, but tedious, manner by counting the number of ways in which a diagram can be constructed by connecting the vertices with the same topological result. Let the diagram consist of V vertices and the corresponding symmetry factor be S_V. In the perturbation expansion (3.49) it is seen that this symmetry factor has to be divided by the permutational factor of each vertex: $(4!)^V$, and by the permutation of the identical vertices: $V!$. In total we get the weight factor:

$$g_V = \frac{S_V}{(4!)^V V!} \ . \tag{3.55}$$

It can be remarked that the occurrence of these numerical factors have not always been clearly noted in the literature.

Chapter 4

Feynman Path Integral

A path integral is a formal expression for the partition function in terms of an integration over a certain function space. This provides both a physically intuitive description of the system and a useful starting point for approximations, such as perturbation theory, and loop expansions around stationary points. The essential idea is due to Dirac (1933) which was developed extensively by Feynman (1948).

4.1 Coherent States

For simplicity we shall start with a bosonic Fock space spanned by the base vectors

$$|n\rangle = |n_1, n_2, \cdots\rangle = \prod_i \frac{(\hat{a}_i^\dagger)^{n_i}}{\sqrt{n_i!}} |0\rangle \ . \tag{4.1}$$

obtained by the repeated action of creation operators on the vacuum state $|0\rangle$. For bosons the values of the occupation numbers $n_i = 0, 1, 2, \cdots$, are unrestricted. Adjoint base vectors $\langle n|$ are created by the action of annihilation operators $\hat{a}_i$. These base vectors span the entire Fock space as expressed by the the completeness relation

$$\sum_{\{n\}} |n\rangle\langle n| = 1 \ . \tag{4.2}$$

Creation and annihilation operators satisfy the commutation relations

$$\left[\hat{a}_i^\dagger, \hat{a}_j^\dagger\right] = 0 \ , \tag{4.3}$$

$$[\hat{a}_i, \hat{a}_j] = 0 \ , \tag{4.4}$$

$$\left[\hat{a}_i, \hat{a}_j^\dagger\right] = \delta_{ij} \ . \tag{4.5}$$

All properties, like the normalization of the base vectors follow from these simple algebraic rules.

Let us now define coherent states. Canonical coherent states are proper eigenstates of $\hat{a}_i$ with continuous complex eigen value z_i defined by

$$|z\rangle = N(z)\ e^{z\cdot\hat{a}^\dagger}|0\rangle \ , \tag{4.6}$$

where $N(z)$ is a normalization factor and the scalar product is shorthand for

$$z \cdot \hat{a}^\dagger = \sum_i z_i \hat{a}_i^\dagger \ . \tag{4.7}$$

Expanding out and using the definition (4.1) we have

$$|z\rangle = N(z) \sum_n \prod_i \frac{(z_i)^{n_i}}{\sqrt{n_i!}} |n\rangle \ . \tag{4.8}$$

The eigenvalue is obtained as

$$\hat{a}_i |z\rangle = N(z) \left[\hat{a}_i, e^{z\cdot\hat{a}^\dagger}\right] |0\rangle = z_i |z\rangle \ . \tag{4.9}$$

The normalization condition

$$\begin{aligned} 1 = \langle z|z\rangle &= |N(z)|^2 \sum_n \prod_i \frac{(z_i^*)^{n_i}(z_i)^{n_i}}{n_i!} &(4.10)\\ &= |N(z)|^2 e^{z^*\cdot z} &(4.11)\end{aligned}$$

determines the normalization factor as

$$N(z) = e^{-\frac{1}{2}z^*\cdot z} \ . \tag{4.12}$$

The coherent states are over-complete in the sense that two states $|z_1\rangle$ and $|z_2\rangle$ are not linearly independent if $z_1 \neq z_2$. On the other hand, $|z\rangle$ has a finite norm and it is a proper element of the Hilbert space, provided $z^* \cdot z, \infty$.

The important feature of coherent states is that they can be used to resolve the identity. To establish this we need the result

$$\int \frac{dz^* dz}{2\pi i} e^{-z\cdot z^*} z^{*n} z^m = \delta_{nm} n! \ . \tag{4.13}$$

It then follows that

$$1 = \sum_n |n\rangle\langle n| = \int \prod_j \frac{dz_j^* dz_j}{2\pi i} \ . \tag{4.14}$$

An almost identical computation gives the trace formula

$$\mathrm{tr}\hat{A} = \int \prod_j \frac{dz_j^* dz_j}{2\pi i} \ .\langle z|\hat{A}|z\rangle \tag{4.15}$$

The overlap of two coherent states is defined as the inner product

$$\begin{aligned} \langle w|z\rangle &= N(w)N(z) \sum_{n,m} \frac{w^{*n}}{\sqrt{n_i!}} \frac{z^{*m}}{\sqrt{m_i!}} \langle n|m\rangle \\ &= \exp -\tfrac{1}{2} w^*\cdot w - \tfrac{1}{2} z^*\cdot z + w^*\cdot z \ . &(4.16)\end{aligned}$$

It is trivial to compute coherent state matrix elements of normal-ordered operators $\hat{A} = A(\hat{a}^\dagger, \hat{a})$. From the formula (4.8) and its adjoint we immediately obtain:

$$\langle w| \ : A(\hat{a}^\dagger, \hat{a}) : \ |z\rangle = A(w^*, z)\langle w|z\rangle \ , \tag{4.17}$$

where $A(w^*, z)$ is a c-number function.

4.2 Field Theory

In field theory the discrete index i is replaced by the continuous one $\mathbf{x}$ labeling the space point. The coherent states are specified by a complex function $z(\mathbf{x})$

$$|z\rangle = N(z) \exp \int d^3x \; \hat{\psi}^\dagger(\mathbf{x}) z(\mathbf{x}) |0\rangle \; . \tag{4.18}$$

We then have

$$\hat{\psi}(\mathbf{x})|z\rangle = z(\mathbf{x})|z\rangle \tag{4.19}$$

and the norm generalizes to

$$N(z) = \exp -\tfrac{1}{2} \int d^3x \, z^*(\mathbf{x}) z(\mathbf{x}) \; , \tag{4.20}$$

which shows that this definition only makes sense if $z(\mathbf{x})$ is in $\mathrm{L}^2(R^3)$, i.e.

$$\int d^3x \, z^*(\mathbf{x}) z(\mathbf{x}) < \infty \; . \tag{4.21}$$

The relevant modification in the overlap function is replacing i by $\mathbf{x}$ and summation by integration:

$$\langle w|z\rangle = \exp -\tfrac{1}{2} \int d^3x [w^*(w-z) - (w^* - z^*)z] \; . \tag{4.22}$$

Formally the discrete integration measure is replaced by a "continuum product"

$$\prod_j dz_j^* z_j \to \prod_{\mathbf{x}} dz(\mathbf{x}) dz^*(\mathbf{x}) \tag{4.23}$$

over all space points $\mathbf{x}$. This product is often written as

$$\prod_{\mathbf{x}} dz(\mathbf{x}) dz^*(\mathbf{x}) = \mathcal{D}z(\mathbf{x}) \mathcal{D}z^*(\mathbf{x}) \tag{4.24}$$

In this way the trace formula (4.15) becomes

$$\mathrm{Tr}A = \int \mathcal{D}z(\mathbf{x}) \mathcal{D}z^*(\mathbf{x}) \langle [z(\mathbf{x})]|A|[z(\mathbf{x})]\rangle \; . \tag{4.25}$$

In general the interpretation of the functional integral is not easy. In this case, however, the integration domain is restricted to functions $z(\mathbf{x})$ in $\mathrm{L}^2(R^3)$, which enables us to give a specific definition. Namely, there exits a countable basis $\{\phi_i(\mathbf{x})\}$, so that any function in $\mathrm{L}^2(R^3)$ can be written as

$$z(\mathbf{x}) = \sum_i c_i \, \phi_i(\mathbf{x}) \tag{4.26}$$

for certain c_i. Since the ϕ_i's are fixed, the freedom in the choice of $z(\mathbf{x})$ resides in the coefficients c_i, so that the integration measure $\mathcal{D}z(\mathbf{x})\mathcal{D}z^*(\mathbf{x})$ may be replaced by $\prod dc_i dc_i^*$, and we are back at the discrete situation handled before.

