
Nonequilibrium Relativistic Quantum Many-Body Theory

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Introduction

The following manuscript aims at an introduction to modern methods in relativistic quantum many-body theory. In the recent years the interest in this topic has been triggered by the developments in **heavy-ion physics**, where the creation of strongly interacting matter in collisions of nuclei and its properties are studied (mostly at the Relativistic Heavy Ion Collider (RHIC) at the Brookhaven National Lab (BNL) and the Large Hadron Collider (LHC) at CERN). There are many indications for the creation of a deconfined state of matter, the **Quark-Gluon Plasma (QGP)**, which quickly thermalizes and can be described with (ideal and viscous) hydrodynamical models, describing the **collective motion** of the particles in the sense of a perfect or nearly perfect fluid. Here, the question of the off-equilibrium properties of the very early phases and the microscopic mechanisms behind the very quick thermalization are of particular interest. In any case, the fireball is a rapidly expanding system, and the medium is undergoing a transition from the deconfined “partonic” state to a hadronic many-body system, and observable are only the **asymptotically free** hadrons, photons, and leptons hitting the detectors. Other interesting questions involve the chiral phase transition in the light-quark sector of QCD and the implications for heavy-ion observables, particularly **electromagnetic probes** (lepton-antilepton pairs, aka. dileptons, photons) and the properties of hadrons in dense and hot hadronic matter. Another important topic is the identification of observables indicating a possible first-order chiral and or deconfinement phase transition in **compressed baryonic matter** which may be achievable in heavy-ion collisions at lower collision energies (beam-energy scan at RHIC, upcoming FAIR and NICA experiments).

In this manuscript we introduce many-body techniques, using relativistic quantum field theory, emphasizing the so-called **real-time formulation**, which allows the investigation of **dynamical properties** of quantum systems. We start with a thorough discussion of **thermal equilibrium**, where the **closed real time-path formalism of Schwinger and Keldysh** is extended by an **imaginary-time path**, leading to a unification of the real-time methods with the older imaginary-time (Matsubara) formalism via analytic continuation. Later, we shall consider more general **off-equilibrium situations**, concentrating on the derivation of semiclassical **transport equations** from the underlying microscopic quantum-field theoretical models. Despite its great practical applicability to the analysis of many-body systems off thermal equilibrium, it also helps to answer the fundamental question, how the classical description of matter and fields (mostly the electromagnetic field) emerges from the underlying fundamental quantum theory.

This manuscript is organized as follows: After a brief reminder about the description of free scalar and spin-1/2 (Dirac) particles in the first chapter, in the second chapter we investigate many-body systems of interacting particles in thermal equilibrium within the **operator formalism of relativistic quantum field theory**, using **canonical quantization**. The main goal is to establish the **thermal Feynman-diagram rules** for the evaluation of **Green’s functions** in the **Schwinger-Keldysh real-time formalism**. To achieve this goal we work from the very beginning with **generating functionals** with simple field theoretical models like ϕ^4 theory or the linear σ model. We shall also introduce the **path-**

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integral methods, which are equivalent to the operator formalism for the simple models studied before, but are of great advantage in the treatment of **gauge theories**, which underly the **standard model of elementary particles** and are thus of particular interest. Here we shall also begin with **quantum electrodynamics** and then generalize to non-abelian gauge theories on the example of QCD.

In chapter 3 we shall generalize all these qft techniques to the off-equilibrium case, starting from the **Baym Φ functional** to derive the **Kadanoff-Baym equations**, which are the “master equations” for quantum transport. Since today they are only (numerically) treatable for the most simple qft models like ϕ^4 theory. For this practical reason, but also the above mentioned fundamental questions, we further derive **semiclassical transport equations**, using the **gradient-expansion method** for “coarse graining” over the microscopic degrees of freedom to achieve an effective description of the “slow” macroscopic collective quantities of interest. As we shall then see, the connection with the equilibrium methods of chapter 2 is given by **linear response theory**, leading to a microscopic foundation of **transport coefficients** like **viscosity, drag- and diffusion coefficients, and heat conductivity**.

Despite the many references in the text, here I mention some more general textbooks and review papers, which of course I also used in preparing this manuscript: Among the many texts on **many-body quantum field theory**, using both the real- and the imaginary-time formalism in the equilibrium case, I recommend [KB61, Mil69, CSHY85, Lv87, LeB96, KG06, Kam11]. An excellent source to learn about the Schwinger-Keldysh formalism is [Dan84], where the methods are used in nonrelativistic qft. For the non-equilibrium methods I used [BM90, KV96, IKV99, GL98, IKV00, KIV01, Ber02, CH08, Cas09].

Part I

Equilibrium Theory

Chapter 1

Introduction to quantum-field theory: Free fields

In this chapter, we shall briefly summarize the basic concepts of **relativistic quantum field theory** within the **canonical operator quantization formalism**. We begin with the basic concept of **Poincaré invariance** and introduce the three types of fields needed in elementary-particle physics: bosons with spin 0 (scalar fields), fermions with spin 1/2 (Dirac fields), and massless bosons with spin 1 (photons). Then we shall remind the reader about basic physical concepts as **cross sections** in **scattering theory**, the notion of **asymptotic states**, and **many-body theory** in thermal equilibrium. Here we shall restrict ourselves to the most simple treatment of ideal gases by calculating the corresponding partition sums within the operator formalism.

1.1 Poincaré invariance

In this section we introduce the most important basics about the special relativistic structure of spacetime, **Minkowski space**. We also define our notation and the use of **natural units**, i.e., we set

$$\hbar = c = 1. \quad (1.1.1)$$

Usually it is customary to measure masses, energies and momenta in MeV or GeV and lengths and times in fm. To convert fm in MeV^{-1} we only need the constant [A⁺08]

$$\hbar c = 197.3269631(49) \text{ MeV fm}. \quad (1.1.2)$$

Special-relativistic spacetime is described as an affine four-dimensional real space, on which a **fundamental bilinear form** (or “pseudo-metric”) with signature (1, 3) is defined. Using a **orthonormalized basis** at an arbitrary point in spacetime, the components (**covariant tensor components** of this bilinear form read

$$(g_{\mu\nu}) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \quad (1.1.3)$$

The pseudo-Euclidean \mathbb{R}^4 with this fundamental form is called **Minkowski space**. In the following we also use column vectors for contravariant vector components,

$$(x^\mu) = \begin{pmatrix} x^0 \\ x^1 \\ x^2 \\ x^3 \end{pmatrix} = \begin{pmatrix} x^0 \\ \vec{x} \end{pmatrix}. \quad (1.1.4)$$

The fundamental form defines the **Minkowski product** for two four-vectors as

$$x \cdot y = g_{\mu\nu} x^\mu y^\nu = x^0 y^0 - \vec{x} \cdot \vec{y}, \quad (1.1.5)$$

where over equal indices is summed (**Einstein's summation convention**). The usual scalar product in Euclidean \mathbb{R}^3 is written as $\vec{x} \cdot \vec{y} = x^1 y^1 + x^2 y^2 + x^3 y^3$ das "übliche Skalarprodukt im Euklidischen \mathbb{R}^3 bezeichnet. The covariant components of a vector are given with help of the covariant components of the fundamental form,

$$(x_\mu) = (g_{\mu\nu} x^\nu) = (x^0, -x^1, -x^2, -x^3) = (x^0, -\vec{x}^t), \quad (1.1.6)$$

where the superscript t denotes transposition of a matrix, i.e., \vec{x}^t is the row vector (x^1, x^2, x^3) .

Accordingly $g^{\mu\nu}$ are the contravariant components of the fundamental form. Since for any four-vector

$$x^\mu = g^{\mu\nu} x_\nu = g^{\mu\nu} g_{\nu\sigma} x_\sigma, \quad (1.1.7)$$

we must have

$$g^{\mu\nu} g_{\nu\sigma} = \delta_\sigma^\mu = \begin{cases} 1 & \text{for } \mu = \nu, \\ 0 & \text{for } \mu \neq \nu, \end{cases} \quad (1.1.8)$$

leading to

$$(g^{\mu\nu}) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \quad (1.1.9)$$

The four-vectors $x \in \mathbb{R}^4$ can be classified into three types,

$$x \cdot x = x^2 \begin{cases} > 0 & \text{time like,} \\ = 0 & \text{light like,} \\ < 0 & \text{space like.} \end{cases} \quad (1.1.10)$$

A linear transformation in Minkowski space that leaves the fundamental form between any pair of four-vectors invariant is a **Lorentz transformation**. As any linear mapping, a Lorenta transformation can be described with respect to an arbitrary basis as a matrix $(\Lambda^\mu{}_\nu)$. Then the contravariant components behave under Lorentz transformations as

$$x'^\mu = \Lambda^\mu{}_\nu x^\nu. \quad (1.1.11)$$

Since the Minkowski products stay unchanged under this transformation, we must have

$$g_{\mu\nu} x'^\mu y'^\nu = g_{\mu\nu} \Lambda^\mu{}_{\mu'} \Lambda^\nu{}_{\nu'} x^{\mu'} y^{\nu'} = g_{\mu'\nu'} x^{\mu'} y^{\nu'}. \quad (1.1.12)$$

Since this should hold true for all $x, y \in \mathbb{R}^4$ we necessarily have

$$g_{\mu\nu} \Lambda^\mu{}_{\mu'} \Lambda^\nu{}_{\nu'} = g_{\mu'\nu'}. \quad (1.1.13)$$

Using the "index-dragging convention" also for Minkowski matrices, this can be written as

$$(g_{\mu\nu} \Lambda^\mu{}_{\mu'} g^{\mu'\sigma}) \Lambda^\nu{}_{\nu'} = \Lambda_\nu{}^\sigma \Lambda^\nu{}_{\nu'} = \delta_{\nu'}^\sigma. \quad (1.1.14)$$

Thus a Lorentz transformation is invertible with the inverse given by

$$(\Lambda^{-1})^\mu{}_\nu = \Lambda_\nu{}^\mu. \quad (1.1.15)$$

In matrix-vector notation this means

$$\Lambda^{-1} = g \Lambda^t g, \quad (1.1.16)$$

where we understand Λ as the matrix given in its form with the first index as superscript and the second as subscript. Obviously describes any matrix Λ which fulfills (1.1.16) a Lorentz transformation.

Obviously the Lorentz transformations build a group with the composition of transformations, i.e., matrix multiplications of the corresponding Lorentz matrices, as the group product. Indeed, if Λ_1 and Λ_2 leave the Lorentz products of any pair of four-vectors invariant so does the composition $\Lambda_1 \Lambda_2$. Obviously for this transformation also (1.1.16) is valid, since because of $g^2 = \mathbb{1}$ we have

$$g(\Lambda_1 \Lambda_2)^t g = g \Lambda_2^t \Lambda_1^t g = (g \Lambda_2^t g)(g \Lambda_1^t g) = \Lambda_2^{-1} \Lambda_1^{-1} = (\Lambda_1 \Lambda_2)^{-1}, \quad (1.1.17)$$

which means that $\Lambda_1 \Lambda_2$ obeys the condition (1.1.16) for representing a Lorentz transformation.

