



Introduction to path-integral Quantum Field Theory – A toolbox

Roland Koberle*¹

¹Universidade de São Paulo, Departamento de Física e Informática, São Carlos, SP, Brasil.

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Lecture notes on path-integrals, suitable for an undergraduate course with prerequisites such as: Classical Mechanics, Electromagnetism and Quantum Mechanics. The aim is to provide the reader, who is familiar with the major concepts of Solid State Physics, to study these topics couched in the language of path integrals. We endeavor to keep the formalism to the bare minimum.

Keywords: Path-integrals, Quantum Field Theory, Solid State Models.

1. Introduction

If you are familiar with some of the major concepts of Solid State Physics, but want to dive into modern topics using the language of Quantum Field Theory these notes are for you. As stated in the subtitle, the notes are only a toolbox and not a complete set of lecture notes. Therefore they are actually a sort of *manual*, as required for any box containing moderately complex tools. It is a common phenomenon, that students often have problems with the mathematical techniques and the notes are supposed to address this and only this issue. We have endeavored to keep them as short as possible, refraining e.g. to include many references, so that the student may dive into the tricks of the trade without distraction. As such the notes are like a skeleton onto which the instructor/student is supposed to attach the flesh.

The material was used in a one-semester, four hours per week, undergraduate course in our institute. Prerequisites being mainly Classical, Statistical and Quantum Mechanics. After digesting the material, you should be able to read books like [6], [7] etc. Of course all these books also present the mathematical techniques we discuss, but the exposition is often incomplete or too complete.

Our journey starts with Gaussian integrals in **section 2**, since these are essentially the only integrals we need to set up the path-integrals used below. **Sections 2.4** and **2.5** on stochastic processes are not prerequisites for the subsequent material, but are included to highlight the unity of the mathematical structure. We introduce path-integrals in **section 3**, generalizing the Gaussian processes of **section 2.2** from the 3-dimensional euclidean space to four dimensions. Upon analytic continuation in the *time* variable, we obtain

a relativistically invariant theory in Minkowski-space in **section 3.3** and show that this theory is identical to the one obtained using the operator-quantum-field-theory formalism. This is too good a bonus to leave out, although our subsequent models are mainly non-relativistic. This formalism is extended to interacting theories in **section 3.5**, where we also introduce integrals over fermionic variables. **Section 4** rewrites quantum mechanical expectation values as path-integrals and **section 5** uses this to express statistical mechanics in the path-integral formalism. Finally **section 6** presents models for ferro-magnetism and superconductivity with emphasis on spontaneous symmetry breaking.

The only possibly new result is the behavior of the order-parameter near criticality within the BCS-model Eq. (354). I added *pointers*, indicated as \rightsquigarrow , which should help you brush up on the physical underpinnings of the math used. To get a flavor of Feynman's original thoughts, you may look at *Feynman & Hibbs*[1].

2. Gaussian Integrals and Gaussian Processes

Gaussian integrals are the basic building blocks for the subsequent material.

2.1. Gaussian integrals in n dimensions

Let us start with the basic 1-dimensional integral¹

$$I_{00} = \int_{-\infty}^{\infty} dx e^{-ax^2/2} = \sqrt{\frac{2\pi}{a}}. \quad (1)$$

For complex a the integral may be defined by analytic continuation. For this to be possible a needs a positive

¹ In case you forgot, recall $I_{00}^2 = \int_{-\infty}^{\infty} dx dy e^{-a(x^2+y^2)/2} = \int_0^{2\pi} d\varphi \int_0^{\infty} \frac{1}{2} dr^2 e^{-ar^2/2}$ etc.

* Correspondence email address: rk@ifsc.usp.br

real part for the integral to be convergent. Complete the square in the exponential to get

$$I_0 = \int_{-\infty}^{\infty} dx e^{-(ax^2/2+bx)} = \sqrt{\frac{2\pi}{a}} e^{+b^2/2a} \quad (2)$$

and use the derivative-trick to integrate powers of x

$$\begin{aligned} I_{0n}(a, b) &= \int_{-\infty}^{\infty} dx x^n e^{-ax^2/2-bx} \\ &= \int_{-\infty}^{\infty} dx \frac{\partial^n}{\partial b^n} e^{-ax^2/2-bx} \\ &= \sqrt{\frac{2\pi}{a}} \frac{\partial^n}{\partial b^n} e^{b^2/2a}. \end{aligned} \quad (3)$$

Here we may set $b = 0$ after taking derivatives to obtain $I_{0n}(a, 0)$.

The generalization to n dimensions is straightforward. x becomes a vector $x = [x_1, x_2, \dots, x_n] \in \mathcal{R}^n$ and the exponent $ax^2/2 + bx$ is replaced by

$$Q(x) = \frac{1}{2} \sum_{i,j=1}^n x_i A_{ij} x_j + \sum_{i=1}^n b_i x_i \quad (4)$$

with A a symmetric, positive matrix and $b \in \mathcal{R}^n$ an auxiliary vector. It is convenient to introduce the inner product notation

$$Q(x) \equiv \frac{1}{2}(x | A | x) + (b | x) \quad (5)$$

The minimum of $Q(x)$ is at $\bar{x} = -A^{-1}b$. We thus have

$$Q(x) = Q(\bar{x}) + \frac{1}{2}(x - \bar{x} | A | x - \bar{x}), \quad (6)$$

with

$$Q(\bar{x}) = -\frac{1}{2}(b | A^{-1} | b). \quad (7)$$

After shifting $x - \bar{x} \rightarrow x$, we have to compute the integral

$$\int_{-\infty}^{\infty} Dx e^{-\frac{1}{2} \sum_{i,j=1}^n x_i A_{ij} x_j}, \quad Dx \equiv d^n x, \quad (8)$$

which is invariant under unitary transformations U or orthogonal transformations for real matrices. We therefore change to a new basis $\{x\} \rightarrow \{z = Ux\}$, which diagonalises the matrix A . A being diagonal, the integral $\int D^n z$ becomes a product of n integrals $\sim \int dz_i e^{-z_i^2 \hat{a}_i} = \sqrt{2\pi/\hat{a}_i}$, where \hat{a}_i is an eigenvalue of $1A$. This yields

$$\begin{aligned} \int_{-\infty}^{\infty} Dz e^{-\frac{1}{2}(z|A|z)} &= \prod_i (2\pi/a_i)^{1/2} \\ &= (2\pi)^{n/2} (\det A)^{-1/2}. \end{aligned} \quad (9)$$

Here we wrote the product of the eigenvalues as a determinant. Since the determinant is invariant under

orthogonal transformations, the result holds true in the original basis $\{x\}$.

Thus we obtain

$$\begin{aligned} \int_{-\infty}^{\infty} Dx e^{-\frac{1}{2}(x|A|x)-(b|x)} \\ = (2\pi)^{n/2} (\det A)^{-1/2} e^{\frac{1}{2}(b|A^{-1}|b)}. \end{aligned} \quad (10)$$

It will be convenient to include the determinant in the exponential as

$$(\det A)^{-1/2} = e^{-1/2 \ln \det A}.$$

Using the identity² $\ln \det A = \text{Tr} \ln A$, where the trace operation instructs us to sum over the diagonal elements, we get

$$\boxed{\int_{-\infty}^{\infty} Dx e^{-\frac{1}{2}(x|A|x)-(b|x)} = (2\pi)^{n/2} e^{\frac{1}{2}[(b|A^{-1}|b) - \text{Tr} \ln A]}. \quad (11)}$$

Using

$$x_j e^{\frac{1}{2} \sum x_i A_{ij} x_j + \sum b_i x_i} = \frac{\partial}{\partial b_j} e^{\frac{1}{2} \sum x_i A_{ij} x_j + \sum b_i x_i}, \quad (12)$$

we conveniently compute integrals with a polynomial $P(x)$ in the integrand as

$$\begin{aligned} \int Dx P(x) e^{-Q(x)} &= \int Dx P \left[\frac{\partial}{\partial b} \right] e^{-Q(x)} \\ &= P \left[\frac{\partial}{\partial b} \right] \int Dx e^{-Q(x)} \\ &= (2\pi)^{n/2} (\det A)^{-1/2} P \\ &\quad \times \left(\frac{\partial}{\partial b} \right) [e^{\frac{1}{2}(b|A^{-1}|b)}]. \end{aligned} \quad (13)$$

For example

$$\begin{aligned} \int_{-\infty}^{\infty} Dx x_i e^{-\frac{1}{2}(x|A|x)} \\ = (2\pi)^{n/2} (\det A)^{-1/2} A^{-1} b_i |_{b_i=0} = 0 \end{aligned} \quad (14)$$

and

$$\begin{aligned} \langle x_i x_j \rangle &\equiv \frac{\int_{-\infty}^{\infty} Dx x_i x_j e^{-\frac{1}{2}(x|A|x)}}{(2\pi)^{n/2} (\det A)^{-1/2}} \\ &= \frac{\partial}{\partial b_j} (A^{-1} b_i) |_{b=0} = A_{ji}^{-1} = A_{ij}^{-1}. \end{aligned} \quad (15)$$

² This is easy to verify in a base, where A is diagonal. Functions with matrix entries, such as $\log A$, $\exp A$, are defined by their power series expansions and we gloss over questions of convergence.

Exercise 2.1

Show that all Gaussian means with even powers of $\langle x_1, x_2, \dots, x_n \rangle$, $n = 1, 2, 3, \dots$, can be expressed in terms of one mean $\langle x_a x_b \rangle$ only.

2.2. Gaussian processes

A deterministic process X may be the evolution of a dynamical system described by Newton’s laws like the trajectory of a point particle $X = x(t)$, i.e. at each time the particle has a precise position.

In a stochastic process³ q we would allow the position of the particle to be random, i.e. at each time we have $q = f(X, t)$, where X is a stochastic variable chosen from some probability density $P(x)$. There are now many possible trajectories for the particle and we can compute a mean over all of them as

$$\langle q(t) \rangle = \int f(x, t)P(x)dx. \tag{16}$$

We will study systems described by a variable $q(t)$, or many variables $q_i(t)$, with $P(x)$ a Gaussian distribution.

If the process is Gaussian, we may define it either by its probability distribution, as any stochastic process, or by its two correlation functions: the one-point function

$$\langle q(t) \rangle = 0, \tag{17}$$

set to zero for simplicity⁴ and the two-point function

$$\langle q(t_1)q(t_2) \rangle = g(t_1, t_2). \tag{18}$$

Here $g(t_1, t_2)$ may be regarded as an infinite, positively defined matrix, since t_1 and t_2 may assume any real values.⁵ Yet if we want this process to represent a physically realizable one, such as a one-dimensional random walk, the time variables have to satisfy the following obvious ordering

$$t_1 \leq t_2. \tag{19}$$

For a Gaussian process all other N -point functions can be expressed in terms of the one- and two-point functions.

Supposing the process to be time-translationally invariant, the two-point function satisfies

$$g(t_1, t_2) = g(t_2 - t_1). \tag{20}$$

We now verify that the probability distribution is given in terms of the two-point function as:

$$P[q(t)] = \frac{1}{Z} e^{-\frac{1}{2} \int q(t_2)g^{-1}(t_2-t_1)q(t_1)dt_1 dt_2}. \tag{21}$$

³ See [3], III.4 for a detailed definition.

⁴ Otherwise just consider the process $q - \langle q(t) \rangle$.

⁵ We use the letter g , since this function will become a *Green* function.

Here $g^{-1}(t_1, t_2)$ is the inverse of the matrix $g(t_1, t_2)$, defined as

$$\int dtg(t_1, t)g^{-1}(t, t_2) = \int dtg^{-1}(t_1, t)g(t, t_2) = \delta(t_1-t_2). \tag{22}$$

The factor Z is responsible for the correct normalization of $P[q(t)]$:

$$\begin{aligned} & \int DQP[q(t)] \\ & \equiv \int \prod_t dq(t) \frac{1}{Z} e^{-\frac{1}{2} \int q(t_1)g^{-1}(t_1-t_2)q(t_2)dt_1 dt_2} = 1. \end{aligned} \tag{23}$$

The distribution $P[q(t)]$ is a *functional*, since it depends on the function $q(t)$. In order to perform explicit computations, like the normalization factor Z , we will discretize the continuous time variable in the next section. This will turn the functional into a function of many variables.

2.3. Discretizing and taking the limit $N \rightarrow \infty$

To make sense of integrals over an infinite number of integration variables, we have to discretise our continuous time axis as

$$t \rightarrow i$$

with $i = 1, 2, \dots, N$. Thus t becomes an integer index and $g(t)$ an N -dimensional matrix

$$\begin{aligned} q(t) & \rightarrow q_i, \\ g(t_1 - t_2) & \rightarrow g(i, j) \equiv g_{i-j}. \end{aligned} \tag{24}$$

The integral in Eq. (23) is now approximated by an integral over the N variables q_i as

$$\int DQP[q(t)] \sim \int dq_1 dq_2 \dots dq_N e^{-\frac{1}{2} \sum_{i,j=1}^N q(i)g^{-1}(i-j)q(j)} \tag{25}$$

After effecting the matrix computations, we will take the continuum limit

$$\prod_t dq(t) \equiv DQ = \lim_{N \rightarrow \infty} \prod_i dq_i \tag{26}$$

The exponent becomes

$$\begin{aligned} & \frac{1}{2} \int q(t_1)g^{-1}(t_1 - t_2)q(t_2)dt_1 dt_2 \\ & = \lim_{N \rightarrow \infty} \frac{1}{2} \sum_{i,j=1}^N q(i)g^{-1}(i - j)q(j), \end{aligned} \tag{27}$$

yielding for Eq. (21)

$$P[q(t)] = \lim_{N \rightarrow \infty} \prod_i dq_i \frac{1}{Z_N} e^{-\frac{1}{2} \sum_{i,j=1}^N q(i)g^{-1}(i-j)q(j)}, \tag{28}$$

where Z_N is the normalization factor for finite N . Again it is convenient to introduce the auxiliary vector b to compute correlation functions as derivatives $\frac{\partial}{\partial b^{(i)}}$ applied to

$$P_b[q(t)] = \lim_{N \rightarrow \infty} \prod_i^N dq_i \frac{1}{Z_N} \times e^{-\frac{1}{2} \sum_{i,j=1}^N q^{(i)} g^{-1}(i-j) q^{(j)} - \sum_{i=1}^N b^{(i)} q^{(i)}}. \tag{29}$$

The correct 2-point function can be read off Eq. (15), yielding Eq. (18), albeit for finite N , with

$$Z_N = (2\pi)^{N/2} (\det g)^{1/2}. \tag{30}$$

Let us verify in detail, that Eqs. (17) e (18) follow from Eq. (21), when we take the limit $N \rightarrow \infty$. Eq. (17) is trivially true, since Gaussian integrals of odd powers are zero. Now compute $\langle q(t_1)q(t_2) \rangle$ in two steps.

1. Calculate first the exponent in Eq. (21), i.e.

$$\int q(t_2)g^{-1}(t_2 - t_1)q(t_1)dt_1dt_2 \equiv \langle q|g^{-1}|q \rangle, \tag{31}$$

directly in the continuum limit. Due to translational invariance the Fourier-transform (FT)⁶

$$q(t) = \int_{-\infty}^{\infty} \tilde{d}\omega e^{-i\omega t} \tilde{q}(\omega), \quad \tilde{d}\omega \equiv \frac{d\omega}{\sqrt{2\pi}}. \tag{32}$$

is the road to take.

The exponent is

$$\begin{aligned} & \int q(t_2)g^{-1}(t_2 - t_1)q(t_1)dt_1dt_2 \\ &= \int \tilde{d}\omega_1 \tilde{d}\omega_2 \tilde{d}\omega_3 e^{-i\omega_1 t_2} e^{-i\omega_2(t_2-t_1)} e^{-i\omega_3 t_1} \\ & \tilde{q}(\omega_1) \tilde{q}(\omega_2) \tilde{q}(\omega_3) \tilde{g}^{-1}(\omega_2) dt_1 dt_2 \\ &= \int \tilde{d}\omega_1 \tilde{d}\omega_2 \tilde{d}\omega_3 2\pi \delta(\omega_1 + \omega_2) \delta(\omega_2 - \omega_3) \\ & \times \tilde{q}(\omega_1) \tilde{q}(\omega_3) \tilde{g}^{-1}(\omega_2) \\ &= \int \tilde{d}\omega |\tilde{q}(\omega)|^2 \tilde{g}^{-1}(\omega). \end{aligned} \tag{33}$$

$\tilde{q}(\omega)$ are complex variables satisfying $\tilde{q}(\omega) = \tilde{q}^*(-\omega)$, since $q(t)$ is real.

$g(\cdot)$ depends only on the difference $t_1 - t_2$. Therefore \tilde{g} is a function of one variable only. Since \tilde{g} is a diagonal matrix⁷, we get for its inverse

$$\tilde{g}^{-1}(\omega) = \frac{1}{\tilde{g}(\omega)}. \tag{34}$$

The diagonal matrix $\tilde{g}(\omega)$ does not couple variables with different ω 's, therefore the $\tilde{q}(\omega)$ are **independent** random variables with probability distribution given by

$$P[\tilde{q}(\omega)] = \frac{1}{Z} e^{-1/2 \int \tilde{d}\omega \frac{|\tilde{q}(\omega)|^2}{\tilde{g}(\omega)}}. \tag{35}$$

2. Let us compute the correlation function

$$\begin{aligned} \langle q(t_1)q(t_2) \rangle &= \int DQ \cdot q(t_2) \cdot q(t_2) \\ &\times \frac{1}{Z} e^{-1/2 \int q(t_2)g^{-1}(t_2-t_1)q(t_1)dt_1dt_2} \end{aligned} \tag{36}$$

We discretize as Eq. (24), but now in Fourier space. Instead of continuous variables $\tilde{q}(\omega)$, due to the discretization we now have discrete variables \tilde{q}_a , where a is an integer index

$$\tilde{q}(\omega) \rightarrow \tilde{q}_a, \tilde{q}(\omega') \rightarrow \tilde{q}_b.$$

Thus we get

$$\begin{aligned} \langle \tilde{q}(\omega) \tilde{q}(\omega') \rangle &\rightarrow \langle \tilde{q}_a \tilde{q}_b \rangle \\ &= \frac{1}{Z} \lim_{N \rightarrow \infty} \\ &\times \left\{ \int \tilde{q}_a \tilde{q}_b \left[\prod_{k=-N}^N d\tilde{q}_k \right] e^{-1/2 \sum_{k=-N}^N \tilde{q}_k^* \frac{1}{\tilde{g}_k} \tilde{q}_k} \right\} \\ &= \frac{1}{Z} \lim_{N \rightarrow \infty} \left\{ \prod_{k=-N}^N \int d\tilde{q}_k \tilde{q}_a \tilde{q}_b e^{-1/2 \tilde{q}_k^* \frac{1}{\tilde{g}_k} \tilde{q}_k} \right\}, \end{aligned} \tag{37}$$

Here we used that the Jacobian $t \rightarrow \omega$ equals unity and replaced the sum $\sum_{k=-N}^N$ in the exponent by the product $\prod_{k=-N}^N$.

Since $\int_{-\infty}^{\infty} x^n e^{-cx^2} dx = 0$ ($n = \text{odd}$) we get a non-zero result only if $\tilde{q}_a = \tilde{q}_{-b}$ or $\tilde{q}_b = \tilde{q}_{-a}$:

$$\begin{aligned} \langle \tilde{q}_a \tilde{q}_{-b} \rangle &= [\langle \tilde{q}_{-a} \tilde{q}_b \rangle]^* \\ &= \frac{1}{Z} \left[\int d\tilde{q}_a |\tilde{q}_a|^2 e^{-1/2 |\tilde{q}_a|^2 / \tilde{g}_a} \right] \\ &\times \lim_{N \rightarrow \infty} \prod_{|k| \neq a}^N \left[\int d\tilde{q}_k e^{-1/2 |\tilde{q}_k|^2 / \tilde{g}_k} \right] \end{aligned}$$

⁶ This is the orthogonal transformation mentioned to get Eq. (9).

⁷ Such as $A(i, j) = a(i - j) \delta_{i,j}$.

Performing the Gaussian integrals⁸ yields

$$\begin{aligned} \langle \tilde{q}_a \tilde{q}_{-b} \rangle &= \lim_{N \rightarrow \infty} \frac{(2\pi)^{N/2}}{Z_N} \{ [\tilde{g}_a]^{1/2} \tilde{g}_a \} \\ &\quad \star \left\{ \prod_{k \neq a}^N [\tilde{g}_k]^{1/2} \right\} \\ &= \lim_{N \rightarrow \infty} \frac{(2\pi)^{N/2}}{Z_N} \tilde{g}_a \prod_{k=-N}^N [\tilde{g}_k]^{1/2} \end{aligned} \quad (38)$$

Here we encounter our first problem with the continuum limit. The **infinite product** $\lim_{N \rightarrow \infty} \prod_k^N$.

Yet performing the same computation without the factors $\tilde{q}_a \tilde{q}_{-b}$, we compute Z as

$$Z = \lim_{N \rightarrow \infty} (2\pi)^{N/2} (\det g)^{1/2} \quad (39)$$

in agreement with Eq. (30). This factor guarantees the equality

$$\int P[q(t)] DQ = 1 = \int P[\tilde{q}(\omega)] D\tilde{Q} \quad (40)$$

with $D\tilde{Q} \equiv dq_1 dq_2 \dots dq_N$ and **cancels out in the correlation function, leaving a finite result.**

We are left only with the factor \tilde{g}_a in Eq. (38) and therefore get

$$\langle \tilde{q}_a \tilde{q}_{-a} \rangle = \tilde{g}_a \quad (41)$$

or

$$\langle \tilde{q}_a \tilde{q}_{-b} \rangle = \delta_{a,b} \tilde{g}_a. \quad (42)$$

The continuum limit results in

$$\langle \tilde{q}(\omega) \tilde{q}(-\omega') \rangle = \delta(\omega - \omega') \tilde{g}(\omega). \quad (43)$$

Using $\tilde{q}(-\omega) = \tilde{q}^*(\omega)$, since $q(t)$ is real, we get its FT as

$$\begin{aligned} \langle q(t_1) q(t_2) \rangle &= \int D\omega_1 D\omega_2 e^{-i(\omega_1 t_1 + \omega_2 t_2)} \langle \tilde{q}(\omega_1) \tilde{q}(\omega_2) \rangle \\ &= \int D\omega_1 e^{-i\omega_1(t_2 - t_1)} \tilde{g}(\omega_1) = g(t_2 - t_1). \end{aligned} \quad (44)$$

⁸ $\tilde{q} = x + iy$ is a complex number. The reality of $q(t)$ implies $\tilde{q}_k = \tilde{q}_{-k}^*$, so that we do not double the number of degrees of freedom, even though k runs over positive and negative values. Since only half of the degrees of freedom of \tilde{q} are independent, we integrate as $D\tilde{q}(\omega) \equiv \prod_{k=1}^{n/2} dx_k dy_k$.

For a complex variable this results in $\int dq e^{-c|q|^2} \equiv \int dx e^{-c|x|^2} \int dy e^{-c|y|^2} = [\sqrt{\frac{\pi}{c}}]^2, \int x^2 dq e^{-c|q|^2} = \int y^2 dq e^{-c|q|^2} = \frac{\pi}{2c^2}, \int |q|^2 dq e^{-c|q|^2} = \frac{\pi}{c^2}, \int q^2 dq e^{-c|q|^2} = 0$.

We realize that the two-point function is the inverse of the function, which couples the variables in the exponent of the Gaussian distribution Eq. (21).

Using Eq. (13) we obtain the n -point functions as

$$\langle q(t_1) q(t_2) \dots q(t_n) \rangle = \frac{\partial_{b_1} \dots \partial_{b_n} [e^{\frac{1}{2} \langle b|g|b \rangle}]}{e^{\frac{1}{2} \langle b|g|b \rangle}} \Big|_{b=0}. \quad (45)$$

Exercise 2.2

Show that all the n -point functions can be expressed in terms of the one- and two-point functions, if the process is Gaussian.

Exercise 2.3

Using a dice, propose a protocol to measure the correlation function $\langle q(t_1) q(t_2) \rangle$. What do you expect to get? Perform a computer experiment to compute this 2-point function. Can you impose some correlations without spoiling time-translation invariance?

Exercise 2.4 (The law of Large Numbers)

In an experiment \mathcal{O} an event \mathcal{E} is given by

$$P(\mathcal{E}) = p, P(\bar{\mathcal{E}}) = 1 - p \equiv q.$$

Repeating the experiment n times, the probability of obtaining \mathcal{E} k times is

$$p_n(k) = \binom{n}{k} p^k q^{n-k},$$

assuming the events \mathcal{E} to be independent. Show that

$$\binom{n}{k} p^k q^{n-k} \sim \frac{1}{\sqrt{2\pi npq}} e^{-(k-np)^2 / 2npq}, npq \gg 1.$$

Verify the *weak law of large numbers*

$$P\left\{ \left| \frac{k}{n} - p \right| \leq \epsilon \right\} \rightarrow 1 \text{ as } n \rightarrow \infty.$$

The *strong law of large numbers* states that the above is even true a.e. (a.e.=almost everywhere).

What is the difference between the weak and strong laws? For a delightful discussion of these non-trivial issues see [2], pg.18, Example 4.

Exercise 2.5 (The Herschel-Maxwell distribution)

Suppose that a joint probability distribution $\rho(x, y)$ satisfies (Herschel 1850)

- 1 - $\rho(x, y) dx dy = \rho(x) dx \rho(y) dy$
- 2 - $\rho(x, y) dx dy = g(r, \theta) r dr d\theta$ with $g(r, \theta) = g(r)$.

Show that this distribution is Gaussian.

Exercise 2.6 (Maximum entropy)

Show that the Gaussian distribution has maximum entropy $S = -\sum_i p_i \ln p_i$ for a given mean and variance.

2.4. *The Ornstein-Uhlenbeck process

We define the **Ornstein-Uhlenbeck** process as a Gaussian process with one-point function $\langle q(t) \rangle = 0$ and two-point correlation function as

$$\langle q(t_1) q(t_2) \rangle = e^{-\gamma(t_2 - t_1)} \equiv \kappa(\tau) \quad (46)$$

with $t_2 - t_1 = \tau > 0$. $\tau_{ou} \equiv 1/\gamma$ is a characteristic relaxation time.

This process was constructed to describe the **stochastic behavior of the velocity of particles in Brownian motion**. It is stationary, since it depends only on the time difference⁹

$$\langle q(t_1)q(t_2) \rangle = \langle q(t_1 + \tau)q(t_2 + \tau) \rangle.$$

Write the probability distribution $P[q_2, q_1]$ to observe q at instant t_1 and at instant t_2 as $P[q_2, q_1] \equiv P[q(t_1), q(t_2)]$. It is convenient to condition this distribution on q_1 , decomposing it as

$$P[q_2, q_1] \equiv T_\tau[q_2|q_1]P[q_1]. \tag{47}$$

Here $P[q_1]$ is the probability to observe q at time t_1 and $T_\tau[q_2|q_1]$ is the transition probability to observe q_2 at instant t_2 given q_1 at instant t_1 with $\tau = t_2 - t_1 > 0$. Note that $T_\tau[q_2|q_1]$ does not depend on the two times, but only on the time difference τ .