4.3 Path Integral

We begin by writing the partition function as a functional integral over the space of complex functions $z(\mathbf{x})$ which are elements of $\mathrm{L}^2(R^3)$:

$$Z = \int \mathcal{D}z(\mathbf{x})\mathcal{D}z^*(\mathbf{x})\ \langle [z(\mathbf{x})]|\, e^{-\beta\hat{H}}\, |[z(\mathbf{x})]\rangle\ . \tag{4.27}$$

The matrix elements of the exponent cannot be calculated for finite β. Thus, the idea is to partition the interval $[0,\beta]$ into M infinitesimal pieces $\epsilon = \beta/M$, so that we can write

$$Z = \int \mathcal{D}z\mathcal{D}z^*\ \langle z|\left(e^{-\epsilon\hat{H}}\right)^M |z\rangle \tag{4.28}$$

with an obvious short-hand notation for the states and the integration measure.

For a reason nobody understands, the inverse temperature $\beta = (k_B T)^{-1}$ in the canonical ensemble plays the role of an imaginary time, and the interval $[0,\beta]$ may be seen as an analytic extension of the time variable t in the complex plane: $t = -i\tau, 0 < \tau < \hbar\beta$; we have explicitly inserted Planck's and Boltzmann's constant so that one may check that the dimension comes out correctly. Hence, the subdivision in elements ϵ may be seen as a discretization of the imaginary time variable τ.

We now insert the completeness relation $M-1$ times. Relabeling $|z_0\rangle = |z\rangle, \langle z_M| = \langle z|$ we get:

$$Z = \int \mathcal{D}z_1 \cdots \mathcal{D}z_n \prod_{n=1}^{M} \langle z_n|e^{-\epsilon\hat{H}}|z_{n-1}\rangle\ . \tag{4.29}$$

The crucial step is to find an approximate expression for the matrix element of the infinitesimal Boltzmann factor. One may show that for small ϵ the operator may be approximated by its normal ordered form:

$$e^{-\epsilon\hat{H}} =: e^{-\epsilon\hat{H}} : +\mathcal{O}(\epsilon^2)\ . \tag{4.30}$$

With this approximation the typical matrix element becomes:

$$\langle z_n|\ e^{-\epsilon\hat{H}}\ |z_{n-1}\rangle = \langle z_n|z_{n-1}\rangle \exp -\epsilon\, \langle z_n|\, \hat{H}\, |z_{n-1}\rangle\ . \tag{4.31}$$

The special properties of the coherent states allow us to calculate the matrix element

$$\langle z_n|\hat{H}(\hat{a}^\dagger,\hat{a})|z_{n-1}\rangle = H(z_n^*, z_{n-1})\ , \tag{4.32}$$

where H is now a function of the c-numbers z_n and z_n^*. Collecting the above results we may write for the partition function

$$Z = \int \prod_{n=1}^{M} \mathcal{D}z_n\mathcal{D}z_n^*\ e^S\ , \tag{4.33}$$

where the exponent, called the *action*, given by the expression:

$$S = \epsilon \sum_{n=1}^{M} \left[\frac{\log\langle z_n|z_{n-1}\rangle}{\epsilon} - H(z_n^*, z_{n-1})\right] \tag{4.34}$$

is a function of the sequence $\{z\} = (z_1, z_2, \cdots, z_M)$.

Let us now define a set of intermediate points $\tau_n = n\epsilon$ on the imaginary time interval $[0, \hbar\beta]$, so that $\tau_M = \beta$ and $\tau_0 = 0$, and relabel: $z_n \to z(\tau_n)$. Then in the limit $M \to \infty$ the sequence of numbers $\{z\}$ becomes a function: $\{z\} \to z(\tau)$ and the product of integrations a functional measure

$$\sum_{n=1}^{M} \mathcal{D}z_n \to \mathcal{D}z(\tau) \; . \tag{4.35}$$

Because of the trace condition $z_0 = z_M$, the functional integral runs over functions $z(\tau)$ subject to the periodicity condition: $z(0) = z(\tau)$. Unfortunately, the formal expressions are almost meaningless. The reason is that the space of all functions $z(\tau)$ is far too large to be tractable. We cannot assign a meaning to $\mathcal{D}z(\tau)$ like we defined $\mathcal{D}z(\mathbf{x})$, because the functions $z(\mathbf{x})$ are elements of $\mathrm{L}^2(R^3)$, whereas the functions $z(\tau)$ need not be measurable, let alone integrable. The functional integral is only properly defined by the discretize (lattice) form for finite M.

Although we cannot assume continuity or differentiability of $z(\tau)$, we can be bold and restrict the integration domain to a subspace of functions having 'good' mathematical properties. In particular we can demand that this subspace consists of differentiable functions, that is, we assume

$$z_n = z_{n-1} + \dot{z}_n \epsilon + \mathcal{O}(\epsilon^2) \tag{4.36}$$

for some well defined sequence $\dot{z}_n$ which may be called the derivative of the sequence $\{z_n\}$. The limit function $z(\tau)$ will then be differentiable:

$$\left.\frac{dz}{d\tau}\right|_{\tau=\tau_n} = \lim \frac{z_n - z_{n-1}}{\epsilon} = \dot{z}_n \; . \tag{4.37}$$

If this holds we can expand the first term of the action (4.34) as follows:

$$\begin{aligned} \log\langle z_n | z_{n-1}\rangle &= -\tfrac{1}{2}\left[z_n^*(z_n - z_{n-1}) - (z_n^* - z_{n-1}^*)z_{n-1}\right] \\ &= -\tfrac{1}{2}\epsilon[z_n^*\dot{z}_n - \dot{z}_n^* z_n] + \mathcal{O}(\epsilon^2) \; . \end{aligned} \tag{4.38}$$

The action (4.34) in the Feynman path integral then takes the form of an action integral

$$\lim_{M\to\infty} S = \int_0^{\hbar\beta} L(\tau) \equiv S[z^*, z] \; , \tag{4.39}$$

where $L(\tau)$ is the Lagrangian

$$L(\tau) = \frac{dz^*(\tau)}{d\tau} z(\tau) - z^*(\tau)\frac{dz(\tau)}{d\tau} - H\left(z^*(\tau), z(\tau)\right) \; . \tag{4.40}$$

Thus, the partition function is the sum over all trajectories $z(\tau)$, beginning and ending at the same point, of the exponential of the action calculated over the finite imaginary time interval $[0, \hbar\beta]$:

$$Z = \int \mathcal{D}z(\tau)\mathcal{D}z^*(\tau)\; e^{S[z^*, z]} \; . \tag{4.41}$$

Recalling now that the functions $z(\tau)$ were in fact also functions on configuration space, we get the complete Feynman path integral for the partition function

$$Z = \int \mathcal{D}\phi(-i\tau, \mathbf{x})\mathcal{D}\phi^*(-i\tau, \mathbf{x})\; e^{S[\phi^*,\phi]} \;, \tag{4.42}$$

where we have renamed $z(\tau, \mathbf{x}) \to \phi(-i\tau, \mathbf{x})$. The action

$$S = \int_0^{\hbar\beta} d\tau \int d^3x\; \mathcal{L}(-i\tau, \mathbf{x}) \tag{4.43}$$

is given in terms of the classical Lagrangian density of the (3+1)-dimensional theory with the time t analytically continued to $-i\tau$.

$$\mathcal{L}(t, \mathbf{x}) = \phi^*(t, \mathbf{x})i\frac{\partial\phi(t, \mathbf{x})}{\partial t} - i\frac{\partial\psi^*(t, \mathbf{x})}{\partial t}\phi(t, \mathbf{x}) - H\left(\phi^*, \phi\right) \;. \tag{4.44}$$

We conclude that the partition function (4.42) can be represented as an Euclidean functional integral over fields $\phi(t, \mathbf{x})$ defined on the time interval $t = -i\tau, 0 < \tau < \hbar\beta$. The path integration is subject to the periodicity condition $\phi(i\hbar\beta, \mathbf{x}) = \phi(0, \mathbf{x})$.