The physical meaning of the Lorentz transformations becomes clear, when we consider the two most significant spacial cases, i.e.,

- (i) rotations of the basis for the spatial part of four-vectors,
- (ii) uniform rectilinear motion of one reference frame with respect to another one, called a **rotation free Lorentz boost**.

An example for spatial rotations is given by the matrix for the rotation around the 3-axis with an angle $\phi \in [0, 2\pi)$:

$$D_3(\phi) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos \phi & \sin \phi & 0 \\ 0 & -\sin \phi & \cos \phi & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \quad (1.1.18)$$

A rotation free Lorentz boost has the parametrization

$$B_3(\eta) = \begin{pmatrix} \cosh \eta & 0 & 0 & -\sinh \eta \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -\sinh \eta & 0 & 0 & \cosh \eta \end{pmatrix} \quad (1.1.19)$$

with the parameter, $\eta \in \mathbb{R}$. To understand the physical meaning of this quantity, called **rapidity**, we use (1.1.19) for the transformation of contravariant four-vector components,

$$x' = B_3(\eta)x = \begin{pmatrix} x^0 \cosh \eta - x^3 \sinh \eta \\ x^1 \\ x^2 \\ -x^0 \sinh \eta + x^3 \cosh \eta \end{pmatrix}. \quad (1.1.20)$$

Consider now the spatial origin of the reference frame Σ' by setting $x'^1 = x'^2 = x'^3 = 0$ we find that this point moves in Σ according to

$$x^1 = x^2 = 0, \quad x^3 = x^0 \tanh \eta = t \tanh \eta. \quad (1.1.21)$$

This means that Σ' with respect to Σ along of its 3-axis with velocity $v = \tanh \eta$. We see immediately that $|v| = |\tanh \eta| < 1$, i.e., one inertial reference frame can move only with a velocity smaller than the speed of light with respect to any other inertial frame.

We can also express the boost (1.1.19) directly in terms of the velocity, using the properties of hyperbolic functions,

$$\cosh \eta = \frac{1}{\sqrt{1-v^2}} := \gamma(v), \quad \sinh \eta = \frac{v}{\sqrt{1-v^2}} = v\gamma(v). \quad (1.1.22)$$

Analogously to (1.1.18) and (1.1.19) we can also write down rotations around or a boost along an arbitrary spatial axis. The latter is given by

$$B(\vec{v}) = \begin{pmatrix} \gamma & -\vec{v}^t \gamma \\ -\vec{v} \gamma & \mathbb{1} + (\gamma - 1) \vec{v} \otimes \vec{v} / v^2 \end{pmatrix}. \quad (1.1.23)$$

Here $\vec{a} \otimes \vec{b}$ denotes the **dyadic** product between two three-vectors, i.e., a matrix with the elements

$$(\vec{a} \otimes \vec{b})_{ij} = a^i b^j, \quad (1.1.24)$$

and the matrix multiplication of this object with a column vector from the left has the meaning

$$(\vec{a} \otimes \vec{b} \vec{c})_i = a^i b^j c^j = a_i \vec{b} \cdot \vec{c}. \quad (1.1.25)$$

The action of a boost (1.1.23) on the components of an arbitrary four-vector is thus given by

$$B(\vec{v})x = \begin{pmatrix} \gamma(x^0 - \vec{v} \cdot \vec{x}) \\ \vec{x} - (\gamma - 1) \vec{v} (\vec{v} \cdot \vec{x}) / v^2 + \gamma \vec{v} x^0 \end{pmatrix}. \quad (1.1.26)$$

Finally we note that rotations around an arbitrary fixed axis or boosts along an arbitrary direction are one-parameter subgroups of the Lorentz group, because according to the rules for the addition of arguments of trigonometric or hyperbolic functions one immediately sees (using the three axis as rotation axis or boost direction, respectively) we find

$$D_3(\phi_1)D_3(\phi_2) = D_3(\phi_1 + \phi_2), \quad B_3(\eta_1)B_3(\eta_2) = B_3(\eta_1 + \eta_2). \quad (1.1.27)$$

In addition to the Lorentz group which describes transformations of space time for which one point (here chosen as the origin of the reference frame) is held fixed. In addition the choice of this origin is physically irrelevant since no space-time point is special compared to any other (homogeneity of space and time). Thus also the translations, $x \rightarrow x' = x - a$ with an arbitrary fixed four-vector, a , are symmetries of space-time. The composition of these space-time translations with Lorentz transformations generate the full symmetry group of Minkowski space-time, the **Poincaré group**, which in this way is defined as the corresponding **semidirect product** of the translation and the Lorentz groups.

A **relativistic description of nature** should respect these fundamental symmetries of nature, at least those that can be continuously deformed from the identity transformation (the Poincaré group's unit element). Without prove we note that the so-called **proper orthochronous Lorentz transformations** are connected continuously with the group identity. A proper orthochronous Lorentz transformation is represented by Lorentz matrices with determinant 1 and the component $\Lambda^0_0 \geq 1$. The latter condition means that the **order of time** is not changed with such Lorentz transformations, i.e., the sign of the time-component of any time-like vector does not change under such Lorentz transformations. The proper orthochronous Lorentz group is denoted as $SO(1,3)^\uparrow$.

Any Lorentz transformation can be composed of a proper orthochronous one and either a spatical reflection (“parity transformation”) $P = \text{diag}(1, -1, -1, -1)$, which keeps the time ordering intact but has determinant -1 , a time reflection, $T = \text{diag}(-1, 1, 1, 1)$ which has determinant -1 , or both (a full reflection) $\text{diag}(-1, -1, -1, -1)$ which has determinant 1 but changes the sign of time order. The subgroup of the full Lorentz group $O(1, 3)$ which keeps the time direction of any timelike four vector is called the orthochronous Lorentz group $O(1, 3)^\uparrow$. The subgroup of $O(1, 3)$ which consists of Lorentz matrices with determinant 1 (but do not keep necessarily the direction of time) is called $SO(1, 3)$. Any of these subgroups together with the translations of space and time build the corresponding subgroup of the Poincaré group. It turns out that in nature only the proper orthochronous Poincaré group, which is connected continuously to the group unity, is a symmetry group. The weak inter action breaks the symmetry under both parity and time reversal.

We shall also need the “infinitesimal transformations”. Writing

$$\Lambda^\mu{}_\nu = \delta^\mu{}_\nu + \delta\omega^\mu{}_\nu, \quad (1.1.28)$$

we can expand the condition (1.1.13) for Λ being a Lorentz matrix up to $\mathcal{O}(\delta\omega^2)$,

$$g_{\mu\rho}\Lambda^\mu{}_\nu\Lambda^\rho{}_\sigma = g_{\nu\sigma} + \delta\omega_{\rho\sigma} + \delta\omega_{\sigma\rho} + \mathcal{O}(\delta\omega^2) \stackrel{!}{=} g_{\rho\sigma}. \quad (1.1.29)$$

This means that

$$\delta\omega_{\rho\sigma} = -\delta\omega_{\sigma\rho}. \quad (1.1.30)$$

An infinitesimal proper orthochronous Lorentz transformation is thus generated by antisymmetric $\delta\omega_{\mu\nu} = g_{\mu\rho}\delta\omega^\rho{}_\nu$. Since there are six linearly independent antisymmetric 4×4 matrices, the proper orthochronous Lorentz group is a six-dimensional Lie group. Natural generators are those for rotation-free boosts $\delta\omega_{0\nu}$ and spatial rotations $\delta\omega_{mn}$ with $m, n \in \{1, 2, 3\}$.

1.2 Free scalar bosons

Now we come to the most simple case of a relativistic quantum field theory. We start with a classical **scalar field** $\phi \in \mathbb{C}$, which behaves under Poincaré transformations as

$$x^\mu \rightarrow x'^\mu = \Lambda^\mu{}_\nu x^\nu - a, \quad \phi'(x') = \phi(x) = \phi[\Lambda^{-1}(x' + a)] \quad \text{with } \Lambda \in SO(1, 3)^\uparrow, \quad a \in \mathbb{R}^4. \quad (1.2.1)$$

The most simple method to develop dynamical field equations that obey given symmetries is to use **Hamilton’s least-action principle**. As we shall see in a moment that has also great heuristical advantages compared to guessing directly such field equations.

Hamilton’s principle in its **Lagrangian form** derives the equations of motion as the stationary points of the action functional

$$S[\phi] = \int_{\mathbb{R}^4} d^4x \mathcal{L}(\phi, \partial_\mu\phi) \quad \text{with} \quad \partial_\mu\phi = \frac{\partial\phi}{\partial x^\mu}. \quad (1.2.2)$$

If we use a Lagrangian density, \mathcal{L} , that is a Lorentz scalar, we will get Poincaré covariant field equations by the stationarity condition

$$\delta S[\phi] = \int_{\mathbb{R}^4} d^4x \left[\delta\phi \frac{\partial\mathcal{L}}{\partial\phi} + \delta(\partial_\mu\phi) \frac{\partial\mathcal{L}}{\partial\dot{\phi}} \right] \stackrel{!}{=} 0. \quad (1.2.3)$$

By definition, in the variation only the fields are varied, while the space-time coordinates are kept fixed. Thus we have

$$\delta(\partial_\mu \phi) = \partial_\mu \delta \phi, \quad (1.2.4)$$

and thus we can integrate the second expression in (1.2.3) by parts to obtain

$$\Delta S[\phi] = \int_{\mathbb{R}^4} d^4x \delta \phi \left[\frac{\partial \mathcal{L}}{\partial \phi} - \partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} \right] \stackrel{!}{=} 0. \quad (1.2.5)$$

Since this stationarity condition must hold for *any* $\delta \phi$, we can conclude that necessarily the field ϕ must obey the **Lagrange equations of motion**

$$\frac{\partial \mathcal{L}}{\partial \phi} - \partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} = 0. \quad (1.2.6)$$

We should note that in principle we have *two* real field-degrees of freedom, namely $\text{Re } \phi$ and $\text{Im } \phi$, and we could vary these two components, or equivalently ϕ and its conjugate complex ϕ^* , independently of each other. However, as long as we choose \mathcal{L} to be **real**, which we essentially have to fulfill in order to get a unitary Hamilton operator in the later derivation of a quantum field theory¹. Then the variation with respect to ϕ^* will only give the conjugate complex of the equation of motion (1.2.6) (*why?*).

Here we consider **free or non-interacting fields**, which are defined as derived from a Lagrange density that is of second order in the fields only. With the field ϕ and its derivative $\partial_\mu \phi$ we can essentially only build one Poincaré invariant real Lagrangian, namely

$$\mathcal{L} = (\partial_\mu \phi^*)(\partial^\mu \phi) - m^2 \phi^* \phi. \quad (1.2.7)$$

The choice of the sign of the terms in this expression will become clear in a moment. The equations of motion (1.2.6) for this Lagrangian reads

$$-m^2 \phi^* - \square \phi^* = 0, \quad -m^2 \phi - \square \phi = 0 \quad \text{with} \quad \square := \partial_\mu \partial^\mu = \partial_t^2 - \Delta. \quad (1.2.8)$$

Here, the first equation is given by the variation of the action functional wrt. ϕ and the second one by variation wrt. ϕ^* . As expected both equations are conjugate complex to each other, and thus we have to deal only with the latter equation, which is the Klein-Gordon equation.