The Gaussian distribution $P[q_2, q_1]$, which depends only on two indices $[t_1, t_2] \rightarrow [i, j]$, is of the form

$$P[q_2, q_1] \sim e^{-\frac{1}{2} \sum_{i,j=1}^2 q_i A_{ij} q_j}.$$

To obtain the matrix A , we insert Eq. (46) into Eq. (15) to get

$$\kappa(\tau) = A_{12}^{-1} = A_{21}^{-1}. \tag{48}$$

In the limit $t_2 \rightarrow t_1$ we have $\kappa(0) = 1$, implying

$$\langle |q_1^2| \rangle = A_{11}^{-1} = \langle |q_2^2| \rangle = A_{22}^{-1} = 1,$$

i.e

$$A_{11}^{-1} = A_{22}^{-1} = 1. \tag{49}$$

The matrix A^{-1} is therefore

$$A^{-1} = \begin{pmatrix} 1 & \kappa \\ \kappa & 1 \end{pmatrix} \tag{50}$$

with the inverse

$$A = \frac{1}{1 - \kappa^2} \begin{pmatrix} 1 & -\kappa \\ -\kappa & 1 \end{pmatrix}. \tag{51}$$

Requiring the correct normalization

$$\int P[q_2, q_1] dq_1 dq_2 = 1. \tag{52}$$

we get

$$P[q_2, q_1] = \frac{1}{2\pi\sqrt{\det A}} e^{-\langle q_2, q_1 | A | q_2, q_1 \rangle}. \tag{53}$$

To compute $P[q_1]$ and $T_\tau[q_2|q_1]$, note that we may factor the exponential in Eq. (53) as follows

$$e^{-\frac{1}{2} \langle q_2, q_1 | A | q_2, q_1 \rangle} = e^{-\frac{q_2^2 - 2\kappa q_2 q_1 + q_1^2}{2(1-\kappa^2)}} = e^{-\frac{(q_2 - \kappa q_1)^2}{2(1-\kappa^2)}} e^{-\frac{1}{2} q_1^2},$$

allowing us to identify

$$P[q_1] = \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2} q_1^2}, \int dq_1 P[q_1] = 1. \tag{54}$$

and

$$T_\tau[q_2|q_1] \equiv \frac{1}{\sqrt{2\pi(1-\kappa^2)}} e^{-\frac{(q_2 - \kappa q_1)^2}{2(1-\kappa^2)}}. \tag{55}$$

You may verify that

$$\int T_\tau[q_2|q_1] dq_2 = 1, \int T_\tau[q_2|q_1] P[q_1] dq_1 = P[q_2]. \tag{56}$$

Since all other correlation functions can be reconstructed from $P[q_1]$ and $T_\tau[q_2|q_1]$, the Ornstein-Uhlenbeck process is *Markovian*. For example, taking $t_3 > t_2 > t_1$,

$$P[q_3, q_2, q_1] = P[q_3|q_2, q_1]P[q_2, q_1] \\ = T_{\tau'}[q_3|q_2]T_\tau[q_2|q_1]P[q_1]$$

with $\tau' = \tau_3 - \tau_2$. Here we used the fact that the transition probability depends only on one previous time-variable, i.e. $P[q_3|q_2, q_1] = P[q_3|q_2]$.

We now model the velocity distribution of *Brownian* particles at temperature T introducing the velocity $V(t)$ of a particle as

$$q(t) = \sqrt{\frac{m}{k_B T}} V(t). \tag{57}$$

Noticing that $P[q]dq = P[V]dV$, this results in the correct Maxwell-Boltzmann distribution at the initial time $t = t_1$

$$P[V_1] = \sqrt{\frac{m}{2\pi k_B T}} e^{-\frac{mV_1^2}{2k_B T}} \text{ with } \int dV_1 P[V_1] = 1. \tag{58}$$

The transition probability becomes

$$T_\tau[V_2|V_1] = \sqrt{\frac{m}{2\pi k_B T(1-\kappa^2)}} e^{-\frac{m}{k_B T} \frac{(V_2 - \kappa V_1)^2}{2(1-\kappa^2)}}. \tag{59}$$

The correlation functions are

$$\langle V(t_2)V(t_1) \rangle = \frac{k_B T}{m} e^{-\gamma(t_2-t_1)}, \langle V(t) \rangle = 0. \tag{60}$$

Exercise 2.7

Generate an Ornstein-Uhlenbeck process and measure the 2-point function using a random-number generator. Use the Yule-Walker equations. You need only two equations.

⁹ It is the only Gaussian, stationary, markovian process (*Doob's Theorem*). For *markovian* see Eq. (55).

Exercise 2.8

Convince yourself, that the transition probability $T_\tau[V_2|V_2]$ satisfies

$$\lim_{\tau \rightarrow 0} T_\tau[V_2|V_2] = \delta(V_2 - V_1). \tag{61}$$

Exercise 2.9

Show that the transition probability $P(V, \tau) \equiv T_\tau[V|V_0]$ satisfies the *Fokker-Planck* equation

$$\frac{\partial P}{\partial \tau} = \gamma \left\{ \frac{\partial VP}{\partial V} + \frac{k_B T}{m} \frac{\partial^2 P}{\partial V^2} \right\}. \tag{62}$$

Exercise 2.10

Using the transition probability $T_\tau[V|V_0]$ compute the one and two-point correlation functions for a fixed initial velocity V_0 , i.e.

$$P[V_1] = \delta(V_1 - V_0).$$

Since the initial distribution is not Gaussian with mean zero, the correlation functions are only stationary for $t \gg 1/\gamma$.

Exercise 2.11

Use Eq. (60) to show that

$$\langle (V(t + \Delta t) - V(t))^2 \rangle \rightarrow \frac{2k_B T}{m} \gamma \Delta t \text{ as } \Delta t \rightarrow 0.$$

Conclude that $V(t)$ is not differentiable.

2.5. *Brownian motion X(t)

Imagine a bunch of identical and independent particles, initially at $X = 0$ with the equilibrium velocity distribution given by the Ornstein-Uhlenbeck process Eq. (58, 59). Now define the *Brownian* process by

$$X(t) = \int_0^t V(t') dt'. \tag{63}$$

This equation is understood as an instruction to compute averages $\langle \cdot \rangle$, since we have not defined $V(t)$ by itself.

As the sum of Gaussian processes $X(t)$ is also Gaussian.¹⁰ The mean vanishes, since

$$\langle X(t) \rangle = \int_0^t \langle V(t') \rangle dt' = 0 \tag{64}$$

and the correlation function is

$$\langle X(t_1) X(t_2) \rangle = \int_0^{t_1} dt' \int_0^{t_2} dt'' \langle V(t') V(t'') \rangle. \tag{65}$$

We get from Eq. (60) for $t_2 > t_1$

$$\langle X(t_1) X(t_2) \rangle = \frac{k_B T}{m} \int_0^{t_1} dt' \int_0^{t_2} dt'' e^{-\gamma|t'-t''|}$$

¹⁰ Consider two independent Gaussian processes. The probability for the sum $Y = X_1 + X_2$ is $P(Y) = \int \int P_1(X_1) P_2(X_2) \delta(X_1 + X_2 - Y) dX_1 dX_2 = \int P_1(X_1) P_2(Y - X_1) dX_1$. This convolution of two Gaussians is again Gaussian.

To compute the above integral $I(t)$, compute first the integral

$$\begin{aligned} I_1(t) &= \int_0^t dt_1 \int_0^t dt_2 e^{-\gamma|t_1-t_2|} \\ &= \int_0^t dt_1 \int_0^{t_1} dt_2 e^{-\gamma(t_1-t_2)} \\ &\quad + \int_0^t dt_2 \int_0^{t_2} dt_1 e^{+\gamma(t_1-t_2)} \\ &= \frac{2}{\gamma^2} (\gamma t + e^{-\gamma t} - 1). \end{aligned}$$

Now use $I_1(t)$ to compute $I(t)$ for $0 \leq t_1 \leq t_2$ as

$$\begin{aligned} I_2 &= \int_0^{t_1} dt' \int_0^{t_2} dt'' e^{-\gamma|t'-t''|} \\ &= \int_0^{t_1} dt' \left(\int_0^{t_1} dt'' + \int_{t_1}^{t_2} dt'' \right) e^{-\gamma|t'-t''|} \\ &= I_1(t_1) + \int_0^{t_1} dt' \int_{t_1}^{t_2} dt'' e^{\gamma(t'-t'')} \\ &= I_1(t_1) + \frac{1}{\gamma^2} (e^{\gamma t_1} - 1) (e^{-\gamma t_1} - e^{-\gamma t_2}) \\ &= \frac{1}{\gamma^2} \left(2\gamma t_1 - 1 + e^{-\gamma t_1} + e^{-\gamma t_2} - e^{-\gamma(t_2-t_1)} \right). \end{aligned}$$

We obtain the correlation function for $0 \leq t_1 \leq t_2$ as

$$\langle X(t_1) X(t_2) \rangle = \frac{k_B T}{m \gamma^2} \left[2\gamma t_1 - 1 + e^{-\gamma t_1} + e^{-\gamma t_2} - e^{-\gamma(t_2-t_1)} \right]. \tag{66}$$

Now this Gaussian process is fully specified, since we know the first two correlation functions. But notice that $X(t)$ is neither stationary nor markovian! Yet for large times

$$t_1 \gg 1/\gamma, \quad t_2 - t_1 \gg 1/\gamma \tag{67}$$

this process reduces to the markovian **Wiener** process¹¹ with

$$\langle W(t_1) W(t_2) \rangle = \frac{2k_B T}{m \gamma} t_1 = \frac{2k_B T}{m \gamma} \min(t_1, t_2) \tag{68}$$

and

$$\langle W^2(t) \rangle = 2 \frac{k_B T}{m \gamma} t \equiv 2Dt. \tag{69}$$

Here D with dimension $[\frac{m^2}{sec}]$ is the *diffusion coefficient* (Einstein 1905)

$$D = \frac{k_B T}{m \gamma}. \tag{70}$$

¹¹ The sample paths of this process, as of the Ornstein-Uhlenbeck process, are very *rough*: they are continuous, but nowhere (*almost never*) differentiable. In fact from Eq. (69) we get $\langle (W(t + \Delta t) - W(t))^2 \rangle = \frac{2k_B T}{m \gamma} \Delta t$, so that the increments ΔW over a time-interval Δt behave as $\Delta W \sim \sqrt{\Delta t}$. Thus $\frac{\Delta W}{\Delta t} \sim \Delta t^{-1/2}$, which diverges as $\Delta t \rightarrow 0$.

This equation says: to reach thermal equilibrium, there has to be a balance between **fluctuations** $k_B T$ and **dissipation** $m\gamma$, i.e. $k_B T \sim m\gamma$.

Inspired by Einstein’s paper on Brownian motion, J.B. Perrin measured $\langle X^2(t) \rangle$ to obtain D and therefore the value of the Boltzmann constant

$$k_B = \frac{m\gamma D}{T}.$$

For γ Einstein used Stoke’s formula $\gamma = 6\pi\eta a$ for a molecule with radius a immersed in a stationary medium with viscosity η . From the perfect gas law $pV = RT = N_A k_B T$, we know $R = N_A k_B$, yielding a value for Avogadro’s number N_A

$$N_A = \frac{RT}{Dm\gamma}. \tag{71}$$

This equation has been verified by Perrin.¹² For the measurement of N_A he received the Nobel price in 1926. His work provided the nail in the coffin enclosing the deniers of the existence of atoms: Boltzmann was finally vindicated.

Exercise 2.12

The Ornstein-Uhlenbeck and the Wiener processes are related as

$$W(t) = \sqrt{2t} V(\ln t/2\gamma), \quad t > 0. \tag{72}$$

Verify that $\sqrt{2t}V(\ln t/2\gamma)$ is also Gaussian and show that Eq. (60) go over into $\langle W(t) \rangle = 0$ and Eq. (68).

Exercise 2.13

Show that the Ornstein-Uhlenbeck transition probability T_τ in Eq. (55) becomes the Wiener transition probability

$$W_\tau[q|q_0] = \frac{1}{\sqrt{4\pi D\tau}} e^{-\frac{(q-q_0)^2}{4D\tau}}, \quad \lim_{\tau \rightarrow 0} W_\tau[q|q_0] = \delta(q - q_0), \tag{73}$$

when we rescale the variables as follow $T_\tau \rightarrow \sqrt{\beta/D}T_\tau, q \rightarrow \alpha q, \tau \rightarrow \beta\tau, \beta = 2D\alpha^2 \rightarrow 0$. Show that it satisfies the diffusion equation

$$\frac{\partial W_\tau}{\partial \tau} = D \frac{\partial^2 W_\tau}{\partial q^2}. \tag{74}$$

Exercise 2.14

$V(t)$ being the Ornstein-Uhlenbeck process given by Eq. (60), use Eq. (66) for $X(t)$, show that

$$\langle (X(t+s) - X(t))^2 \rangle = \frac{2D}{\gamma} (e^{-\gamma s^2} + \gamma s - 1), \quad s > 0. \tag{75}$$

Therefore

$$\langle (X(t + \Delta t) - X(t))^2 \rangle \sim D\gamma\Delta t^2, \quad \Delta t \rightarrow 0. \tag{76}$$

From its definition, we expect $X(t)$ to be differentiable (almost everywhere). This is born out due to the $(\Delta t)^2$

¹² For a discussion of this point see ref. [4], pg. 51.

in Eq. (76), as opposed to the Wiener process, in which we have a $(\Delta t)^1$. Yet for large t , $X(t)$ goes over into the non-differentiable Wiener process. Clarify!

Exercise 2.15

For the *Langevin* approach to Brownian motion see [3], chapt. VIII,8.

3. Path Integrals

The integral $\int DQ$ in the correlation function Eq. (36)

$$\langle q(t_1)q(t_2) \rangle = \int DQ \cdot q(t_1) \cdot q(t_2) P[q(t)] = g(t_2 - t_1) \tag{77}$$

with

$$P[q(t)] = \frac{1}{Z} e^{-1/2 \int dt_1 q(t_2) g^{-1}(t_2-t_1) q(t_1) dt_2} \tag{78}$$

is in fact a sum over all trajectories, a **path integral**. In Fig. 1 we show two possible paths for a discrete time axis and discrete $q(t)$. The probability distribution $P[q(t)]$ is a *functional*, since it depends¹³ on a whole function $q(t)$.

We define the *Generating Function* as

$$Z[j] \equiv \frac{1}{Z} \int DQ \times e^{-1/2 \int dt_2 q(t_2) g^{-1}(t_2-t_1) q(t_1) dt_1 + \int dt_1 j(t_1) q(t_1)} \tag{79}$$

and using Eq. (10) to integrate over DQ

$$Z[j] = e^{1/2 \int dt_2 j(t_2) g(t_2-t_1) j(t_1) dt_1}. \tag{80}$$

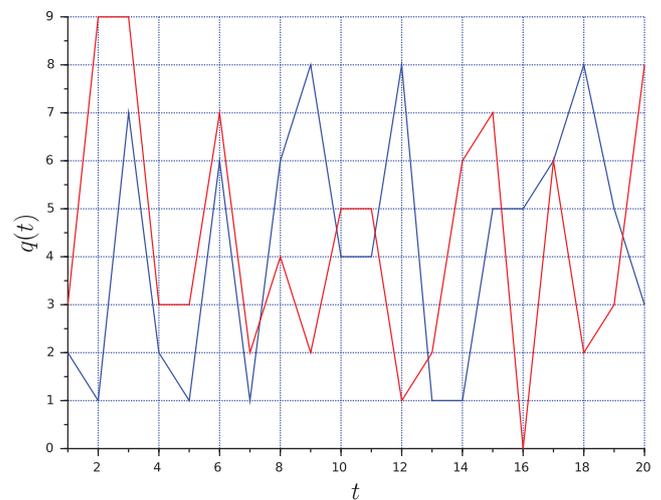


Figure 1: The integral DQ is discretized into a sum. Summing over all paths means adding the contribution of possible lines with the proper weight. Here we show only two paths for discretized time $t = 0, 1, 2, \dots, 20$. The dynamical variable q is also discretized $0 \leq q(t) < 10$.

¹³ Notice the difference to section 2.4, where $P[q_1]$ there depends only on the real number q_1 .

Here we chose the normalization factor Z such that $Z(j = 0) = 1$.

Use Eq. (45) with b_i replaced by $j(t)$, to obtain the correlation functions as¹⁴

$$\langle q(t_1) \dots q(t_N) \rangle = \frac{\delta^N Z[j]}{\delta j(t_1) \dots \delta j(t_N)} \Big|_{j=0}. \quad (81)$$

All correlation functions are actually compositions of the 2-point function $g(t)$ (See exercise 2.1).

3.1. A Gaussian field in one dimension

Consider an Ornstein-Uhlenbeck type process with the correlation function

$$g_{t_2, t_1} = g(t_2 - t_1) = e^{-|t_2 - t_1|/\tau}.$$

Due to the absolute value in the exponent, the correlation function $\langle q(t_2)q(t_1) \rangle$ is defined for any time-ordering, although only for $t_1 < t_2$ does it describe the Brownian motion of particles.

Let us compute the matrix-inverse g_{t_2, t_1}^{-1} . This will deliver a convenient operator expression for $g^{-1}(t)$, easily generalizable to higher dimensions.

The Fourier transform $g(t) \equiv \int \frac{d\omega}{2\pi} e^{-i\omega t} \tilde{g}(\omega)$ of $g(t)$ is

$$\begin{aligned} \tilde{g}(\omega) &= \int_0^\infty dt e^{-i\omega t - t/\tau} + \int_{-\infty}^0 dt e^{-i\omega t + t/\tau} \\ &= \frac{1}{-i\omega + 1/\tau} - \frac{1}{-i\omega - 1/\tau} = \frac{2}{\tau} \frac{1}{\omega^2 + \tau^{-2}}. \end{aligned} \quad (82)$$

Since this is a diagonal matrix, the inverse is

$$\tilde{g}^{-1}(\omega) = \frac{\tau}{2} (\omega^2 + \tau^{-2}). \quad (83)$$

In t-space we get

$$g^{-1}(t) = \int \frac{d\omega}{2\pi} e^{+i\omega t} \frac{\tau}{2} (\omega^2 + \tau^{-2}).$$

Using $\delta(t) = \int_{-\infty}^\infty \frac{d\omega}{2\pi} e^{i\omega t}$, this results in¹⁵

$$g^{-1}(t) = \frac{\tau}{2} \left(-\frac{d^2}{dt^2} + \tau^{-2} \right) \delta(t). \quad (84)$$

We check this equation using partial integration with vanishing boundary terms and respecting the symmetry

¹⁴ The definition of the functional derivative of the functional $F[\varphi(x)]$, generalizing the index i in $\partial/\partial b_i$ to a continuous variable, is

$$\frac{\partial F[\varphi(x)]}{\partial \varphi(y)} \equiv \lim_{\epsilon \rightarrow 0} \frac{F[\varphi(x) + \epsilon \delta(x - y)] - F[\varphi(x)]}{\epsilon}.$$

In particular we have $\frac{\partial \varphi(x)}{\partial \varphi(y)} = \delta(x - y)$, generalizing the discrete Kronecker δ_{ij} .

¹⁵ This identity is easily shown using $\theta(t) = \int_{-\infty}^\infty \frac{d\omega}{2\pi} \frac{e^{i\omega t}}{i\omega + \epsilon}$ and taking the derivative d/dt before the limit $\epsilon \downarrow 0$.

$$g(t) = g(-t)^{16};$$

$$\begin{aligned} &\int_{-\infty}^\infty dt g^{-1}(t_1 - t) g(t - t_2) \\ &= \frac{\tau}{2} \int_{-\infty}^\infty dt \left\{ \left(-\frac{d^2}{dt^2} + \tau^{-2} \right) \delta(t_1 - t) \right\} e^{-|t - t_2|/\tau} \\ &= \frac{\tau}{2} \int_{-\infty}^\infty dt \delta(t_1 - t) \left(-\frac{d^2}{dt^2} + \tau^{-2} \right) \\ &\quad \times \{ \theta(t - t_2) e^{-(t - t_2)/\tau} + \theta(t_2 - t) e^{+(t - t_2)/\tau} \} \\ &= \frac{\tau}{2} \int_{-\infty}^\infty dt \delta(t_1 - t) \left\{ \tau^{-2} e^{-|t - t_2|/\tau} \right. \\ &\quad - \left(\frac{1}{2} \delta'_t(t - t_2) - \frac{1}{2} 2\delta(t - t_2)/\tau + \theta(t - t_2)/\tau^2 \right) \\ &\quad \times e^{-(t - t_2)/\tau} \\ &\quad - \left(\frac{1}{2} \delta'_t(t_2 - t) - \frac{1}{2} 2\delta(t_2 - t)/\tau + \theta(t_2 - t)/\tau^2 \right) \\ &\quad \times e^{+(t - t_2)/\tau} \left. \right\} \\ &= \delta(t_1 - t_2), \end{aligned}$$

i.e.

$$\int dt g^{-1}(t_1 - t) g(t - t_2) = \delta(t_1 - t_2). \quad (85)$$

Recognize $g(t) \equiv g_{OU}(t)$ as the Green function of the differential operator $\mathcal{O}_{OU}[t]$ (also called the *resolvent*) with Dirichlet boundary conditions at $t = \pm\infty$

$$\mathcal{O}_{OU}[t] \equiv \frac{\tau}{2} \left(-\frac{d^2}{dt^2} + \tau^{-2} \right), \quad (86)$$

satisfying¹⁷

$$\begin{aligned} \mathcal{O}_{OU}[t] g(t - t') &= \frac{\tau}{2} \left(-\frac{d^2}{dt^2} + \tau^{-2} \right) g(t - t') \\ &= \delta(t - t'). \end{aligned} \quad (87)$$

For the physically realizable process the time-variables are restricted to $t_2 > t_1$. The corresponding *retarded* Green function

$$\hat{g}_{t_2, t_1} = \hat{g}(t_2 - t_1) = e^{-(t_2 - t_1)/\tau} \theta(t_2 - t_1) \quad (88)$$

is the solution of the *diffusion* equation

$$\hat{\mathcal{O}}_{OU}(t) \hat{g}(t) \equiv \left(\tau \frac{d}{dt} + 1 \right) \hat{g}(t) = \delta(t).$$

¹⁶ This means in particular, that the singularities generated by d/dt applied to the θ -functions are equally distributed, acquiring each a factor 1/2 to avoid double counting.

¹⁷ The matrix product is $\int dt_1 g^{-1}(t - t_1) g(t_1 - t') = \int dt_1 \frac{\tau}{2} \left(-\frac{d^2}{dt_1^2} + \tau^{-2} \right) \delta(t - t_1) g(t_1 - t') = \delta(t - t')$, the $\delta(t - t_1)$ eating up the integral to get Eq. (87).

Writing $g(t)$ as

$$g(t) = \hat{g}(t) + \hat{g}(-t) = e^{-t/\tau}\theta(t) + e^{+t/\tau}\theta(-t). \quad (89)$$

Up to boundary conditions, this shows this expression to be a one-dimensional analog of the Feynman propagator – to be introduced below Eq. (133).

3.2. Gaussian field in Euclidean 4-dimensional space

Let us extend the path integral formalism to four dimensions. Consider a *field* $\phi(x, y, z, t)$ living in this four-dimensional space and suppose it to be random. An example could be the surface of a wildly perturbed ocean and the field $\phi(x, y, z, t)$ would be the height of the ocean’s surface at point x, y, z at time t . Notice the height ϕ is a random variable, whereas x, y, z, t are coordinates, which under discretisation become integer indices.

We generalize the 1-dimensional operator in Eq. (86) to four Euclidean dimensions $[x_1, x_2, x_3, x_4]$, renaming $\tau^{-1} \equiv m$

$$\begin{aligned} \mathcal{O}'_{OU}(t) &\equiv -\frac{d^2}{dt^2} + \tau^{-2} \\ &\rightarrow -\frac{\partial^2}{\partial x_1^2} - \frac{\partial^2}{\partial x_2^2} - \frac{\partial^2}{\partial x_3^2} - \frac{\partial^2}{\partial x_4^2} + m^2 \\ &\equiv -\square_x^2 + m^2. \end{aligned}$$

The one-dimensional field $q(t)$ becomes a four-dimensional *euclidean field* $\varphi(x_1, x_2, x_3, x_4)$

$$q(t) \rightarrow \varphi(x_1, x_2, x_3, x_4) \quad (90)$$

with a *mass-type* parameter m . Denote $x = [x_1, x_2, x_3, x_4]$ the coordinate in the four-dimensional euclidean space \mathcal{E}_4 .

Applying the substitution

$$\mathcal{O}'_{OU}(t) = \frac{-d^2}{dt^2} + \tau^{-2} \rightarrow \mathcal{O}_E(x) = \square_x^2 - m^2 \quad (91)$$

to Eq. (87), requires the 2-point function $D_E(x)$ of the Euclidean theory to satisfy the four-dimensional equation

$$\boxed{(\square_x^2 - m^2)D_E(x) = \delta^{(4)}(x)}. \quad (92)$$

We therefore have the following correspondences

$$\begin{aligned} q &\rightarrow \phi \\ t &\rightarrow x = [x_1, x_2, x_3, x_4] \\ \langle q(t_2)q(t_1) \rangle &\rightarrow \langle \varphi(y)\varphi(z) \rangle \\ \mathcal{O}'_{OU}(t)\delta(t) &\rightarrow \mathcal{O}_E(x)\delta^{(4)}(x). \end{aligned} \quad (93)$$

We now **define** the Euclidean generating functional, as

$$\begin{aligned} Z_E[J] &= \frac{1}{Z} \int_E D\varphi \\ &e^{1/2 \int d^4x \varphi(x) (\square_x - m^2) \delta^{(4)}(x-y) \varphi(y) d^4y + \int d^4x J(x) \varphi(x)}. \end{aligned} \quad (94)$$

where the subscript E reminds us that we are in Euclidean space.

In the next section we will relate our Euclidean theory to a relativistic Minkowskian one. The variable x_4 will go over into a time variable as $x_4 \rightarrow ct$ with c the light velocity. Without the $\delta^{(4)}(x - y)$ in Eq. (94), this would lead to a non-local Lagrangian density, which for a local relativistic field theory an unacceptable situation. Such things as action-at-a-distance potentials as $\sim 1/r$ would violate special relativity. Using $\delta^{(4)}(x - y)$ to eliminate one integral, we get

$$Z_E[J] = \frac{1}{Z} \int_E D\varphi e^{1/2 \int d^4x \varphi(x) (\square_x - m^2) \varphi(x) + \int d^4x J(x) \varphi(x)}. \quad (95)$$

We now trade $\int d^4x \varphi(x) \square_x \varphi(x)$ for $-\int d^4x \partial_\mu \varphi(x) \partial_\mu \varphi(x)$ by a partial integration and use Gauss’s theorem under the assumption that the boundary terms vanish. This is true, if the field $\varphi(x)$ and its first derivatives vanish at the boundary or for periodic boundary conditions. We get

$$\begin{aligned} Z_E[J] &= \frac{1}{Z} \int_E D\varphi \\ &e^{1/2 \int d^4x (-\partial_\nu \varphi(x) \partial_\nu \varphi(x) - m^2) \varphi^2(x) + \int d^4x J(x) \varphi(x)} \end{aligned}$$

with $\partial_\nu \equiv \partial/\partial x^\nu \equiv [\partial_{x_1}, \partial_{x_2}, \partial_{x_3}, \partial_{x_4}]$ and sum over $\nu = 1, 2, 3, 4$ implied,

The generating functional can be expressed in terms to the Euclidean Lagrangian density

$$\mathcal{L}_E(\varphi) \equiv \frac{1}{2} [\partial_\nu \varphi(x) \partial_\nu \varphi(x) + m^2 \varphi^2(x)] \quad (96)$$

as

$$Z_E[J] = \frac{1}{Z} \int_E D\varphi e^{-\int d^4x \mathcal{L}_E(\varphi) + \int d^4x J\varphi} \quad (97)$$

Integrating out $D\varphi$ as in Eq. (80), we obtain the generating functional defining our theory

$$\boxed{Z_E[J] = e^{1/2 \int_E d^4x J(x) [\square_x - m^2]^{-1} J(x)}}. \quad (98)$$

Again normalized as $Z(0) = 1$. We have constructed a **local** theory, involving only fields and their derivatives at the single point x .