A similar derivation can be given for fermionic fields. Because fermionic fields anti-commute, it turns out to be necessary to replace the complex numbers z, z^* by new quantities, called Grassman variables, that satisfy different calculational rules. In particular they anti-commute among themselves, and commute with all bosonic quantities, like bosonic operators and ordinary c-numbers. The point of these rules is that the whole coherent state formalism, including the derivation of the path integral, can be taken over almost literally. The only essential difference is that the boundary condition on fermionic fields in the path integral is anti-periodic: $\psi(i\hbar\beta, \mathbf{x}) = -\psi(0, \mathbf{x})$.

Although the expression for the partition function (4.42) has a great formal beauty, we should not forget that it was derived by the rather arbitrary prescription that the sequence $\{z\}$ approach a differentiable function. Even with this prescription, the path integral is mathematically ill defined. The point is that the subspace of smooth functions is so exceedingly small in the total space of functions that it is impossible to find a measure $\mathcal{D}\phi\mathcal{D}\phi^*$ that picks only contributions from these smooth functions. This is the paradox of the continuum path integral: either one restricts it to smooth functions but then it is identically zero or one allows more functions, but then the continuum action is undefined. One way is to go back to the discrete form; this is the method of lattice field theories. Another way is to normalize the formal path integral to an analytically solvable reference problem. In practice this means that the Gaussian path integral for a free system is prescribed.

Chapter 5

BCS-Theory of Superconductivity

As understood today, superconductivity is explained by a spontaneous break down of electromagnetic gauge invariance. All important qualitative features, like the fact that electrical resistance is so low that currents can circulate for years, can be understood as exact consequences of this breakdown. However, to give a physical basis to the mechanism of symmetry breakdown, and as a starting point for approximate quantitative calculations, one needs a model. In this chapter we will study the microscopic model introduced by Bardeen, Cooper and Schrieffer (BCS) in 1957. This model has been highly successful in correlating and explaining the properties of simple superconductors in terms of a few experimental parameters.

In the BCS-model electrons appear explicitly, but it is assumed in advance that only electrons near the Fermi surface have an interaction, which is supposedly weak and attractive in nature. This effective electron-electron interaction arises from the exchange of phonons associated with the crystal lattice. The effects of this interaction on a normal solid are remarkably small and are described by simply replacing non-interacting particles by quasi-particles with slightly modified properties.

However, the introduction of an attractive interaction, no matter how weak, also leads to a bound state consisting of a pair of electrons at the Fermi surface with equal but opposite, momenta and spins. Once a macroscopic number of such Cooper pairs with a lower net energy appears, a description of the system in terms of single-particle states does no longer correspond to the state of lowest energy, and a transition to a new equilibrium state must take place. This qualitative different state cannot be obtained by a perturbative scheme which develops continuously from the original single particle states, and one has to include the possibility of pairing from the beginning.

5.1 Order Parameter

The phenomena of superconductivity and superfluidity have a similar origen which is the breaking of $U(1)$ symmetry. The specific mechanism by which the breakdown occurs in superconductors is "Cooper pairing". Two electrons in a metal may feel an effective attractive force due to "over screening" by the ions of the metal. The bare Coulomb

potential between the electrons is repulsive, of course. The ions of the system respond to the motion of the electrons and, in certain circumstances, cam produce an effective interaction between electrons which is attractive. This discovery is due to Frölich (1950). Later, Cooper (1956) showed that this attractive interaction could produce a two-electron bound state in the presence of a Fermi sphere of Bloch electrons. These bound pairs have properties which are similar to bosons and , at sufficiently low temperatures, condense in the superconducting state.

The basic dynamical variable of the problem is the field operator $\hat{\psi}_\sigma(\mathbf{x})$ describing an electron with spin state up ($\sigma =\uparrow$) or down ($\sigma =\downarrow$), satisfying the anti-commutation relations:

$$\left[\hat{\psi}_\sigma(\mathbf{x}), \hat{\psi}^\dagger_{\sigma'}(\mathbf{x}')\right]_+ = \delta_{\sigma\sigma'}\delta\left(\mathbf{x}-\mathbf{x}'\right) \ , \tag{5.1}$$

$$\left[\hat{\psi}_\sigma(\mathbf{x}), \hat{\psi}_{\sigma'}(\mathbf{x}')\right]_+ = \left[\hat{\psi}^\dagger_\sigma(\mathbf{x}), \hat{\psi}^\dagger_{\sigma'}(\mathbf{x}')\right]_+ = 0 \ . \tag{5.2}$$

In terms of these fields the electron charge density and corresponding current density are given by

$$\hat{q}(\mathbf{x}) = e\sum_\sigma \hat{\psi}^\dagger_\sigma(\mathbf{x})\hat{\psi}_\sigma(\mathbf{x}) \ , \tag{5.3}$$

$$\hat{\mathbf{j}}(\mathbf{x}) = \frac{e}{2m}\sum_\sigma \left[\hat{\psi}^\dagger_\sigma(\mathbf{x})(-i\nabla)\hat{\psi}_\sigma(\mathbf{x}) + h.c.\right] \ , \tag{5.4}$$

where e and m are the electron charge and mass, respectively. Charge and current density $\hat{j}^\mu = (\hat{q}, \hat{\mathbf{j}})$ satisfy the continuity equation

$$\partial_\mu \hat{j}^\mu\left(x\right) = 0 \ , \tag{5.5}$$

which comprises the conservation of charge

$$\frac{d\hat{Q}}{dt} = \frac{d}{dt}\int d^3x\, \hat{q}\left(x\right) = 0 \tag{5.6}$$

in local form.

The Pauli principle as expressed by

$$\hat{\psi}_\sigma(\mathbf{x})\hat{\psi}_\sigma(\mathbf{x}) = 0 \ , \tag{5.7}$$

forbids more than one electron from condensing into the same quantum state. Therefore, Bose-Einstein condensation of electrons is not physically possible. However, if the electrons were to form pairs, i.e. composite entities having boson properties, there is no contradiction in assuming that these pairs may accumulate in the same macroscopic state. It was shown in 1956 by Cooper that the effective attraction between electrons near the Fermi surface, due to electron-phonon interaction, must lead to bound states of electrons, regardless of how weak the attraction may be. With this idea as a starting point, it has been possible to construct a successful theory of superconductivity (Bardeen, Cooper,

Schrieffer, 1957). In this theory a superconductor is characterized by a non-vanishing value of the electron-pair amplitude

$$F_{\sigma\sigma'}(\mathbf{x}-\mathbf{x}') = \langle\hat{\psi}_\sigma(\mathbf{x})\hat{\psi}_{\sigma'}(\mathbf{x}')\rangle \neq 0 \ . \tag{5.8}$$

In the homogeneous problem (i.e. in the absence of an external field), the expectation value depends only on the coordinate difference. In the normal state the expectation value (5.8) must vanish because all states and operators are gauge invariant, that is, commute with the number operator $\hat{N}$. Hence, in the superconducting state gauge invariance must be broken.