We will not go into the issue of whether one can interpret this **Klein-Gordon equation** in the sense of a single-particle wave equation as with the Schrödinger equation in the non-relativistic case. For a discussion of this see, e.g., [PS95]. Here we will immediately **quantize** this classical field theory canonically. The corresponding **quantum field theory** is a many-body theory including the possibility of particle creation and destruction processes as is common for reactions at relativistic energies and momenta².

The canonical formalism is derived in close analogy to the case of classical mechanics. First we define the **conjugate field momenta**, one for each *real* field-degree of freedom. In our case we use the formalism

¹One should note that this is not a necessary condition since a given set of equations of motion for a set of fields can be derived from different Lagrangians, \mathcal{L} . Indeed, it is easy to show that any Lagrangian density \mathcal{L}' which differs from \mathcal{L} only by a total four-divergence of a vector function $\Omega^\mu(\phi)$ of the fields ϕ only (*exercise!*).

²A reaction with a “relativistic energy” is by definition one, where the total kinetic energy of the reacting particles become at the order of the mass of at least one of the particle species involved in the model.

to vary ϕ and ϕ^* as independent fields, which is somewhat more convenient than to work with real and imaginary part of ϕ . Thus we define

$$\Pi = \frac{\partial \mathcal{L}}{\partial \dot{\phi}} = \dot{\phi}^*, \quad \Pi^* = \frac{\partial \mathcal{L}}{\partial \dot{\phi}^*} = \dot{\phi}. \quad (1.2.9)$$

One should note that at this point we leave the manifest covariant formalism since the canonical description treats the time derivatives of the fields differently from the spatial derivatives. The Hamilton density is then given by

$$\begin{aligned} \mathcal{H}(\phi, \Pi, \vec{\nabla}\phi) &= \dot{\phi}\Pi + \dot{\phi}^*\Pi^* - \mathcal{L} = 2|\dot{\phi}|^2 - \left[|\dot{\phi}|^2 - (\vec{\nabla}\phi^*) \cdot (\nabla\phi) - m^2|\phi|^2 \right] \\ &= |\Pi|^2 + (\vec{\nabla}\phi^*) \cdot (\nabla\phi) + m^2|\phi|^2. \end{aligned} \quad (1.2.10)$$

Now we “quantize” the system by taking the fields as operators on a Hilbert space, fulfilling the **canonical equal-time commutation relations**

$$\begin{aligned} [\phi(t, \vec{x}), \phi(t, \vec{y})] &= [\Pi(t, \vec{x}), \Pi(t, \vec{y})] = 0, \quad [\phi(t, \vec{x}), \Pi(t, \vec{y})] = i\delta^{(3)}(\vec{x} - \vec{y}), \\ [\phi^\dagger(t, \vec{x}), \phi(t, \vec{y})] &= [\Pi^\dagger(t, \vec{x}), \Pi(t, \vec{y})] = [\phi^\dagger(t, \vec{x}), \Pi(t, \vec{y})] = 0. \end{aligned} \quad (1.2.11)$$

Furthermore, for the following it is convenient to consider the fields on a **finite spatial volume**, which we chose as the cube $C_L = [0, L] \times [0, L] \times [0, L]$ with the edge of length L . Since we are finally interested in the limit $L \rightarrow \infty$, the choice of the boundary conditions at the edges of the cube is irrelevant for the final results. Thus we choose periodic boundary conditions, i.e., for all fields we assume

$$\phi(t, \vec{x}) = \phi(t, \vec{x} + L\vec{e}_j) \quad \text{for } j \in \{1, 2, 3\}. \quad (1.2.12)$$

The equations of motion for the field operators in the **Heisenberg picture** of time evolution follows from

$$\dot{\phi} = \frac{1}{i} [\phi, \mathbf{H}] = \frac{\delta \mathbf{H}}{\delta \Pi} = \Pi^\dagger, \quad \dot{\Pi} = \frac{1}{i} [\Pi, \mathbf{H}] = -\frac{\delta \mathbf{H}}{\delta \phi} = \Delta\phi^\dagger - m^2\phi^\dagger, \quad (1.2.13)$$

where the Hamilton operator is given by

$$\mathbf{H} = \int_{C_L} d^3\vec{x} \mathcal{H}. \quad (1.2.14)$$

Here, we do not care about the problem of operator ordering in field-operator products at the same space-time point. As we shall see soon, such products are not well defined a priori since because of the equal-time commutation relations (1.2.11) the field operators are distribution valued operators rather than proper linear operators on Hilbert space.

Taking the conjugate complex of the first equation in (1.2.13) and use it in the second equation, we find again that ϕ^\dagger (and through hermitean conjugation thus also ϕ) fulfills the Klein-Gordon equations (1.2.8), now as equations for the field operators.

In order to solve the equations of motion and come to a **many-particle interpretation** of the Hilbert space, we first look for **plane-wave solutions** of the Klein-Gordon equation, i.e., we set

$$\phi(x) = u_{\vec{k}}(t) \exp(i\vec{k} \cdot \vec{x}). \quad (1.2.15)$$

The momenta are constrained to the discrete set $\vec{k} \in 2\pi/L\vec{n}$ with $\vec{n} \in \mathbb{Z}^3$. We find

$$(\square + m^2)\phi(x) = \left[\ddot{u}_{\vec{k}}(t) + \omega_{\vec{k}}^2 u_{\vec{k}}(t) \right] \exp(i\vec{k} \cdot \vec{x}) \stackrel{!}{=} 0 \quad \text{with} \quad \omega_{\vec{k}} = +\sqrt{m^2 + \vec{k}^2}. \quad (1.2.16)$$

The general solution of the equation for the mode function $u_{\vec{k}}$ is given as the superposition of

$$u_{\vec{k}}(t) = N_{\vec{k}} \exp(-i\omega_{\vec{k}} t) \quad \text{and} \quad u_{\vec{k}}(t)^* = N_{\vec{k}} \exp(+i\omega_{\vec{k}} t), \quad (1.2.17)$$

where $N_{\vec{k}} > 0$ is normalization constant to be determined in a moment.

Now we use the corresponding Fourier decomposition for the field *operators*. The “positive-frequency solutions” $u_{\vec{k}}$ corresponds to a particle-annihilation field operator in non-relativistic many-body theory. As we shall see also in a moment, we cannot neglect the “negative-frequency solutions” $u_{\vec{k}}^*$ in building the field operator since (a) we must have a field with two real degrees of freedom corresponding to two species of particles, namely the “particle” and its “antiparticle”, and (b) we want to fulfill the *local* commutation relations (1.2.11). In addition, as we shall prove later, this is also the only possibility to (c) have a **unitary realization of the Poincaré group** which acts locally on the field operators as on the classical counterparts cf. Eq. (1.2.1). The time dependence of $u_{\vec{k}}^*$ however suggests that this “negative-frequency mode” must be related in the mode decomposition of the field operator with a creation operator for a particle moving in direction $-\vec{k}$. Thus we write

$$\phi(x) = \sum_{\vec{k}} \frac{1}{\sqrt{V}} \left[\mathbf{a}(\vec{k}) u_{\vec{k}}(t) + \mathbf{b}^\dagger(-\vec{k}) u_{\vec{k}}^*(t) \right] \exp(i\vec{k} \cdot \vec{x}). \quad (1.2.18)$$

Here $V = L^3$ denotes the quantization volume. Now we note that

$$u_{\vec{k}}(t) \overleftrightarrow{\partial}_t u_{\vec{k}}(t) = 0, \quad u_{\vec{k}}^*(t) \overleftrightarrow{\partial}_t u_{\vec{k}}(t) = -2i\omega_{\vec{k}} N_{\vec{k}}^2 \quad \text{mit} \quad a \overleftrightarrow{\partial}_t b := a \partial_t b - (\partial_t a) b. \quad (1.2.19)$$

Thus we find

$$\begin{aligned} \mathbf{a}(\vec{k}) &= \frac{i}{2\omega_{\vec{k}} N_{\vec{k}}^2} \int_{C_L} \frac{d^3\vec{x}}{\sqrt{V}} \exp(-i\vec{k} \cdot \vec{x}) u_{\vec{k}}^*(t) \overleftrightarrow{\partial}_t \phi(x), \\ \mathbf{b}(-\vec{k}) &= \frac{i}{2\omega_{\vec{k}} N_{\vec{k}}^2} \int_{C_L} \frac{d^3\vec{x}}{\sqrt{V}} \exp(-i\vec{k} \cdot \vec{x}) u_{\vec{k}}^*(t) \overleftrightarrow{\partial}_t \phi^\dagger(x), \end{aligned} \quad (1.2.20)$$

From the canonical equal-time commutation relations (1.2.11) we find

$$\left[\mathbf{a}(\vec{k}), \mathbf{a}^\dagger(\vec{k}') \right] = \left[\mathbf{b}(\vec{k}), \mathbf{b}^\dagger(\vec{k}') \right] = \frac{1}{(2\omega_{\vec{k}})^2 N_{\vec{k}}^4} \delta_{\vec{k}, \vec{k}'}, \quad (1.2.21)$$

where

$$\delta_{\vec{k}, \vec{k}'} = \begin{cases} 1 & \text{for } \vec{k} = \vec{k}', \\ 0 & \text{for } \vec{k} \neq \vec{k}' \end{cases} \quad (1.2.22)$$

denotes the Kronecker symbol for the discrete set of momenta. The similar commutators of all other combinations of annihilation and destruction operators vanishing. The most convenient commutation relations are thus given by the choice

$$N_{\vec{k}} = \frac{1}{\sqrt{2\omega_{\vec{k}}}}. \quad (1.2.23)$$

Thus defining

$$u_{\vec{k}}^-(x) = \frac{1}{\sqrt{2\omega_{\vec{k}}}} u_{\vec{k}}^-(t) \exp(i\vec{k} \cdot \vec{x}), \quad (1.2.24)$$

we can write (1.2.18) after substitution of $\vec{k} \rightarrow -\vec{k}$ in the part with the destruction operator and using $u_{-\vec{k}}^-(t) = u_{\vec{k}}^-(t)$ in the more convenient form

$$\phi(x) = \sum_{\vec{k}} \frac{1}{\sqrt{V}} \left[\mathbf{a}(\vec{k}) u_{\vec{k}}^-(x) + \mathbf{b}^\dagger(\vec{k}) u_{\vec{k}}^{*-}(x) \right]. \quad (1.2.25)$$

The non-trivial commutation relations for the creation and destruction operators are

$$\left[\mathbf{a}(\vec{k}), \mathbf{a}^\dagger(\vec{k}') \right] = \left[\mathbf{b}(\vec{k}), \mathbf{b}^\dagger(\vec{k}') \right] = \delta_{\vec{k}, \vec{k}'}. \quad (1.2.26)$$