Notice that the above construction works for any Green function, not only for the relativistic case. In fact we will use non-relativistic models of electrons in the applications sects.(6.1,6.3) with

$$\mathcal{O} = i\hbar\partial_t - \frac{\hbar^2\nabla^2}{2m} - \mu. \quad (99)$$

We constructed a field theory in four dimensions based on a Gaussian probability distribution and the question arises: **What does it describe?** To answer this question we will

1. Morph one of its coordinates into a *time* variable, so that the resulting theory lives in Minkowski space.
2. Show that this theory equals the usual *Operator Quantum Field Theory* (OQFT) of a free bosonic quantum field.
3. Show that this equivalence carries over to interacting fields.

3.3. Wick rotation to Minkowski space

Start from a 4-dimensional Euclidean space \mathcal{E}_4 with points being indexed as $x^\mu = [x_1, x_2, x_3, x_4]$ and metric

$$ds_E^2 = dx_1^2 + dx_2^2 + dx_3^2 + dx_4^2. \tag{100}$$

Although we could have defined our theory directly in Minkowski space \mathcal{M}_4 , it is instructive to go from \mathcal{E}_4 to \mathcal{M}_4 by an analytic continuations¹⁸ in x_4 , since this automatically yields the 2-point function with the correct boundary condition. In fact to go from an Euclidean theory with metric ds_E^2 to a Minkowskian theory with metric

$$-ds_M^2 = dx_1^2 + dx_2^2 + dx_3^2 - dt^2 \equiv -dx^\mu dx_\mu \tag{101}$$

we perform the analytic continuation

$$t \equiv x_0 = -ix_4, \tag{102}$$

where t is now our time-variable.¹⁹

In the case of a Gaussian theory it is sufficient to perform this for the 2-point function, also called the *propagator*. The Fourier transform of the defining Eq. (92) in 4-dimensional Euclidean space, is

$$-(p^2 + m^2)\tilde{D}_E(p) = 1, \quad p^2 = p_1^2 + p_2^2 + p_3^2 + p_4^2 = \mathbf{p}^2 + p_4^2, \tag{103}$$

i.e.

$$\tilde{D}_E(p) = \frac{-1}{p^2 + m^2}. \tag{104}$$

Therefore going to x -space yields

$$D_E(x) = \int \frac{d^3p}{(2\pi)^3} \frac{dp_4}{2\pi} \frac{e^{-ip \cdot x}}{\mathbf{p}^2 + p_4^2 + m^2}. \tag{105}$$

This integral is well defined and is the unique solution of Eq. (92).

To obtain a theory living in Minkowski space analytically²⁰ continue $\tilde{D}_E(p)$ to complex momentum p_4 . The

¹⁸ The *Osterwalder-Schrader* theorem states the very general conditions under which this analytic continuation is possible.

¹⁹ Whenever a time variable has the same dimension as a space variable, it means that we are using unities in which $c = 1$.

²⁰ For our Gaussian theory there are no problems with analytic continuation.

Wick rotation in the complex p_4 plane

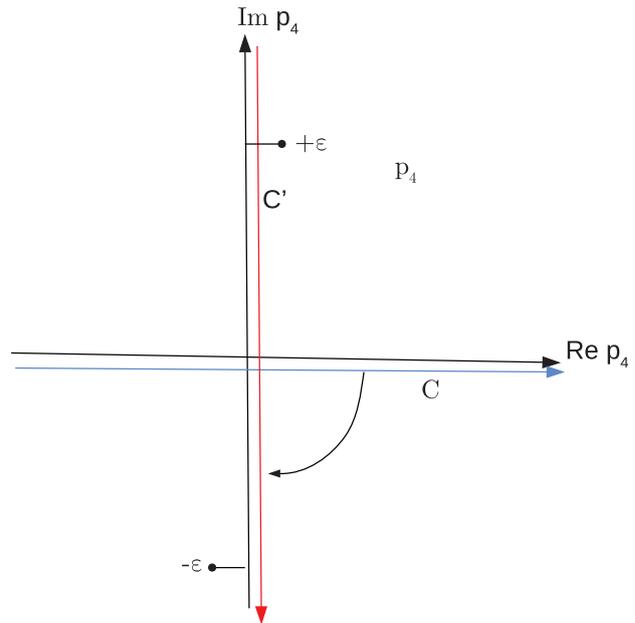


Figure 2: Wick rotation of the blue contour C , running along the real p -axis, into the red contour C' , running along the imaginary p -axis, without crossing the poles. These are shown as blobs, whose distance to the vertical axis is $\pm\epsilon$.

p_4 -dependent integral in Eq. (105) is

$$\begin{aligned} I_4(x_4) &= \int_{-\infty}^{\infty} \frac{dp_4}{2\pi} \frac{e^{-ip_4 x_4}}{p_4^2 + E(\mathbf{p})^2} \\ &= \int_{-\infty}^{\infty} \frac{dp_4}{2\pi} \frac{e^{-ip_4 x_4}}{(p_4 + iE(\mathbf{p}))(p_4 - iE(\mathbf{p}))} \end{aligned}$$

with $E(\mathbf{p}) = \sqrt{\mathbf{p}^2 + m^2}$. The integrand is a meromorphic function with two poles on the imaginary axis at $\pm iE(\mathbf{p})$.²¹ Now move the integration path C to the vertical axis of the complex p_4 -plane by a rotation of $-\pi/2$ as shown in Fig. 2. To avoid hitting the poles under the rotation, displace them by an infinitesimal amount to the left and right of the vertical axis. To avoid the blowup of $e^{ip_4 x_4}$ under rotation also rotate x_4 by $\pi/2$ and introduce a new coordinate

$$x_0 = t = -ix_4. \tag{106}$$

$I_4(x_4)$ now becomes

$$\begin{aligned} I_4(x_0) &= \lim_{\epsilon \rightarrow 0} \int_{C'} \frac{ds}{2\pi} \\ &\times \frac{e^{p_4(s)x_0}}{(p_4(s) + iE(\mathbf{p}) + \epsilon)(p_4(s) - iE(\mathbf{p}) - \epsilon)}, \end{aligned} \tag{107}$$

²¹ In Minkowski space the poles are along the real axis as you may see in references [6, 7].

where s is a real coordinate running along the contour \mathcal{C}' . Since along this contour $p_4(s)$ is purely imaginary define the real variable k_0 as

$$k_0 = ip_4 \tag{108}$$

and trade s for k_0 as integration variable. With this change of variables, the integral along the new path \mathcal{C}' becomes²²

$$\begin{aligned} I_4(x_0) &= \lim_{\epsilon \rightarrow 0} \int_{-\infty}^{\infty} \frac{dk_0}{2\pi} \frac{e^{-ik_0x_0}}{(k_0 + E(\mathbf{k}) - i\epsilon)(k_0 - E(\mathbf{k}) + i\epsilon)} \\ &= \lim_{\epsilon \rightarrow 0} \int_{-\infty}^{\infty} \frac{dk_0}{2\pi} \frac{e^{-ik_0x_0}}{k^2 - m^2 + i\epsilon}, \end{aligned} \tag{109}$$

where

$$k^2 \equiv k_0^2 - \mathbf{k}^2. \tag{110}$$

After this analytic continuation of the Euclidean propagator $D_E(x)$ of Eq. (105) becomes the **Feynman propagator**

$$D_F(x) = \int_{-\infty}^{\infty} \frac{d^4k}{(2\pi)^4} \frac{e^{-ik \cdot x}}{k^2 - m^2 + i\epsilon}, \tag{111}$$

the scalar product in Minkowski space being defined as $k \cdot x \equiv k_0x_0 - \mathbf{k} \cdot \mathbf{x}$. The propagator satisfies

$$\begin{aligned} (\partial^2 + m^2)D_F(x - y) &= -\delta^{(4)}(x - y), \\ \partial^2 &\equiv \partial^\nu \partial_\nu = \partial_t^2 - \nabla^2 \end{aligned} \tag{112}$$

where $\partial_\nu \equiv \partial/\partial x^\nu \equiv [\partial_t, \partial_{x_1}, \partial_{x_2}, \partial_{x_3}], \partial^\nu \equiv [\partial_t, -\partial_{x_1}, -\partial_{x_2}, -\partial_{x_3}]$, repeated indices $\nu = [0, 1, 2, 3]$ being summed over.

To explicitly compute $I_4(x_0)$, we close the integration path by a contour in the complex plane, choosing always the decreasing exponential in Eq. (109) to get

$$I_4(x_0) = i \begin{cases} \frac{e^{-ix_0 E(\mathbf{k})}}{2E(\mathbf{k})}, & x_0 > 0 \\ \frac{e^{ix_0 E(\mathbf{k})}}{2E(\mathbf{k})}, & x_0 < 0 \end{cases} \tag{113}$$

with $E(\mathbf{k}) = \sqrt{\mathbf{k}^2 + m^2}$.

In the following section we show, that the Feynman propagator obtained by the the analytic continuation of the euclidean one, is **identical to the Feynman propagator of the Operator Quantum Field Theory** (OQFT). This great advantage is the reason we started from the Euclidean formulation.

Apply now the substitution

$$\int_E d^4x \rightarrow i \int d^4x, \quad \square \rightarrow -\partial^2, \tag{114}$$

²² Since $E(\mathbf{p}) > 0$, $2E(\mathbf{p})\epsilon$ is an equivalent stand-in for the limit $\epsilon \rightarrow 0$.

to the Euclidean functional Eq. (97), to get the generating functional for the Minkowskian theory as

$$Z[J] = \frac{1}{Z} \int D\varphi e^{i \int d^4x (\mathcal{L}_0(\varphi) + J\varphi)} \tag{115}$$

with

$$\mathcal{L}_0(\varphi) \equiv \frac{1}{2} (\partial_\nu \varphi \partial^\nu \varphi - m^2 \varphi^2). \tag{116}$$

and $d^4x = dx dy dz dt$. Notice that whenever an i appears in the exponent multiplying \mathcal{L}_0 , we are in Minkowski space \mathcal{M}_4 . Integrating over φ we get in analogy to Eq. (98)

$$\begin{aligned} Z[J] &= \frac{1}{Z} \int D\varphi e^{\frac{i}{2} \int d^4x (\varphi(-\partial^2 - m^2)\varphi + J\varphi)} \\ &= e^{-\frac{i}{2} \int d^4x J(x) [\partial^2 + m^2]^{-1} J(x)} \\ &= e^{-\frac{i}{2} \int d^4x d^4y J(x) \frac{\delta^{(4)}(x-y)}{\partial^2 + m^2} J(y)} \end{aligned}$$

where we set the normalization factor Z such that $Z(0) = 1$. Upon using Eq. (112) this yields

$$Z[J] = e^{\frac{i}{2} \int d^4x d^4y J(x) D_F(x-y) J(y)}. \tag{117}$$

The Minkowskian generating functional Eq. (115) produces the correct correlation function as

$$\langle \varphi(x_1) \dots \varphi(x_n) \rangle = \frac{\delta^n Z[J]}{i^n \delta J(x_1) \dots \delta J(x_n)} \Big|_{J=0}. \tag{118}$$

In particular for $n = 2$ we get

$$\langle \varphi(x_1) \varphi(x_2) \rangle = i D_F(x_1 - x_2). \tag{119}$$

Since the equation of motion Eq. (92) is linear, it describes a *free* field propagation in space-time. To get some interesting physics we will have to turn interactions on in Sect. 3.5.

3.4. Quantizing a complex scalar field

In this section we will compute the two-point function of a free complex scalar field using the operator approach of Quantum Field Theory (OQFT) in order to show that this yields the same Feynman propagator. In this section we will always work in Minkowski space with coordinate $[x_1, x_2, x_3, x_0 = t]$.

In OQFT the propagator is defined to be the vacuum expectation value of the following time-ordered 2-point function

$$iD_F^{(OQFT)}(x - y) = \langle \Omega | T \phi(x) \phi^*(y) | \Omega \rangle \tag{120}$$

of the quantized operator field $\phi(\vec{x}, t)$ – actually an *operator valued distribution*. Here $|\Omega\rangle$ is the vacuum state and T means *time-ordered* – see Eq. (133). The quantized field $\phi(\vec{x}, t)$ will turn out to be a collection of harmonic operators.

Consider a complex scalar field, whose Lagrangian density is

$$\mathcal{L}_0(\phi) \equiv \frac{1}{2} (\partial_\alpha \phi^* \partial^\alpha \phi - m^2 \phi^* \phi), \quad (121)$$

where $\partial_\alpha \equiv [\partial_t, \partial_{x_1}, \partial_{x_2}, \partial_{x_3}]$, $\partial^\alpha \equiv [\partial_t, -\partial_{x_1}, -\partial_{x_2}, -\partial_{x_3}]$ and we sum over the repeated indices α , so that

$$\mathcal{L}_0(\phi) = \frac{1}{2} (\partial_0 \phi^* \partial_0 \phi - \nabla \phi^* \cdot \nabla \phi - m^2 \phi^* \phi).$$

The equations of motion are

$$\frac{\partial}{\partial x^\alpha} \frac{\partial \mathcal{L}_0}{\partial(\partial \phi / \partial x^\alpha)} - \frac{\partial \mathcal{L}_0}{\partial \phi} = 0,$$

$$\frac{\partial}{\partial x^\alpha} \frac{\partial \mathcal{L}_0}{\partial(\partial \phi^* / \partial x^\alpha)} - \frac{\partial \mathcal{L}_0}{\partial \phi^*} = 0$$

i.e.

$$(\partial^2 + m^2) \left\{ \begin{array}{l} \phi(x) \\ \phi^*(x) \end{array} \right\} = 0 \quad (122)$$

with $\partial^2 \equiv \partial_t^2 - \partial_{x_1}^2 - \partial_{x_2}^2 - \partial_{x_3}^2$. This so called *Klein-Gordon* equation, is a four-dimensional wave equation familiar from the study of Maxwell's equations, in which case $m = 0$.

The canonical quantization rules are – in units where $c = \hbar = 1$ –

$$[\phi(x, t), \phi(x', t)] = 0, \quad [\pi(x, t), \pi(x', t)] = 0$$

$$\phi(x, t), \pi(x', t) = -i\delta^{(3)}(x - x') \quad (123)$$

with the conjugate momenta

$$\pi = \partial \mathcal{L}_0 / \partial \dot{\phi} = \dot{\phi}^* \quad \text{and} \quad \pi^* = \partial \mathcal{L}_0 / \partial \dot{\phi}^* = \dot{\phi}.$$

Expand this field in energy-momentum *eigenstates*,²³ satisfying Eq. (122)

$$\phi(\mathbf{x}, t) = \int \frac{d^3 k}{\sqrt{(2\pi)^3 2E_k}} \times [a_+(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{x} - iE_k t} + a_-^\dagger(\mathbf{k}) e^{-i\mathbf{k} \cdot \mathbf{x} + iE_k t}]$$

$$\equiv \int d^3 k [a_+(\mathbf{k}) f_{\mathbf{k}}(x) + a_-(\mathbf{k})^\dagger f_{\mathbf{k}}^*(x)], \quad (124)$$

where

$$E_k = \sqrt{\mathbf{k}^2 + m^2}, \quad f_{\mathbf{k}}(x) = \frac{e^{-ik \cdot x}}{\sqrt{(2\pi)^3 2E_k}}$$

with $k = \{\mathbf{k} = [k_1, k_2, k_3], k_0 = E_k\}$ and $k \cdot x = E_k x_0 - \mathbf{k} \cdot \mathbf{x}$. Here $a_-^\dagger(\mathbf{k})$ is the hermitian conjugate of $a_-(\mathbf{k})$, since we are dealing with operators.

We easily solve for $a_\pm(\mathbf{k})$. For this we use the orthogonality relations

$$i \int d^3 x f_{\mathbf{k}}^*(\mathbf{x}, t) \overleftrightarrow{\partial}_t f_{\mathbf{l}}(\mathbf{x}, t) = \delta^3(\mathbf{k} - \mathbf{l}) \quad (125)$$

$$\int d^3 x f_{\mathbf{k}}(\mathbf{x}, t) \overleftrightarrow{\partial}_t f_{\mathbf{l}}(\mathbf{x}, t) = 0, \quad (126)$$

where

$$f(t) \overleftrightarrow{\partial}_t g(t) \equiv f(t) \frac{dg}{dt} - \frac{df}{dt} g(t),$$

such that, inter alia, the $\overleftrightarrow{\partial}_t$ kills the $E_{\mathbf{k}}$ factors from $f_{\mathbf{k}}(x)$ and allows the cancellation necessary for Eq. (126) to be true. Using these in Eq. (124) we get

$$a_+(\mathbf{k}) = i \int d^3 x f_{\mathbf{k}}^*(\mathbf{x}, t) \overleftrightarrow{\partial}_t \phi(\mathbf{x}, t),$$

$$a_-(\mathbf{k}) = i \int d^3 x f_{\mathbf{k}}^*(\mathbf{x}, t) \overleftrightarrow{\partial}_t \phi^*(\mathbf{x}, t).$$

Executing the operation $\overleftrightarrow{\partial}_t$ we get

$$a_+(\mathbf{k}) = \int d^3 x f_{\mathbf{k}}^*(\mathbf{x}, t) [E_{\mathbf{k}} \phi(\mathbf{x}, t) + i\dot{\phi}(\mathbf{x}, t)]$$

and using Eq. (123), this yields the commutator

$$[a_+(\mathbf{k}), a_+^\dagger(\mathbf{l})]$$

$$= - \int d^3 x d^3 y [f_{\mathbf{k}}^*(\mathbf{x}, t) \overleftrightarrow{\partial}_t \phi(\mathbf{x}, t), f_{\mathbf{l}}(\mathbf{y}, t) \overleftrightarrow{\partial}_t \phi^*(\mathbf{y}, t)]$$

$$= i \int d^3 x f_{\mathbf{k}}^*(\mathbf{x}, t) \overleftrightarrow{\partial}_t f_{\mathbf{l}}(\mathbf{x}, t) = \delta^{(3)}(\mathbf{k} - \mathbf{l}). \quad (127)$$

Proceeding analogously, we get for the whole set

$$[a_+(\mathbf{k}), a_+^\dagger(\mathbf{k}')] = [a_-(\mathbf{k}), a_-^\dagger(\mathbf{k}')] = \delta^{(3)}(\mathbf{k} - \mathbf{k}'),$$

$$[a_\pm(\mathbf{k}), a_\pm(\mathbf{k}')] = 0, \quad [a_\pm^\dagger(\mathbf{k}), a_\pm^\dagger(\mathbf{k}')] = 0,$$

$$[a_+(\mathbf{k}), a_-^\dagger(\mathbf{k}')] = 0, \quad [a_-(\mathbf{k}), a_+^\dagger(\mathbf{k}')] = 0. \quad (128)$$

These commutation relations show, that we have **two independent harmonic oscillators** $a_\pm(\mathbf{k})$ for each momentum \mathbf{k} . Defining the vacuum for each \mathbf{k} as

$$a_\pm(\mathbf{k})|0_{\mathbf{k}}\rangle = 0, \quad \forall \mathbf{k}, \quad (129)$$

we build a product-Hilbert space applying the creation operators $a_\pm^\dagger(\mathbf{k})$ to the ground state $|\Omega\rangle = \prod_{\mathbf{k}} |0_{\mathbf{k}}\rangle$.

We have the usual harmonic oscillator operators like energy, momentum etc, but here just highlight the charge operator. Due to the symmetry

$$\phi(x) \rightarrow e^{i\eta} \phi(x) \quad (130)$$

for constant η , Noether's theorem tells us that the current

$$j^\mu = i(\phi^* \partial^\mu \phi - \phi \partial^\mu \phi^*) \quad (131)$$

²³ The factor $\sqrt{2E_k}$ is included, so that e.g. the commutation relations Eq. (128) are the usual harmonic oscillator ones.

is conserved: $\partial_\mu j^\mu = 0$. The conserved charge is²⁴

$$Q = i \int d^3x j^0 = \int d^3k [a_+^\dagger(k) a_+(k) - a_-^\dagger(k) a_-(k)], \quad (132)$$

the operator $a_+^\dagger(k)$ creating a positively charged particle of mass m and the $a_-^\dagger(k)$ a negatively charged one.

Now compute the time-ordered product

$$\begin{aligned} \langle \Omega | T \phi(x') \phi^*(x) | \Omega \rangle & \\ & \equiv \theta(t' - t) \langle 0 | \phi(x') \phi^*(x) | 0 \rangle \\ & \quad + \theta(t - t') \langle 0 | \phi^*(x) \phi(x') | 0 \rangle. \end{aligned} \quad (133)$$

Both terms above create a charge $Q = +1$ at (x, t) and destroy this charge at $(x', t' > t)$. The first term does the obvious job, whereas the second term creates a charge $Q = -1$ at (x', t') and destroys it at $(x, t > t')$. This justifies the name *propagator*, since it propagates stuff from x to x' and vice-versa.²⁵ Since the fields $\phi(x), \phi^*(x')$ commute for space-like distances $x - x'$, the θ -functions don't spoil relativistic invariance.

Inserting the expansions Eq. (124) into Eq. (133), we get

$$\begin{aligned} \langle \Omega | T \phi(x') \phi^*(x) | \Omega \rangle & \\ & = \int d^3k [f_{\mathbf{k}}(x') f_{\mathbf{k}}^*(x) \theta(t' - t) \\ & \quad + f_{\mathbf{k}}^*(x') f_{\mathbf{k}}(x) \theta(t - t')] \\ & = \int \frac{d^3k}{(2\pi)^3 2E_k} [\theta(t' - t) e^{-ik \cdot (x' - x)} \\ & \quad + \theta(t - t') e^{ik \cdot (x' - x)}] \end{aligned}$$

The time-dependent part of the integrand in square brackets equals the rhs of Eq. (113).²⁶ Using Eq. (109) we get

$$\langle \Omega | T \phi(x) \phi^*(y) | \Omega \rangle = i \int \frac{d^4k}{(2\pi)^4} \frac{e^{-ik \cdot (x - y)}}{k^2 - m^2 + i\epsilon}. \quad (134)$$

Therefore conclude with Eq. (111), that

$$\begin{aligned} \langle \Omega | T \phi(x) \phi^*(y) | \Omega \rangle & \\ & = i D_F^{(OQFT)}(x - y) \\ & = i D_F(x - y) = \langle \varphi(x) \varphi^*(y) \rangle. \end{aligned} \quad (135)$$

²⁴ Going from Eq. (131) to Eq. (132) we actually subtracted in infinite constant. The presence of an infinite number of oscillators requires this redefinition of the charge! This simple subtraction is sufficient for a free theory. The interacting case requires a whole new machinery called *renormalization*.

²⁵ To be able to follow the propagating charge, was to reason to use a complex field and not a real, neutral field.

²⁶ Although this equation was computed for a real scalar field, the integrand is the same for our complex field.

The other time-ordered products are

$$\langle \Omega | T \phi(x) \phi(y) | \Omega \rangle = \langle \Omega | T \phi^*(x) \phi^*(y) | \Omega \rangle = 0. \quad (136)$$

Upon expanding in terms of real, hermitian fields ϕ_1, ϕ_2 as

$$\phi(x) = \frac{1}{\sqrt{2}} (\phi_1(x) + i\phi_2(x)),$$

yields

$$\begin{aligned} \langle \Omega | T \phi_i(x) \phi_j(y) | \Omega \rangle & = i \delta_{ij} D_F^{(OQFT)}(x - y) \\ & = i \delta_{ij} D_F(x - y). \end{aligned} \quad (137)$$

Thus Eqs. (115, 119) show, that the path-integral yields the time-ordered correlation functions of OQFT

$$\langle \Omega | T \phi(x_1) \phi(x_2) | \Omega \rangle = \int D\varphi \varphi(x_1) \varphi(x_2) e^{i \int d^4x \mathcal{L}_0(\varphi)}. \quad (138)$$

Since our theory is Gaussian, this is all we need to specify the whole theory and we therefore have for any number of fields

$$\begin{aligned} \langle \Omega | T \phi(x_1) \phi(x_2) \dots \phi(x_N) | \Omega \rangle & \\ & = \int D\phi \varphi(x_1) \varphi(x_2) \dots \varphi(x_N) \\ & \quad \times e^{i \int d^4x \mathcal{L}_0(\varphi)}. \end{aligned} \quad (139)$$

We have therefore shown, that the **path-integral formulation is equivalent to the OQFT description**. In section 3.5 we will extend this to a theory with interactions.

Aside: On- & Off-shell

A field is called *on-shell*, if its energy-momentum operator eigenvalues satisfy $E_k = +\sqrt{\mathbf{k}^2 + m^2}$. If this is not true, the field is *off-shell*.²⁷

Explicit relativistic invariance is a **must** in QFT, especially in the old days, when non-invariant cut-offs abounded to tame ultraviolet divergences. If we use traditional non-relativistic perturbation theory, we maintain conservation of momentum, but abandon conservation of energy, to allow the appearance of intermediate states. This results in the ubiquitous presence of energy denominators. This procedure, although yielding correct results, breaks explicit relativistic invariance. In QFT we

²⁷ We may impose the on-shell condition with positive energy in a manifestly relativistic invariant way as

$$\int \frac{d^3k}{(2\pi)^3 2E_k} = \int d^4k \delta(k^2 - m^2) 2\pi \theta(k_0).$$

want to maintain explicit invariance and therefore impose conservation of energy **and** momentum. But now, in order to allow the appearance of intermediate states, we have to place the particles *off-shell*.

Exercise 3.1

For a discussion of Feynman’s propagator theory \rightsquigarrow BD1[8], Section 6.4. What is the difference between retarded, advanced and Feynman propagators, all of which satisfy Eq. (112)?

3.5. Generating functional for interacting theories

We turn interactions on²⁸ adding an interaction term to the free quadratic Lagrangian $\mathcal{L}_0(\varphi)$ in Eq. (115)

$$\mathcal{L}_0(\varphi) \rightarrow \mathcal{L}(\varphi) = \mathcal{L}_0(\varphi) + \mathcal{L}_{int}(\varphi) \quad (140)$$

and **define** our interacting theory via the generating functional

$$Z[J] = \int D\varphi e^{\int d^4x (\mathcal{L}_0(\varphi) + \mathcal{L}_{int}(\varphi) + J\varphi)} \quad (141)$$

with the normalization factor $\int D\varphi e^{\int d^4x (\mathcal{L}_0(\varphi) + \mathcal{L}_{int}(\varphi))}$ included into the measure $D\varphi$, so that $Z(0) = 1$.

Equation (139) written now for interacting fields becomes

$$\begin{aligned} &\langle \Omega | T\phi(x_1)\phi(x_2) \dots \phi(x_N) | \Omega \rangle \\ &= \int D\phi \varphi(x_1)\varphi(x_2) \dots \varphi(x_N) e^{\int d^4x (\mathcal{L}_0(\varphi) + \mathcal{L}_{int}(\varphi))}. \end{aligned} \quad (142)$$

This looks, but only looks, similar to the **Gell-Mann Low** formula of OQFT

$$\begin{aligned} &\langle \Omega | T\phi(x_1)\phi(x_2) \dots \phi(x_N) | \Omega \rangle \\ &= \frac{1}{Z} \langle 0 | T\phi^0(x_1)\phi^0(x_2) \dots \phi^0(x_N) \\ &\quad \times e^{\int d^4x (\mathcal{L}_{int}(\phi^0) + J\phi^0)} | 0 \rangle, \end{aligned} \quad (143)$$

where $\phi, |\Omega\rangle$ are the operator field and the vacuum of the interacting theory, $|0\rangle, \phi^0$ the corresponding free field quantities²⁹ and \tilde{Z} , as usual, equals the numerator with $J = 0$. But here we deal with time-ordered products, as in Eq. (133), of operator-valued-distributions. In the

rhs of Eq. (142) the operator-valued-distributions have morphed into mere integration variables at the price of performing path-integrals.