Two particles with spin 1/2 can pair in a singlet state with total spin $S = 0$, or in a triplet state with total spin $S = 1$ and spin projections $S_z = 0, \pm 1$. If we assume spherical symmetry, the electrons can only form pairs with opposite spins. In this case of so-called s-wave pairing, we need only consider

$$F(|\mathbf{x}-\mathbf{x}'|) = \langle\hat{\psi}_\uparrow(\mathbf{x})\hat{\psi}_\downarrow(\mathbf{x}')\rangle \ . \tag{5.9}$$

This function describing the correlation between two electrons has a spatial range ξ_0, called the coherence length, and falls off rapidly beyond. By relating this length to the smallest size wave packet the electrons can form, one arrives at the estimate

$$\xi_0 = a\frac{v_F}{T_c} \ , \tag{5.10}$$

where $v_F = p_F/m$ is the Fermi velocity and where a is a numerical constant for which the BCS-theory gives the value $a = 0.18$. For real superconductors the order of magnitude of ξ_0 is 10^{-4} cm, much larger that the interparticle distance.

If we confine ourselves to phenomena that vary only slightly over distances ξ_0, we may define th order parameter of the superconductor as the expectation value of the local product of two electron operators with opposite spins

$$F(|\mathbf{x}|) = \lambda \ \langle\hat{\psi}_\downarrow(\mathbf{x})\hat{\psi}_\uparrow(\mathbf{x})\rangle \ . \tag{5.11}$$

This order parameter characterizes the simplest (BCS)-type of superconductors with s-wave pairing. The normalization shall be given a physical meaning in the BCS-model. As we will see, the order parameter F is directly proportional to the order parameter of the Ginzburg-Landau theory.

5.2 BCS model

The BCS theory starts from the following model Hamiltonian for an electron gas

$$\hat{H} = \sum_\sigma \int d^3x \left[\hat{\psi}^\dagger_\sigma(\mathbf{x}) \ \epsilon(\mathbf{p})\,\hat{\psi}_\sigma(\mathbf{x}) - \tfrac{1}{2}\lambda\hat{\psi}^\dagger_\sigma(\mathbf{x})\,\hat{\psi}^\dagger_{-\sigma}(\mathbf{x})\,\hat{\psi}_{-\sigma}(\mathbf{x})\,\hat{\psi}_\sigma(\mathbf{x})\right] \ , \tag{5.12}$$

with kinetic energy

$$\epsilon(\mathbf{p}) = -\frac{\hbar^2\nabla^2}{2m} - \epsilon_{\rm F} \ , \tag{5.13}$$

which is measured relative to the Fermi energy $\epsilon_{\rm F}$. The electron fields satisfy the standard anti-commutation relations. As shown by Cooper, the exchange of phonons leads to an effective attraction between electrons close to the Fermi surface. In the Hamiltonian (5.12) this interparticle potential has been approximated by an attractive delta-function-like potential with coupling constant $\lambda > 0$.

Given the Hamiltonian we can immediately write down the corresponding partition function. We replace operator fields $\hat{\psi}_\sigma(\mathbf{x})$ by Grassman variables $\psi_\sigma(-i\tau, \mathbf{x})$ defined on the Euclidean time interval $t = -i\tau, 0 < \tau < \hbar\beta$ and construct the corresponding Euclidean action

$$S = \int_0^{\hbar\beta} d\tau \int d^3x \ \mathcal{L}(-i\tau, \mathbf{x}) \tag{5.14}$$

with Lagrangian density

$$\begin{aligned} \mathcal{L} &= \mathcal{L}_0 + \mathcal{L}_I \ , & (5.15)\\ \mathcal{L}_0 &= \psi_\uparrow^* \left[p_0 - \epsilon(\mathbf{p})\right] \psi_\uparrow + \psi_\downarrow^* \left[p_0 - \epsilon(\mathbf{p})\right] \psi_\downarrow \ , & (5.16)\\ \mathcal{L}_I &= \lambda \psi_\uparrow^* \psi_\downarrow^* \psi_\uparrow \psi_\downarrow \ , & (5.17) \end{aligned}$$

where we introduced the abbreviation $p_0 = -\hbar\partial/\partial\tau$ as a short hand for the time derivative. The partition function then takes the form:

$$Z = \int \mathcal{D}\psi \mathcal{D}\psi^* \ e^S \ . \tag{5.18}$$

The functional integration is over all fields $\psi_\sigma(-i\tau, \mathbf{x}), \psi_\sigma^*(-i\tau, \mathbf{x})$, which satisfy the anti-periodicity conditions:

$$\begin{aligned} \psi_\sigma^*(0, \mathbf{x}) &= \psi_\sigma^*(-i\hbar\beta, \mathbf{x}) \ , & (5.19)\\ \psi_\sigma(0, \mathbf{x}) &= \psi_\sigma(-i\hbar\beta, \mathbf{x}) \ , & (5.20) \end{aligned}$$

on the imaginary time-interval $[0, \hbar\beta]$.

Before we go further it is important to emphasize that the BCS-theory serves as a model rather than as a valid microscopic theory. For example, what is missing is the repulsive Coulomb interaction between the electrons. The total interaction, which is the balance of the phonon-electron attraction and the Coulomb repulsion, may be either attractive or repulsive. In its general form, the problem of taking both interactions into account for actual models is very complicated, especially since real superconductor are anisotropic.

The main reason why the BCS -model works so well is that it allows for the possibility that two electrons of opposite spins form a self-bound Cooper pair, which below some critical temperature condense. This results in the breaking of $U(1)$ gauge invariance and a non-zero value of the order parameter (5.11). The field $F(\mathbf{x})$ is an order parameter

for the SC-state and represents the essential degrees of freedom of the ordered phase. Therefore, our program will be to express the partition function as a functional integral over an auxiliary field $\Delta(-i\tau, \mathbf{x})$ that has a direct relation to the order parameter F.

At this point it is convenient to introduce the Nambu notation and rewrite the Lagrangian in terms of doublet fields:

$$\psi = \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow^* \end{pmatrix}, \quad \psi^\dagger = \left(\psi_\uparrow^*, \psi_\downarrow\right) . \tag{5.21}$$

With this compact notation the non-interacting part (5.16) of the Lagrangian density can be written in the bilinear form

$$\mathcal{L}_0 = \psi^\dagger \begin{pmatrix} p_0 - \epsilon(\mathbf{p}) & 0 \\ 0 & p_0 + \epsilon(\mathbf{p}) \end{pmatrix} \psi \tag{5.22}$$

In arriving at this expression we took the anti-commuting character of the fields into account and performed a partial integration, neglecting terms that are a total derivative.

The next step is to rewrite the quartic interaction as a Gaussian path integral over auxiliary fields Δ and $\Delta^\dagger$ with the help of the identity

$$\exp \lambda \int d\tau d^3x \psi_\uparrow^* \psi_\downarrow^* \psi_\uparrow \psi_\downarrow = \int \mathcal{D}\Delta \mathcal{D}\Delta^\dagger \exp \int d\tau d^3x \left(\Delta^\dagger \psi_\downarrow \psi_\uparrow + \psi_\uparrow^\dagger \psi_\downarrow^\dagger \Delta - \frac{1}{\lambda} \Delta^\dagger \Delta \right) , \tag{5.23}$$

which is the functional analogon of the identity

$$e^{AB} = \int_{-\infty}^{\infty} \frac{d^2 z}{\pi} e^{-|z|^2 + Az + Bz^*} \tag{5.24}$$

for ordinary variables $z = x + iy, d^2 z = dx\, dy$. The identity (5.23) is known as the Hubbard-Stratonovich (HS) transformation. We employ this transformation to rewrite the partition function in the form:

$$Z = \int \mathcal{D}\Delta \mathcal{D}\Delta^\dagger e^{-\Gamma[\Delta, \Delta^\dagger]} , \tag{5.25}$$

where the effective action is given by the expression

$$e^{-\Gamma[\Delta, \Delta^\dagger]} = \int \mathcal{D}\psi \mathcal{D}\psi^\dagger \exp \int_0^{\hbar\beta} d\tau d^3x \, \left(\psi^\dagger K \psi - \frac{1}{\lambda} |\Delta|^2 \right) . \tag{5.26}$$

The kernel in the last expression is the 2×2 matrix operator

$$K = \begin{pmatrix} p_0 - \epsilon(\mathbf{p}) & \Delta \\ \Delta^\dagger & p_0 + \epsilon(\mathbf{p}) \end{pmatrix} \tag{5.27}$$

in the space of the Nambu doublet fields. By the HS transformation we have achieved that in the action fermionic fields only appear bi-linearly, at the expense of the introduction of two new fields. As we will see, these two fields are closely related to the order parameter.