Since these are the commutation relations of an infinite set of independent harmonic oscillators, the construction of the Hilbert space is now straight forward. It is spanned by the **occupation-number basis** $\left\{ |N(\vec{k}), \bar{N}(\vec{k})\rangle \right\}$ with $N(\vec{k}), \bar{N}(\vec{k}) \in \mathbb{N}_0 = \{0, 1, 2, \dots\}$. The occupation-number operator for particles and antiparticles are given by

$$\mathbf{N}(\vec{k}) = \mathbf{a}^\dagger(\vec{k}) \mathbf{a}(\vec{k}), \quad \bar{\mathbf{N}}(\vec{k}) = \mathbf{b}^\dagger(\vec{k}) \mathbf{b}(\vec{k}), \quad (1.2.27)$$

and there is one state with all occupation numbers vanishing, the **vacuum state** $|\Omega\rangle$, characterized by

$$\forall \vec{k}: \quad \mathbf{a}(\vec{k}) |\Omega\rangle = \mathbf{b}(\vec{k}) |\Omega\rangle = 0. \quad (1.2.28)$$

The other **normalized** (*check!*) states are given by

$$\left\{ |N(\vec{k}), \bar{N}(\vec{k})\rangle \right\} = \prod_{\vec{k}} \frac{1}{\sqrt{N(\vec{k})! \bar{N}(\vec{k})!}} \left[\mathbf{a}^\dagger(\vec{k}) \right]^{N(\vec{k})} \left[\mathbf{b}^\dagger(\vec{k}) \right]^{\bar{N}(\vec{k})} |\Omega\rangle. \quad (1.2.29)$$

The so constructed Hilbert space is called the **Fock space** and the occupation-number basis also **Fock basis**. Since the creation operators obey *commutation* relations, The Fock states (1.2.29) are symmetric under exchange of these operators, corresponding to a reordering of any particles within the occupation-number state. Thus our formalism with *commutation* relations for the field operators describes **bosons**.

As a final step we have to define **observables** like energy, momentum, and angular momentum. To this end we apply Noether's theorem to the classical field theory (see Appendix A) to the Poincaré symmetry of the action. We start with the translations, i.e.,

$$x'^\mu = x^\mu - \delta a^\mu = x^\mu - \delta a^\nu \delta_\nu^\mu, \quad \phi'(x') = \phi(x). \quad (1.2.30)$$

In the notation of (A.1.1) this means

$$t_\nu^\mu = -\delta_\nu^\mu, \quad T_\nu = 0. \quad (1.2.31)$$

Here we have identified $\delta \eta_a$ with δa^μ . To find the Noether currents, it is most easy to use (A.1.8), which leads to

$$\partial_\nu \Theta_\mu^\nu = \partial_\nu \left[\frac{\partial \mathcal{L}}{\partial (\partial_\nu \phi)} \partial_\mu \phi - \mathcal{L} \delta_\mu^\nu \right]. \quad (1.2.32)$$

Here in the first term a summation over ϕ and ϕ^* is implied. The Noether currents are thus given by the **energy-momentum tensor** of the scalar field (*check!*),

$$\Theta_{\mu}^{\nu} = \frac{\partial \mathcal{L}}{\partial (\partial_{\nu} \phi)} \partial_{\mu} \phi - \mathcal{L} \delta_{\mu}^{\nu} = \partial^{\nu} \phi \partial_{\mu} \phi^* + \partial_{\nu} \phi^* \partial_{\mu} \phi - (\partial_{\rho} \phi^* \partial^{\rho} \phi - m^2 |\phi|^2) \delta_{\mu}^{\nu}. \quad (1.2.33)$$

The tensor $\Theta_{\mu\nu}$ is called the **canonical energy-momentum tensor**. For $\nu = 0$ we get the **densities of energy and momentum**,

$$\mathcal{H} = \Theta_0^0 = |\dot{\phi}|^2 + (\vec{\nabla} \phi^*) \cdot (\vec{\nabla} \phi) + m^2 |\phi|^2, \quad (1.2.34)$$

$$\vec{\mathcal{P}} = \vec{e}_j \Theta^{j0} = -\dot{\phi}^* \vec{\nabla} \phi - \dot{\phi} \vec{\nabla} \phi^*. \quad (1.2.35)$$

Now investigate the corresponding quantized quantities and calculate the operators of total energy (i.e., the Hamilton operator) and momentum in terms of annihilation and creation operators. Without caring about the issue of operator ordering we first write

$$\mathbf{H}' = \int_{C_V} d^3 \vec{x} \left(|\dot{\phi}|^2 + (\vec{\nabla} \phi^*) \cdot (\vec{\nabla} \phi) + m^2 |\phi|^2 \right). \quad (1.2.36)$$

Then we plug in the mode decomposition (1.2.25), leading after some simple manipulations with the integrals

$$\mathbf{H}' = \sum_{\vec{k}} \omega_{\vec{k}} \left[\mathbf{a}^{\dagger}(\vec{k}) \mathbf{a}(\vec{k}) + \mathbf{b}(\vec{k}) \mathbf{b}^{\dagger}(\vec{k}) \right] = \sum_{\vec{k}} \omega_{\vec{k}} \left[\mathbf{N}(\vec{k}) + \bar{\mathbf{N}}(\vec{k}) + \mathbb{1} \right]. \quad (1.2.37)$$

In the last step we have used the commutation relations (1.2.26) and the definition of the occupation-number operators (1.2.27). We see that in (1.2.37) the first two terms in the bracket lead to a physically meaningful interpretation of the quantum-field theoretical formalism in terms of particles: Each particle or antiparticle with momentum \vec{k} carries a *positive energy* of $\omega_{\vec{k}} = \sqrt{\vec{k}^2 + m^2}$, and the total energy is the sum of all these single-particle energies, which is to be expected for *non-interacting particles*. The remaining term, however leads to a **divergence** of the total energy. It is due to the *zero-point energy* of each harmonic oscillator of the field modes, leading to an infinite contribution to the total energy.

On the other hand, the absolute value of the total energy has no physical meaning, and thus we can simply subtract this contribution and **renormalize the total energy** to vanish for the **vacuum state**, i.e., we *define* the proper Hamilton operator of the many-body system as

$$\mathbf{H} = \sum_{\vec{k}} \omega_{\vec{k}} \left[\mathbf{N}(\vec{k}) + \bar{\mathbf{N}}(\vec{k}) \right]. \quad (1.2.38)$$

This procedure of renormalizing observables can be formalized by defining **normal ordering**. This means in the expansion of an operator expression in terms of annihilation and creation operators in any term one brings all annihilation operators of an expression to the right of all creation operators without taking into account the contributions $\propto \mathbb{1}$ from the commutators. This is noted by enclosing the expression into colons. Thus for the **renormalized Hamilton operator** instead of (1.2.36) we write

$$\mathbf{H} = \int_{C_V} d^3 \vec{x} : \left(|\dot{\phi}|^2 + (\vec{\nabla} \phi^*) \cdot (\vec{\nabla} \phi) + m^2 |\phi|^2 \right) :. \quad (1.2.39)$$

We apply the same procedure for the operator of **total momentum**. Using normal ordering we find (*check it*)

$$\vec{\mathbf{P}} = - \int_{C_L} d^3 \vec{x} : \left(\dot{\phi}^* \vec{\nabla} \phi + \dot{\phi} \vec{\nabla} \phi^* \right) : = \sum_{\vec{k}} \vec{k} \left[\mathbf{N}(\vec{k}) + \bar{\mathbf{N}}(\vec{k}) \right]. \quad (1.2.40)$$

This is exactly the expected expression: The quantum of each mode carries the corresponding momentum \vec{k} , and the vacuum has vanishing total momentum. Also the fact that both total energy and momentum are time independent according to (1.2.38) and (1.2.40) is not surprising because of Noether's theorem.

Another important aspect is that also the converse of Noether's theorem is true. In fact, there is another theorem by Noether, which says that any conserved quantity induces a corresponding symmetry of the action. Within classical mechanics or field theory this is most naturally seen in the **Hamiltonian canonical formulation**. In quantum theory it is thus also a very simple concept: The operators of energy and momentum should be generators of a representation of the spacetime translation group.

We shall show now that this is indeed the case. The spacetime translation (1.2.30) in the quantized theory should be represented by the **unitary transformation**

$$\mathbf{U}_{\text{trans}}(a) = \exp(ia^\mu \mathbf{P}_\mu) \quad \text{with} \quad (\mathbf{P}^\mu) = \begin{pmatrix} \mathbf{H} \\ \vec{\mathbf{P}} \end{pmatrix}. \quad (1.2.41)$$

That this is indeed a unitary transformation follows from the hermiticity of the operators, \mathbf{H} and $\vec{\mathbf{P}}$. For an infinitesimal transformation $a^\mu \rightarrow \delta a^\mu$ we find

$$\phi'(x') = \mathbf{U}_{\text{trans}}(\delta a) \phi(x') \mathbf{U}_{\text{trans}}^\dagger(\delta a) = \phi(x') + \delta a^\mu i [\mathbf{P}_\mu, \phi(x')] + \mathcal{O}(\delta a^2). \quad (1.2.42)$$

Here it is more convenient to use the space-time version of energy and momentum (1.2.39) and (1.2.40) instead of the mode decomposition. It is also clear that we can neglect the normal ordering when calculating the commutator since the normal ordering differs from the naive expression only by a contribution $\propto \mathbb{1}$, which cancels in the commutator. We can also evaluate the integrals for \mathbf{P}_μ at the same time $t = t'$ as in the argument of the field operator in (1.2.42), because \mathbf{P}_μ is time independent. With help of the equal-time commutation relations for the field operators (1.2.11), using (1.2.9) for the canonical field momenta, after some manipulations we find (*check it!*)

$$\phi'(x') = \phi(x') + \delta a^\mu \partial'_\mu \phi(x') + \mathcal{O}(\delta a^2) = \phi(x) + \mathcal{O}(\delta a^2), \quad (1.2.43)$$

where in the final step we have used the definition of the spacetime-translation operation $x' = x - \delta a$. Eq. (1.2.43) tells us that our formalism indeed defines a unitary representation of the spacetime translation subgroup of the Poincaré group that acts on the field operators of the quantized theory in the same local way as the corresponding operation in classical field theory.