Generally we are unable to perform the $\int D\varphi$ integral, since the interaction Lagrangian is not quadratic in the field variables. But we may rewrite $Z[j]$ using our old trick equ(15). Expand the exponential $e^{\int d^4x \mathcal{L}_{int}(\varphi)}$ in powers of $\varphi(y)$. A linear term would be

$$\int D\varphi \varphi(y) e^{\int d^4x (\mathcal{L}_0(\varphi) + J\varphi)}$$

Replace $\varphi(y)$ by the operation $\frac{1}{i} \frac{\delta}{\delta J(y)}$ as

$$\begin{aligned} &\int D\varphi \varphi(y) e^{\int d^4x (\mathcal{L}_0(\varphi) + J\varphi)} \\ &= \int D\varphi \frac{1}{i} \frac{\delta}{\delta J(y)} e^{\int d^4x (\mathcal{L}_0(\varphi) + J\varphi)} \\ &= \frac{1}{i} \frac{\delta}{\delta J(y)} \int D\varphi e^{\int d^4x (\mathcal{L}_0(\varphi) + J\varphi)} \end{aligned}$$

We can perform this substitution for all the powers of $\varphi(y)$ and reassemble the exponential to get

$$\begin{aligned} Z[j] &= \int D\varphi e^{\int \mathcal{L}(\varphi) + \int J\varphi} \\ &= e^{\int \mathcal{L}_{int}(\frac{1}{i} \frac{\delta}{\delta J})} \int D\varphi e^{\int \mathcal{L}_0(\varphi) + \int J\varphi}. \end{aligned} \quad (144)$$

Performing the Gaussian integral over $D\varphi$ we obtain

$$Z[J] = e^{\int \mathcal{L}_{int}(\frac{1}{i} \frac{\delta}{\delta J})} e^{\frac{i}{2} \int d^4x J(x) \Delta_F(x-y) J(y) d^4y} \quad (145)$$

and correlation functions as

$$\begin{aligned} &\langle \varphi(x_1)\varphi(x_2) \dots \varphi(x_n) \rangle \\ &= \frac{\delta^n Z[J]}{i^n \delta J(x_1)\delta J(x_2) \dots \delta J(x_n)} \Big|_{J=0} \end{aligned} \quad (146)$$

Eq. (145) is a **closed formula for the fully interacting theory**. Yet it is in general unknown how to compute

$$e^{\mathcal{L}_{int}(\frac{1}{i} \frac{\delta}{\delta J})} \langle \dots \rangle,$$

except expanding the exponential.

Furthermore our *manipulations* are formal and the integrals in general turn out to be divergent! Yet there is a well-defined mathematical scheme – not some mysteriously dubious instructions – to extract finite results for *renormalizable* field theories e.g. the BPHZ³⁰ renormalization scheme [16]. Renormalizable roughly

²⁸ This process often leads to misunderstandings. We started with a chimera: a free charged field, which is not the source of an electromagnetic field. The interaction now has to change this chimera into a real-world particle with a new mass, charge etc. A very non-trivial process indeed, which we don’t discuss here.

²⁹ Like the free scalar field of Eq. (124).

³⁰ The acronym stands for N. Bogoliubov and O. Parasiuk, who invented it; K. Hepp, who showed its correctness to all orders in perturbation theory and W. Zimmermann, who turned it into a highly efficient machinery.

means that the Lagrangian contains only products of fields, whose total mass-dimension is less or equal to the space-time dimension $D = 4$ and the theory includes all interactions of this type. The symmetries of the thus constructed quantum field theory may be different from the classical version. In particular it may have even **more** or less conservation laws – in which case *anomalies* are said to arise.

Let us obtain the **path-integral version of the equation of motion** like Eq. (122). For this purpose use the following simple identity

$$\int D\varphi \frac{\delta}{\delta\varphi} = 0, \tag{147}$$

assuming as usual boundary conditions with vanishing boundary terms. Applying this to the integrand of the generating functional $Z[j]$ of Eq. (144)

$$Z[J] = \int D\varphi e^{\imath \int d^4x (\mathcal{L}(\varphi) + J\varphi)} = \int D\varphi e^{\imath S(\varphi) + \imath \int d^4x J\varphi},$$

we get

$$\begin{aligned} & \int D\varphi \frac{\delta}{\delta\varphi} e^{\imath S(\varphi) + \imath \int d^4x J\varphi} \\ &= \int D\varphi \imath \left[\frac{\delta S(\varphi)}{\delta\varphi} + J \right] e^{\imath S(\varphi) + \imath \int d^4x J\varphi} = 0. \end{aligned} \tag{148}$$

Remember that

$$\frac{\delta S(\varphi)}{\delta\varphi} = \frac{\partial \mathcal{L}}{\partial\varphi} - \partial_\mu \frac{\partial \mathcal{L}}{\partial\partial_\mu\varphi}, \tag{149}$$

which set to 0 yields the classical equation of motion.

In fact, since the action depends both on $\varphi(x)$ and its derivative $\varphi'(x) = d\varphi(x)/dx$, we have

$$\begin{aligned} \delta S &= \delta \int dy \mathcal{L}[\varphi(y), \varphi'(y)] \\ &= \int dy \left[\frac{\partial \mathcal{L}}{\partial\varphi(y)} \delta\varphi + \frac{\partial \mathcal{L}}{\partial\varphi'(y)} \delta\varphi' \right] \\ &= \int dy \left[\frac{\partial \mathcal{L}}{\partial\varphi(y)} - \frac{d}{dy} \frac{\partial \mathcal{L}}{\partial\varphi'(y)} \right] \delta\varphi(y), \end{aligned} \tag{150}$$

where we performed a partial integration, assuming that the boundary terms vanish. Thus

$$\frac{\delta S}{\delta\varphi(x)} = \frac{\partial \mathcal{L}}{\partial\varphi(x)} - \frac{d}{dx} \frac{\partial \mathcal{L}}{\partial\varphi'(x)} \tag{151}$$

with Eq. (149) its four-dimensional version.

Setting $J = 0$ in Eq. (148) yields the equation of motion

$$\begin{aligned} & \int D\varphi e^{\imath S(\varphi)} \frac{\delta S}{\delta\varphi(y)} \\ &= \int D\varphi e^{\imath S(\varphi)} \left(\frac{\partial \mathcal{L}}{\partial\varphi} - \partial_\mu \frac{\partial \mathcal{L}}{\partial\partial_\mu\varphi} \right) = 0. \end{aligned} \tag{152}$$

Here the classical equation of motion shows up in the integrand.

Taking one derivative of Eq. (148) with respect to J , we get

$$\begin{aligned} 0 &= \frac{\delta}{\delta J_{x_1}} \int D\varphi e^{\imath S(\varphi) + \imath \int d^4x J(x)\varphi(x)} \left(\frac{\delta S}{\delta\varphi(y)} + J(y) \right) \\ &= \imath \int D\varphi \varphi(x_1) e^{\imath S(\varphi) + \imath \int d^4x J(x)\varphi(x)} \left(\frac{\delta S}{\delta\varphi(y)} + J(y) \right) \\ &\quad + \int D\varphi e^{\imath S(\varphi) + \imath \int d^4x J(x)\varphi(x)} \delta^{(4)}(y - x_1) \end{aligned}$$

Setting $J = 0$ yields

$$\int D\varphi e^{\imath S(\varphi)} \left(\varphi(x_1) \frac{\delta S}{\delta\varphi(y)} - \imath \delta^{(4)}(y - x_1) \right) = 0. \tag{153}$$

Exercise 3.2

Taking two derivatives of Eq. (148) with respect to J , show that

$$\begin{aligned} & \int D\varphi \varphi(x_2) \varphi(x_1) e^{\imath S(\varphi)} \left(\frac{\delta S}{\delta\varphi(y)} \right) \\ &= \imath \int D\varphi e^{\imath S(\varphi)} \\ &\quad \times \left(\varphi(x_1) \delta^{(4)}(y - x_2) + \varphi(x_2) \delta^{(4)}(y - x_1) \right). \end{aligned} \tag{154}$$

Exercise 3.3

Write Eq. (148) as

$$\left[\delta S'(-\imath \frac{\delta}{\delta J}) + J \right] Z[j] = 0. \tag{155}$$

This **Schwinger-Dyson** equation is an exact equation. $Z[j]$ may now be expanded in a power series to obtain perturbation theory results.

3.6. Connected correlation functions and the effective action

We have been using the auxiliary source field $J(x)$ to generate correlation functions from $Z[j]$ via Eq. (146). As such $J(x)$ actually is a sort of outsider, since we are really interested in the field $\varphi(x)$. It is therefore extremely useful to have a generating functional, which permits direct access to the field $\varphi(x)$.

For this purpose we first define a new generating functional $W(J)$ as

$$Z[J] = e^{\imath W[J]}, \quad W[J] = -\imath \ln Z[J]. \tag{156}$$

Using the cumulant expansion of exercise 3.3 or by direct computation, it is straightforward to verify, that $W[J]$

generates the connected correlation functions

$$\langle \varphi(x_1)\varphi(x_2)\dots\varphi(x_n) \rangle_c = \frac{i^n \delta^n W[J]}{i^n \delta J(x_1)\delta J(x_2)\dots\delta J(x_n)} \Big|_{J=0} \tag{157}$$

E.g.

$$\begin{aligned} \langle \varphi(x) \rangle_c &= \langle \varphi(x) \rangle, \\ \langle \varphi(x_1)\varphi(x_2) \rangle_c &= \frac{\delta^2 W[J]}{i\delta J(x_1)\delta J(x_2)} \Big|_{J=0} \\ &= \left[-\frac{1}{Z[j]} \frac{\delta^2 Z[j]}{\delta J(x_1)\delta J(x_2)} \right. \\ &\quad \left. + \frac{1}{Z[j]^2} \frac{\delta Z[j]}{\delta J(x_1)} \frac{\delta Z[j]}{\delta J(x_2)} \right] \Big|_{J=0} \\ &= \langle \varphi(x_1)\varphi(x_2) \rangle - \langle \varphi(x_1) \rangle \langle \varphi(x_2) \rangle, \end{aligned} \tag{158}$$

where we used Eq. (146). Now trade the auxiliary source $J(x)$ for the one-point correlation function³¹

$$\tilde{\varphi}(x) \equiv \langle \varphi(x) \rangle = \langle \varphi(x) \rangle_c = \frac{\delta W}{\delta J(x)} \tag{159}$$

by a functional Legendre transformation

$$\Gamma[\tilde{\varphi}] \equiv W[J] - \int d^4x J(x)\tilde{\varphi}(x) \tag{160}$$

and use $\tilde{\varphi}(x)$ as the **independent field**. The field $\tilde{\varphi}(x)$ is directly related to physical properties as opposed to auxiliary field $J(x)$.

As Eq. (156) shows, $\Gamma[\tilde{\varphi}]$ is an *effective action*. $J(x)$ is now a variable dependent of $\tilde{\varphi}(x)$, given by

$$\frac{\delta \Gamma[\tilde{\varphi}]}{\delta \tilde{\varphi}(x)} = -J(x). \tag{161}$$

Using Eq. (159) it also follows that

$$\frac{\delta \Gamma[\tilde{\varphi}]}{\delta J(x)} = 0.$$

Differentiating Eqs. (159, 161), we get

$$\begin{aligned} \langle \tilde{\varphi}(x)\tilde{\varphi}(y) \rangle_c &= \frac{-i\delta^2 W}{\delta J(x)\delta J(y)} = -i \frac{\delta \varphi(x)}{\delta J(y)} \\ \Gamma^{(2)}(x, y) &\equiv \frac{\delta^2 \Gamma}{\delta \varphi(x)\delta \varphi(y)} = -\frac{\delta J(y)}{\delta \varphi(x)}. \end{aligned} \tag{162}$$

The functional $\Gamma[\tilde{\varphi}]$ is useful, inter alia, for the study of phase transitions. If $\tilde{\varphi}(x)$ is not zero, even if $J(x) = 0$, **spontaneous symmetry breaking**³² occurs. Due to Eq. (161), this means

$$\delta \Gamma[\tilde{\varphi}]/\delta \tilde{\varphi}(x) = 0. \tag{163}$$

³¹ In the presence of the external source $J(x)$ the one-point correlation functions $\langle \varphi(x) \rangle$ does not vanish!

³² See e.g. [11], Eq. (3.18) for details, after reading section 6.1.

Exercise 3.4 (The cumulant expansion)

Show that

$$\ln \langle e^{-x} \rangle = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \langle x^n \rangle_c, \tag{164}$$

where the subscript c stands for *connected*. We have

$$\langle x \rangle_c = \langle x \rangle, \langle x^2 \rangle_c = \langle x^2 \rangle - \langle x \rangle^2, \dots$$

Exercise 3.5 (Proper vertex functions)

The functions

$$\Gamma^{(n)}(x_1, x_2, \dots, x_n) \equiv \frac{\delta^n \Gamma[\tilde{\varphi}]}{\delta \tilde{\varphi}(x_1) \dots \delta \tilde{\varphi}(x_n)} \Big|_{\tilde{\varphi}=0} \tag{165}$$

are called *proper vertex functions*. Verify, that for the free field case the only proper vertex is

$$\Gamma_0^{(2)}(x, y) = -(\partial^2 + m^2)\delta^{(4)}(x - y), \quad \Gamma_0^{(2)}(p) = p^2 - m^2. \tag{166}$$

Exercise 3.6

Show that

$$\int d^4y \Gamma_0^{(2)}(x, y) D_F(y - z) = \delta^{(4)}(x - z), \tag{167}$$

i.e. the Feynman propagator is the Green function of the proper vertex $\Gamma_0^{(2)}$. Show that the analogous relation

$$\int d^4y \Gamma^{(2)}(x, y) [-i\langle \varphi(y)\varphi(z) \rangle_c] = \delta^{(4)}(x - z) \tag{168}$$

holds for the interacting case. Multiply Eqs. (162) like matrices, paying attention to the repeated indices summed/integrated over.

Exercise 3.7 (The free field case)

Eq. (117) states

$$W_0[J] = \frac{1}{2} \int d^4x d^4y J(x) D_F(x - y) J(y).$$

Verify

$$\tilde{\varphi}_0(z) = \int d^4z' D_F(z - z') J(z'). \tag{169}$$

Insert this in Eq. (160) to get

$$\begin{aligned} \Gamma_0[\tilde{\varphi}] &= - \int d^4y J(y) \tilde{\varphi}_0(y) \\ &= \int d^4x d^4y J(x) (-\delta^{(4)}(x - y)) \tilde{\varphi}_0(y). \end{aligned}$$

Use the equation for the Feynman propagator (Eq. (112))

$$(\partial_x^2 + m^2) D_F(x - y) = -\delta^{(4)}(x - y)$$

to get rid of the $(-\delta^{(4)}(x - y))$ -factor. Show using Eq. (169), that

$$\Gamma_0[\tilde{\varphi}] = -\frac{1}{2} \int d^4x \tilde{\varphi}_0(x) (\partial^2 + m^2) \tilde{\varphi}_0(x), \tag{170}$$

$$J(x) = (\partial^2 + m^2) \tilde{\varphi}_0(x).$$

You will perform usual matrix multiplications with continuous indices and perform a partial integration.

Apply a partial integration on the $\partial^2 \tilde{\varphi}$ -term³³ to show that the effective action $\Gamma_0[\tilde{\varphi}]$ coincides with the classical free action $S_0(\varphi) = \int \mathcal{L}_0(\varphi)$.

At this point notice, that we had to execute the path-integral $\int D\varphi$ in Eq. (95) with the classical action $S_0(\varphi)$ figuring in the integrand, to obtain $\Gamma_0[\tilde{\varphi}] = S_0(\tilde{\varphi})$. In the interacting case $\Gamma[\tilde{\varphi}]$ is very different from the interacting classical action $S(\varphi) = \int \mathcal{L}(\varphi)$!

Exercise 3.8(The effective potential)

Let us compute the first order quantum correction to the classical action[11, 13, 18]. For this purpose we expand around the classical saddle point Eq. (149), where $\phi(x)|_{saddle\ point} = \phi_0$. The saddle-point equation is

$$\frac{\delta(S[\phi] + \int J\phi)}{\delta\phi} \Big|_{\phi=\phi_0} = 0 \tag{171}$$

or

$$\frac{\delta S[\phi]}{\delta\phi(x)} \Big|_{\phi=\phi_0} = -J(x), \tag{172}$$

which expresses ϕ_0 as a functional of $J \rightarrow \phi_0[J]$. Expanding about the saddle-point, we have up to second order

$$S[\phi] = S[\phi_0] - \int d^4x J(x)\Delta_\phi(x) + \frac{1}{2} \int d^4x d^4y \Delta_\phi(x) A \Delta_\phi(y) \tag{173}$$

with $\Delta_\phi = \phi - \phi_0$ and the expansion coefficient A is a functional of ϕ_0 :

$$A[\phi] = \frac{\delta^2 S[\phi]}{\delta\phi(x)\delta\phi(y)} \Big|_{\phi=\phi_0}. \tag{174}$$

To simplify notation write this as

$$S[\phi] = S[\phi_0] - (J, \Delta_\phi) + \frac{1}{2}(\Delta_\phi, A\Delta_\phi). \tag{175}$$

Eq. (156) tells us to compute

$$Z[J] = \int D\phi e^{i(S[\phi] + (J, \phi))} = e^{iW[J]}. \tag{176}$$

We perform this in the Euclidean version

$$Z_E[J] = \int D\phi e^{-(S_E[\phi] + (J, \phi))} = e^{-W_E[J]}, \tag{177}$$

where $(,)$ are now Euclidean integrals. Shifting ϕ to $\phi + \phi_0$, we have

$$Z_E[J] = \int D\phi e^{-(S_E[\phi_0] + (J, \phi_0) + \frac{1}{2}(\phi, A\phi))} = e^{-S_E[\phi_0] - (J, \phi_0)} \int D\phi e^{-\frac{1}{2}(\phi, A\phi)} \tag{178}$$

³³ See the comments after Eq. (97).

Integrate over ϕ , to get

$$W_E[J] = S_E[\phi_0] + (J, \phi_0) + \frac{1}{2} \log \det A. \tag{179}$$

The corresponding effective action is

$$\Gamma_E[\tilde{\phi}] = W_E[J] - (J, \tilde{\phi}) = S_E[\phi_0] + (J, (\phi_0 - \tilde{\phi})) + \frac{1}{2} \log \det A. \tag{180}$$

We still have to trade J for $\tilde{\phi}_0$. This means solving the implicit Eq. (172) and Eq. (159). Fortunately it is only necessary to expand S_E to first order to get with Eq. (172)

$$S_E[\tilde{\phi}] = S_E[\phi_0] + \int (\tilde{\phi} - \phi_0) \frac{\delta S_E}{\delta\phi} \Big|_{\phi=\phi_0} = S_E[\phi_0] - \int (\tilde{\phi} - \phi_0) J.$$

Therefore we find the effective action including a first order quantum correction as

$$\Gamma_E[\tilde{\phi}] = S_E[\tilde{\phi}] + \frac{1}{2} \log \det A[\tilde{\phi}]. \tag{181}$$

Reinstating the factors of \hbar , convince yourself that the additional term is first order in \hbar .

To get some feeling for this formula, we compute the effective potential V_{eff} , which is the effective action $\Gamma[\phi]$ computed for constant ϕ . Since $\Gamma[\phi]$ is an extensive quantity, we also will extract the space-time volume Ω to obtain an intensive quantity for V_{eff} . Computing in Euclidean space we get for the action

$$S_E[\phi] = \int d^4x \left[\frac{1}{2}(\partial\phi)^2 + V(\phi) \right] \tag{182}$$

and expand it to second order in η with $\tilde{\phi} = v + \eta(x)$ and v constant. After a partial integration we get

$$S_E[\phi] = \int d^4x \left[\frac{1}{2}(\partial\eta)^2 + V(v) + \eta V'(v) + \frac{1}{2}\eta^2 V''(v) \right] = \Omega V(v) + \int d^4x \times \left\{ \eta V'(v) + \frac{1}{2}\eta [-\partial^2 + V''(v)]\eta \right\}. \tag{183}$$

Eq. (172) and Eq. (174) now yield at the saddle-point $\phi = v$

$$V'(v) = -J$$

$$A[x, y] = [-\partial^2 + V''(v)]\delta^{(4)}(x - y). \tag{184}$$

Thus integrating over η , we obtain from Eq. (179)

$$W_E[J] = \Omega V(v) + (J, v) + \frac{1}{2} Tr \log A[v].$$

In Fourier space the trace is

$$Tr \log A[\tilde{\phi}] = \Omega \int \frac{d^4 k}{(2\pi)^4} \log[k^2 + V''(v)]. \quad (185)$$

Now expand the effective action in powers of momentum around a constant $\phi = v$ as

$$\Gamma[\phi] \equiv \int d^4 x \left[V_{eff}(v) + \frac{1}{2}(\partial\phi)^2 Z(v) + \dots \right], \quad (186)$$

where V_{eff} is now a function of v , not a functional.

Thus we finally get from Eq. (181)

$$V_{eff}(v) = V(v) + \frac{1}{2} \int \frac{d^4 k}{(2\pi)^4} \log[k^2 + V''(v)]. \quad (187)$$

This integral is ultraviolet divergent for large k . Integrating up to a cut off at Λ , one obtains neglecting an irrelevant constant

$$V_{eff}(v) = V(v) + \frac{\Lambda^2}{32\pi^2} V''(v) + \frac{(V''(v))^2}{64\pi^2} \left(\log \frac{(V''(v))^2}{\Lambda^2} - \frac{1}{2} \right). \quad (188)$$

If we choose for the potential the expression

$$V(\phi) = \frac{\lambda}{4!} \phi(x)^4 \quad (189)$$

our model is renormalizable,³⁴ allowing us to obtain a cut-off independent result. It has the symmetry

$$\phi(x) \rightarrow -\phi(x). \quad (190)$$

After the dust of the renormalization has settled, we are left with the following effective potential

$$V_{eff}(v) = \frac{\lambda}{4!} v^4 + (a_1 \lambda^2 + a_2) v^4 \left(\log \frac{v^2}{M^2} - a_3 \right), \quad (191)$$

where $a_i, i = 1, 2, 3$ are numerical constants. Notice that the action $S_E[\phi]$ does not contain any dimensional parameter. Yet in order to obtain a non-trivial result when implementing the renormalization, one is obliged to introduce a mass-parameter M in order to avoid infrared divergencies at $k = 0$.

Although $V(\phi)$ has a minimum at $\phi = 0$, $V_{eff}(v)$ has a maximum there and two minima at $\pm v_{min}$

$$\frac{\partial \Gamma[v]}{\partial v} \Big|_{v_{min}} = \frac{\partial V[v]}{\partial v} \Big|_{v_{min}} = 0, v_{min}^2 > 0. \quad (192)$$

In accordance with Eq. (163), the quantum corrections induce the **spontaneous breaking** of the symmetry Eq. (190) in the limit³⁵ $\Omega \rightarrow \infty$ – see sect. 6 explaining this concept.

³⁴ See the comments after Eq. (146).

³⁵ For finite Ω the two states centered at $\pm v_{min}$ would overlap, creating either a symmetric or an anti-symmetric state. For infinite Ω the overlap vanishes exponentially and we have to choose either $+v_{min}$ or $-v_{min}$ with identical physics.

4. Path Integrals in Quantum Mechanics

We now rewrite the usual formulation of non-relativistic Quantum Mechanics in terms of path-integrals. Although this is just a special 1-dimensional case of sect. 3.3, it is instructive, because we start from scratch and obtain the path-integral formulation also for the interacting case.

Consider the hamiltonian

$$H = \frac{1}{2m} P^2 + V(Q) \quad (193)$$

with

$$[Q, P] = i\hbar. \quad (194)$$

Time evolution is given by

$$\langle b(t')|a(t) \rangle = \langle b|e^{-iH(t'-t)/\hbar}|a \rangle \quad (195)$$

Using the usual *non-normalizable* states, we have

$$Q|q \rangle = q|q \rangle, P|p \rangle = p|p \rangle, \quad (196)$$

$$\langle q'|q \rangle = \delta(q' - q), \langle p'|p \rangle = \delta(p' - p) \quad (197)$$

$$\langle q|p \rangle = \langle p|q \rangle^* = \frac{e^{ipq}}{\sqrt{2\pi}} \quad (198)$$

$$\langle q|P|p \rangle = p\langle q|p \rangle = \frac{1}{i} \frac{\partial}{\partial q} \langle q|p \rangle. \quad (199)$$

The completeness relation is

$$\mathcal{I} = \int_{-\infty}^{\infty} dq |q \rangle \langle q|. \quad (200)$$

We have in the Heisenberg representation

$$q_{\mathcal{H}}(t)|q, t \rangle = e^{tH/\hbar} q e^{-tH/\hbar} e^{tH/\hbar} |q \rangle = q|q, t \rangle. \quad (201)$$

For a time-dependent Hamiltonian the Heisenberg operators $q_{\mathcal{H}}(t_1)$ and $q_{\mathcal{H}}(t_2)$ do in general not commute for $t_1 \neq t_2$. Therefore, if we want to use completeness for different times, we have to choose a different basis $|q, t \rangle$ for each t in which $q(t)$ is diagonal.

Use the unitary time evolution operator $U(t_I, t_F)$ to propagate the wave function as

$$\psi(t_F) = U(t_F, t_I) \psi(t_I). \quad (202)$$

Therefore $U(t_F, t_I)$ has to satisfy the Schrödinger equation

$$i\hbar \frac{\partial U(t_F, t_I)}{\partial t_F} = H(t_F) U(t_F, t_I) \quad (203)$$

with the initial condition $U(t_I, t_I) = \mathcal{I}$. For a time-independent Hamiltonian H the evolution operator $U(t_I, t_I)$ is given by

$$U(t_F, t_I) = e^{-i/\hbar(t_F-t_I)H}, \quad (204)$$

whereas for a time-dependent Hamiltonian it is expressed in terms of the time-ordered exponential as

$$U(t_F, t_I) = T e^{-i/\hbar \int_{t_I}^{t_F} dt' H(t')} \quad (205)$$

We can decompose the time-evolution into steps due to

$$U(t_F, t_I) = U(t_F, t)U(t, t_I), \text{ for } t_F > t > t_I. \quad (206)$$

The matrix elements

$$K(q_F, q_I; t_F - t_I) \equiv \langle q_F | U(t_F, t_I) | q_I \rangle \equiv \langle q_F, t_F | q_I, t_I \rangle \quad (207)$$

are called the *kernel*. We will compute it in the position-space representation in order to express it in terms of Path-integrals. Use Eq. (206) to evolve from t_I to t_F in N consecutive steps (for notational simplicity only for the time-independent case)

$$\begin{aligned} K(q_F, q_I; t_F - t_I) \\ = \langle q_F | U(t_F, t_{N-1}) U(t_{N-1}, t_{N-2}) \dots U(t_1, t_I) | q_I \rangle. \end{aligned} \quad (208)$$

Insert the identity Eq. (200) N times splitting our time interval into N small intervals $\Delta t = (t_F - t_I)/N$ to get

$$K(q_F, q_I; t_F - t_I) = \prod_{i=1}^{N-1} \int_{-\infty}^{\infty} dq_i \prod_{i=0}^{N-1} K(q_{i+1}, q_i; \Delta t) \quad (209)$$

with $t_0 = t_I, t_N = t_F$ and we do not integrate over $q_0 = q_I$ and $q_N = q_F$! Now compute the kernel for a small time step (with $\hbar = 1$)

$$K(q_{i+1}, q_i; \Delta t) = \langle q_{i+1} | e^{-iH\Delta t} | q_i \rangle \quad (210)$$

with

$$K(q_{i+1}, q_i; \Delta t) \rightarrow \delta(q_{i+1} - q_i) \text{ for } \Delta t \rightarrow 0.$$

Although q does not commute with p , for small Δt we may ignore³⁶ this and write

$$e^{-iH\Delta t} = e^{-i\frac{p^2}{2m}\Delta t} e^{-iV(q)\Delta t} \quad (211)$$

Therefore

$$\begin{aligned} \langle q_{i+1} | e^{-iH\Delta t} | q_i \rangle &= \langle q_{i+1} | e^{-i\frac{p^2}{2m}\Delta t} e^{-iV(q)\Delta t} | q_i \rangle \\ &= \langle q_{i+1} | e^{-i\frac{p^2}{2m}\Delta t} | q_i \rangle e^{-iV(q_i)\Delta t} \\ &= \int dp_i \langle q_{i+1} | p_i \rangle e^{-i\frac{p_i^2}{2m}\Delta t} \langle p_i | q_i \rangle e^{-iV(q_i)\Delta t} \\ &= \frac{1}{2\pi} \int dp_i e^{ip_i(q_{i+1}-q_i)-i\Delta t[\frac{p_i^2}{2m}+V(q_i)]}. \end{aligned} \quad (212)$$

³⁶ The commutant of the kinetic and potential energy is of order $\mathcal{O}(e^2)$. If this were untrue, and if $[H(t), H(t')] \neq 0$ we would have to use the Baker-Hausdorff formula – see [5], section 10.2.5 and Wikipedia.