5.3 Landau approximation

The above derivation is exact, at least in so far as the formal algebraic manipulations are allowed. However, at this point, we confine ourselves to the mean-field-approximation. In MFA we set the partition function equal to the maximum term

$$\log Z = -\Gamma\left[\bar{\Delta}, \bar{\Delta}^\dagger\right] \ , \tag{5.28}$$

where $\bar{\Delta}, \bar{\Delta}^\dagger$ are the solutions of the MFA equations:

$$\frac{\delta\Gamma}{\delta\Delta} = 0 \ , \qquad \frac{\delta\Gamma}{\delta\Delta^\dagger} = 0 \ . \tag{5.29}$$

As we have argued before, the corrections to MFA describe fluctuations of the order parameter. Because of the large number of particles involved, the fluctuations about the expectation value should be small. In the BCS-theory these fluctuations are ignored. MFA breaks down only in a small region very close to the critical temperature, the so-called Ginzburg region.

Non-trivial solutions of MFA determine the order parameter of the BCS-theory. From the definition of the effective action (5.26), we get

$$\bar{\Delta}(\mathbf{x}) = \lambda\langle\psi_\downarrow(\mathbf{x})\psi_\uparrow(\mathbf{x})\rangle \ . \tag{5.30}$$

This identifies $\bar{\Delta}$ as the proper order parameter of the SC-state, since a non-zero value breaks $U(1)$ invariance.

Through the effective action, the partition function is given as a functional of the order parameter. To calculate the effective action (5.26) we have to evaluate the Gaussian path integral

$$I[\Delta, \Delta^\dagger] = \int \mathcal{D}\psi\mathcal{D}\psi^\dagger \exp \psi^\dagger \cdot K \cdot \psi \ , \tag{5.31}$$

where the exponent reads explicitly

$$\psi^\dagger \cdot K \cdot \psi = \int_0^\beta d\tau d^3x \int_0^\beta d\tau' d^3x' \psi_\sigma^\dagger(-i\tau, \mathbf{x})\, K_{\sigma\rho}(\tau, \mathbf{x}|\tau', \mathbf{x}')\, \psi_\rho(-i\tau', \mathbf{x}') \tag{5.32}$$

with Nambu indices $\sigma, \rho = 1, 2$ and kernel

$$K_{\sigma\rho}(\tau, \mathbf{x}|\tau', \mathbf{x}') = K_{\sigma\rho}\delta(\tau - \tau')\delta(\mathbf{x} - \mathbf{x}') \tag{5.33}$$

determined by the 2×2 differential operator (5.27); we have set $\hbar = 1$.

For fermions the general formula for the Gaussian integral (5.31) is

$$I[\Delta, \Delta^\dagger] = \det K = \exp[\mathrm{Tr} \log K] \ , \tag{5.34}$$

where K is to be regarded as a matrix in the infinite dimensional space labeled by $(\tau, \mathbf{x}, \sigma)$. The second member of the last equation is an obvious mathematical identity for any matrix that can be diagonalized.

To get further we assume that the order parameter is a constant. It is then convenient to introduce an expansion in terms of plane-wave eigenfunctions of the operator K satisfying the completeness relation:

$$\delta(\tau-\tau')\delta(\mathbf{x}-\mathbf{x}') = \frac{1}{\beta}\sum_n \int \frac{d^3p}{(2\pi)^3} \exp -i\omega_n(\tau-\tau') \exp i\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}') \; . \tag{5.35}$$

The frequencies ω_n are determined by the boundary conditions on the fermion fields which may be expanded in a Fourier series on the finite interval $[0,\beta]$ as

$$\psi_\sigma(-i\tau,\mathbf{x}) = \frac{1}{\beta}\sum_n \frac{d^3p}{(2\pi)^3}\tilde{\psi}_\sigma(i\omega_n,\mathbf{p})\exp -i\omega_n\tau + i\mathbf{p}\cdot\mathbf{x} \; . \tag{5.36}$$

On account of the anti-periodicity conditions (5.20) on the fermion fields, the so-called Matsubara frequencies take the odd values $\omega_n = (2n+1)\pi\beta^{-1}$ for fermions.

For the effective action (5.26) we have substituting (5.34)

$$\Gamma[\Delta,\Delta^\dagger] = -\mathrm{Tr}\log K + \frac{1}{\lambda}\int_0^\beta d\tau d^3x|\Delta|^2 \; . \tag{5.37}$$

The logarithm is defined by its expansion in powers of K. The first term we calculate as:

$$\begin{aligned} \mathrm{Tr}K &= \int_0^\beta d\tau d^3x K_{\sigma\sigma}\; \delta(\tau-\tau')\delta(\mathbf{x}-\mathbf{x}')|_{\tau=\tau',\mathbf{x}=\mathbf{x}'} \\ &= \int_0^\beta d\tau d^3x \frac{1}{\beta}\sum_n \frac{d^3p}{(2\pi)^3}\tilde{K}_{\sigma\sigma}(p) \\ &= \beta V \mathrm{Tr}\tilde{K}(p) \; . \end{aligned} \tag{5.38}$$

The momentum-space operator in the last line is

$$\tilde{K}(i\omega_n,\mathbf{p}) = \begin{pmatrix} i\omega_n - \epsilon(\mathbf{p}) & \Delta \\ \Delta^\dagger & i\omega_n + \epsilon(\mathbf{p}) \end{pmatrix} \tag{5.39}$$

and the trace in the last line of (5.38) must be understood as

$$\mathrm{Tr} \equiv \frac{1}{\beta}\sum_n \int \frac{d^3p}{(2\pi)^3}\mathrm{tr} \; , \tag{5.40}$$

where tr indicates the trace in Nambu space.

Similarly, we get for the quadratic term

$$\mathrm{Tr}K^2 = \beta V \mathrm{Tr}\tilde{K}^2(p) \; . \tag{5.41}$$

Hence, as it should be, the effective action is an extensive quantity

$$\Gamma[\Delta,\Delta^\dagger] = -\beta V\left(\mathrm{Tr}\log\tilde{K} - \frac{1}{\lambda}|\Delta|^2\right) \; . \tag{5.42}$$

This is an exact representation of the effective action for the case of a constant order parameter. In this case we may assume Δ to be real, without loss of information, since the arbitrary constant phase can be absorbed into the definition of the field operators.