Now we turn to **proper orthochronous Lorentz transformations**. According to (1.1.28) and (1.1.30) an infinitesimal Lorentz transformation for a scalar field is given by six independent infinitesimal parameters $\delta \omega_{\mu\nu} = -\delta \omega_{\nu\mu}$,

$$x'^\mu = x^\mu + \delta \omega^\mu{}_\nu x^\nu, \quad \phi'(x') = \phi(x). \quad (1.2.44)$$

In the convention of (A.1.1) this transformation reads

$$x'^\mu = x^\mu - \frac{1}{2} \delta \omega^{\rho\sigma} t_{\rho\sigma}^\mu \quad \text{with} \quad t_{\rho\sigma}^\mu = x_\rho \delta_\sigma^\mu - x_\sigma \delta_\rho^\mu, \quad T_{\rho\sigma} = 0. \quad (1.2.45)$$

Plugging this into (A.1.8) we find as the six Noether currents, labeled by the Lorentz indices ρ and σ , the angular-momentum density tensor (*check it!*)

$$J^{\rho\sigma\mu} = x^\rho \Theta^{\sigma\mu} - x^\sigma \Theta^{\rho\mu}. \quad (1.2.46)$$

The generators for boosts in the quantized theory are thus given by

$$\mathbf{K}^m = \int_{C_L} d^3\vec{x} : \mathbf{J}^{0m0} := {}_t\mathbf{P}^m - \int_{C_L} d^3\vec{x} x^m \mathcal{H} \quad \text{with } m \in \{1, 2, 3\}. \quad (1.2.47)$$

The generators of rotations are usually written in terms of **angular-momentum operators**,

$$\mathbf{J}^m = \frac{1}{2} \epsilon^{mab} \int_{C_L} d^3\vec{x} : \mathbf{J}^{ab0} := \int_{C_L} d^3\vec{x} : (\vec{x} \times \vec{\mathcal{P}})^m : \quad \text{with } a, b, m \in \{1, 2, 3\}. \quad (1.2.48)$$

In (1.2.47) and (1.2.48) we have used the definitions of the energy and momentum density operators from (1.2.34) and (1.2.35), implying normal ordering.

Parametrizing the infinitesimal Lorentz-transformation matrix in terms of two three-vectors $\delta\vec{\eta}$ (boosts) and $\delta\vec{\varphi}$ (rotations) as

$$(\delta\omega^\mu{}_\nu) = \begin{pmatrix} 0 & -\delta\eta_1 & -\delta\eta_2 & -\delta\eta_3 \\ -\delta\eta_1 & 0 & \delta\varphi_3 & -\delta\varphi_2 \\ -\delta\eta_2 & -\delta\varphi_3 & 0 & \delta\varphi_1 \\ -\delta\eta_3 & \delta\varphi_2 & -\delta\varphi_1 & 0 \end{pmatrix} \quad (1.2.49)$$

the unitary operator representing proper orthochronous Lorentz transformations thus should read

$$\mathbf{U}_\Lambda(\vec{\eta}, \vec{\varphi}) = \exp(-i\vec{\eta} \cdot \vec{\mathbf{K}} - i\vec{\varphi} \cdot \vec{\mathbf{J}}). \quad (1.2.50)$$

Using again the canonical equal-time commutation relations (1.2.11) and (1.2.13), indeed we find after some calculation (*check it!*)

$$\begin{aligned} \phi'(x') &= \phi(x') + i \left[\phi(x'), \delta\vec{\eta} \cdot \vec{\mathbf{K}} + \delta\vec{\varphi} \cdot \vec{\mathbf{J}} \right] + \mathcal{O}(\delta\omega^2) \\ &= \phi(x') + \delta\vec{\eta} \cdot \left[{}_t\vec{\nabla}' \phi(x') + \vec{x}' \dot{\phi}(x') \right] + \delta\vec{\varphi} \cdot (\vec{x}' \times \vec{\nabla}') \phi(x') \\ &= \phi(x) + \mathcal{O}(\delta\omega^2), \end{aligned} \quad (1.2.51)$$

where in the second step we have used (1.2.44) for the transformation of the space-time coordinates. The \mathbf{U}_Λ thus provide a **unitary representation of the proper orthochronous Lorentz group** on the Hilbert space of the quantized free scalar field. The field operators transform in a local way as the corresponding classical fields.

All together we have constructed a quantum-field theory with the following properties

- (a) The field operators obey equations of motion according to a Hamiltonian that is built by the spatial integral over a local Hamilton-density operator, where locality means that it is a polynomial of the fields, their conjugate field momenta, and their spatial gradients.
- (b) The energy is bounded from below, i.e., the energy eigenvalues are positive semi-definite. The vacuum state $|\Omega\rangle$ is an energy eigenvector with eigenvalue 0 and thus the ground state of the quantum-field theoretical system.
- (c) The Hilbert space admits a unitary representation of the proper orthochronous Lorentz group, under which the field operators transform locally as the analogous classical fields.

- (d) Local observables like energy, momentum, and angular momentum densities at a space-time point x commute with the energy density at any space-time argument y that is spacelike wrt. x , i.e., which fulfills $(x - y)^2 < 0$.

The latter property can be proved by checking it for the special case of equal time arguments, $x^0 = y^0$, using the equal-time commutation relations (1.2.11) for the field operators. Then the statement must hold true for any other space-like separated space-time arguments, because one can always find a proper orthochronous Lorentz transformation such that $[\Lambda(x - y)]^0 = 0$ (*check it!*).

Property (d) is known as the **microcausality condition** and is a sufficient condition for the existence of a Lorentz-invariant S matrix (for details, see [Wei95]). We note that (b), i.e., the existence of a stable ground state is compatible with all the other mentioned constraints on a physically meaning full quantum field theory if we use canonical *commutation* relations when quantizing the field theory, i.e., when we describe **bosons** with our scalar field theory. Had we used anticommutation relations for fermions instead of the bosonic commutation relations (1.2.11), the normal-ordering procedure would have introduced a sign change in the expression for the energy of the antiparticles in (1.2.37), and the energy would not come out to be positive definite. This is a special case of the **spin-statistics theorem**, according to which any local quantum field theory of fields with integer (half-integer) spin necessarily must be quantized with boson-commutation (fermion-anticommutation) rules.

Finally we consider the symmetry of the Lagrangian (and thus also of the action) under **changes of the phase of the field**, directly for the quantized fields

$$\phi'(x) = \exp(i\alpha)\phi(x), \quad \phi'^{\dagger}(x) = \exp(-i\alpha)\phi^{\dagger}(x) \quad \text{mit } \alpha \in \mathbb{R}. \quad (1.2.52)$$

This is the most simple example for **global gauge symmetry**. The symmetry group is the $U(1)$. In terms of (A.1.1) the infinitesimal transformation reads

$$\delta x^{\mu} = 0, \quad \delta \phi = i\delta\alpha\phi, \quad \delta \phi^{\dagger} = -i\delta\alpha\phi^{\dagger}, \quad (1.2.53)$$

i.e., we have

$$t(x) = 0, \quad \mathbf{T} = i\phi, \quad \mathbf{T}^{\dagger} = -i\phi^{\dagger}. \quad (1.2.54)$$

To find the corresponding Noether current we use (A.1.9). Again we have to treat the fields ϕ and ϕ^{\dagger} as independent field-degrees of freedom. First we find

$$\frac{\partial \mathcal{L}}{\partial \phi} \mathbf{T} + \frac{\partial \mathcal{L}}{\partial \phi^{\dagger}} \mathbf{T}^{\dagger} = i\phi^{\dagger}\phi - i\phi\phi^{\dagger} = 0, \quad (1.2.55)$$

where we have used the canonical commutation relations (1.2.11) Further we find (up to singular expressions that are $\propto \mathbb{1}$)

$$-\partial_{\nu} \frac{\partial \mathcal{L}}{\partial (\partial_{\nu} \phi)} \mathbf{T} - \partial_{\nu} \frac{\partial \mathcal{L}}{\partial (\partial_{\nu} \phi^{\dagger})} \mathbf{T}^{\dagger} = -i(\square \phi^{\dagger})\phi + i(\square \phi)\phi^{\dagger} = \partial_{\nu} \left(i\phi^{\dagger} \overleftrightarrow{\partial}^{\nu} \phi \right). \quad (1.2.56)$$

Applying the normal-ordering description we thus obtain the **Noether current**

$$\mathbf{j}^{\mu} = i : \phi^{\dagger} \overleftrightarrow{\partial}^{\mu} \phi :, \quad (1.2.57)$$

which, for the solution of the Klein-Gordon equation is conserved, i.e., it obeys the continuity equation (*check it!*)

$$\partial_{\mu} \mathbf{j}^{\mu} = 0. \quad (1.2.58)$$

Using the mode decomposition (1.2.25) For the corresponding **Noether charge**, we find

$$\mathbf{Q} = \int_{C_L} d^3\vec{x} : \mathbf{j}^0(t, \vec{x}) := \sum_{\vec{k}} [\mathbf{N}(\vec{k}) - \overline{\mathbf{N}}(\vec{k})]. \quad (1.2.59)$$

This adds further confirmation of the many-particle interpretation of the canonical field formalism: Obviously (1.2.59) means that each particle carries a charge-quantum number 1 and each antiparticle a charge-quantum number 2, because the occupation-number Fock states are obviously also eigenstates of the charge operator.

Finally we note, how to take the limit $L \rightarrow 0$, i.e., considering the whole space as “quantization volume”. For any spatial integral we have simply to make the substitution $C_L \rightarrow \mathbb{R}^3$. The momentum sums go into momentum integrals. We have to take care of the corresponding density of single-particle states. At finite L , a momentum volume $\Delta^3\vec{k}$ contains $L^3/(2\pi)^3 \Delta^3\vec{k}$ states, because $\vec{k} \in \frac{L}{2\pi}\mathbb{Z}^3$. Thus we have to substitute

$$\sum_{\vec{k}} \rightarrow V \int_{\mathbb{R}^3} \frac{d^3\vec{k}}{(2\pi)^3}. \quad (1.2.60)$$

Of course the volume $V = L^3$ does not make much sense in the limit $L \rightarrow \infty$. However, since the larger the volume becomes, the less important the boundary conditions become. This means that we simply can build **density operators** out of the number operators,

$$\mathbf{n}(\vec{k}) = \frac{\mathbf{N}(\vec{k})}{V}, \quad \overline{\mathbf{n}}(\vec{k}) = \frac{\overline{\mathbf{N}}(\vec{k})}{V}. \quad (1.2.61)$$

Then, e.g., from (1.2.60), we read off that the operator for the total **charge density** is given by

$$\rho = \int_{\mathbb{R}^3} d^3\vec{x} : \mathbf{j}^0(t, \vec{x}) := \int_{\mathbb{R}^3} \frac{d^3\vec{k}}{(2\pi)^3} [\mathbf{n}(\vec{k}) - \overline{\mathbf{n}}(\vec{k})]. \quad (1.2.62)$$

Obviously the mode decomposition (1.2.25) now becomes

$$\phi(t, \vec{x}) = \int_{\mathbb{R}^3} \frac{d^3\vec{k}}{(2\pi)^{3/2}} \left[\mathbf{a}(\vec{k}) u_{\vec{k}}(x) + \mathbf{b}^\dagger(\vec{k}) u_{\vec{k}}^*(x) \right], \quad (1.2.63)$$

while the non-trivial commutation relations (1.2.26) for the become Dirac- δ distributions,

$$[\mathbf{a}(\vec{k}), \mathbf{a}^\dagger(\vec{k}')] = [\mathbf{b}(\vec{k}), \mathbf{b}^\dagger(\vec{k}')] = \delta^{(3)}(\vec{k} - \vec{k}'). \quad (1.2.64)$$

1.3 Free Dirac fermions

1.3.1 The classical Dirac field

With the goal to construct a consistent relativistic wave mechanics with a single-particle interpretation as in the non-relativistic case, Dirac looked for a wave equation that is in first order with respect to time derivatives like the non-relativistic Schrödinger equation. Due to Lorentz symmetry then also the spatial derivatives should appear only in first order and for free particles the mass-shell condition,

1.3 · Free Dirac fermions

$-(\square + m^2)\psi(x) = 0$, should follow. As it turned out this property could be reached by using a **four-component spinor field**, which we now call a **Dirac-spinor field**. This admits the first-order field equation

$$(i\partial_\mu\gamma^\mu - m\mathbb{1}_4)\psi = 0, \quad (1.3.1)$$

where γ^μ are complex 4×4 matrices, the **Dirac matrices**. As a short-hand notation, later Feynman introduced his “slash convention”, $\not{\partial} := \gamma^\mu\partial_\mu$.