Here we chose to replace $\langle q_{i+1} | e^{-iV(q)\Delta t} | q_i \rangle$ by $e^{-iV(q=q_i)\Delta t}$. For eventual problems with this choice see [5], section 4.

Performing the p -integrals, we get

$$\begin{aligned} \frac{1}{2\pi} \int dp_i e^{ip_i(q_{i+1}-q_i)-i(\frac{p_i^2}{2m})\Delta t} \\ = \left(\frac{m}{2\pi i \Delta t} \right)^{1/2} e^{im(q_{i+1}-q_i)^2/(2\Delta t)}. \end{aligned} \quad (213)$$

Therefore the small time-step kernel is

$$\begin{aligned} K(q_{i+1}, q_i; \Delta t) &= \left(\frac{m}{2\pi i \Delta t} \right)^{1/2} \\ &\times \exp\left(i\frac{m}{2} \frac{(q_{i+1}-q_i)^2}{\Delta t} - i\Delta t V(q_i) \right) \end{aligned} \quad (214)$$

For $q_{i+1} = q(t+\Delta t), q_i = q(t)$ and $\Delta t \sim 0$ we manipulate as³⁷ Thus

$$\begin{aligned} \frac{m}{2} \frac{(q(t+\Delta t) - q(t))^2}{\Delta t} &= \frac{m}{2} \left(\frac{q(t+\Delta t) - q(t)}{\Delta t} \right)^2 \Delta t \\ &= \frac{m}{2} \int_t^{t+\Delta t} dt \dot{q}^2. \end{aligned} \quad (215)$$

Therefore we get

$$\frac{m}{2} \frac{(q(t+\Delta t) - q(t))^2}{\Delta t} - \Delta t V(q_1) = \int_t^{t+\Delta t} dt L(q, \dot{q}), \quad (216)$$

where the systems Lagrangian is

$$L(q, \dot{q}) = \frac{1}{2} m \dot{q}^2 - V(q). \quad (217)$$

This yields

$$\langle q(t+\Delta t) | q(t) \rangle = \left(\frac{m}{2\pi i \Delta t} \right)^{1/2} e^{i \int_t^{t+\Delta t} dt L(q, \dot{q})}. \quad (218)$$

Inserting this into Eq. (209) (now with \hbar inserted),

$$\begin{aligned} \langle q_F, t_F | q_I, t_I \rangle \\ &= K(q_F, q_I; t_F - t_I) \\ &= \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi i \hbar \Delta t} \right)^{N/2} \\ &\times \left[\prod_{k=1}^{N-1} \int_{-\infty}^{\infty} dq_k \right] e^{i \int_{t_I}^{t_F} dt L(q, \dot{q})}. \end{aligned} \quad (219)$$

With the notation

$$\lim_{N \rightarrow \infty} \left[\prod_{k=1}^{N-1} \int_{-\infty}^{\infty} dq_k \right] = \int_{q(t_I)}^{q(t_F)} D[q(t)] = \int Dq, \quad (220)$$

³⁷ Regarding the differentiability of $q(t)$, refer to the discussion at Eq. (68) of the Wiener process. Thus our manipulations are formal, but we know how to compute before the limit $N \rightarrow \infty$.

we have

$$\langle q_F, t_F | q_I, t_I \rangle = \int_{q(t_I)}^{q(t_F)} D[q(t)] e^{i/\hbar \int dt L(q, \dot{q})} = \int Dq e^{iS/\hbar}, \tag{221}$$

with the action

$$S = \int_{t_I}^{t_F} L(q, \dot{q}) dt. \tag{222}$$

This equation is the one-dimensional version of Eq. (141) with $J = 0$.

Although we have shown Eq. (221) to be true for a non-relativistic one-body Hamiltonian with a potential $V(q)$, Eq. (221) does not make any reference to this particular form and it is in fact true generally.

We can also leave the p -integrals undone³⁸ in Eq. (213) and write

$$\langle q_F, t_F | q_I, t_I \rangle = \lim_{N \rightarrow \infty} \left[\prod_{k=1}^{N-1} \int_{-\infty}^{\infty} dq_k \right] \left[\prod_{k=1}^{N-1} \int_{-\infty}^{\infty} dp_k \right] e^{i/\hbar \int dt (p(t)\dot{q}(t) - H(p(t), q(t)))}.$$

or

$$\langle q_F, t_F | q_I, t_I \rangle = \int_{q(t_I)}^{q(t_F)} D[q(t)] \int \frac{D[p(t)]}{2\pi\hbar} \times e^{i/\hbar \int_{t_I}^{t_F} dt [p(t)\dot{q}(t) - H(p(t), q(t))]} \tag{223}$$

This formulation is called the *phase space integral*, since the integration measure is the Liouville measure $D[q(t)]D[p(t)]$.

In our computation it was necessary that $t_F > t_I$, so that we could use the kernel-decomposition property Eq. (206) in Eq. (208). Suppose, we want to compute the expectation value of two operators, e.g. $\hat{q}(t_1), \hat{q}(t_2)$. In their path-integral computation we would necessarily have to insert $q(t_1), q(t_2)$ in their correct Δt -interval, the later operator to the left and the earlier to the right. Therefore the path-integral

$$\int Dq q(t_1)q(t_2) e^{iS/\hbar}$$

always represents the expectation value of the **time-ordered** operators

$$\int Dq q(t_1)q(t_2) e^{iS/\hbar} = \langle q_F, t_F | T \hat{q}(t_1) \hat{q}(t_2) | q_I, t_I \rangle.$$

One outstanding property of the path integral representation Eq. (221) is the ease in obtaining **the classical**

limit, which means taking $\hbar \rightarrow 0$. For small \hbar the exponent fluctuates wildly and the integrals will vanish, unless the action S assumes its minimum, implying

$$\delta S[q(t), \dot{q}(t)] / \delta q = 0, \tag{224}$$

which yields the classical equations of motion, to be compared with the exact equation (152).

We quote several relevant properties of K

1. The kernel $K(q_F, q_I, t_F - t_I)$ satisfies the Schrödinger equation

$$[i\hbar \partial_{t_F} - H(q_F, p_F)] K(q_F, q_I, t_F - t_I) = 0. \tag{225}$$

2. We can expand the kernel using energy eigenstates $\psi_n(x) \equiv \langle x | n \rangle$

$$\begin{aligned} K(q_F, q_I, t_F - t_I) &= \langle q_F | e^{-i(t_F - t_I)H} | q_I \rangle \\ &= \sum_n \langle q_F | e^{-i(t_F - t_I)H} | n \rangle \langle n | q_I \rangle \\ &= \sum_n e^{-i(t_F - t_I)E_n} \psi_n^*(q_F) \psi_n(q_I) \end{aligned} \tag{226}$$

3. The *kernel* is also called *propagator*, since it propagates the system from t_I to t_F . We can construct the *retarded* propagator as

$$K_R(q_F, q_I; t_F - t_I) = \theta(t_F - t_I) K(q_F, q_I; t_F - t_I) \tag{227}$$

where $\theta(t) = 1$ for $t > 0$ and zero elsewhere. Since $d\theta(x)/dx = \delta(x)$, the retarded propagator satisfies

$$\begin{aligned} [i\hbar \partial_{t_F} - H(q_F, p_F)] K_R(q_F, q_I; t_F - t_I) \\ = i\hbar \delta(t_F - t_I) \delta(q_F - q_I), \end{aligned} \tag{228}$$

i.e. the retarded propagator is the Green function of the Schrödinger equation.

Exercise 4.1

Obtain Eq. (205) for a time-dependent Hamiltonian. To show this rewrite Eq. (203) as an integral equation, using the identity

$$\begin{aligned} \int_{t_I}^t dt' \partial_{t'} U(t', t_I) &= U(t, t_I) - U(t_I, t_I) \\ &= -i/\hbar \int_{t_I}^t dt' H(t') U(t', t_I). \end{aligned}$$

Therefore

$$U(t, t_I) = 1 - i/\hbar \int_{t_I}^t dt' H(t') U(t', t_I).$$

³⁸ The first and last p -integrals are different, but we have not indicated this.

Now we iterate this as

$$\begin{aligned}
 U(t, t_I) &= 1 - \imath/\hbar \int_{t_I}^t dt' H(t') \\
 &\quad \times \left(1 - \imath/\hbar \int_{t_I}^{t'} dt'' H(t'') U(t', t_I) \right) + \dots \\
 &= 1 + (-\imath/\hbar) \int_{t_I}^t dt' H(t') \\
 &\quad + (-\imath/\hbar)^2 \int_{t_I}^t dt' \int_{t_I}^{t'} dt'' H(t') H(t'') + \dots
 \end{aligned}$$

We express the integrands in terms of the *time-ordered products* defined as

$$\begin{aligned}
 T[H(t_1)H(t_2) \dots H(t_n)] \\
 \equiv \theta(t_1 - t_2)\theta(t_2 - t_3) \dots \theta(t_{n-1} - t_n) \\
 \quad H(t_1)H(t_2) \dots H(t_n) \\
 + n! \text{ permutations.}
 \end{aligned}$$

Show that

$$\begin{aligned}
 \frac{1}{2} \int_{t_I}^t dt_1 \int_{t_I}^{t_1} dt_2 T[H(t_1)H(t_2)] \\
 = \int_{t_I}^t dt_1 \int_{t_I}^{t_1} dt_2 H(t_2)H(t_1)
 \end{aligned}$$

Therefore

$$\begin{aligned}
 U(t, t_I) &= 1 + (-\imath/\hbar) \int_{t_I}^t dt_1 T[H(t_1)] \\
 &\quad + \frac{(-\imath/\hbar)^2}{2!} \int_{t_I}^t dt_1 \int_{t_I}^{t_1} dt_2 T[H(t_1)H(t_2)] + \dots
 \end{aligned}$$

Going on like this get Eq. (205).

Exercise 4.2

Obtain the kernel for the free particle with $H = \frac{p^2}{2m}$

$$K_0(q_F, q_I, t_F - t_I) = \sqrt{\frac{m}{2\pi\imath\hbar(t_F - t_I)}} e^{\frac{\imath}{\hbar} \frac{m(q_F - q_I)^2}{2(t_F - t_I)}}, \tag{229}$$

using its path-integral representation Eq. (221). This can also easily be obtained directly as

$$\begin{aligned}
 K_0(q_F, q_I, t_I - t_I) &= \langle q_f | e^{-\imath H(t_F - t_I)/\hbar} | q_I \rangle \\
 &= \langle q_f | \int \frac{dp}{2\pi} e^{-\imath H(t_F - t_I)/\hbar} | p \rangle \langle p | q_I \rangle \\
 &= \int \frac{dp}{2\pi} e^{-\imath [\frac{p^2}{2m}](t_F - t_I)/\hbar} \langle q_f | p \rangle \langle p | q_I \rangle \\
 &= \int \frac{dp}{2\pi} e^{-\imath [\frac{p^2}{2m}](t_F - t_I)/\hbar + \imath (q_F - q_I)p/\hbar}.
 \end{aligned}$$

Performing this Gaussian integral yields Eq. (229).

Exercise 4.3

Show that the kernel for the harmonic oscillator with action

$$S_h[q] = \frac{m}{2} \int_{t_I}^{t_F} dt [\dot{q}(t)^2 - \omega_h^2 q(t)^2] \tag{230}$$

is given by

$$K_h(q_F, q_I, T = t_I - t_I) = \sqrt{\frac{m\omega_h}{2\pi\imath\hbar \sin \omega_h T}} e^{\imath S_h[q_c(T)]/\hbar}, \tag{231}$$

where q_c is the classical path and

$$S_h[q_c(T)] = \frac{m\omega_h}{2 \sin \omega_h T} [(q_F^2 + q_I^2) \cos \omega_h T - 2q_F q_I]. \tag{232}$$

For details see e.g. [1], Problem 3-8.

5. Statistical Mechanics in Terms of Path Integrals

The statistical partition function is

$$Z(\beta) = \sum_n e^{-\beta E_n} \equiv Tr e^{-\beta H}, \quad \beta = \frac{1}{k_B T}. \tag{233}$$

For systems to be in thermal equilibrium, the Hamiltonian has to be time-independent. This looks like the quantum mechanical $Tr U(t_F - t_I)$ of Sect. 4, after replacing β by $\imath(t_F - t_I)/\hbar$. We will therefore use the quantum-mechanical path-integral formulation for $U(t_F - t_I)$ and after that introduce a fictitious *time* variable τ to label our paths.

To start with write

$$\tilde{Z}(t_F - t_I) \equiv Tr e^{-\frac{\imath}{\hbar}(t_F - t_I)H} \tag{234}$$

in terms of the position-representation using Eq. (226). The trace operation becomes an integral over $|x\rangle$ states with $x_F = x_I = x$, i.e. we do not integrate over all paths, but only over all closed loops coming back to x and then integrate over x

$$\begin{aligned}
 \tilde{Z}(t_F - t_I) &= \int_{-\infty}^{\infty} dx \langle x | U(t_F, t_I) | x \rangle \\
 &= \int_{-\infty}^{\infty} dx K(x, x, t_F - t_I).
 \end{aligned} \tag{235}$$

Using Eq. (219) with $x(t_F) = x(t_I)$, i.e. **periodic boundary conditions** and the product now running up to $k = N$, we get

$$\begin{aligned}
 \tilde{Z}(t_F - t_I) &= \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi\imath\hbar\Delta t} \right)^{N/2} \\
 &\quad \times \left[\prod_{k=0}^N \int_{-\infty}^{\infty} dq_k \right] e^{(\imath/\hbar) \int_t^{t+\Delta t} dt L(x, \dot{x})} \\
 &= \int_{-\infty}^{\infty} dx \int_{x(t_I)=x}^{x(t_F)=x} D[x(t)] e^{\imath/\hbar S[x(t)]}
 \end{aligned}$$

or

$$\tilde{Z}(t_F - t_I) = \int_{pbc} D[x(t)] e^{i/\hbar S[x(t)]}. \tag{236}$$

We now set $t_I = 0$ and $t_F = i\hbar\beta$ and $t = -i\tau$. The exponent becomes for a particle subject to a potential

$$\begin{aligned} iS[x(t)] &= i \int dt \left[\frac{m}{2} \left(\frac{dx}{dt} \right)^2 - V(x) \right] \\ &= - \int_0^{\hbar\beta} d\tau \left[\frac{m}{2} \left(\frac{dx}{d\tau} \right)^2 + V(x) \right] \end{aligned}$$

with the Euclidean Lagrangian

$$L_E[x] \equiv \frac{m}{2} \left(\frac{dx}{d\tau} \right)^2 + V(x). \tag{237}$$

In terms of the Euclidean Lagrangian density in four dimensions as in Eq. (96), we get

$$Z(\beta) = \int_{pbc} D\varphi e^{-\int_0^{\hbar\beta} d\tau \int d^3x \mathcal{L}_E(\varphi, \partial\varphi)}. \tag{238}$$

The imposition of periodic boundary conditions imposes a constraint on the Fourier transforms $g(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \tilde{g}(\omega) e^{-i\omega t}$. Requiring $g(t) = g(t + \beta)$ implies $e^{i\omega\beta} = 1$ or

$$\omega_n = \frac{2\pi n}{\beta} \quad (\text{bosons}) \tag{239}$$

for integer n . The integral becomes a *Matsubara* sum

$$\int \frac{d\omega}{2\pi} \tilde{g}(\omega) \rightarrow \frac{1}{\beta} \sum_{n=-\infty}^{\infty} \tilde{g}(\omega_n). \tag{240}$$

5.1. Fermions

For fermionic fields we have to impose **anti-periodic** boundary conditions. We therefore need to set $e^{i\omega\beta} = -1$ or

$$\omega_n = \frac{(2n + 1)\pi}{\beta}, \quad (\text{fermions}). \tag{241}$$

To get this tricky point clear, we will look at a **one-dimensional fermionic oscillator**. We will compute the trace e^{-iHt} using elementary quantum mechanics and path-integrals to compare the results. But first we have to learn how to integrate over fermionic variables!

5.1.1. Fermionic integrals

We need a fermionic path-integral formalism analogous to the bosonic case. Since we don't have the least idea how to get this, we proceed the following way.

For a quadratic Lagrangian we know how to perform the path-integral. We will therefore invent integration rules, which for the known free quadratic case give the

same results as OQFT. Then we will use these rules for interacting Lagrangians, guaranteeing that they give the OQFT results in perturbation theory. We may of course then use our path-integral formalism to obtain non-perturbative results.

Consider real-valued quantities obeying the following anti-commutation rules

$$\{\theta_i, \theta_j\} = 0 \rightarrow \theta_i^2 = 0, \quad i, j = 1, 2, \dots, N. \tag{242}$$

Thus any function of one variable is at most linear in θ

$$g(\theta) = g_0 + g_1\theta \tag{243}$$

and for two variables

$$g(\theta_1\theta_2) = g_0 + g_1\theta + g_2\theta_2 + g_{12}\theta_1\theta_2.$$

E.g. for the exponential we have

$$e^{A\theta_1\theta_2} = 1 + A\theta_1\theta_2.$$

The variables θ_i are called **Grassmann fermions**.

Define differentiation and integration rules as

$$\frac{d}{d\theta_i} \theta_j = \delta_{ij}, \quad \int d\theta_i = 0, \quad \int \theta_j d\theta_i = \delta_{i,j}, \tag{244}$$

where $d\theta_i$ are also anti-commuting Grassmann variables, anti-commuting also with θ_j . Although differentiation and integration rules are the same³⁹, therefore redundant, having both is still convenient in order to maintain similarity to the bosonic calculations. We will go on and use most of the usual calculus rules without proving them.

The only big difference will be the rule for changing variables⁴⁰. In fact we have with Eq. (243)

$$\int g(\theta) d\theta = g_1$$

and for a real number a using linearity

$$g(a\theta) = g_0 + ag_1\theta.$$

Therefore $\int g(a\theta) d\theta = \int (g_0 + ag_1\theta) d\theta = ag_1 = a \int g(\theta) d\theta$ i.e.

$$\int g(a\theta) d\theta = a \int g(\theta) d\theta. \tag{245}$$

For the bosonic case we would have instead

$$\int f(ax) dx = \frac{1}{a} \int f(x) dx.$$

The ubiquitous determinant also moves to the numerator. Consider a real, positive definite matrix $A_{i,j}$

³⁹ It necessarily follows, that there is no geometric interpretation for $\int d\theta$ and no integration limits etc.

⁴⁰ The Jacobian in a transformation of variables also changes place.

composed of four sets of all anti-commuting variables $\theta_i, \theta_j^*, \eta_i, \eta_i^*$ with $i, j = 1, 2, \dots, M$ and the quadratic form

$$Q(\theta, \theta^*) \equiv \sum_{[i,j]=1}^M \theta_i^* A_{i,j} \theta_j - \sum_{i=1}^M \eta_i^* \theta_i - \sum_{i=1}^M \theta_i^* \eta_i$$

$$\equiv Q(\theta, \theta^*) = \theta^* A \theta - \eta^* \theta - \theta^* \eta, \quad (246)$$

where the $*$ just distinguishes different independent anti-commuting sets.

Notice that

$$\frac{\partial e^Q}{\partial \theta_i} = -\theta_i e^Q, \quad \frac{\partial e^Q}{\partial \theta_i^*} = +\theta_i^* e^Q.$$

With the convention

$$\int [D\theta D\theta^*] \theta_1^* \theta_1 \theta_2^* \theta_2 \dots \theta_M^* \theta_M = +1, \quad (247)$$

where $D\theta D\theta^* = d\theta_1 d\theta_1^* d\theta_2 d\theta_2^* \dots d\theta_M d\theta_M^*$, we have the following identity

$$I_F = \int D\theta D\theta^* e^{Q(\theta, \theta^*)} = \det A e^{-\eta^* A^{-1} \eta}. \quad (248)$$

This can be shown with some combinatorics. To compute

$$I_F = \int [D\theta D\theta^*] e^{\sum_{[i,j]=1}^M \theta_i^* A_{i,j} \theta_j}$$

for the case $\eta = 0, \eta^* = 0$, we go to the diagonal representation of A

$$I_F = \int [D\theta D\theta^*] e^{\sum_{i=1}^M \theta_i^* a_i \theta_i}.$$

Expand the exponential and notice that one factor of θ, θ^* is needed for each $d\theta, d\theta^*$ to get a non vanishing result after integration. Thus only the term

$$a_1 \theta_1^* \theta_1 a_2 \theta_2^* \theta_2 \dots a_M \theta_M^* \theta_M$$

survives in the integral. But there are $M!$ ways to obtain this term and all have the same sign, since the pair $\theta_i^* \theta_i$ commutes with all other pairs. Thus we get⁴¹ with Eq. (247)

$$I_F = \int [D\theta D\theta^*] e^{\sum_{[i,j]=1}^M \theta_i^* A_{i,j} \theta_j} = \prod_{i=1}^M a_i = \det A.$$

For η, η^* nonzero we complete the square as in the bosonic case.

We will generate correlation functions applying $\partial/\partial\eta_i$ as in the bosonic case.

⁴¹ Had we integrated only over $\int d\theta$ with an anti-symmetric matrix A – therefore with purely imaginary eigenvalues – and an even number of variables, the result would be the Pfaffian of A with $\text{Pf}(A) = \sqrt{\det A}$.

Exercise 5.1

Show that the definition of the integral as $\int d\theta = 0$ is required by shift invariance, which we of course want to maintain. For this purpose consider $g(\theta) = g_0 + g_1 \theta$ and compute $\int g(\theta + \eta) d\theta$, assuming $\int \theta d\theta = 1$. Invoke linearity to conclude that $\int g(\theta) d\theta = \int g(\theta + \eta) d\theta$ requires $(f_1 \eta) \int d\theta = 0$.

Exercise 5.2

Show that the Jacobian’s position is inverted, when compared to the bosonic case.

5.1.2. The fermionic harmonic oscillator

To compute path-integrals we need the classical description of the oscillator for a fermionic field $\psi(t)$. Define its Lagrangian density to be

$$\mathcal{L}(\psi, \psi^*) = \psi^* i \partial_t \psi - \omega \psi^* \psi, \quad (249)$$

where ω is some constant parameter and we set $\hbar = 1$. Here ψ and ψ^* are independent fields. This Lagrangian is the one-dimensional version of the relativistic 3-dimensional Dirac Lagrangian, see e.g. \rightsquigarrow [12], chapter 3.

Since $\mathcal{L}(\psi, \psi^*)$ is independent of $\partial_t \psi^*$, the equation motion for ψ reduces to $\frac{\partial \mathcal{L}}{\partial \psi^*} = 0$, i.e.

$$i \partial_t \psi - \omega \psi = 0 \quad \rightarrow \quad \psi(t) = b e^{i\omega t}. \quad (250)$$

The equation of motion for ψ^* yields

$$\psi^*(t) = b^\dagger e^{-i\omega t}, \quad (251)$$

where the peculiar naming of the initial condition as b^\dagger for $\psi^*(t)$ foreshadows its role as creation operator. Here it is just another constant.

The momentum conjugate to ψ is $\pi_\psi = \partial \mathcal{L} / \partial \dot{\psi} = i \psi^*$ and we compute the Hamiltonian as

$$H_F = \pi_\psi \dot{\psi} - \mathcal{L} = \omega \psi^* \psi. \quad (252)$$

Now quantize this fermionic system. In accordance with Pauli’s principle b becomes an **anti-commuting** operator satisfying

$$\{b, b^\dagger\} = 1, \quad \{b, b\} = 0 \quad \{b^\dagger, b^\dagger\} = 0,$$

where now b^\dagger is the hermitian conjugate of b .

This one-dimensional fermionic system has only two eigenstates: the fermionic state being either empty or occupied

$$b|0\rangle = 0, \quad |1\rangle = b^\dagger|0\rangle.$$

We thus have a two-dimensional Hilbert space with Hamiltonian

$$H_F = \omega b^\dagger b + \text{constant},$$

where we used the equations of motion Eq. (250). Hermiticity of H_F correctly identifies b^\dagger as the hermitian conjugate of b . Due to possible operator ordering ambiguities, when going from the classical to the quantum hamiltonian, the energy levels are only given up to an arbitrary off-set. We set the *constant* so that

$$H_F = \omega(b^\dagger b - 1/2). \tag{253}$$

Compare H_F with the bosonic Hamiltonian $H_B = \omega(a^\dagger a + 1/2)$.

The two energy eigenvalues of H_F are

$$\epsilon_0 = \langle 0|H_F|0\rangle = -\omega/2, \quad \epsilon_1 = \langle 1|H_F|1\rangle = +\omega/2.$$

We now compute the **normalized trace** of $e^{-iH_F T}$ for some time variable T , summing over the two eigenvalues

$$\begin{aligned} \text{tr}[e^{-iH_F T}] &= \frac{\sum_{i=0}^1 e^{-i\epsilon_i T}}{Z} \\ &= \frac{e^{i\omega T/2} + e^{-i\omega T/2}}{2} = \cos \frac{\omega T}{2}, \end{aligned} \tag{254}$$

where the normalization factor $Z = 2$ has been chosen as to satisfy the normalization condition

$$\text{tr}[e^{-iH_F T}]_{\omega=0} = 1. \tag{255}$$

Now compute the same trace with the path-integral method. Use Eq. (236), integrating over the anti-commuting Grassmann variables ψ, ψ^* . The normalized trace with normalization factor \tilde{Z} is

$$\text{tr} e^{-iHT} = \frac{1}{\tilde{Z}} \int D\psi D\psi^* e^{i \int_0^T \mathcal{L} dt}$$

Inserting Eq. (249) we have

$$\begin{aligned} \text{tr} e^{-iHT} &= \frac{1}{\tilde{Z}} \int D\psi D\psi^* e^{i \int d\tau \psi^*(t) [i d_t - \omega] \psi(t)} \\ &= \frac{1}{\tilde{Z}} \det[i d/dt - \omega]. \end{aligned}$$

Adopting the same normalization Eq. (255) we get

$$\tilde{Z} = \det[i d/dt - \omega]_{\omega=0} = \det[i d/dt],$$

yielding

$$\text{tr} e^{-iHT} = \frac{\det[i d/dt - \omega]}{\det[i d/dt]} \equiv \frac{\det[D_\omega]}{\det[i d/dt]}. \tag{256}$$

We compute the determinants in momentum-space, where the operators are diagonal and the determinant is the product of the eigenvalues $e_n(\omega)$. Compute them solving the classical equations of motion to get a complete set of eigenfunctions

$$D_\omega f_n(t) \equiv [i d/dt - \omega] f_n(t) = e_n(\omega) f_n(t).$$

With the appropriate *anti-periodic* boundary conditions $f_n(t + T) = -f_n(t)$ the eigenvalues are

$$e_n(\omega) = -\frac{(2n + 1)\pi}{T} - \omega \equiv -\omega_n - \omega, \quad n = 0, \pm 1, \pm 2, \dots$$

This yields

$$\text{tr} e^{-iH(\omega)T} = \prod_{n=-\infty}^{\infty} \frac{e_n(\omega)}{e_n(0)} = \prod_{n=0}^{\infty} \left(1 - \frac{\omega^2}{\omega_n^2} \right).$$

The product is

$$\prod_{n=0}^{\infty} \left(1 - \frac{\omega^2 T^2}{(2n + 1)^2 \pi^2} \right) = \cos \frac{\omega T}{2}. \tag{257}$$

This agrees with the **fermionic partition function** Eq. (254)

$$Z_F(\omega) = \cos \frac{\omega T}{2}, \tag{258}$$

vindicating the use of **anti-periodic** boundary conditions. Although we used the proverbial slash-hammer to kill the fly Eq. (254), path-integrals prove to be extremely expedient in the field-theoretical case.