5.4 Gap Equation

The partition function of the BCS-model is completely determined by the 2×2-matrix $\tilde{K}$. The determinant is:

$$\begin{aligned} \det \tilde{K} &= -\omega_n^2 - \epsilon^2(\mathbf{p}) - \Delta^2 \\ &= \left(-i\omega_n + \sqrt{\epsilon^2 + \Delta^2}\right)\left(-i\omega_n - \sqrt{\epsilon^2 + \Delta^2}\right) . \end{aligned} \tag{5.43}$$

For real energies E the determinant has zero's for the pair of energies

$$E_\pm = \pm\sqrt{\epsilon^2 + \Delta^2} . \tag{5.44}$$

This implies that the energy spectrum of the Fermi excitations exhibits a gap, that is, the excitation energy cannot be less than Δ. The gap value is reached for

$$\epsilon(\mathbf{p}) = \frac{\mathbf{p}^2}{2m} - \epsilon_F . \tag{5.45}$$

The gap is qualitatively explained as the finite binding energy of the Cooper pair formed by two electrons close to the Fermi surface.

The value of the gap may be obtained from the mean field equations (5.29). For constant Δ functional differentiation becomes ordinary differentiation which is easily performed with the help of the relation

$$\delta \mathrm{Tr} \log A = \mathrm{Tr} A^{-1} \delta A . \tag{5.46}$$

In this way we obtain from (5.42)

$$\frac{\partial \Gamma}{\partial \Delta^*} = -\beta V \left\{ \mathrm{Tr}\left[\tilde{S}(p) \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix} \right] - \frac{1}{\lambda}\Delta \right\} = 0 , \tag{5.47}$$

where the so-called propagator $\tilde{S}(p)$ is the inverse of $\tilde{K}(p)$

$$\tilde{S}(p) = \frac{1}{\omega_n^2 + \epsilon^2 + |\Delta|^2} \begin{pmatrix} i\omega_n + \epsilon(\mathbf{p}) & -\Delta \\ -\Delta^\dagger & i\omega_n - \epsilon(\mathbf{p}) \end{pmatrix} . \tag{5.48}$$

From (5.47) we get the celebrated (finite temperature) BCS gap equation

$$\Delta = \frac{\lambda}{\beta} \sum_n \int \frac{d^3p}{(2\pi)^3} \frac{\Delta}{\omega_n^2 + \epsilon^2 + |\Delta|^2} . \tag{5.49}$$

This equation can have a solution $\Delta \neq 0$ for a positive coupling constant, which is the crucial result of the BCS-theory.

The sum over the Matsubara frequencies may be performed with the help of a contour integral. The basic formula is

$$\begin{aligned} \frac{1}{\beta} \sum_n \frac{1}{i\omega_n - x} &= \frac{1}{\beta} \frac{1}{2\pi i} \oint dz \frac{1}{e^{\beta x} + 1} \frac{1}{z - x} \\ &= n(x) - \tfrac{1}{2} . \end{aligned} \tag{5.50}$$

with $n(x) = 1/(e^{\beta x}+1)$ the Fermi-Dirac distribution function. The contour integral circles the poles at $z = i\omega_n$ on the imaginary axis. This gives

$$1 = \lambda \int \frac{d^3p}{(2\pi)^3} \frac{\tanh \frac{1}{2}\beta E}{2E} \ . \tag{5.51}$$

The last equation is a non-linear integral equation for the gap parameter as a function of the temperature $\Delta = \Delta(T)$. One may note immediately that this equation would have no solution if $\lambda < 0$, i.e. in the case of repulsion, since then the two sides would have an opposite sign.

Since the general solution of the gap equation requires numerical methods we shall confine ourselves to some limiting behavior. For that purpose it is convenient to introduce the *density of states* according to the formal definition

$$\nu(\varepsilon) = 2 \int \frac{d^3p}{(2\pi)^3} \, \delta(\varepsilon - \varepsilon(\mathbf{p})) \ . \tag{5.52}$$

When integrands are peaked near the Fermi surface $\epsilon(\mathbf{p}) = 0$, we may use the approximation $\nu(\varepsilon) \cong \nu(0) =: \nu_F$. The symmetry of the integrand of (5.51) then allows us to write

$$1 = \lambda \nu_F \int_0^{\omega_D} d\varepsilon \, \frac{\tanh \frac{1}{2}\beta E}{2E} \ . \tag{5.53}$$

The integral must be cut off at some value ω_D to render it convergent. In the present model the interaction with the crystal lattice leads to an attractive force between the electrons. Since the Debije energy ω_D is a measure for the inverse lattice spacing, this leads to the condition that only electrons with energies of thickness $2\omega_D$ about the Fermi surface participate. In all practical cases we have $\omega_D << \epsilon_F$. Typical values are $\omega_D \sim 100$K and $\epsilon_F \sim 10.000$K.

In the zero-temperature limit equation (5.53) reduces to

$$1 = \lambda \nu_F \int_0^{\omega_D} \frac{d\varepsilon}{2E} \ . \tag{5.54}$$

The integral is elementary and gives

$$\Delta(0) = \frac{2\omega_D}{\sinh(2/\lambda\nu_F)} \ . \tag{5.55}$$

For many superconductors the dimensionless coupling constant $g = \frac{1}{2}\lambda\nu_F$ is small: $g \cong 0.2 - 0.3$. In the weak-coupling limit we obtain

$$\Delta(0) = 2\,\omega_D \, e^{-\frac{1}{g}}, \tag{5.56}$$

which depends sensitively on the value of coupling constant. One may note that the point $g = 0$ is an essential singularity. This non-analyticity means that the above results can never be obtained by a perturbation expansion in the small parameter g.

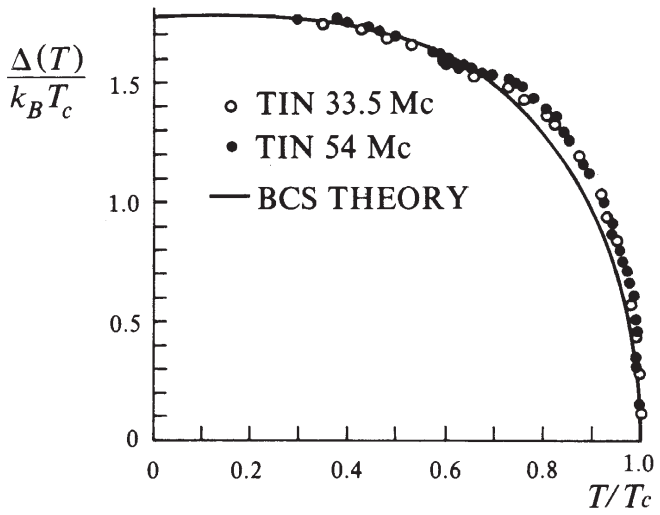


Figure 5.1: Temperature dependence of the energy gap in the BCS theory

In the opposite limit $T \to T_c$ the gap vanishes by definition and we find

$$1 = g \int_0^{\omega_D} \frac{d\varepsilon}{2\varepsilon} \tanh \frac{\varepsilon}{2T_c} \,. \tag{5.57}$$

It is possible to solve this implicit equation for T_c (see e.g. reference [FW]). The result is

$$T_c = 1.13\,\omega_D\, e^{-\frac{1}{g}} \,. \tag{5.58}$$

We see that T_c and the zero-temperature gap both depend in the same way on the coupling constant g. This dependence cancels in forming the ratio

$$\frac{\Delta\,(0)}{T_c} = 1.76 \,, \tag{5.59}$$

which is a universal constant independent of the material. Experimental results give reasonable agreement with this value.

The temperature dependence of the gap can be computed numerically. For weak coupling superconductors $\Delta(0) << \omega_D$, the ratio $\Delta(T)/\Delta(0)$ is a universal function determined by

$$\log \frac{\Delta\,(T)}{\Delta\,(0)} = -2 \int_0^{\omega_D} \frac{d\varepsilon}{E} \quad \frac{1}{e^{\beta E}+1} \,, \tag{5.60}$$

which decreases monotonically to zero at T_c, as shown in figure 5.1.