Multiplying the Dirac equation (1.3.1) with $i\not{\partial} + m\mathbb{1}_4$, we obtain

$$(-\not{\partial}^2 - m^2\mathbb{1}_4)\psi = 0. \quad (1.3.2)$$

To make this the mass-shell condition for free particles with mass m , we demand

$$\not{\partial}^2 = \square \quad (1.3.3)$$

or, more generally,

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}\mathbb{1}_4. \quad (1.3.4)$$

From (1.3.4) indeed (1.3.3) immediately follows:

$$\not{\partial}^2 = \gamma^\mu\gamma^\nu\partial_\mu\partial_\nu = \frac{1}{2}\{\gamma^\mu, \gamma^\nu\}\partial_\mu\partial_\nu = g^{\mu\nu}\partial_\mu\partial_\nu\mathbb{1}_4 = \square\mathbb{1}_4. \quad (1.3.5)$$

Writing the Dirac matrices in a 2×2 block notation, a convenient concrete realization, the so-called **chiral or Weyl representation** reads

$$\gamma^0 = \begin{pmatrix} 0 & \mathbb{1}_2 \\ \mathbb{1}_2 & 0 \end{pmatrix}, \quad \gamma^j = \begin{pmatrix} 0 & \sigma^j \\ -\sigma^j & 0 \end{pmatrix} \quad (1.3.6)$$

with the Pauli matrices

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (1.3.7)$$

The anticommutation relations (1.3.4) immediatly follow from the anticommutation realions for the Pauli Matrices,

$$\{\sigma^j, \sigma^k\} = 2\delta^{jk}\mathbb{1}_2. \quad (1.3.8)$$

Further we note the **pseudohermitezity of the Dirac matrices**,

$$\gamma^0\gamma^{\mu\dagger}\gamma^0 = \gamma^\mu \Leftrightarrow \gamma^{\mu\dagger} = \gamma^0\gamma^\mu\gamma^0. \quad (1.3.9)$$

Now we have to consider the behavior of the **Dirac-spinor field under Lorentz transformations**. We come to the transformation rule by assuming that the field transforms linearly under Lorentz transformations in a local way, i.e., according to

$$x' = \Lambda x, \quad \psi'(x') = S(\Lambda)\psi(x). \quad (1.3.10)$$

To find $S(\Lambda)$ we note that

$$\partial'_\mu = \frac{\partial}{\partial x'^\mu} = \frac{\partial x^\nu}{\partial x'^\mu}\partial_\nu = (\Lambda^{-1})^\nu{}_\mu\partial_\nu. \quad (1.3.11)$$

Using this in the Dirac equation for the transformed field, we obtain

$$(i\mathcal{D}' - m)\psi'(x') = [i(\Lambda^{-1})^\nu{}_\mu \gamma^\mu \partial_\nu - m] S(\Lambda)\psi(x). \quad (1.3.12)$$

Multiplication of this equation from the left with $S^{-1}(\Lambda)$, we see that the Dirac equation holds for the new field if

$$(\Lambda^{-1})^\nu{}_\mu S^{-1}(\Lambda)\gamma^\mu S(\Lambda) = \gamma^\nu \Rightarrow S^{-1}(\Lambda)\gamma^\mu S(\Lambda) = \Lambda^\mu{}_\nu \gamma^\nu. \quad (1.3.13)$$

To determine $S(\Lambda)$, we first consider infinitesimal Lorentz transformations as defined by (1.1.28-1.1.30),

$$\Lambda = \mathbb{1} + \delta\omega, \quad \Lambda^\mu{}_\nu = \delta^\mu{}_\nu + \delta\omega^\mu{}_\nu. \quad (1.3.14)$$

Now, up to $\mathcal{O}(\delta\omega^2)$ we have

$$S(\Lambda) = \mathbb{1}_4 + \frac{1}{8}\delta\omega_{\mu\nu}\gamma^{\mu\nu}, \quad S^{-1}(\Lambda) = \mathbb{1}_4 - \frac{1}{8}\delta\omega_{\mu\nu}\gamma^{\mu\nu}, \quad (1.3.15)$$

where $\gamma^{\mu\nu} = -\gamma^{\nu\mu}$ denotes an appropriate set of six 4×4 matrices, which acts in Dirac-spinor space. To find these matrices, we use this ansatz in (1.3.13) and expand up to linear order in $\delta\omega$, leading to

$$\begin{aligned} [\gamma^\mu, \gamma^{\rho\sigma}] &= 4(g^{\mu\rho}\gamma^\sigma - g^{\mu\sigma}\gamma^\rho) = 2(\{\gamma^\mu, \gamma^\rho\}\gamma^\sigma - \gamma^\rho\{\gamma^\mu, \gamma^\sigma\}) \\ &= 2[\gamma^\mu, \gamma^\rho\gamma^\sigma] = [\gamma^\mu, [\gamma^\rho, \gamma^\sigma]] \end{aligned} \quad (1.3.16)$$

In the final step, we have used $\gamma^{\rho\sigma} = -\gamma^{\sigma\rho}$. Thus we find

$$\gamma^{\rho\sigma} = [\gamma^\rho, \gamma^\sigma]. \quad (1.3.17)$$

For finite Lorentz transformations we only need to use matrix exponentiation to get

$$S(\Lambda) = \exp\left(\frac{1}{8}\omega_{\mu\nu}\gamma^{\mu\nu}\right). \quad (1.3.18)$$

Using the pseudohermiteicity (1.3.9) and $(\gamma^0)^2 = 1$, we get

$$\gamma^0(\gamma^{\rho\sigma})^\dagger\gamma^0 = \gamma^{\sigma\rho} = -\gamma^{\rho\sigma} \quad (1.3.19)$$

and thus

$$S^{-1}(\Lambda) = \gamma^0 S^\dagger(\Lambda) \gamma^0, \quad (1.3.20)$$

i.e., $S(\Lambda)$ is pseudounitary. It is important to note that $S(\Lambda)$ is only pseudounitary but not really unitary. This already gives a hint that a one-particle interpretation also of the Dirac equation as a quantum mechanical wave equation is inconsistent since for a Lorentz-invariant quantum theory Lorentz transformations should be represented by unitary (ray) representations. To explicitly see that (1.3.18) is not unitary, we consider a **boost** in an arbitrary direction \vec{n} with $\vec{n}^2 = 1$. The corresponding Lorentz matrix is of the form

$$\Lambda(\vec{n}) = \begin{pmatrix} \cosh \eta & -\vec{n}^t \sinh \eta \\ -\vec{n} \sinh \eta & \cosh \eta P_{\parallel}(\vec{n}) + P_{\perp}(\vec{n}) \end{pmatrix} \quad (1.3.21)$$

with the $\mathbb{R}^{3 \times 3}$ projection matrices,

$$P_{\parallel}(\vec{n}) = \vec{n} \otimes \vec{n}, \quad P_{\perp} = \mathbb{1}_3 - \vec{n} \otimes \vec{n}. \quad (1.3.22)$$

The boost velocity is $v = \tanh \eta$. Expanding (1.3.21) for infinitesimal $\delta\eta$ to first order we find the exponential form

$$\Lambda_B(\vec{\eta}) = \exp(i\vec{\eta} \cdot \vec{K}) \quad \text{with} \quad \vec{\eta} = \eta \vec{n}, \quad (1.3.23)$$

with

$$K^j = i \begin{pmatrix} 0 & \vec{e}_j^t \\ \vec{e}_j & 0 \end{pmatrix}. \quad (1.3.24)$$

Thus for the infinitesimal transformation we find

$$\begin{aligned} \delta x^0 = -\delta\vec{\eta} \cdot \vec{x}, \quad \delta x^j = -\delta\eta^j x^0 \Rightarrow \omega_{\rho 0} = -\omega_{0\rho} = \begin{cases} 0 & \text{for } \rho = 0, \\ \eta^\rho & \text{for } \rho \in \{1, 2, 3\}, \end{cases} \\ \omega_{00} = \omega_{jk} = 0 \quad \text{for } j, k \in \{1, 2, 3\}. \end{aligned} \quad (1.3.25)$$

For the Dirac representation $S(\Lambda_B)$ we thus need

$$\gamma^{0\mu} = \gamma^0 \gamma^\mu - \gamma^\mu \gamma^0 = \begin{cases} 0 & \text{for } \mu = 0, \\ 2\gamma^0 \gamma^\mu & \text{for } \mu \in \{1, 2, 3\}. \end{cases} \quad (1.3.26)$$

so we find

$$\frac{1}{8} \omega_{\mu\nu} \gamma^{\mu\nu} = \frac{1}{4} \omega_{0\rho} \gamma^{0\rho} = -\frac{1}{2} \gamma^0 \vec{\eta} \cdot \vec{\gamma} =: -i\vec{\eta} \cdot \vec{x}. \quad (1.3.27)$$

Using the chiral representation (1.3.6) of the Dirac matrices, we have

$$\vec{x} = \frac{i}{2} \vec{\gamma} \gamma^0 = \frac{i}{2} \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & -\vec{\sigma} \end{pmatrix}. \quad (1.3.28)$$

It is important to note that this matrix is **antihermitean**, and thus the Dirac representation of the boosts,

$$S_B[\vec{\eta}] =: S_{\vec{n}}(\eta) = \exp(-i\eta \vec{n} \cdot \vec{x}), \quad (1.3.29)$$

is **not unitary**.³ We shall see in the next chapter that the full orthochronous Lorentz group is realized as a unitary representation within the quantum-field theoretical framework. Now we can evaluate (1.3.29) explicitly since

$$(i\vec{n} \cdot \vec{x})^2 = \frac{1}{4} (\gamma^0 \vec{n} \cdot \vec{\gamma})^2 = -\frac{1}{4} (\vec{n} \cdot \vec{\gamma})^2 = \frac{\vec{n}^2}{4}. \quad (1.3.30)$$

Summation of the exponential series in (1.3.29) finally leads to

$$S_B(\vec{\eta}) = \gamma^0 \left[\cosh\left(\frac{\eta}{2}\right) \gamma^0 - \sinh\left(\frac{\eta}{2}\right) \vec{n} \cdot \vec{\gamma} \right]. \quad (1.3.31)$$

This is more conveniently written in the compact form,

$$S_B(\vec{\eta}) = \gamma^0 \Psi \quad \text{with} \quad U = \begin{pmatrix} \cosh(\eta/2) \\ \sinh(\eta/2) \vec{n} \end{pmatrix}, \quad (1.3.32)$$