Remember that we had to use particular boundary conditions to write the path-integral in terms of the Lagrangian in Eq. (96). This is not necessary for fermionic Lagrangians linear in the derivatives, so that anti-periodic boundary conditions are no roadblock here.

Exercise 5.3

Repeat the computation of the trace for the bosonic oscillator.

Exercise 5.4

Show that **Matsubara-sums** may be evaluated as

$$\sum_n f(\omega_n) = \sum_{Res_f} f(-iz)g(z) \tag{259}$$

with

$$g(z) = \begin{cases} +\frac{\beta}{e^{\beta z} - 1} & \text{bosons} \\ -\frac{\beta}{e^{\beta z} + 1} & \text{fermions} \end{cases} \tag{260}$$

and Res_f instructs us to sum over the residues of the poles of $f(-iz)$. If $f(z)$ has cuts, we have to include the discontinuity across them.

For ω_n =fermionic and ω_m =bosonic show

$$\frac{1}{\beta} \sum_{n=-\infty}^{\infty} \frac{1}{i\omega_n - \epsilon} = \frac{1}{e^{\beta\epsilon} + 1},$$

$$\frac{1}{\beta} \sum_{m=-\infty}^{\infty} \frac{1}{i\omega_m - \epsilon} = -\frac{1}{e^{\beta\epsilon} - 1}$$

The bosonic sum has $\lim_{\epsilon \rightarrow 0} \rightarrow -\infty$, so we may use this limit to check the sign.

If you use the function $g(z) = -\frac{\pi}{2} \tanh(\frac{\pi z}{2})$ for fermions or $g(z) = \frac{\pi}{2} \coth(\frac{\pi z}{2})$ for bosons, do you get the same result?

Exercise 5.5

Show the following identities for fermions

$$\frac{1}{\beta} \sum_n \frac{1}{(i\omega_n - \epsilon_q)(i\omega_n + i\omega - \epsilon_{p+q})} = \frac{-n_F(\epsilon_q) - n_F(\epsilon_{q+p})}{i\omega + \epsilon_p - \epsilon_{q+p}} \tag{261}$$

and

$$\frac{1}{\beta} \sum_n \frac{1}{(i\omega_n - \epsilon_q)(i\omega_n - i\omega_m - \epsilon_{p-q})} = \frac{1 - n_F(\epsilon_q) - n_F(\epsilon_{p-q})}{i\omega + \epsilon_p - \epsilon_{p-q}},$$

using $n_F(-x) = 1 - n_F(x)$, $n_F(x + i\omega) = n_F(x)$.

Exercise 5.6

For ω_n =fermionic and ω_m =bosonic frequencies show

$$\frac{1}{\beta} \sum_n \frac{1}{(i\omega_n - \epsilon_q)(i\omega_n + i\omega_m - \epsilon_{q+p})} = \frac{n_F(\epsilon_q) - n_F(\epsilon_{q+p})}{i\omega_m - \epsilon_{q+p} + \epsilon_q} \tag{262}$$

6. Non-relativistic Electron Models

Let us consider non-relativistic electrons coupled by a 4-fermion interaction. This is one of the simplest models, yet sufficiently rich to contain extremely interesting physics, such as *spontaneous symmetry breaking*.

Since this model includes fermions, we will use two independent set of Grassmann variables: $\psi(x)$ and $\psi^*(x)$ with $x = [x_1, x_2, x_3, t]$. We append a binary variable to describe the electron’s spin $\psi_i^*(x), \psi_i(x), i = \pm$. We will integrate over ψ and ψ^* , indicating the measure as $D[\psi, \psi^*]$, using the results of Sect. (5.1.1), in particular Eq. (248). As usual path-integrals will be performed in their discrete version. A finite hyper-cube in \mathcal{R}^4 of length $L = N$, we will have N^4 space-time points with two variables at each point, yielding $M = 2 * N^4$ degrees of freedom in e.g. Eq. (248).

The total Lagrangian density is the sum of the free density⁴² and an additional 4-fermion interaction

$$\mathcal{L} = \sum_{i=\pm} \psi_i^*(i\partial_t + \frac{1}{2m} \nabla^2 + \mu) \psi_i + G \psi_+^* \psi_-^* \psi_- \psi_+ \tag{263}$$

where μ is the chemical potential and G is a coupling constant.

With one electron per site, a half-filled band, this interaction is the only **local** four-fermion interaction possible. Yet this simple model is rich enough to describe several important systems undergoing phase transitions. The free parameter G is a coupling constant with dimension $\sim m^{-2}$, supposed to encapsulate all physics, such as non-local effects due to some potential $V(\mathbf{r} - \mathbf{r}')$, which are swept under the rug by our simple 4-fermion interaction. Of course this model cannot describe situations, where particular properties of the Fermi-surface are important like high temperature superconductors, graphene etc.

The generating functional

$$Z = \int D[\psi, \psi^*] e^{\int d^4x \mathcal{L}} \tag{264}$$

with $d^4x = dt d^3x$. The generating functional is translationally and rotationally invariant, although in condensed matter physics we typically want to describe crystals. In crystals these symmetries are broken down to sub-symmetries and we have invariance only to subgroups, depending on the crystal’s symmetry. Since we will concentrate on phase transitions, these details are not relevant.

In the following sections we will manipulate this Lagrangian in several ways, each one exposing the feature we are looking for. In other words, we will find different minima of the generating functional above \rightsquigarrow [7], chapter 6. This of course means, that we know what we want to get: how to introduce additional fields $\mathbf{m}(x), \mathbf{\Delta}(x)$ to tame the 4-fermion interaction, morphing it to a bilinear form. This will allow us to exactly integrate over the fermions, leaving an action involving only these new fields $\mathbf{m}(x)$ and $\mathbf{\Delta}(x)$.

6.1. Ferromagnetism

We will rewrite the generating functional Eq. (264) to extract a model describing the ferromagnetic phase transition.

In order to describe spin, we need the three traceless Pauli matrices

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ +i & 0 \end{pmatrix}, \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{265}$$

satisfying the identity

$$\sigma_{ij}^\alpha \sigma_{kl}^\beta = \frac{\delta^{\alpha\beta}}{3} [2\delta_{il}\delta_{jk} - \delta_{ij}\delta_{kl}] + i\epsilon^{\alpha\beta\gamma} [\delta_{jk}\sigma_{il}^\gamma - \delta_{ik}\sigma_{jl}^\gamma] \tag{266}$$

with $\alpha, \beta = 1, 2, 3$ and $i, j, k, l = \pm$. In particular we set $\alpha = \beta$ and sum to get

$$\sigma_{ij} \cdot \sigma_{kl} = 2\delta_{il}\delta_{jk} - \delta_{ij}\delta_{kl}. \tag{267}$$

⁴² We will set $\hbar = 1$ in the following.

Use it to rewrite the 4-fermion interaction as⁴³

$$\psi_+^* \psi_-^* \psi_- \psi_+ = -2\mathbf{s}(x) \cdot \mathbf{s}(x) \tag{268}$$

with

$$\mathbf{s}(x) = \sum_{ij=\pm} \psi_i^* \boldsymbol{\sigma}_{ij} \psi_j. \tag{269}$$

The action becomes

$$\begin{aligned} S[\psi, \mathbf{s}] &= \int d^4x \mathcal{L} \\ &= \int d^4x \left(\sum_{i=\pm} \psi_i^* (\imath \partial_t + \frac{1}{2m} \nabla^2 + \mu) \psi_i \right. \\ &\quad \left. - 2G \mathbf{s}(x) \cdot \mathbf{s}(x) \right). \end{aligned} \tag{270}$$

Now linearize the $\mathbf{s}(x) \cdot \mathbf{s}(x)$ term introducing the field \mathbf{m} , called *magnetization*. The name is justified, since \mathbf{m} couples with the spin-density $\mathbf{s}(\mathbf{x})$ due to the term $\mathbf{m} \cdot \mathbf{s}$. In fact, with $g = \sqrt{G}$, use

$$\begin{aligned} &\int D[\mathbf{m}] e^{\imath \int d^4x (\mathbf{m}^2 - 2g\mathbf{m} \cdot \mathbf{s})} \\ &= \int D[\mathbf{m}] e^{\imath \int d^4x (\mathbf{m} - g\mathbf{s})^2} e^{-\imath \int d^4x G \mathbf{s}^2} \\ &= \left[\int D[\mathbf{m}'] e^{\imath \int d^4x \mathbf{m}'^2} \right] e^{-\imath G \int d^4x \mathbf{s} \cdot \mathbf{s}}. \end{aligned} \tag{271}$$

The integral over \mathbf{m}' yields the constant determinant \mathcal{N} and we get the identity

$$e^{-\imath G \int d^4x \mathbf{s}(x) \cdot \mathbf{s}(x)} = \frac{1}{\mathcal{N}} \int D[\mathbf{m}] e^{\imath \int d^4x (\mathbf{m}^2 - 2g\mathbf{m} \cdot \mathbf{s})}. \tag{272}$$

Using $\mathbf{m} \cdot \mathbf{s} = \mathbf{m} \cdot \psi_i^* \boldsymbol{\sigma}_{ij} \psi_j$, the generating functional becomes

$$\begin{aligned} Z_{\psi, \mathbf{m}} &= \frac{1}{\mathcal{N}} \int D[\psi, \psi^*] D[\mathbf{m}] \\ &\quad \times e^{\imath \int d^4x \left\{ \sum_{i,j} \psi_i^* \left[(\imath \partial_t + \frac{1}{2m} \nabla^2 + \mu) \delta_{ij} - 2g\mathbf{m} \cdot \boldsymbol{\sigma}_{ij} \right] \psi_j + \mathbf{m}^2 \right\}} \end{aligned} \tag{273}$$

Now use Eq. (248) to integrate over the bilinear fermions, to get

$$Z[\mathbf{m}] = \frac{1}{\mathcal{N}} \int D[\mathbf{m}] (\det \mathcal{O}[\mathbf{m}]) e^{\imath \int d^4x \mathbf{m}^2},$$

where

$$\mathcal{O}[\mathbf{m}] = (\imath \partial_t + \frac{1}{2m} \nabla^2 + \mu) \delta_{ij} - 2g\mathbf{m}(x) \cdot \boldsymbol{\sigma}. \tag{274}$$

Putting the determinant into the exponent with $\det \mathcal{O} = e^{Tr \ln \mathcal{O}}$, we get for the generating functional in terms of the action $S[\mathbf{m}]$

$$\begin{aligned} Z[\mathbf{m}] &= \frac{1}{\mathcal{N}} \int D[\mathbf{m}] e^{\imath S[\mathbf{m}]} \\ &= \frac{1}{\mathcal{N}} \int D[\mathbf{m}] e^{\imath \int d^4x g \mathbf{m}^2 + Tr \ln \mathcal{O}[\mathbf{m}]}. \end{aligned} \tag{275}$$

\mathcal{O} is the infinite-dimensional matrix with indices $[x, i]$, so that the trace is to be taken over all the indices x in x -space and i in σ -space: $Tr \equiv Tr_{[x, \sigma]}$. Eventually we will have to expand the log and we therefore factor out $\mathcal{O}[0]$ to get a structure like $\ln(1 - x)$

$$Tr \ln \mathcal{O}[\mathbf{m}] = Tr \ln \{ \mathcal{O}[0] (1 - 2D_S g \mathbf{m} \cdot \boldsymbol{\sigma}) \} \tag{276}$$

with

$$D_S^{-1} \equiv \mathcal{O}[0] = (\imath \partial_t + \frac{1}{2m} \nabla^2 + \mu) \delta_{ij}. \tag{277}$$

To ease the notation we renamed $\mathcal{O}^{-1}[0]$ as D_S , which is the Schrödinger propagator of the free fermionic theory.

Let us flesh out the structure of the above equation, writing out the indices. As a matrix $\mathcal{O}[\mathbf{m}]$ needs two indices a and c

$$\mathcal{O}[\mathbf{m}]_{ac} = \mathcal{O}[0]_{a,b} (\delta_{b,c} - 2g[D_S]_{b,c} [\mathbf{m} \cdot \boldsymbol{\sigma}]_{b,c}), \tag{278}$$

where Latin indices are compound indices as $\{a, b, \dots\} \equiv \{[x, i], [y, j], \dots\}$. The $\delta_{b,c}$ is a product of a Kronecker delta in σ -space and a Dirac delta in x -space. $\mathcal{O}[0]$ is a local operator – see Eq. (86) for a 1-dimensional example. But an operator containing derivatives will become non-local in the discrete/finite version of the path-integral, since derivatives have support in neighboring bins. Its inverse, the propagator D_S , due to translational invariance depends only on the difference in x -space, as $\hat{g}(t_2 - t_1)$ in Eq. (87). It is diagonal in σ -space: $D_S \equiv D_S(x - y) \delta_{ij}$. \mathbf{m} is a diagonal matrix in x -space: $\mathbf{m}_{x,y} = \mathbf{m}(x) \delta(x - y)$. Products of $\mathbf{m}(x)$ are local in x -space, but non-local in momentum space.

We now compute the trace tr_σ in spin-space. In order to get rid of the logarithm, we use a convenient trick. Take the derivative of

$$Tr \ln \mathcal{O}[\mathbf{m}] = Tr \ln \mathcal{O}[0] (1 - 2gD_S \boldsymbol{\sigma} \cdot \mathbf{m})$$

as

$$\frac{\partial Tr_{x,\sigma} \ln \mathcal{O}[\mathbf{m}]}{\partial g} Tr_{x,\sigma} \left\{ \frac{-2D_S \boldsymbol{\sigma} \cdot \mathbf{m}}{1 - 2gD_S \boldsymbol{\sigma} \cdot \mathbf{m}} \right\}, \tag{279}$$

where we have displayed the matrix-inverse as a fraction to emphasize, that positions don't matter. Using

$$[1 - \mathbf{B} \cdot \boldsymbol{\sigma}]^{-1} = \frac{1 + \mathbf{B} \cdot \boldsymbol{\sigma}}{1 - B^2},$$

⁴³ Remember the anti-commutativity of ψ !

we compute

$$\begin{aligned} tr_\sigma \frac{2D_S \boldsymbol{\sigma} \cdot \mathbf{m}}{1 - 2gD_S \boldsymbol{\sigma} \cdot \mathbf{m}} &= tr_\sigma \frac{2D_S \boldsymbol{\sigma} \cdot \mathbf{m} [1 + 2gD_S \mathbf{m} \cdot \boldsymbol{\sigma}]}{(1 - 4g^2 [D_S \mathbf{m}]^2)} \\ &= \frac{8gD_S \mathbf{m} \cdot D_S \mathbf{m}}{1 - 4g^2 D_S \mathbf{m} \cdot D_S \mathbf{m}}, \end{aligned} \quad (280)$$

where we used $tr \boldsymbol{\sigma} = 0$. Inserting this into the derivative of Eq. (275), we get

$$\frac{\partial S[\mathbf{m}]}{\partial g} = tr_x \frac{-8gD_S \mathbf{m} \cdot D_S \mathbf{m}}{1 - 4g^2 D_S \mathbf{m} \cdot D_S \mathbf{m}}. \quad (281)$$

Integrating we get the action with the tr_σ already taken

$$\begin{aligned} S[\mathbf{m}] &= i \int d^4x m^2(x) \\ &+ tr_x \ln \{ \mathcal{O}[0] [1 - 4GD_S \mathbf{m} \cdot D_S \mathbf{m}] \} \end{aligned} \quad (282)$$

where we adjusted the g -independent constant to correctly reproduce the limit $G \rightarrow 0$.

Up to here we have **not made any approximations**, but only rewritten Eq. (264). Yet it is not known how to **compute** the tr_x or compute the integral $\int D[\mathbf{m}]$ without some approximation, such as expanding the ln.

Eq. (282) shows that our system is **rotationally invariant**. In fact the measure $D[\mathbf{m}]$ and $\int d^3x, d^3k$ are invariant and $S[\beta, \mathbf{m}]$ depends only on scalar products of bona fide vectors.⁴⁴ **Therefore any mathematically correct result deduced from this action has to respect this symmetry.** Dear reader: please **never** forget this statement!

When describing **phase-transitions**, we are looking for an *order parameter*, in the present case the magnetization, which is zero in the paramagnetic and non-zero in the ferromagnetic phase. As mentioned in Eq. (163) we require, that

$$\frac{\delta \Gamma[\tilde{\mathbf{m}}(x)]}{\delta \tilde{\mathbf{m}}(x)} = 0 \quad (283)$$

for some non-zero $\tilde{\mathbf{m}}(x) \equiv \langle \mathbf{m}(x) \rangle$. We do want to preserve translational invariance, so that momentum conservation is not spontaneously broken. Therefore we require Eq. (283) to hold for a constant non zero value of the magnetization $\tilde{\mathbf{m}}$

$$\langle \mathbf{m}(x) \rangle = \tilde{\mathbf{m}} \neq 0. \quad (284)$$

Since we did not compute $\Gamma[\tilde{\mathbf{m}}(x)]$, we will resort to the **mean field** approximation or Ginzburg-Landau effective action in the next section.

6.2. The Ginzburg-Landau effective action: ferromagnetic spontaneous symmetry breaking

To model a simple ferromagnetic phase transition, we will expand the logarithm of $S[\mathbf{m}]$ in Eq. (282). It is

⁴⁴ We actually should show that \mathbf{m} transforms as a vector: see exercise 6.1 below.

sufficient to keep terms up to g^4 . We therefore compute

$$\begin{aligned} tr \ln \{ 1 - 4g^2 D_S \mathbf{m} \cdot D_S \mathbf{m} \} \\ = \sum_{n=1}^{\infty} \frac{(-4g^2)^n}{n} tr \{ [D_S \mathbf{m} \cdot D_S \mathbf{m}]^n \}. \end{aligned}$$

Thus $S[\mathbf{m}]$ is given up to order g^4 by

$$\begin{aligned} S_4[\mathbf{m}] &= \int_0^\beta d\tau \int d^3x m^2(x) - 4g^2 tr \{ D_S \mathbf{m} \cdot D_S \mathbf{m} \} \\ &+ 8g^4 tr \{ [D_S \mathbf{m}]^4 \}. \end{aligned} \quad (285)$$

In the instruction to take the trace tr_x , \mathbf{x} is an **integration variable** and we may therefore change to any other convenient variables, but let us not forget the Jacobian J of the transformation. We will compute the determinants/traces in momentum-space, using their invariance under this unitary transformation, which guarantees $J = 1$

$$\begin{aligned} det_x(A) &= det_x \{ \mathcal{U} \mathcal{U}^{-1} A \mathcal{U} \mathcal{U}^{-1} \} \\ &= det_x \{ \mathcal{U} \} det_x \{ \mathcal{U}^{-1} A \mathcal{U} \} det_x \{ \mathcal{U}^{-1} \} \\ &= det_x \{ \mathcal{U} \} det_x \{ \mathcal{U}^{-1} \} det_x \{ \mathcal{U}^{-1} A \mathcal{U} \} \\ &= det_x \{ \mathcal{U} \mathcal{U}^{-1} \} det_x \{ \mathcal{U}^{-1} A \mathcal{U} \} = det_{\mathbf{k}} A. \end{aligned}$$

With $t = -i\tau$ and taking the Fourier transform as

$$\mathbf{m}(\omega, \mathbf{k}) = \int d^4x e^{i(\omega\tau + \mathbf{k} \cdot \mathbf{x})} \mathbf{m}(\tau, \mathbf{x}),$$

we get for the free propagator from Eq. (277)

$$D_S(k) = \frac{1}{i\omega - \epsilon(\mathbf{k})} \quad (286)$$

with $\epsilon(\mathbf{k}) = \frac{\mathbf{k}^2}{2m} - \mu$.

We compute the g^2 -term as

$$\begin{aligned} tr_x \{ D_S m_i \cdot D_S m_i \} \\ = Tr_x \{ m_i D_S \cdot m_i D_S \} \\ = \int d^4x d^4y m_i(x) D_S(x-y) m_i(y) D_S(y-x) \\ = \int d^4x d^4y \frac{d^4k_1}{(2\pi)^4} \frac{d^4k_2}{(2\pi)^4} \frac{d^4k_3}{(2\pi)^4} \frac{d^4k_4}{(2\pi)^4} \\ \star e^{i[k_1 \cdot x + k_2 \cdot (x-y) + k_3 \cdot y + k_4 \cdot (y-x)]} m_i(k_1) \\ D_S(k_2) m_i(k_3) D_S(k_4) \\ = \int \frac{d^4k_1}{(2\pi)^4} \frac{d^4k_2}{(2\pi)^4} \frac{d^4k_3}{(2\pi)^4} \frac{d^4k_4}{(2\pi)^4} \end{aligned} \quad (287)$$

$$\begin{aligned} & \star \delta(k_1 + k_2 - k_4)\delta(-k_2 + k_3 + k_4))m_i(k_1) \\ & D_S(k_2)m_i(k_3)D_S(k_4) \\ & = \int \frac{d^4k_1}{(2\pi)^4} \frac{d^4k_2}{(2\pi)^4} m_i(k_1) \\ & D_S(k_2)m_i(-k_1)D_S(k_1 + k_2). \end{aligned} \tag{288}$$

Thus

$$\text{tr}\{D_S m_i D_S m_i\} = \int \frac{d^4k}{(2\pi)^4} m_i(k) \Pi_2(k) m_i(-k). \tag{289}$$

with the *polarization function*

$$\Pi_2(k) = \int \frac{d^4q}{(2\pi)^4} D_S(q)D_S(k+q). \tag{290}$$

This process is illustrated in Fig. 3. We can easily read off the resulting Eq. (289) without tedious Fourier transforms. Notice that translational invariance in x -space implies energy-momentum conservation.

To describe statistical mechanics, the ω -integral in $\int d^4q$ has to morph into a sum over Matsubara frequencies Eq. (240) for fermions as

$$\int \frac{d\omega}{2\pi} g(\omega) \rightarrow \frac{1}{\beta} \sum_{n=-\infty}^{\infty} g(\omega_n), \quad \omega_n = \frac{(2n+1)\pi}{\beta}.$$

Remembering from Eq. (277) that ω_n are fermionic, whereas ω are bosonic frequencies coming from $m_i(k)$, we get from Eq. (262)

$$\begin{aligned} & \frac{1}{\beta} \sum_n D_S(q)D_S(k+q) \\ & = \frac{1}{\beta} \sum_n \frac{1}{(i\omega_n - \epsilon_q)(i\omega_n + i\omega - \epsilon_{k+q})} \\ & = \frac{n_F(\epsilon_q) - n_F(\epsilon_{k+q})}{i\omega - \epsilon_{k+q} + \epsilon_q} \end{aligned} \tag{291}$$

Below we will need the expansion of $\Pi(\mathbf{k}^2, \omega)$ to first order in \mathbf{k}^2

$$\Pi_2(\mathbf{k}, \omega) \sim \Pi_2(\mathbf{0}, 0) + \alpha_2 \mathbf{k}^2, \tag{292}$$

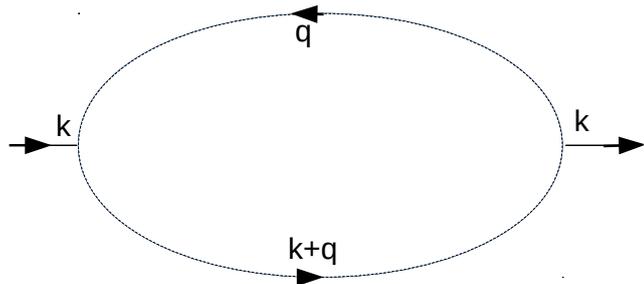


Figure 3: $\Pi_2(k)$: second order contribution to the trace. The thin lines stand for the propagators D_S . Notice momentum conservation at the vertices.

with e.g.

$$\begin{aligned} \Pi_2(\mathbf{0}, 0) & = \lim_{k \rightarrow 0} \int \frac{d^3q}{(2\pi)^3} \sum_n D_S(q)D_S(k+q) \\ & = \int \frac{d^3q}{(2\pi)^3} \frac{e^{\beta\epsilon_q}}{(\epsilon_q + 1)^2}. \end{aligned}$$

Similarly we get for the g^4 term - indicating convolutions by the symbol \otimes ,

$$\text{tr}\{(D_S \mathbf{m} \cdot D_S \mathbf{m})^2\} = a_4(\beta) \{\mathbf{m} \otimes\}^4. \tag{293}$$

Hence we get to order g^4 or G^2

$$\begin{aligned} S_4[\mathbf{m}] & = 8G^2 \alpha_4 \{\mathbf{m} \otimes\}^4 + \int \frac{d^4k}{(2\pi)^4} m_i(k) \\ & \times [1 - 4G(\Pi_2(\mathbf{0}, 0) + \alpha_2 \mathbf{k}^2)] m_i(-k). \end{aligned} \tag{294}$$

This model is supposed to describe the Fe-phase transition occurring at some critical temperature T_c . The magnetization vanishes above T_c and is non-zero below T_c . Therefore it is called **order parameter**. The particular value of T_c depends on the physical details of the ferro-magnetic material. We will not model some particular system, but rather leave T_c as well as $\alpha_2, \Pi_2(\mathbf{0}, 0)$ and α_4 as free parameters.

Yet in the vicinity of the critical point a **universal** behaviour of the order parameter sets in. Universal quantities do not depend on the details, but only on stuff like the spatial dimension ($d = 3$ in our case), the symmetry of the order parameter (rotational symmetry in our case) etc. Which properties are universal has to be discovered in each case and it is those our model has a chance to describe. We therefore simply dump non-universal properties into the free parameters [$G, \alpha_2, \Pi_2(\mathbf{0}, \alpha_4)$] and hope for the best.⁴⁵ We will expand all the temperature-dependent variables around the critical temperature T_c . As we will see, the value of T_c is determined by the vanishing of the coefficient of the \mathbf{m}^2 -term.

All this can be subsumed into the **Ginzburg-Landau effective action** as an approximation to $\Gamma[\mathbf{m}]$ of Eq. (160). Notice that at this point we have abandoned performing the path integral $\int D[\mathbf{m}]$, neglecting the associated quantum effects. We therefore drop the mean value symbol and set $\langle \mathbf{m}(x) \rangle \sim \mathbf{m}(x)$. Transferring $S_4[\mathbf{m}]$ to Euclidean τ, \mathbf{x} -space, we get the Ginzburg-Landau effective action

$$\Gamma_{GL}[\mathbf{m}] = \int d\tau d^3x [c_1 \nabla \mathbf{m} \cdot \nabla \mathbf{m} + c_2 \mathbf{m}^2 + c_4 \mathbf{m}^4]. \tag{295}$$

with some free parameters $c_2, c_i > 0, i = 1, 4$. The gradient term damps out high frequency spatial variations of the order-parameter.

⁴⁵ For more details see [13], sect. 15.2.