Near $T = 0$ the temperature variation is exponentially slow

$$\Delta\,(T) \approx \Delta\,(0) - \sqrt{2\pi\Delta\,(0)\,T} e^{-\Delta(0)/T} \,, \tag{5.61}$$

so that the hyperbolic tangent is nearly unity and insensitive to T. This means that Δ is nearly constant until a significant number of excitations is thermally excited. On the other hand, near $T_c, \Delta(T)$ drops to zero approximately as

$$\Delta(T) \approx \pi \left[\frac{8T_c}{7\zeta(3)}\right]^{\frac{1}{2}} (T_c - T)^{\frac{1}{2}} \ . \tag{5.62}$$

The variation of the order parameter with the square root of $T_c - T$ is characteristic of all mean field theories.

5.5 Thermodynamics

The calculation of the thermodynamic properties of a BCS-superconductor, proceeds from the thermodynamic potential in the mean-field-approximation (5.28), which in virtue of (5.42) for a constant gap becomes

$$\Phi \equiv \frac{1}{\beta V} \log Z = -\mathrm{Tr} \log \tilde{K} + \frac{1}{\lambda}\Delta^2 \ . \tag{5.63}$$

We will now show that the first term is nothing but the thermodynamic potential of an ideal gas of fermionic excitations (quasi-particles) with energies (5.44). First we note that the trace over Nambu space degrees of freedom gives:

$$\begin{aligned} \mathrm{tr} \log \tilde{K} &= \log \det{}_2 \tilde{K} \\ &= \log\left(-\omega_n^2 - \epsilon^2 - \Delta^2\right) \ . \end{aligned} \tag{5.64}$$

The fact that the argument of the logarithm has the wrong sign is no problem because it merely adds an irrelevant constant to the thermodynamic potential. This implies that we have:

$$\Phi = -\frac{1}{\beta} \int \frac{d^3p}{(2\pi)^3} \log\left(\omega_n^2 + \epsilon^2 + \Delta^2\right) + \frac{1}{\lambda}\Delta^2 \ . \tag{5.65}$$

The summation over Matsubara frequencies can be performed by contour integration. However, it is simpler to make use of the formula for the gap equation (5.51) derived earlier

$$\frac{1}{\beta}\frac{\partial}{\partial\Delta} \log\left(\omega_n^2 + \epsilon^2 + \Delta^2\right) = \frac{1}{\beta}\sum_n \frac{2\Delta}{\omega_n^2 + E^2} = \frac{\Delta}{E} \tanh \tfrac{1}{2}\beta E \ . \tag{5.66}$$

By integrating with respect to Δ, we arrive at

$$\Phi = -\sum_{s=\pm} \int \frac{d^3p}{(2\pi)^3} \log\left(1 + e^{-s\beta E_s}\right) + \frac{1}{\lambda}\Delta^2 \ . \tag{5.67}$$

As might be expected, the thermodynamic potential has the form of the partition function for an ideal gas of two types of particles with energies given by (5.44). The reasoning applies to a constant gap, but a generalization to a gap function which depends on $|\mathbf{p}|$ can easily be incorporated.

Appendix
Propagator in d-dimensions

In the neighborhood of T_c we may assume the correlation function in coordinate space to have the form:

$$G(\mathbf{r}) = \int \frac{d^d k}{(2\pi)^d} \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\alpha^2\mathbf{k}^2 + \mu^2} \; . \tag{5.68}$$

To calculate this expression we use the "proper time" representation

$$\frac{1}{\alpha^2\mathbf{k}^2 + \mu^2} = \int_0^\infty ds \; \exp -(\alpha^2\mathbf{k}^2 + \mu^2)\, s \tag{5.69}$$

to obtain:

$$G(\mathbf{r}) = \int_0^\infty ds \int \frac{d^d k}{(2\pi)^d} \exp -(\alpha^2\mathbf{k}^2 + \mu^2)\, s + i\mathbf{k}\cdot\mathbf{r} \; . \tag{5.70}$$

The variable shift $\mathbf{k} \to \mathbf{k} + i\mathbf{r}/2\alpha^2 s$ gives

$$G(\mathbf{r}) = \int_0^\infty ds e^{-\mu^2 s - \mathbf{r}^2/4\alpha^2 s} \int \frac{d^d k}{(2\pi)^d} e^{-\alpha^2 s \mathbf{k}^2} \; . \tag{5.71}$$

The Gaussian integral can be performed

$$G(\mathbf{r}) = \frac{1}{(4\pi\alpha^2)^{d/2}} \int_0^\infty ds \; s^{-d/2} e^{-\mu^2 s - \mathbf{r}^2/4\alpha^2 s} \; . \tag{5.72}$$

We may now use the representation for the Bessel functions:

$$\int_0^\infty dx \, x^{\nu-1} e^{-\frac{\beta}{x} - \gamma x} = 2 \left(\frac{\beta}{\gamma}\right)^{\nu/2} K_\nu(2\sqrt{\beta\gamma}) \tag{5.73}$$

This yields:

$$G(\mathbf{r}) = \frac{\mu^{d/2-1}}{\alpha^{d/2+1}(2\pi)^{d/2}} \frac{K_{d/2-1}\left(\frac{\mu r}{\alpha}\right)}{r^{d/2-1}} \; . \tag{5.74}$$

The asymptotic behavior of the Bessel functions is exponential

$$K_{d/2-1}\left(\frac{\mu r}{\alpha}\right) \sim \frac{e^{-\mu r/\alpha}}{\sqrt{2\pi\mu r/\alpha}} \; . \tag{5.75}$$

Hence we find exponential decay

$$G(\mathbf{r}) \sim \frac{e^{-r/\xi}}{r^{\frac{1}{2}(d-1)}} \tag{5.76}$$

with the correlation length

$$\xi = \frac{\alpha}{\mu} \tag{5.77}$$

This quantity plays a crucial role because it relates the length scale to the temperature.

In the case that $\mu = 0$ (massless case) the correlation length diverges and the decay is no longer exponential. On dimensional grounds we must have

$$G(\mathbf{r}) \sim \frac{1}{r^{d-2}} \ . \tag{5.78}$$

This follows directly from the definition (5.68) by changing to dimensionless integration variables $\mathbf{x} = \mathbf{k}r$.

Appendix
Gaussian Integrals

Gaussian integrals have some important applications. One of those is that they form the basis of perturbation theory in quantum field theory. In this appendix some algebraic identities about Gaussian integrals are briefly described for a finite number of integration variables.

Throughout the appendix the *Einstein summation convention* is used, that is, summation is understood to be carried out over repeated index symbols.

A general Gaussian integral has the form:

$$Z(j_1, \cdots, j_n) = \int_{-\infty}^{\infty} \prod_{i=1}^{n} d\phi_i \exp\left(-\frac{1}{2}\phi_i A_{ij} \phi_j + j_i \phi_i\right) \ , \tag{5.79}$$

in which A is a *symmetric positive definite* matrix, that is, its eigenvalues λ_i satisfy $\mathrm{Re}(\lambda_i) \geq 0, \ \lambda_i \neq 0$.