³The full group theoretical analysis of the finite-dimensional linear representations of the proper orthochronous Lorentz group or its corresponding covering group, $SL(2, \mathbb{C})$, show that only the trivial representation is unitary. Any non-trivial representation is not equivalent to a unitary representation. The reason for this is that these groups are *not* compact. Contrary to this, the rotation group, $SO(3)$, and its covering group $SU(2)$, are compact. As we shall see below, the chiral representation of the γ matrices lead indeed to a unitary representation of the rotation group as a subgroup of the Lorentz group.

which can be expressed also in terms of the four-velocity components,

$$u = \begin{pmatrix} \cosh \eta \\ \vec{n} \sinh \eta \end{pmatrix} = \frac{1}{\sqrt{1-v^2}} \begin{pmatrix} 1 \\ \vec{v} \end{pmatrix} = \gamma \begin{pmatrix} 1 \\ \vec{v} \end{pmatrix}, \quad (1.3.33)$$

using simple relations for hyperbolic functions like $\sinh \eta = 2 \sinh(\eta/2) \cosh(\eta/2)$, etc.

$$U = \begin{pmatrix} \sqrt{\frac{\gamma+1}{2}} \\ \vec{n} \sqrt{\frac{\gamma-1}{2}} \end{pmatrix}. \quad (1.3.34)$$

Now we investigate the Dirac representation of rotations, which transform only the spatial components of the four vectors, i.e., in (1.3.18) we have to set

$$\omega_{00} = \omega_{0j} = -\omega_{j0} = 0, \quad \omega_{jk} = -\epsilon_{jkl} \varphi^l \quad \text{for } j, k \in \{1, 2, 3\}. \quad (1.3.35)$$

For infinitesimal rotations we indeed get

$$x'^0 = x^0, \quad x'^j = x^j + \epsilon^{jkl} \delta \varphi^l x^k = x^j - (\delta \vec{\varphi} \times \vec{x})^j. \quad (1.3.36)$$

Exponentiation leads to

$$\vec{x}' = \vec{n} (\vec{n} \cdot \vec{x}) - \sin \varphi \vec{n} \times \vec{x} + \cos \varphi P_{\perp}(\vec{n}) \vec{x} \quad \text{with } \vec{n} = \frac{\vec{\varphi}}{\varphi}. \quad (1.3.37)$$

Further we have

$$\gamma^{jk} = - \begin{pmatrix} [\sigma^j, \sigma^k] & 0 \\ 0 & [\sigma^j, \sigma^k] \end{pmatrix} = -2i \epsilon^{jkl} \begin{pmatrix} \sigma^l & 0 \\ 0 & \sigma^l \end{pmatrix} =: -4i \epsilon^{jkl} \Sigma^l. \quad (1.3.38)$$

In explicit matrix form this leads to

$$\Sigma^l = \frac{i}{8} \epsilon^{jkl} \gamma^{jk} = \frac{i}{4} \epsilon^{jkl} \gamma^j \gamma^k = \frac{1}{2} \begin{pmatrix} \sigma^l & 0 \\ 0 & \sigma^l \end{pmatrix}. \quad (1.3.39)$$

Using (1.3.35) we find

$$S_D(\vec{\varphi}) = \exp\left(\frac{1}{8} \omega_{\mu\nu} \gamma^{\mu\nu}\right) = \exp(i \vec{\varphi} \cdot \vec{\Sigma}). \quad (1.3.40)$$

The chiral representation is convenient for the representation of rotations since the spin matrix is block diagonal, and the two upper and the two lower components of the Dirac field transform as usual two-dimensional **Weyl spinors**. Thus the spinor representation is also called Weyl representation. Since the $\vec{\Sigma}$ are **hermitean matrices**, the rotations are indeed represented by unitary transformations according to (1.3.40). Because of

$$(\vec{n} \cdot \vec{\Sigma})^2 = \mathbb{1}_4 \quad \text{with } \vec{n} = \frac{\vec{\varphi}}{\varphi}, \quad \varphi = |\vec{\varphi}| \quad (1.3.41)$$

we find by using the exponential series for (1.3.40)

$$S_D(\vec{\varphi}) = \cos\left(\frac{\varphi}{2}\right) \mathbb{1}_4 + i \sin\left(\frac{\varphi}{2}\right) \vec{n} \cdot \vec{\Sigma}. \quad (1.3.42)$$

1.3 · Free Dirac fermions

Usually one defines instead of the $\gamma^{\mu\nu}$

$$\sigma^{\mu\nu} = \frac{i}{4}\gamma^{\mu\nu} = \frac{i}{4}[\gamma^\mu, \gamma^\nu], \quad (1.3.43)$$

so that the representation matrix of an arbitrary $\text{SO}(1,3)^\uparrow$ transformation reads in terms of the six covariant parameters

$$S(\omega_{\mu\nu}) = \exp\left(\frac{1}{8}\omega_{\mu\nu}\gamma^{\mu\nu}\right) = \exp\left(-\frac{i}{2}\omega_{\mu\nu}\sigma^{\mu\nu}\right). \quad (1.3.44)$$

The connection with to above introduced generators for boosts (1.3.28) and rotations (1.3.39) is given by

$$\chi^a = \frac{i}{4}[\gamma^a, \gamma^0] = \sigma^{a0} = -\sigma^{0a}, \quad \Sigma^a = \frac{i}{8}\epsilon^{abc}\gamma^{bc} = \frac{1}{2}\epsilon^{abc}\sigma^{bc}. \quad (1.3.45)$$

Now we come back to the Dirac equation (1.3.1) and the Dirac spinor ψ . As already noted above, with respect to rotations, it is composed in terms of two **Weyl spinors** according to

$$\psi = \begin{pmatrix} \xi_L \\ \xi_R \end{pmatrix}, \quad (1.3.46)$$

where $\xi_{L,R} \in \mathbb{C}^2$ are two-component Weyl spinors which transform under rotations accordingly because of (1.3.40-1.3.46). Thus, a Dirac field always describes **two spin-1/2 particles**. As we shall see in the next section, within the QFT formalism this corresponds to a spin-1/2 particle and its antiparticle. From the structure of the Dirac representation of the Lorentz group, which is generated by arbitrary products of boost and rotation matrices (1.3.32) and (1.3.40), one sees that we can built **Lorentz scalars** from the Dirac fields by multiplication with the **Dirac adjoint spinor**

$$\bar{\psi}(x) = \psi^\dagger(x)\gamma^0. \quad (1.3.47)$$

Indeed from (1.3.10) and (1.3.20) one finds

$$\bar{\psi}'(x') = \psi'^\dagger(x')\gamma^0 = \psi^\dagger(x)S^\dagger(\Lambda)\gamma^0 = \bar{\psi}(x)\gamma^0 S^\dagger(\Lambda)\gamma^0 = \bar{\psi}(x)S^{-1}(\Lambda). \quad (1.3.48)$$

From this we immediately conclude

$$\bar{\psi}'(x')\psi(x') = \bar{\psi}(x)\psi(x), \quad (1.3.49)$$

i.e., $\bar{\psi}\psi$ is a **scalar field**. In the same way, using (1.3.13) we see that

$$j^\mu(x) = \bar{\psi}(x)\gamma^\mu\psi(x) \quad (1.3.50)$$

behaves as a **vector field** under Lorentz transformations.

We find the equation for the Dirac adjoint by hermitean conjugation of the Dirac equation (1.3.1),

$$\bar{\psi}(x)\gamma^0(-i\overleftarrow{\mathcal{D}}^\dagger - m) = 0. \quad (1.3.51)$$

By multiplying this equation from the right with γ^0 we find, using the pseudohermitezity relation (1.3.9),

$$\bar{\psi}(x)(-i\overleftarrow{\mathcal{D}} - m) = 0. \quad (1.3.52)$$

By taking the four divergence of (1.3.50) from the Dirac equation (1.3.1) and its adjoint (1.3.52) we find

$$\partial_\mu j^\mu = 0, \quad (1.3.53)$$

i.e., the charge

$$Q = \int d^3\vec{x} j^0(x) = \int d^3\vec{x} \psi^\dagger(x)\psi(x) \quad (1.3.54)$$

is **conserved**. In this sense Dirac thought to have found the desired relativistic wave equation for a single particle of spin 1/2 since this conserved charge is obviously positive definite, and one would think that a single-particle interpretation in the sense of Born's probabilistic interpretation of the wave function is possible as in the case of the non-relativistic Schrödinger equation. However, as we shall see soon, for plane waves, describing particles with a certain momentum, one finds always solutions of the Dirac equation with both positive and negative frequencies, $\omega = \pm E(\vec{k}) = \pm\sqrt{\vec{k}^2 + m^2}$. Also Dirac found that for any relativistically meaningful interaction scattering solutions with purely positive-frequency solutions, which could be properly interpreted as particles with positive energy, in the initial state, always has contributions from negative-frequency solutions in the final state, and these would correspond to particles with a negative energy. But then the energy spectrum would not be bounded from below, and the whole system would be unstable, since one could produce states of arbitrarily low energy by just producing an arbitrary number of negative-energy particles.

Dirac's solution for this dilemma was to give up the single-particle interpretation and consider a many-body theory, where the "vacuum state" is given by the state, where all negative-energy single-particle states are occupied and assuming that spin-1/2 particles are fermions (which is the case for electrons, which where the particles Dirac wanted to describe with his equation anyway). Now by high-energy collisions, one could also kick out such an electron from this **Dirac sea**, and this would manifest itself as this additional negatively charged electron and a hole in the **Dirac sea**, which behaved in any way like an electron with the opposite charge of an electron. This led, after some initial misconceptions, to the prediction of "antielectrons" (now called a **positron**), which have the same mass and spin as an electron but carry one positive elementary charge.

The same conclusion follows also from the more natural quantum-field theoretical treatment, which we shall present in the next section. As a first step for the canonical quantization program, which is analogous to the quantization of the Klein-Gordon field in the previous section, we first construct a **Lorentz invariant Lagrangean** and then translate it into the (not manifestly covariant) Hamilton formalism. As we shall see, here the assumption of canonical equal-time commutators does not lead to a quantum field theory with a Hamiltonian that is bounded from below. However, using **equal-time anticommutation relations**, corresponding to **fermions** leads to a properly interpretable many-body theory for spin-1/2 particles and their antiparticles. This is another manifestation of the already mentioned spin-statistics theorem, according to which fields with half-integer spin must be quantized as fermions.

To find the free-particle Lagrangean, which should be bilinear or sesquilinear in the fields, we note that it must contain only one derivative in each term since the Dirac equation is a first-order differential equation. Further it should be a Lorentz scalar. From our analysis of the transformation properties of the Dirac spinor, we find the ansatz,

$$\mathcal{L} = \bar{\psi}(i\cancel{D} - m)\psi. \quad (1.3.55)$$

Since $\psi \in \mathbb{C}^4$ we can consider ψ and $\bar{\psi}$ as independent field-degrees of freedom and vary them independently. The Euler-Lagrange equations from varying $\bar{\psi}$ immediately lead to the Dirac equation (1.3.1).

Varying with respect to ψ leads to the Dirac-adjoint equation (1.3.51) as expected.