Using Eq. (283) we get the **gap equation** for $\mathbf{m}(x)$

$$\frac{\delta\Gamma_{GL}[\mathbf{m}]}{\delta\mathbf{m}(y)} = [-2c_1\nabla^2\mathbf{m} + 2c_2\mathbf{m} + 4c_4\mathbf{m}^3] = 0. \quad (296)$$

As a first approximation, we neglect fluctuations and look for constant

$$\mathbf{m}(x) = \bar{\mathbf{m}} \neq 0 \quad (297)$$

as required by Eq. (284). The magnetization $\bar{\mathbf{m}}$ becomes the **order parameter of the ferromagnetic phase transition**. Since our model is rotationally invariant, it is of course unable to provide a particular direction for the magnetization to point to! At most it may yield a non-zero value for the **length** of the magnetization vector. This is called **Spontaneous Symmetry Breaking (SSB)**. In fact under a rotation the magnetization vector \mathbf{m} transforms as

$$\bar{m}_i \rightarrow \mathcal{R}_{ij}\bar{m}_j, \quad \text{summed over } j, \quad (298)$$

where \mathcal{R} is an anti-symmetric 3×3 - matrix. It satisfies $\mathcal{R}_{ij}\mathcal{R}_{ik} = \delta_{jk}$, so that the original vector and the rotated one have the same length. This means that the **angle** of $\bar{\mathbf{m}}$ is arbitrary, the partition function being independent of this angle! We have now **two possibilities**

1. Either $\bar{\mathbf{m}} = 0$, in which case the angle is irrelevant.
2. Or $\bar{\mathbf{m}} \neq 0$, in which case we have identical physics for all values of the angle, i.e. SSB. The theory only tells us **that \mathbf{m} lies on a sphere of radius $|\bar{\mathbf{m}}| \neq 0$** . If the reader needs a bona fide magnetization vector with a direction, it is up to him to choose this direction. Due to the symmetry, all eventually chosen directions will produce identical results!

Comment 1

Symmetry arguments like the one used at Eq. (298) are millennia old. Aristoteles resorted to symmetry to prove that the vacuum does not exist. In the middle ages this was called **horror vacui** - nature abhors the vacuum.

The argument goes as follows: If the vacuum existed, a body travelling in it with constant velocity would never stop! Due to translational invariance this is true, since all the places are equivalent and the body can't do anything except going on[20]. Now he concludes: but this is absurd, therefore the vacuum does not exist⁴⁶.

Notice that Aristoteles lived ~ 2000 years before Galileo! If you want the body to stop, you have to somehow break translational

invariance. In our system you have to somehow break rotational invariance. You could take resource to some magnetic field pointing in a particular direction and adding a corresponding interaction to our model. This would be **explicit symmetry breaking**. But SSB is much more subtle!

For a constant order parameter the gap equation Eq. (296) becomes

$$2\bar{\mathbf{m}} \{c_2 + 4c_4\bar{\mathbf{m}}^2\} = 0. \quad (299)$$

If $\bar{\mathbf{m}}^2 \neq 0$, we say that the system undergoes spontaneous symmetry breaking. This requires c_2 to change sign at some $T = T_c$. The simplest assumption is

$$c_2 = a(T - T_c), \quad a > 0$$

such that

$$\bar{\mathbf{m}}^2 = \frac{a(T_c - T)}{4c_4}. \quad (300)$$

The solutions of our gap-equation are then

$$|\bar{\mathbf{m}}| = \begin{cases} a'[T_c - T]^{1/2}, & T \leq T_c \\ 0 & T > T_c \end{cases} \quad (301)$$

with the constant $a' = \sqrt{a/(4c_4)}$.

Here we encounter the **critical index** γ , which controls how the magnetization vanishes at the critical temperature

$$\bar{\mathbf{m}} \sim (T_c - T)^\gamma \quad (302)$$

with $\gamma = 1/2$. We also notice that the derivative $d\bar{\mathbf{m}}/dT$ diverges at the critical temperature, signaling a **singularity**.

Now we observe

1. The critical temperature T_c depends on the details of the physics to be described. Since this would be a tall order for our model to live up to, we left T_c a free, unknown parameter.
2. Unless forbidden by some special requirement, the lowest order terms in the expansion of the determinant are $\mathbf{m}(x) \cdot \mathbf{m}(x)$, $[\mathbf{m}(x) \cdot \mathbf{m}(x)]^2$. These terms are **required by the rotational symmetry** of our model, which excludes all the odd powers of $\mathbf{m}(x)$. This fixes the value of critical exponent γ to be $\frac{1}{2}$. We therefore trust this value to have a rather general validity: it is called **universal**. See \rightsquigarrow [7], pgs. 285, 351.

We now include fluctuations to compute the \mathbf{x} -dependence of the 2-point correlation function. This is actually an inconsistent procedure. We first neglect fluctuations, which forced us to set $\langle \mathbf{m}(x) \rangle \sim \mathbf{m}(x) = \bar{\mathbf{m}}$. But we include them now, to compute $\langle \mathbf{m}(\mathbf{x})\mathbf{m}(\mathbf{0}) \rangle$.

⁴⁶ Do you agree or do you feel cheated?

Yet the results provide valuable insights into the physics of phase transitions.

In analogy to Eq. (92), we use Eq. (168) – with no factor of ι since our setting is in our Euclidean. This shows, that the two point correlation function $g_{GL}(\mathbf{x}) = \langle \mathbf{m}(\mathbf{x})\mathbf{m}(\mathbf{0}) \rangle - \bar{\mathbf{m}}^2$ satisfies the equation

$$\{2c_2 + 4c_4\mathbf{m}(x)^2 - 2c_1\nabla^2\}g_{GL}(\mathbf{x}) = \delta^{(3)}(\mathbf{x}). \quad (303)$$

Inserting $\mathbf{m}(x)$ from Eq. (301), we get

$$\{-2c_1\nabla^2 + 2\lambda a'(T_c - T)\}g_{GL}(\mathbf{x}) = \delta^{(3)}(\mathbf{x}) \quad (304)$$

with $\lambda = 2$ for $T < T_c$ and $\lambda = -1$ for $T > T_c$. The solution with the boundary condition $g_{GL}(\infty) = 0$ is

$$g_{GL}(\mathbf{x}) = \frac{1}{8\pi c_1} \frac{e^{-|\mathbf{x}|/\xi}}{|\mathbf{x}|} \quad (305)$$

with

$$\xi = \begin{cases} a_+(T - T_c)^{-1/2}, & T > T_c \\ a_-(T_c - T)^{-1/2}, & T < T_c \end{cases} \quad (306)$$

where $a_+ = \sqrt{c_1/a'}$, $a_- = \sqrt{c_1/2a'}$. ξ is called **correlation length**. It diverges at $T = T_c$ with the **universal** critical exponent $\nu = \frac{1}{2}$. The ratio a_+/a_- is also a universal parameter.

If you want to go beyond the mean-field picture, use e.g. the **Renormalization Group** approach, which is beyond this note. You may check out [10, 17], besides the books already mentioned.

Exercise 6.1

Consider a massless boson in $d = 2$ euclidean dimensions. In analogy to Eq. (92) its propagator satisfies

$$\nabla^2 D_{E_2}(x) = \delta^{(2)}(x). \quad (307)$$

Solve this equation and notice divergences for both small and large distances. The small distance behavior is not relevant, if the system lives on a solid lattice. The large distance divergence illustrates, why SSB of a continuous symmetry does not exist in two dimensions. The small number of neighbors is insufficient to prevent the large distance fluctuations from destroying the coherence in the ordered phase. $d = 1$ is even worse in this respect. $d = 2$ is the *lower critical dimension* for spontaneously breaking a continuous symmetry at a temperature $T > 0$. Yet a discrete symmetry may be broken in $d=2$, but not in $d=1$.

Exercise 6.2

Show that $c_4 > 0$.

Exercise 6.3

Show that \mathbf{m} transforms as a vector under rotations. Choose a coordinate system, whose z -axis coincides with the rotation axis. By definition ψ transforms under a rotation around this axis by an angle φ as

$$\psi'(\mathbf{x}') = S_3\psi(\mathbf{x}),$$

with

$$S_3 = e^{i\frac{\sigma_3}{2}\varphi}$$

and the vector \mathbf{x} transforms as

$$\mathbf{x}' = \mathcal{A}\mathbf{x}$$

$$\mathcal{A} = \begin{pmatrix} \cos \varphi & \sin \varphi & 0 \\ \sin \varphi & \cos \varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Show that \mathbf{m} transforms as \mathbf{x} , i.e.

$$\begin{aligned} m'_i(\mathbf{x}') &= (\psi^*)'(\mathbf{x}')\sigma_i\psi'(\mathbf{x}') \\ &= \mathcal{A}_{ij}\psi^*(\mathbf{x})\sigma_j\psi(\mathbf{x}) = \mathcal{A}_{ij}m_j(\mathbf{x}). \end{aligned} \quad (308)$$

6.3. Superconductivity

Consider again the Lagrangian density Eq. (263)

$$\mathcal{L} = \sum_{i=\pm} \psi_i^* (\iota\partial_t - \frac{1}{2m}\nabla^2 - \mu)\psi_i + G\psi_+^*\psi_-^*\psi_-\psi_+. \quad (309)$$

with the partition function

$$Z = \int D[\psi, \psi^*] e^{\int d^4x \mathcal{L}}. \quad (310)$$

We will again integrate over the fermions, but now in a way different from the previous section. **The order parameter will be a charged field!** In the OQFT language, instead of the Hartree-Fock approximation with the charge-conserving break-up

$$\langle \psi_+^\dagger \psi_-^\dagger \psi_+ \psi_- \rangle \sim \langle \psi_+^\dagger \psi_- \rangle \langle \psi_+^\dagger \psi_+ \rangle,$$

Bardeen-Cooper-Schrieffer(BCS) took the **revolutionary** step to decouple the 4-fermion interaction as

$$\langle \psi_+^\dagger \psi_-^\dagger \psi_+ \psi_- \rangle \sim \langle \psi_+^\dagger \psi_-^\dagger \rangle \langle \psi_+ \psi_- \rangle,$$

requiring the introduction of a complex charged order parameter $\Delta(x)$.

First convert the quartic fermion interaction to a bilinear one, a little different from the analogous computation in Eq. (272). Notice that the integral

$$\int D\Delta D\Delta^* e^{-G\Delta\Delta^*} = C_G$$

where Δ, Δ^* are two independent bosonic fields, is the G -dependent irrelevant constant C_G . Shifting the fields Δ, Δ^* as

$$\Delta \rightarrow \Delta - G\psi_+\psi_-, \quad \Delta^* \rightarrow \Delta^* - G\psi_-^*\psi_+^*, \quad (311)$$

and noticing that this leaves the measure invariant, we get,

$$\begin{aligned} C_G e^G \int d^4x \psi_+^* \psi_-^* \psi_- \psi_+ \\ = \int D[\Delta, \Delta^*] e^{\int d^4x [-\frac{\Delta^* \Delta}{G} + \Delta^* \psi_+ \psi_- + \Delta \psi_-^* \psi_+^*]}. \end{aligned} \quad (312)$$

Inserting Eq. (312) into Eq. (310) yields

$$Z = \int D[\psi, \psi^*] D[\Delta, \Delta^*] e^{\int d^4x \mathcal{L}[\psi, \Delta]} \quad (313)$$

with the Lagrangian density

$$\begin{aligned} \mathcal{L}[\psi, \Delta] = \sum_{i=\pm} \psi_i^* (i\partial_t - \frac{1}{2m} \nabla^2 - \mu) \psi_i \\ + \Delta^* \psi_+ \psi_- + \Delta \psi_-^* \psi_+^* - \frac{\Delta^* \Delta}{G}. \end{aligned} \quad (314)$$

From their coupling to the electrons, we infer that $\Delta(x), \Delta^*(x)$ have spin zero and electric charge

$$Q_\Delta = -2, Q_{\Delta^*} = 2. \quad (315)$$

From Eq. (309) it easily follows that our theory does conserve the electric charge

$$\partial_t \rho + \nabla \cdot \mathbf{j} = 0 \quad (316)$$

with $\rho = \sum_\sigma \psi_\sigma^* \psi_\sigma, \mathbf{j} = \sum_\sigma \psi_\sigma^* \nabla \psi_\sigma$. This conservation law also follows from symmetry arguments. The classical Noether theorem tells us: *To every continuous symmetry there corresponds a conservation law.* Although this is true in classical physics it may fail in the quantum domain. Yet in our case it is true. Our Lagrangian density $\mathcal{L}[\psi, \Delta]$ Eq. (314) is invariant under the following $U(1)$ transformations

$$\begin{aligned} \Delta_i &\rightarrow e^{2i\alpha} \Delta_i \\ \Delta_i^* &\rightarrow e^{-2i\alpha} \Delta_i^* \\ \psi_i &\rightarrow e^{i\alpha} \psi_i \\ \psi_i^* &\rightarrow e^{-i\alpha} \psi_i^*, \end{aligned} \quad (317)$$

the starred variables transforming as complex conjugates of the un-starred ones.

To address the statistical-mechanical description of superconductivity, perform the analytic continuation $t = -i\tau$ to obtain the finite temperature partition function using Eq. (238)

$$Z(\beta) = \int D[\psi, \psi^*] D[\Delta, \Delta^*] e^{-S[\beta, \psi, \Delta]} \quad (318)$$

with the action

$$S[\beta, \psi, \Delta] = \int_0^\beta d\tau \int d^3x \mathcal{L}_E[\psi, \Delta], \quad (319)$$

where

$$\begin{aligned} \mathcal{L}_E[\psi, \Delta] = \sum_{i=\pm} \psi_i^* (\partial_\tau + \frac{1}{2m} \nabla^2 + \mu) \psi_i \\ - \Delta^* \psi_+ \psi_- - \Delta \psi_-^* \psi_+^* + \frac{\Delta^* \Delta}{G}. \end{aligned} \quad (320)$$

Assemble the fermions into *Nambu-spinors*, as

$$\bar{\Psi} = (\psi_+^*, \psi_-), \Psi = \begin{pmatrix} \psi_+ \\ \psi_-^* \end{pmatrix}. \quad (321)$$

In terms $\bar{\Psi}, \Psi$ we get

$$S[\beta, \psi, \Delta] = \int_0^\beta d\tau \int d^3x \left[\bar{\Psi} \mathcal{O} \Psi + \frac{\Delta^* \Delta}{G} \right] \quad (322)$$

with

$$\mathcal{O}(\tau, \mathbf{x}) = \begin{pmatrix} \mathcal{O}_+ & \Delta \\ \Delta^* & \mathcal{O}_- \end{pmatrix}, \quad (323)$$

where

$$\begin{aligned} \mathcal{O}_+ &= \partial_\tau + \left(\frac{\nabla^2}{2m} + \mu \right) \\ \mathcal{O}_- &= \partial_\tau - \left(\frac{\nabla^2}{2m} + \mu \right). \end{aligned}$$

With respect to \mathcal{O}_- notice that

$$\begin{aligned} \psi_-^* \partial_\tau \psi_- &= \partial_\tau (\psi_-^* \psi_-) - (\partial_\tau \psi_-^*) \psi_- \\ \mu \psi_-^* \psi_- &= -\mu \psi_- \psi_-^* \\ \psi_-^* \nabla^2 \psi_- &= \nabla (\psi_-^* \nabla \psi_-) - (\nabla \psi_-^*) (\nabla \psi_-) \\ &= \nabla (\psi_-^* \nabla \psi_-) + (\nabla^2 \psi_-^*) \psi_- - \nabla (\nabla \psi_-^*) \psi_- \end{aligned}$$

Although the ψ 's satisfy anti-periodic boundary condition, the $\psi\psi^*$ -terms satisfy periodic ones. Therefore the total derivative terms cancel in the action and we get

$$\begin{aligned} \psi_-^* (\partial_\tau + \frac{1}{2m} \nabla^2 + \mu) \psi_- \\ = \psi_- \{ \partial_\tau - (\frac{1}{2m} \nabla^2 + \mu) \} \psi_-^* = \mathcal{O}_-. \end{aligned}$$

Since $S[\beta, \psi, \Delta]$ is quadratic in the fermion variables, we integrate them out using Eq. (248) and include the determinant in the exponent to get

$$Z[\beta] = \int D[\Delta, \Delta^*] e^{-S[\beta, \Delta]} \quad (324)$$

with the action

$$S[\beta, \Delta] = \int_0^\beta d\tau \int d^3x \frac{|\Delta|^2}{G} - \ln \det \mathcal{O}[\Delta]. \quad (325)$$

From here proceed as in the previous *ferromagnetic* section, except for the different $\mathcal{O}[\Delta]$. In the Fe-case the

system had rotational symmetry in \mathcal{R}^3 , whereas now we have rotational symmetry in a two-dimensional complex plane, as seen from Eqs. (317). We again factor out $\mathcal{O}[0]$, which now involves σ_3 , as

$$\mathcal{O}[0] = \partial_\tau + \left(\frac{\nabla^2}{2m} + \mu\right) \sigma_3, \tag{326}$$

to get

$$\mathcal{O}[\Delta] = \mathcal{O}[0] + \boldsymbol{\sigma} \cdot \boldsymbol{\Delta} = \mathcal{O}[0](1 + \mathcal{O}[0]^{-1} \boldsymbol{\sigma} \cdot \boldsymbol{\Delta}), \tag{327}$$

where for notational convenience we changed

$$\boldsymbol{\Delta} \rightarrow \boldsymbol{\Delta} = [\mathcal{R}e\Delta, -\mathcal{I}m\Delta, 0]. \tag{328}$$

The propagator

$$D_S = \mathcal{O}[0]^{-1} = \left[\partial_\tau + \left(\frac{\nabla^2}{2m} + \mu\right) \sigma_3\right]^{-1} \tag{329}$$

has the momentum-space representation $D_S(k) = \int d^4x e^{i(\omega\tau + \mathbf{k}\cdot\mathbf{x})} D_S(x)$

$$D_S(k) = \frac{-i\omega - \epsilon_{\mathbf{k}}\sigma_3}{\omega_k^2 + \epsilon_{\mathbf{k}}^2} \tag{330}$$

with $\epsilon_{\mathbf{k}} = \frac{\mathbf{k}^2}{2m} - \mu$.

There is no closed form available for the generating functional $Z(\beta)$ Eq. (324). We therefore have to resort to a perturbation analysis or some other approximation. Before discussing these, we add the following comments

- $\Delta = \rho e^{i\phi}$ is complex and therefore not an observable quantity.
- Using OQFT-parlance: since $\boldsymbol{\Delta}$ has charge two, yet the Hamiltonian conserves charge, it follows that $\boldsymbol{\Delta}$ does not commute with the Hamiltonian. Therefore there does not exist a common set of eigenvectors.
- If we select a particular value for Δ , we have also have to choose a particular value for its phase: **we are spontaneously breaking charge conservation. Yet any value for the phase will give equivalent results!** Due to the symmetry, the action does not depend on the phase ϕ .
- In the ferromagnetic case we had to choose a particular value for the direction of the magnetization, thereby breaking rotational symmetry. We are used to a ferromagnet pointing in a particular direction, blaming all kinds of small external fields for the breaking. Yet in the present case, who is supplying the charge, since charge conservation is broken?

We can argue as follows. SSB occurs only in the thermodynamic limit $M \rightarrow \infty$. Nature may be very large, yet she is finite.⁴⁷ In real life, we may therefore approximate to any precision the SSB-state by a superposition of charge-conserving states and nobody will create charges from the vacuum!

⁴⁷ For small enough samples one observes finite-size effects!

6.4. The BCS model for spontaneous symmetry breaking

We will study the phase transition, using a **saddle-point approximation** for $Z(\beta)$. Thus we look for extrema of the action $S[\beta, \Delta]$, where the integrand dominates the integral $\int D[\Delta]$. This selects the $\boldsymbol{\Delta}(x)$'s, which satisfy

$$\frac{\delta S[\beta, \Delta]}{\delta \boldsymbol{\Delta}(y)} = 0. \tag{331}$$

Here $S[\beta, \Delta]$ is given by Eq. (325)

$$S[\beta, \Delta] = \int_0^\beta d\tau \int d^3x \frac{|\boldsymbol{\Delta}(x)|^2}{G} - Tr_{x,\sigma} \ln \mathcal{O}[\Delta]. \tag{332}$$

The derivative of the first term as

$$\frac{\int d^4y |\boldsymbol{\Delta}(y)|^2 / G}{\partial \boldsymbol{\Delta}(x)} = 2\boldsymbol{\Delta}^*(x) / G.$$

To illustrate, how to compute the derivative of a term like $tr_x \ln(1 + \mathcal{A}[z])$ with $z = \boldsymbol{\Delta}(x)$, take an arbitrary function $f(\mathcal{A}[z])$, expand it in a Taylor series and take the derivative $d_z \equiv d/dz$ term by term

$$\begin{aligned} d_z tr(f(\mathcal{A})) &= d_z \sum_{n=0}^\infty \frac{f(0)^{(n)}}{n!} tr(\mathcal{A}^n) \\ &= \sum_{n=1}^\infty \frac{f^{(n)}(0)}{n!} tr[d_z \mathcal{A} \mathcal{A} \dots \mathcal{A} \\ &\quad + \mathcal{A} d_z \mathcal{A} \dots \mathcal{A} + \dots \mathcal{A} \mathcal{A} \dots d_z \mathcal{A}]. \end{aligned}$$

Now use the circular property of the trace get

$$\begin{aligned} d_z tr(f(\mathcal{A})) &= \sum_{n=1}^\infty \frac{f^{(n)}(0)}{(n-1)!} tr\{\mathcal{A}^{n-1} d_z \mathcal{A}\} \\ &= tr(f'(\mathcal{A}) d_z \mathcal{A}), \end{aligned} \tag{333}$$

where $f'(\mathcal{A}) d_z \mathcal{A}$ is a matrix product with a sum/integral over common indices!

Thus we obtain – with $\boldsymbol{\Delta}(x) \equiv \boldsymbol{\Delta}_x$ for notational simplicity – for the functional derivative

$$\frac{\delta}{\delta \boldsymbol{\Delta}_x} tr_y \{ \ln(\mathcal{A}[\boldsymbol{\Delta}_y]) \} = tr_y \left\{ \left(\mathcal{A}[\boldsymbol{\Delta}_y] \right)^{-1} \frac{\partial \mathcal{A}[\boldsymbol{\Delta}_y]}{\partial \boldsymbol{\Delta}_x} \right\}. \tag{334}$$

This yields with the trace taken in x - and σ -space

$$\begin{aligned} &\frac{\delta}{\delta \boldsymbol{\Delta}_x} Tr \{ \ln(\mathcal{O}[\boldsymbol{\Delta}_y]) \} \\ &= \frac{\delta}{\delta \boldsymbol{\Delta}(x)} Tr \ln \{ [\mathcal{O}[0] + \boldsymbol{\Delta}(y) \cdot \boldsymbol{\sigma}] \} \\ &= Tr \left\{ \left(\mathcal{O}[0] + \boldsymbol{\Delta}(y) \cdot \boldsymbol{\sigma} \right)^{-1} \begin{pmatrix} 0 & \delta^{(4)}(x-y) \\ 0 & 0 \end{pmatrix} \right\} \\ &= Tr \left\{ \left(\mathcal{O}[0] + \boldsymbol{\Delta}(x) \cdot \boldsymbol{\sigma} \right)^{-1} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \right\}. \end{aligned} \tag{335}$$

to get the gap-equation

$$\frac{2\Delta^*(x)}{G} = Tr \left\{ \left(\mathcal{O}[0] + \Delta(x) \cdot \sigma \right)^{-1} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \right\}. \tag{336}$$

We first seek solutions for constant $\Delta(x) = \bar{\Delta}$. To compute the trace in the rhs, we go to Fourier space and use Eq. (330) for $D_S(k)$. The matrix $\mathcal{O}[\bar{\Delta}]$ in the trace to be inverted is block diagonal in momentum space, so that the inversion replaces the 2×2 blocks by their inverses. We have recalling Eq. (323)

$$\begin{aligned} Tr_{x\sigma} & \left\{ \left(\mathcal{O}[0] + \bar{\Delta} \cdot \sigma \right)^{-1} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \right\} \\ &= Tr_{k\sigma} \left\{ \left(\mathcal{O}[0] + \bar{\Delta} \cdot \sigma \right)^{-1} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \right\} \\ &= Tr_{k\sigma} \left\{ \begin{pmatrix} i\omega - \epsilon_k & \bar{\Delta} \\ \bar{\Delta}^* & i\omega + \epsilon_k \end{pmatrix}^{-1} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \right\} \\ &= Tr_{k\sigma} \left\{ \begin{pmatrix} i\omega + \epsilon_k & -\bar{\Delta} \\ -\bar{\Delta}^* & i\omega - \epsilon_k \end{pmatrix} \Big|_{21} \frac{-1}{\omega^2 + \epsilon_k^2 + |\bar{\Delta}|^2} \right\} \\ &= tr_k \frac{\bar{\Delta}^*}{\omega^2 + \epsilon_k^2 + |\bar{\Delta}|^2}, \end{aligned} \tag{337}$$

where the indices $i = 1, j = 2$ label the matrix element in the 2×2 matrix selecting $-\bar{\Delta}$. The expression $\xi_k^2 = \epsilon_k^2 + |\bar{\Delta}|^2$ is called the dispersion relation for the *Bogoliubov quasi-particles* \rightsquigarrow [7], pg. 272.

Thus the mean-field gap equation is

$$\frac{2\bar{\Delta}}{G} = tr_k \frac{\bar{\Delta}}{\omega^2 + \xi_k^2} \tag{338}$$

The ω -integral in the $tr_k \equiv \int d\omega \int d^3k$ is actually a fermionic Matsubara sum⁴⁸. With $\omega \rightarrow \omega_n = \frac{\pi(2n+1)}{\beta}$ we get

$$tr_k \rightarrow \frac{1}{\beta} \sum_{n=-\infty}^{\infty} \int \frac{d^3k}{(2\pi)^3}.$$

If we want to describe the phase transition occurring in some real material, we have to inject here some information about its physical details. They are thus **non-universal** inputs. To execute the $\int d^3k$, recall that the attractive phonon-mediated interaction responsible for the BCS superconductivity, occurs only in a thin shell of the order of the Debye frequency $\omega_D \ll \epsilon_F$ around the Fermi surface \rightsquigarrow [7], pg. 269. Therefore we have

$$\int \frac{d^3k}{(2\pi)^3} \equiv \int \nu(\epsilon) d\epsilon \sim \nu(\epsilon_F) \int_{-\omega_D}^{\omega_D} d\epsilon, \tag{339}$$

where $\nu(\epsilon_F)$ is the electron density of states at the Fermi surface.

⁴⁸ Remember that $\mathcal{O}[0]$ and therefore D_S are fermionic operators!

The gap-equation in this saddle-point or mean field approximation is

$$0 = \bar{\Delta} \left\{ -\frac{1}{G'} + k_B T \nu(\epsilon_F) \int_{-\omega_D}^{\omega_D} d\epsilon \sum_{n=-\infty}^{\infty} \left(\frac{1}{\omega_n^2 + \xi_k^2} \right) \right\} \tag{340}$$

with $G' = G/2$ required to be positive and $\xi_k^2 = \epsilon_k^2 + |\bar{\Delta}|^2$. The solution of this non-linear integral equation yields the temperature dependence $\bar{\Delta}(T)$ of the order parameter. Concerning the **phase** of $\bar{\Delta}$, we again have now **two possibilities**

1. Either $\bar{\Delta} = 0$, in which case the phase is irrelevant.
2. Or $\bar{\Delta} = \rho e^{i\phi} \neq 0$, in which case we have identical physics for all values of the phase ϕ . The theory only tells us **that $\bar{\Delta}$ lies on a circle of radius $\rho \neq 0$** . In the jargon of the trade we say: the selection of a particular phase ϕ **spontaneously breaks charge conservation!** We choose the phase of $\bar{\Delta}$ to be zero for convenience.