To calculate Z one first determines the maximum contribution of the integrand to the integral from the extremum of the exponent:

$$\frac{d}{d\phi_k}\left(\frac{1}{2}\phi_i A_{ij} \phi_j - j_i \phi_i\right) = 0 \ . \tag{5.80}$$

Using the solution of this equation, we shift integration variables according to:

$$\phi_i = (A^{-1})_{ij} j_j + y_i \ . \tag{5.81}$$

The integral (5.79) now becomes:

$$Z(j_1, \cdots, j_n) = \exp \frac{1}{2} j_i (A^{-1})_{ij} j_j \int_{-\infty}^{\infty} \prod_{i=1}^{n} dy_i e^{-\frac{1}{2} y_i A_{ij} y_j} \ , \tag{5.82}$$

which can be calculated by diagonalizing the matrix A. One finally obtains:

$$Z(j_1, \cdots, j_n) = (2\pi)^{\frac{n}{2}} (\mathrm{det} A)^{-\frac{1}{2}} \exp \frac{1}{2} j_i (A^{-1})_{ij} j_j \tag{5.83}$$

The last expression can be used to calculate any Gaussian average:

$$\langle \phi_{k_1}\phi_{k_2}...\phi_{k_l}\rangle \equiv \mathcal{N}\int_{-\infty}^{\infty}\left(\prod_{i=1}^{n}d\phi_i\right)\phi_{k_1}\phi_{k_2}...\phi_{k_l}e^{-\frac{1}{2}\phi_i A_{ij}\phi_j} \tag{5.84}$$

in which the normalization $\mathcal{N}$ is chosen in such a way that $<1>=1$, i.e. $\mathcal{N}^{-1}=Z(0)$. Consider the general Gaussian integral (5.79). Repeated differentiation with respect to the sources leads to the identity:

$$\langle \phi_{k_1}\phi_{k_2}...\phi_{k_l}\rangle = (2\pi)^{-\frac{n}{2}}(\det A)^{\frac{1}{2}}\frac{\partial}{\partial j_{k_1}}\frac{\partial}{\partial j_{k_2}}...\frac{\partial}{\partial j_{k_l}}Z(j_1,\cdots,j_n)\Big|_{\mathbf{j}=0} . \tag{5.85}$$

Insertion of the explicit form (5.83) then gives

$$\begin{aligned}\langle \phi_{k_1}...\phi_{k_l}\rangle &= \frac{\partial}{\partial j_{k_1}}...\frac{\partial}{\partial j_{k_l}}e^{\frac{1}{2}j_i(A^{-1})_{ij}j_j}\Big|_{\mathbf{j}=0} &(5.86)\\ &= \frac{\partial}{\partial j_{k_1}}...\frac{\partial}{\partial j_{k_l}}\frac{1}{n!}\frac{1}{2^n}\left(j_i(A^{-1})_{ij}j_j\right)^n , &(5.87)\end{aligned}$$

with $l=2n$; the number of variables and indices must be even. In principle the differentiations yield $2n!$ different terms. However, since the matrix A is symmetric, 2^n of these terms are equal. Furthermore, we are differentiating a monomial of order n, which implies that there are $n!$ permutations that also yield the same terms. Hence the total number of different terms is $(2n!)/2^n n! = (2n-1)!!$. This is simply the number of all possible pairings of $l=2n$ indices. Thus one finds:

$$\langle \phi_{k1}...\phi_{kl}\rangle = \sum_{\substack{\text{pairings of}\\(k_1,...,k_l)}} A^{-1}_{k_{p_1}k_{p_2}}...A^{-1}_{k_{p_{l-1}}k_{p_l}} . \tag{5.88}$$

The rule is:

- consider all possible pairings of the indices $k_1,...,k_l$ (l even),
- associate to each pair k_pk_q a matrix element of the matrix A^{-1}

Identity (5.88) states that all moments of a Gaussian distribution can be expressed in terms of the second moment alone. Indeed, consider the second moment

$$\langle \phi_{k1}\phi_{k2}\rangle = \left(A^{-1}\right)_{k_1k_2} . \tag{5.89}$$

It is simply equal to the inverse of the matrix A. Therefore an alternative way of writing (5.88) is

$$\langle \phi_{k1}...\phi_{kl}\rangle = \sum_{\substack{\text{pairings of}\\(k_1,...,k_l)}} \langle \phi_{k_{p_1}}\phi_{k_{p_2}}\rangle...\langle \phi_{k_{p_{l-1}}}\phi_{k_{p_l}}\rangle \tag{5.90}$$

In quantum field theory this result is known as *Wick's theorem* and the basis of perturbative calculations.

Appendix
Functional Differentiation

We first give a general definition: a functional F is a mapping from functions $\eta(x)$ on R^d onto the real or complex numbers (or in general on vectors). One writes $F[\eta]$ with square brackets to emphasize that the argument is a function rather than a number. A simple example of a functional is

$$F[\eta] = \int dx\ f(x)\eta(x) \tag{5.91}$$

with $f(x)$ some generalized function on R^d.

Next, we introduce the notion of the functional derivative of a functional. It is defined as a linear functional on a space of suitable test functions $\varphi(x)$ according to

$$\int dx\ \varphi(x)\frac{\delta F[\eta]}{\delta\eta(x)} = \lim_{\epsilon\to 0}\frac{1}{\epsilon}\{F[\eta+\epsilon\varphi] - F[\eta]\} \tag{5.92}$$

Applying this definition to the functional (5.91) , we get

$$\frac{\delta F[\eta]}{\delta\eta(x)} = f(x) \tag{5.93}$$

In a similar manner we derive

$$\frac{\delta\eta(x)}{\delta\eta(y)} = \delta(x-y) \tag{5.94}$$

The rules for functional differentiation are very much like the ones for ordinary derivatives. For, instance, under some mild continuity conditions we have

$$\frac{\delta}{\delta\eta(x)}\frac{\delta F[\eta]}{\delta\eta(y)} = \frac{\delta}{\delta\eta(y)}\frac{\delta F[\eta]}{\delta\eta(x)} = \frac{\delta^2 F[\eta]}{\delta\eta(x)\delta\eta(y)} \tag{5.95}$$

or

$$\left[\frac{\delta}{\delta\eta(x)}, \frac{\delta}{\delta\eta(y)}\right] = 0 \tag{5.96}$$

Other rules one may use are

$$\frac{\delta}{\delta\eta(x)}F^n[\eta] = nF^{n-1}[\eta]\frac{\delta F[\eta]}{\delta\eta(x)} \tag{5.97}$$

$$\frac{\delta}{\delta\eta(x)}e^{F[\eta]} = e^{F[\eta]}\frac{\delta F[\eta]}{\delta\eta(x)} \tag{5.98}$$

which imply

$$\left[\frac{\delta}{\delta\eta(x)}, \eta(y)\right] = \delta(x-y) \tag{5.99}$$

These rules suffice for our purpose.

Under suitable differentiability conditions there also exists an analogue of the Taylor expansion for a functional. Indeed, by Taylor's formula we have

$$F[\eta + z\varphi] = F[\eta] + z\frac{\partial F}{\partial z}\bigg|_{z=0} + \tfrac{1}{2}z^2\frac{\partial^2 F}{\partial z^2}\bigg|_{z=0} + \cdots \tag{5.100}$$

regarding F as an ordinary function of z. Using the definition (5.92) of the functional derivative, we may write

$$F[\eta + z\varphi] = F[\eta] + \sum_{n=1}^{\infty}\frac{z^n}{n!}\int dx^n \varphi(x_1)\cdots\varphi(x_n)\frac{\delta^n F[\eta]}{\delta\eta(x)\cdots\delta\eta(y)} \tag{5.101}$$

Taking $\eta = 0, z = 1$, and changing φ to η, we obtain the so-called Volterra series:

$$F[\eta] = F[0] + \sum_{n=1}^{\infty}\frac{1}{n!}\int dx^n \eta(x_1)\cdots\eta(x_n)\ \frac{\delta^n F[\eta]}{\delta\eta(x)\cdots\delta\eta(y)}\bigg|_{\eta=0} \tag{5.102}$$

If this series converges, the functional $F[\eta]$ is completely specified by giving the infinite set of symmetric functions

$$G(x_1,\cdots,x_n) = \frac{\delta^n F[\eta]}{\delta\eta(x_1)\cdots\delta\eta(x_n)}\bigg|_{\eta=0} \tag{5.103}$$

for which $F[\eta]$ is said to be the generating functional. This formalism is very useful as a starting point for perturbation theory.

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