Choosing the solution with $\bar{\Delta} \neq 0$, we have

$$\frac{1}{G'} = k_B T \nu(\epsilon_F) \int_{-\omega_D}^{\omega_D} d\epsilon \sum_{n=-\infty}^{\infty} \frac{1}{\omega_n^2 + \epsilon^2 + |\bar{\Delta}|^2}$$

Using

$$\sum_{k=-\infty}^{\infty} \frac{1}{x^2 + (2k-1)^2} = \frac{\pi \tanh(\pi x/2)}{4x}, \tag{341}$$

yields with $g = \nu(\epsilon_F)G'$

$$1 = g \int_0^{\omega_D} d\epsilon \frac{\tanh\left(\frac{\sqrt{\epsilon^2 + |\bar{\Delta}|^2}}{2k_B T}\right)}{2\sqrt{\epsilon^2 + |\bar{\Delta}|^2}}. \tag{342}$$

The superconducting phase is characterized by $\bar{\Delta} \neq 0$ and it vanishes at the critical temperature T_c .

Setting $\bar{\Delta} = 0$ in Eq. (342) we get an equation for the critical temperature

$$1 = g \int_0^{\omega_D} d\epsilon \frac{\tanh\left(\frac{\epsilon}{2k_B T_c}\right)}{2\epsilon}. \tag{343}$$

Since in many cases of interest ω_D is large, we would like to make our life easier setting $\omega_D = \infty$. But the integral in Eq. (343) would be divergent. In order to extract the offending term, we integrate by part obtaining a tame log-term and an exponentially convergent $1/\cosh^2$ term as

$$\int_0^{\omega_D} dx \frac{\tanh x}{x} = \ln \omega_D \tanh \omega_D - \int_0^{\omega_D} dx \frac{\ln x}{\cosh^2 x}. \tag{344}$$

We approximate the second term, extending the integral to ∞ to get for large ω_D

$$\int_0^{\omega_D} dx \frac{\ln x}{\cosh^2 x} \cong \int_0^{\infty} dx \frac{\ln x}{\cosh^2 x} = -\log(4B), \tag{345}$$

with $B = e^C/\pi$. Further using $\tanh(\omega_D) \simeq \tanh(\infty) = 1$ we obtain

$$\int_0^{\omega_D} dx \frac{thx}{x} \cong \ln \omega_D + \ln(4B) \simeq \ln(4\omega_D B). \tag{346}$$

This yields

$$T_c \cong \frac{2e^C}{\pi} \hbar \omega_D e^{-\frac{1}{g}}, \tag{347}$$

with \hbar reinstated to highlight the quantum effect. Notice the non-analytic dependence on g . This equation for T_c explicitly shows its **non-universal** characteristic.

To obtain the zero-temperature gap $\bar{\Delta}(0)$ set $T = 0$ in Eq. (342)

$$1 = g \int_0^{\omega_D} \frac{d\epsilon}{2\sqrt{\epsilon^2 + \bar{\Delta}^2(0)}} = \frac{1}{2} \ln \frac{\omega_D + \sqrt{\omega_D^2 + \bar{\Delta}^2(0)}}{\bar{\Delta}(0)}. \tag{348}$$

or

$$\bar{\Delta}(0)e^{g/2} = \omega_D + \sqrt{\omega_D^2 + \bar{\Delta}^2(0)}. \tag{349}$$

Comparing with Eq. (349) we get for large ω_D

$$\bar{\Delta}(0) \simeq \frac{k_B T_c}{B}. \tag{350}$$

We now extract the critical behavior of the order parameter straightforwardly and without approximations[21]. For this purpose we choose $\bar{\Delta}$ real and parametrize as⁴⁹

$$\bar{\Delta}(\beta) = a \left(\frac{\beta - \beta_c}{\beta_c} \right)^\alpha; \beta \sim \beta_c. \tag{351}$$

This yields for the derivative $\partial_\beta \Delta^2 \equiv \frac{\partial \bar{\Delta}^2}{\partial \beta}$ as

$$\lim_{T \rightarrow T_c} \partial_\beta \Delta^2 = \begin{cases} 0 & \alpha > 1/2 \\ a^2/\beta_c & \alpha = 1/2 \\ \infty & \alpha < 1/2 \end{cases} \tag{352}$$

The non-linear integral equation Eq. (342) for the order parameter has the solution $\Delta(\beta, \omega_D, g)$, depending on three parameters. Substituting this solution into

Eq. (342) yields an identity. Differentiating this identity with respect to β easily yields the following relation

$$\partial_\beta \Delta^2(\beta, \omega_D, g) = \frac{\int_0^{\omega_D} \frac{d\epsilon}{\cosh^2 \frac{\beta E}{2}}}{\int_0^{\omega_D} \frac{d\epsilon}{E^3} \left(\tanh \frac{\beta E}{2} - \frac{\beta E}{2 \cosh^2 \frac{\beta E}{2}} \right)} \tag{353}$$

with $E = \sqrt{\epsilon^2 + \bar{\Delta}^2}$.

Taking the limit $T \rightarrow T_c, \Delta \rightarrow 0$, we obtain

$$0 < a^2 = \frac{2(k_B T_c)^2 \tanh \frac{\omega_D \beta_c}{2}}{\int_0^{\omega_D \beta_c} \frac{dx}{x^3} \left(\tanh \frac{x}{2} - \frac{x}{2 \cosh^2 \frac{x}{2}} \right)} < \infty \tag{354}$$

implying $\alpha = 1/2$, as is to be expected for a mean-field theory. Notice that the above integrand is finite at $x = 0$. As illustration we evaluate the integral for $\omega_D \beta_c = 10$ to get

$$\bar{\Delta}(T) = 3.10 \cdot k_B T_c \left(1 - \frac{T}{T_c} \right)^{\frac{1}{2}}, T \sim T_c. \tag{355}$$

We therefore obtain the same universal critical exponents as in the Fe-case as is expected for mean-field models.

Also for the superconducting case, we can write an effective action analogous to Eq. (295), which includes lowest order spatial derivatives of $\Delta(x)$. Using $\ln \det \mathcal{O} = Tr \ln \mathcal{O}$, we expand the log in Eq. (325) as

$$Tr \ln (1 + D_S(x) \Delta \cdot \sigma) = \sum_{n=1}^{\infty} \frac{1}{n} Tr \{ [D_S(x) \Delta \cdot \sigma]^n \}. \tag{356}$$

Due to the tracelessness of σ - or just by symmetry - all odd terms are forbidden. We therefore get including only the even terms

$$Tr \ln (1 + D_S(x) \Delta \cdot \sigma) = \frac{1}{2} \sum_{n=1}^{\infty} \frac{1}{n} Tr \{ [D_S \Delta \cdot \sigma D_S \Delta \cdot \sigma]^n \}. \tag{357}$$

Reintroducing the log, the action is

$$S[\beta, \Delta] = \int_0^\beta d\tau \int d^3x \frac{|\Delta(x)|^2}{G} - \frac{1}{2} Tr_{x,\sigma} \ln \left\{ \mathcal{O}[0] \times \left[1 + (D_S \Delta \cdot \sigma D_S \Delta \cdot \sigma)(x) \right] \right\}. \tag{358}$$

Here we only compute the second order term in the log.

⁴⁹ Although the standard nomenclature for the order parameter's critical exponent is β , we use α to avoid confusion with $\beta = 1/k_B T$.

Referring to Eq. (289), we trade $\mathbf{m}(k)$ for $\boldsymbol{\sigma} \cdot \boldsymbol{\Delta}(k)$ to get

$$\begin{aligned} & Tr_{k,\sigma} [D_S \boldsymbol{\sigma} \cdot \boldsymbol{\Delta} D_S \boldsymbol{\sigma} \cdot \boldsymbol{\Delta}] \\ &= tr_\sigma \int \frac{d^4 k}{(2\pi)^4} \\ &\quad \times \left[\int \frac{d^4 q}{(2\pi)^4} \boldsymbol{\sigma} \cdot \boldsymbol{\Delta}^*(k) D_S(q+k) \boldsymbol{\sigma} \cdot \boldsymbol{\Delta}(k) D_S(q) \right]. \end{aligned}$$

Here we have replaced $\boldsymbol{\sigma} \cdot \boldsymbol{\Delta}(-k)$ by $\boldsymbol{\sigma} \cdot \boldsymbol{\Delta}^*(k)$ to expose **charge conservation**. In Fig.(3) $\boldsymbol{\sigma} \cdot \boldsymbol{\Delta}^*(k)$ creates a charge $Q_{\Delta^*} = 2$ at the left vertex, which is destroyed by $\boldsymbol{\sigma} \cdot \boldsymbol{\Delta}(k)$ at the right vertex.

Inserting the momentum-space propagator $D_S(q)$ from Eq. (330) yields

$$\begin{aligned} & D_S(q) \boldsymbol{\sigma} \cdot \boldsymbol{\Delta}^*(k) D_S(q+k) \boldsymbol{\sigma} \cdot \boldsymbol{\Delta}(k) \\ &= \int \frac{d^4 q}{(2\pi)^4} \left\{ \frac{-i\omega_q - \epsilon_q \sigma_3}{\omega_q^2 + \epsilon_q^2} \boldsymbol{\sigma} \right. \\ &\quad \cdot \boldsymbol{\Delta}^*(k) \left. \frac{-i\omega_{q+k} - \epsilon_{q+k} \sigma_3}{\omega_{q+k}^2 + \epsilon_{q+k}^2} \boldsymbol{\sigma} \cdot \boldsymbol{\Delta}(k) \right\}. \quad (359) \end{aligned}$$

To take the tr_σ , we choose axes such that $\mathcal{I}m\Delta = 0$ and only Δ_1 -terms survive.⁵⁰ Using $\sigma_3 \sigma_i \sigma_3 \sigma_j = -1$ for $i = j = 1$ we get

$$\begin{aligned} & [D_S \boldsymbol{\sigma} \cdot \boldsymbol{\Delta}^* D_S \boldsymbol{\sigma} \cdot \boldsymbol{\Delta}](k) \\ &= - \int \frac{d^4 q}{(2\pi)^4} \frac{\Delta_i^*(k) \Delta_j(q)}{(\omega_q^2 + \epsilon_q^2)(\omega_{q+k}^2 + \epsilon_{q+k}^2)} \\ &\quad \times \left(\delta_{ij} (\omega_q \omega_{q+k} + \epsilon_q \epsilon_{q+k}) \right. \\ &\quad \left. + i[\sigma_3]_{[ij]} (\epsilon_q \omega_{q+k} - \omega_q \epsilon_{q+k}) \right). \end{aligned}$$

The trace over $\boldsymbol{\sigma}$ kills the σ_3 -term, resulting in

$$\begin{aligned} & Tr_{k,\sigma} [D_S \boldsymbol{\sigma} \cdot \boldsymbol{\Delta} D_S \boldsymbol{\sigma} \cdot \boldsymbol{\Delta}] \\ &= - \int \frac{d^4 k}{(2\pi)^4} \Delta_i^*(k) \Pi_{ij}^{(2)}(k) \Delta_j(k) \quad (360) \end{aligned}$$

with the *polarization tensor* up to second order

$$\Pi_{ij}^{(2)}(k) = \delta_{ij} \int \frac{d^4 q}{(2\pi)^4} \frac{\omega_q \omega_{q-k} + \epsilon_q \epsilon_{q-k}}{(\omega_q^2 + \epsilon_q^2)(\omega_{q-k}^2 + \epsilon_{q-k}^2)}. \quad (361)$$

Expanding $\Pi^{(2)}(k)$ to second order in \mathbf{k} , we get the quadratic terms $|\boldsymbol{\Delta}|^2, |\nabla \boldsymbol{\Delta}|^2$ in a Ginzburg-Landau action for $\boldsymbol{\Delta}$, analogous to Eq. (295). We complete the Ginzburg-Landau action adding the zero-momentum fourth order term $|\boldsymbol{\Delta}|^4$.

⁵⁰ At any time we may invoke rotational symmetry to restore general axes.

Comment 2

Here we are dealing with equilibrium statistical mechanics, so that we have no time-dependence. Therefore the absence of time-dependence is not a shortcoming of the saddle point, as is sometimes implied in the literature. For example the classical saddle point in Eq. (149) obviously does not exclude time-dependent dynamics.

The gap equation Eq. (336) selects one particular trajectory, meaning we abandon doing the path integral. Since in our approach **quantisation** is effected by path integrals, the gap equation is always a **classical** statement and we neglect quantum effects associated with the path-integral over $\boldsymbol{\Delta}$. Quantum effects associated with ψ were treated exactly.

So you may ask yourself how we got a quantum result with \hbar showing up explicitly in e.g. the critical temperature Eq. (347)? Recall, that an enormous amount of physics was smuggled in, when we were required to do the integral in Eq. (347) over $d^3 k$. Stuff like the Fermi surface, Debye frequencies etc. All of these are quantum effects.

Why in contrast to this in our modeling ferromagnetism Eqs. (296) no quantum vestige shows up? The quantum effects there are hidden in the non-universal quantities c_1, c_2, c_4 .

Exercise 6.4

Expand $\Pi^{(2)}(k)$ to second order in ∇k . Extract the Δ^4 -term in the \ln to obtain the **Ginzburg-Landau** action.

Exercise 6.5 (The Meissner effect)

We use the Ginzburg-Landau model for the doubly charged field $\boldsymbol{\Delta}(x)$, renamed φ to unclutter notation, of the previous exercise to study how an applied magnetic field penetrates the superconducting region.

As we are dealing with equilibrium statistical mechanics, there is no time-coordinate. Thus we take as our effective superconducting Euclidean Lagrangian for the doubly charged field φ

$$\mathcal{L}_{GL} = \frac{1}{2M} |\imath \nabla \varphi|^2 + V(\varphi),$$

$$V(\varphi) = -\frac{1}{2} a(T) |\varphi|^2 + \frac{1}{4} b(T) |\varphi|^4, \quad (362)$$

where $M = 2m$. The coefficients a, b are non-universal, but obey

$$a(T) = a'(T_c - T), \quad a' > 0, \quad b(T) > 0.$$

\mathcal{L}_{GL} is invariant under the $U(1)$ -symmetry

$$\varphi(x) \rightarrow \varphi(x) e^{i q \theta}, \quad \theta = \text{constant}. \quad (363)$$

The standard way to couple an electromagnetic field to charged matter, e.g. the charged field of sect. 3.4, is the *minimal coupling*. This replaces the ordinary derivative⁵¹ ∂_μ by the covariant derivative

$$\partial_\mu \rightarrow D_\mu = \partial_\mu + iqA_\mu, \tag{364}$$

where q is the charge of the matter field. Here we only use the spatial part $\nabla \rightarrow \nabla + iq\mathbf{A}$.

Show that under the gauge transformation

$$A_\alpha(x) \rightarrow A_\alpha(x) - \partial_\alpha\eta(x), \varphi(x) \rightarrow \varphi(x)e^{iq\eta(x)} \tag{365}$$

$D_\mu\varphi$ transforms as $\varphi(x)$ and therefore the combination $|D_\mu\varphi|^2$ is invariant. This extends the symmetry of Eq. (130) to the local gauge symmetry as required by the electromagnetic Maxwell Lagrangian $\mathcal{L} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} = \frac{1}{2}(\mathbf{E}^2 - \mathbf{B}^2)$ with $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ and its Euclidean version $\mathcal{L}_E = \frac{1}{2}(\mathbf{E}^2 + \mathbf{B}^2)$.

Under minimal coupling our Euclidean Lagrangian Eq. (362) becomes

$$\mathcal{L}_s = \frac{1}{2M} |(\nabla - q\mathbf{A})\varphi|^2 + V(\varphi) + \frac{1}{2}(\nabla \times \mathbf{A})^2, \tag{366}$$

where $M = 2m, q = 2e$ and $\mathbf{B} = \nabla \times \mathbf{A}$ and we added a magnetic, but not an electric term.

We now make two comments.

Comment 3

Whatever transformation or field expansions we perform, the gauge invariance Eq. (365) **will always hold**. Otherwise we would not even be able to compute the gauge-invariant magnetic field as $\mathbf{B} = \nabla \times \mathbf{A}$. A gauge transformation just changes the way we describe the system, leaving the physics invariant.

Comment 4

We will use our gauge freedom to choose particular gauges for our convenience. Recall that choosing the Coulomb gauge $\nabla \cdot \mathbf{A} = 0$, instead of the relativistically invariant gauge $\partial_\mu A^\mu = 0$, is convenient, because the field \mathbf{A} will be transversal in this gauge. Yet this does not mean that we are obliged to break relativistic invariance.

Only gauge-invariant quantities are observables. Statements involving gauge dependent fields like \mathbf{A}, φ , may be true in one gauge, but not in another: they are gauge dependent and may therefore be misleading.

Show that the equation of motion for \mathbf{A} is

$$\nabla^2 \mathbf{A} - \nabla(\nabla \cdot \mathbf{A}) = -\nabla \times \mathbf{B} = -\mathbf{j} \tag{367}$$

with the gauge invariant current

$$\mathbf{j} = \frac{iq}{2}(\varphi^*\nabla\varphi - \varphi\nabla\varphi^*) - \frac{q^2}{M}|\varphi|^2\mathbf{A}. \tag{368}$$

For $T > T_c$ the potential $V(\varphi)$ has a minimum at $|\varphi| = 0$, but for $T < T_c$ the minimum is at

$$|\varphi|^2 = a/b = n_s,$$

where n_s is the density of the superconducting carriers. This minimum condition leaves the phase $\theta(x)$ of the complex field $\varphi(x) = \rho(x)e^{i\theta(x)}$ undetermined.

To simplify our life, we choose the particular gauge in which $\varphi(x)$ is real, i.e. we set $\theta(x) = 0$. Choosing this phase for $\varphi(x)$, we have spontaneously broken the $U(1)$ -symmetry Eq. (363), although this is a gauge-dependent statement. For $T < T_c$ we expand around the minimum as

$$\varphi(x) = \sqrt{n_s} + \chi(x), \chi = real. \tag{369}$$

The Lagrangian now becomes

$$\begin{aligned} \mathcal{L}_s &= \frac{1}{2M} [(\nabla\chi)^2 + q^2(\sqrt{n_s} + \chi)^2\mathbf{A}^2] \\ &\quad - V(\sqrt{n_s} + \chi) + \frac{1}{2}(\nabla \times \mathbf{A})^2 \\ &= \frac{1}{2M}(\nabla\chi)^2 + a(T)\chi^2 + \frac{m^2}{2}\mathbf{A}^2 + \frac{1}{2}(\nabla \times \mathbf{A})^2 \\ &\quad + \frac{q^2}{2M}(2\sqrt{n_s}\chi + \chi^2)\mathbf{A}^2 + (higher\ order\ \chi\ terms) \end{aligned} \tag{370}$$

with $m^2 = \frac{q^2 a}{Mb} = \frac{q^2 n_s}{M}$.

Taking the rotational of Eq. (367) yields, upon neglecting fluctuations of the field χ

$$\nabla^2 \mathbf{B} = m^2 \mathbf{B}. \tag{371}$$

Consider a superconducting material confined to the half-space $z > 0$ with a magnetic field applied parallel to the bounding surface, e.g. $\mathbf{B} = B\hat{x}$. Show that inside the superconducting medium, the magnetic field decreases exponentially with *magnetic length*

$$\xi_B = \frac{1}{m^2} = \sqrt{\frac{bM}{aq^2}} = \sqrt{\frac{bM}{a'q^2}}(T_c - T)^{-1/2}. \tag{372}$$

The χ -dependent quadratic part of \mathcal{L}_s shows, that the *coherence length* of the order parameter field χ is

$$\xi_\chi = [2Ma'(T_c - T)]^{-1/2}. \tag{373}$$

Show that the equation of motion for φ is

$$\frac{1}{2M}(\nabla - q\mathbf{A})^2\varphi - a(T)\varphi + b(T)|\varphi|^2\varphi = 0. \tag{374}$$

⁵¹ We are using units $c = \hbar = 1$.

Using this equation show that

$$\nabla \cdot \mathbf{j} = -\frac{q^2 |\varphi|^2}{M} \nabla \cdot \mathbf{A}. \quad (375)$$

In our gauge Eq. (368) becomes London's equation

$$\mathbf{j} = -\frac{q^2}{M} (\sqrt{n_s} + \chi)^2 \mathbf{A}. \quad (376)$$

To check what happens, if we keep the θ -field, let us neglect fluctuations in ρ and set $\rho = \sqrt{n_s}$

$$\varphi(x) = \sqrt{n_s} e^{i\theta(x)}. \quad (377)$$

The Lagrangian then becomes, up to a constant

$$\mathcal{L}_s = \frac{n_s}{2M} (\nabla\theta - q\mathbf{A})^2 + \frac{1}{2} (\nabla \times \mathbf{A})^2. \quad (378)$$

We define a new gauge-invariant field $\tilde{\mathbf{A}}$ as

$$q\tilde{\mathbf{A}} = q\mathbf{A} - \nabla\theta \quad (379)$$

to get

$$\mathcal{L}_s = \frac{m^2}{2} \tilde{\mathbf{A}}^2 + \frac{1}{2} (\nabla \times \tilde{\mathbf{A}})^2. \quad (380)$$

The θ -field has disappeared into the massive $\tilde{\mathbf{A}}$ -field and there is no trace left of gauge transformations.

Exercise 6.6

Obtain the Lagrangian analogous to Eq. (378), keeping a fluctuating ρ -field.

Exercise 6.7 (Resistance conduction)

The designation *superconductor* calls to mind the absence of resistance to current flow. Current flow, unless stationary, is a time-dependent phenomenon, outside of equilibrium statistical mechanics. Yet, let us suppose Eq. (368) to be true for slowly varying time-dependent phenomena. Consider the situation, when the order parameter is φ is constant – $\nabla\varphi = 0$ – and take the time-derivative of Eq. (368)

$$\frac{d\mathbf{j}}{dt} = -\frac{q^2 n_s}{M} \frac{d\mathbf{A}}{dt}. \quad (381)$$

Since we have not included the scalar potential A_0 in our formulation, we are obliged to use a gauge in which $A_0 = 0$ yielding $\mathbf{E} = -\partial_t \mathbf{A}$. Hence we get

$$\frac{d\mathbf{j}}{dt} = \frac{q^2 n_s}{M} \mathbf{E}. \quad (382)$$

Check that from Newton's equation $\mathbf{F} = q\mathbf{E} = M \frac{\partial \mathbf{v}}{\partial t}$ and $\mathbf{J} = qn_s \mathbf{v}$, we get exactly Eq. (382): current flows without resistance! Resistive flow would modify Newton's equation as

$$M \frac{\partial \mathbf{v}}{\partial t} = -M/\tau \mathbf{v} + \mathbf{E}, \quad (383)$$

where τ is a time constant characterizing the friction.

Comment 5

Suppose we include a τ dependence in our GL model Eq. (366), adding the terms⁵²

$$\frac{1}{2M} |(\partial_\tau - qA_0)\varphi|^2, \quad \frac{1}{4} F_{0i} F^{0i},$$

which are dictated by gauge-invariance. One then argues that this leads to the appearance of an electric field through $\mathbf{E} = -i\partial_\tau \mathbf{A}$ and taking the τ -derivative of Eq. (368) one gets

$$-i\partial_\tau \mathbf{J} = \frac{q^2 n_s}{M} \mathbf{E}.$$

Then, appealing to analytic continuation, use $-i\partial_\tau = \partial_t$ to recover Eq. (382).

But notice, that we started from a theory indexed by $[t, x, y, z]$ and analytically continued to $[\tau, x, y, z]$, having traded time for temperature: we cannot have both! In fact, if we now continue back reinstating a time variable, we would describe a theory, where our potential $V(\varphi)$ would have time-dependent coefficients a, b . This is not what you want!

You may see many papers in the literature about GL models including time dependence, quantising them etc. Nothing wrong with this, but this is not supported by our microscopic model (which actually may not mean that much, given that our model is extremely simple, probably as simple as possible with a lot of physics injected by hand).

Exercise 6.8 (The Higgs Mechanism)

The Higgs mechanism is the relativistic analog of the Meissner effect of the previous exercises. To illustrate it, we will use our singly charged complex scalar field φ with Lagrangian

$$\mathcal{L}_M = \frac{1}{2} (\partial_\alpha \varphi)^* (\partial^\alpha \varphi) - V(\varphi) \quad (384)$$

where $V(\varphi) = -\frac{1}{2} \mu^2 \varphi^* \varphi + \frac{1}{4} \lambda (\varphi^* \varphi)^2$, $\lambda > 0$. \mathcal{L}_M is invariant under the $U(1)$ symmetry given by Eq. (130), namely

$$\varphi \rightarrow \varphi e^{i\eta} \quad (385)$$

with constant η . Minimally coupling φ to an electromagnetic field with the substitution

$$\partial_\alpha \rightarrow D_\alpha = \partial_\alpha + iqA_\alpha, \quad (386)$$

⁵² Notice that these time-dependent terms are unrelated the non-commutativity of q and p . In fact in Eq. (211) we chose Δt small enough, in order to be able to ignore this effect.

we get

$$\mathcal{L} = -\frac{1}{4}F_{\alpha\beta}F^{\alpha\beta} + \frac{1}{2}(D_\alpha\varphi)^*(D^\alpha\varphi) - V(\varphi). \tag{387}$$

\mathcal{L} is now invariant under the gauge transformation (365).

For $\mu^2 < 0$ the potential $V(\varphi)$ has a minimum at $\varphi = 0$, but for $\mu^2 > 0$ the minimum is at the constant non-zero value

$$|\varphi|^2 = \frac{\mu^2}{\lambda} \equiv v^2. \tag{388}$$

We therefore expand the field $\varphi(x)$ around this minimum as

$$\varphi(x) = e^{i\chi(x)/v} (v + \sigma(x)) = v + \sigma + i\chi(x) + \dots \tag{389}$$

The field $\chi(x)$ is called *Nambu-Goldstone* and $\sigma(x)$ the *Higgs* boson. Obviously we explicitly maintain gauge invariance.

Show that the Lagrangian becomes

$$\begin{aligned} \mathcal{L} = & -\frac{1}{4}\tilde{F}_{\alpha\beta}\tilde{F}^{\alpha\beta} \\ & + \partial_\alpha\sigma\partial^\alpha\sigma + (v + \sigma)^2(qA_\alpha + \partial_\alpha\chi/v)^2 - V(v + \sigma). \end{aligned} \tag{390}$$

As before we introduce the **gauge-invariant** field \tilde{A}_α as

$$q\tilde{A}_\alpha = qA_\alpha - \frac{1}{v}\partial_\alpha\chi. \tag{391}$$

This absorbs the Nambu-Goldstone boson into the \tilde{A}_α -field and the Lagrangian becomes

$$\begin{aligned} \mathcal{L} = & -\frac{1}{4}\tilde{F}_{\alpha\beta}\tilde{F}^{\alpha\beta} + \frac{m_A^2}{2}\tilde{A}_\alpha\tilde{A}^\alpha \\ & + \frac{1}{2}\partial_\alpha\sigma\partial^\alpha\sigma - \frac{1}{2}m_\sigma^2\sigma^2 \\ & + \frac{1}{2}e^2\sigma(2v + \sigma)\tilde{A}_\alpha\tilde{A}^\alpha - \lambda v\sigma^3/16 - \lambda\sigma^4/4, \end{aligned} \tag{392}$$

with the vector and boson field's masses

$$\begin{aligned} m_A^2 &= (ev)^2 = e^2\mu^2/\lambda, \\ m_\sigma^2 &= \mu^2 + 3\lambda v^2/4 = 7\mu^2/4. \end{aligned} \tag{393}$$

The Nambu-Goldstone boson has disappeared from the Lagrangian and we are left with a massive vector field and no gauge freedom.

Exercise 6.9

Repeat the previous exercise using the gauge in which φ is real.

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