To convert this to the Hamilton formalism, we need the canonically conjugated field momenta, which results in

$$\Pi = \frac{\partial \mathcal{L}}{\partial \dot{\psi}} = i\bar{\psi}\gamma^0 = i\psi^\dagger, \quad \bar{\Pi} = \frac{\partial \mathcal{L}}{\partial \dot{\bar{\psi}}} = 0. \quad (1.3.56)$$

On the first glance this looks bad since the canonical momentum of the adjoint Dirac field vanishes. However, we can proceed further in the naive way by just calculating the Hamiltonian in the formal way as usual, i.e., we write

$$\mathcal{H} = \Pi\dot{\psi} - \mathcal{L} = i\bar{\psi}\gamma^0\partial_t\psi - i\bar{\psi}(\not{\partial} + im)\psi = \bar{\psi}(-i\vec{\gamma}\cdot\vec{\nabla} + m)\psi = -\Pi\gamma^0(\vec{\gamma}\cdot\vec{\nabla} + im)\psi. \quad (1.3.57)$$

The canonical Hamiltonian equations of motion then read

$$\dot{\psi} = \frac{\delta H}{\delta \Pi} = -\gamma^0(\vec{\gamma}\cdot\vec{\nabla} + im)\psi, \quad \dot{\bar{\Pi}} = -\frac{\delta H}{\delta \psi} = \Pi\left(-\gamma^0\vec{\gamma}\cdot\vec{\nabla} + im\right). \quad (1.3.58)$$

Multiplication of the first equation from the left with $i\gamma^0$ and bringing all terms to one side of the equations leads to the Dirac equation. Multiplication of the second equation from the right with $i\gamma^0$ and again writing all terms to one side of the equation leads to (1.3.51) for $\Pi\gamma^0$. Thus, although we have no connection between ψ and Π by the canonical field equations, we can simply use the relation (1.3.56) as a **constraint**, i.e., we can set

$$\Pi = i\bar{\psi}\gamma^0 = i\psi^\dagger \quad (1.3.59)$$

without contradiction.

1.3.2 Quantization of the free Dirac field

To quantize the Dirac field we substitute the “classical” c-number field by a field operator ψ . As we shall see, here we have to use the quantization for fermionic particles, i.e., canonical equal-time **anticommutation relations**. As we shall see, this does not lead to a contradiction with the general principles of quantum dynamics as long as all **local physical observables** are given by an *even* number of Dirac-field operator products. Particularly we shall show that in the here considered case of free fields the Hamilton operator is given by a sesquilinear form of the Dirac fields. As it will turn out, the quantum dynamics given by the commutator of the quantities with the Hamiltonian will lead back to the Dirac equation for the Dirac-field operators. Thus we postulate the **equal-time anticommutation relations**,

$$\{\psi_a(t, \vec{x}), \psi_b(t, \vec{y})\} = 0, \quad \{\psi_a(t, \vec{x}), \Pi_b(t, \vec{y})\} = i\{\psi_a(t, \vec{x}), \psi_b^\dagger(t, \vec{y})\} = i\delta_{ab}\delta^{(3)}(\vec{x} - \vec{y}). \quad (1.3.60)$$

Here, $a, b \in \{1, 2, 3, 4\}$ run over the Dirac-spinor components of the quantum fields.

Now we look for a mode decomposition of the field operator with respect to plane waves, corresponding to the momentum representation of the corresponding Fock space. As usual in relativistic quantum theory, the spin of a particle is defined in the rest frame of the particle⁴. Let $\sigma = \pm 1/2$ denote the eigenvalues of the spin matrix Σ^3 for a single-particle momentum eigenstate with $\vec{k} = 0$. Then it is very

⁴Here we consider *massive* Dirac particles. We shall come back to the massless case as the limit $m \rightarrow 0$.

customary to define the other single-particle spinors by a rotation-free Lorentz boost in direction of \vec{k} , which is given by the condition

$$\Lambda_{\text{B}}(-\eta\vec{n}) \begin{pmatrix} m \\ 0 \\ 0 \\ 0 \end{pmatrix} = k \quad \text{mit} \quad \eta = \text{arcosh}\left(\frac{E(\vec{k})}{m}\right), \quad \vec{n} = \frac{\vec{k}}{K}. \quad (1.3.61)$$

In the following we shall construct the corresponding mode functions for the Dirac fields. First we define **field modes with positive frequencies** by

$$u_{\vec{k},+}(x) = \frac{1}{\sqrt{(2\pi)^3 2E(\vec{k})}} \exp(-ik \cdot x) \Big|_{k^0=E(\vec{k})} \quad (1.3.62)$$

and make an ansatz for the mode decomposition of the Dirac field using the **Feynman-Stückelberg trick** as in the analogous case for bosons, i.e., we use an annihilation operator as coefficient of the positive-frequency modes and a creation operator for the negative-frequency modes (corresponding to antiparticles). Since here the Dirac-field components in the classical case are complex, we assume that particles and antiparticles are distinguishable and thus write

$$\psi(x) = \int_{\mathbb{R}^3} d^3\vec{k} \sum_{\sigma} \left[\mathbf{a}(\vec{k}, \sigma) u(\vec{k}, \sigma) u_{\vec{k},+}(x) + \mathbf{b}^{\dagger}(\vec{k}, \sigma) v(\vec{k}, \sigma) u_{\vec{k},+}^*(x) \right]. \quad (1.3.63)$$

To fulfill the Dirac equation for this ansatz, the spinors u and v must satisfy the equations

$$(\not{k} - m)u(\vec{k}, \sigma) = 0, \quad (\not{k} + m)v(\vec{k}, \sigma) = 0 \quad \text{mit} \quad k^0 = E(\vec{k}). \quad (1.3.64)$$

It is clear that both equations are compatible with the on-shell condition $k^0 = E(\vec{k})$, because when multiplying the equations with $\not{k} \pm m$ one finds the condition $k^2 = (k^0)^2 - \vec{k}^2 = m^2$.

For $\vec{k} = 0$ Eqs. (1.3.64) read

$$\gamma^0 u(0, \sigma) = u(0, \sigma), \quad \gamma^0 v(0, \sigma) = -v(0, \sigma). \quad (1.3.65)$$

Using the above Weyl representation (1.3.6) for γ^0 we find the linearly independent set of solutions

$$\begin{aligned} u(0, +1/2) &= \sqrt{m} \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix} =: \sqrt{m} u'(0, +1/2), & u(0, -1/2) &= \sqrt{m} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix} =: \sqrt{m} u'(0, -1/2), \\ v(0, +1/2) &= \sqrt{m} \begin{pmatrix} 1 \\ 0 \\ -1 \\ 0 \end{pmatrix} =: \sqrt{m} v'(0, +1/2), & v(0, -1/2) &= \sqrt{m} \begin{pmatrix} 0 \\ 1 \\ 0 \\ -1 \end{pmatrix} =: \sqrt{m} v'(0, -1/2). \end{aligned} \quad (1.3.66)$$

Obviously these spinors are eigenvectors of Σ_3 with the denoted eigenvalues, cf. (1.3.39). The somewhat unusual normalization will turn out to be convenient in the following. Now we use (1.3.34) to

apply the boost (1.3.61) to these solutions. With help of the eigenvector properties (1.3.65) and with $\gamma = E(\vec{k})/m := E/m$ we find

$$\begin{aligned} u(\vec{k}, \sigma) &= \sqrt{\frac{1}{2(E+m)}}(m + \not{k})u'(0, \sigma), \\ v(\vec{k}, \sigma) &= \sqrt{\frac{1}{2(E+m)}}(m - \not{k})v'(0, \sigma). \end{aligned} \quad (1.3.67)$$

It is important to note that these usually are *not* eigenstates of Σ^3 since Σ^3 is generally *not commuting* with the boost-representation matrix $S_B(\vec{\eta})$. Thus, σ labels the spin-three component if observed in the rest frame of the particle.

We see that (1.3.67) is compatible with the definition (1.3.66) for $\vec{k} = 0$, and the limit $m \rightarrow 0$ does not pose any additional problems. In the massless limit we simply have

$$\begin{aligned} u(\vec{k}, \sigma) &= \sqrt{\frac{1}{2E}}\not{k}u'(0, \sigma), \\ v(\vec{k}, \sigma) &= \sqrt{\frac{1}{2E}}(-\not{k})v'(0, \sigma). \end{aligned} \quad (1.3.68)$$

For particles that travel in z direction, these spinors represent states of definite **helicity**, which is defined as the projection of the spin at the direction of momentum. The corresponding operator thus reads

$$\mathbf{h} = \frac{\vec{k} \cdot \vec{\Sigma}}{|\vec{k}|}. \quad (1.3.69)$$

It is easy to show that \mathbf{h} commutes with γ^μ . For $\vec{k} = k\vec{e}_3$ we have

$$\mathbf{h}u(k^3\vec{e}_3, \sigma) = \sigma u(k^3\vec{e}_3, \sigma), \quad \mathbf{h}v(k^3\vec{e}_3, \sigma) = \sigma v(k^3\vec{e}_3, \sigma). \quad (1.3.70)$$

For massless particles thus u and v are helicity eigenstates in any reference frame, where $\vec{k} \parallel \vec{e}_3$, and the eigenvalue is given by $\sigma \in \{-1/2, +1/2\}$.

For the following we shall need the **pseudoorthogonality and orthogonality** relations,

$$\bar{u}(\vec{k}, \sigma)u(\vec{k}, \sigma') = 2m\delta_{\sigma, \sigma'}, \quad \bar{v}(\vec{k}, \sigma)v(\vec{k}, \sigma') = -2m\delta_{\sigma, \sigma'}, \quad (1.3.71)$$

$$\bar{u}(\vec{k}, \sigma)v(\vec{k}, \sigma') = \bar{v}(\vec{k}, \sigma)u(\vec{k}, \sigma') = 0, \quad (1.3.72)$$

$$u(\vec{k}, \sigma)^\dagger u(\vec{k}, \sigma') = 2E\delta_{\sigma, \sigma'}, \quad v(\vec{k}, \sigma)^\dagger v(\vec{k}, \sigma') = 2E\delta_{\sigma, \sigma'}, \quad (1.3.73)$$

$$u(\vec{k}, \sigma)^\dagger v(-\vec{k}, \sigma') = v(\vec{k}, \sigma)^\dagger u(-\vec{k}, \sigma') = 0, \quad (1.3.74)$$

which are easily proven with help of the commutation properties of Dirac matrices using (1.3.68) and the eigenvalue equations (1.3.65). For the last equation (1.3.74) it is important to note that the momentum arguments are to be taken with opposite sign!

To evaluate the anticommutation relations for the creation and annihilation operators in the mode decomposition (1.3.63) we try to solve this equation for $\mathbf{a}(\vec{k}, \sigma)$ and $\mathbf{b}^\dagger(\vec{k}, \sigma)$. From the definition (1.3.62) of the mode functions one immediately finds

Zur Berechnung der Antikommutatorrelationen for die Erzeugungs- und Vernichtungsoperatoren versuchen wir, die Modenentwicklung (1.3.63) nach $\mathbf{a}(\vec{k}, \sigma)$ und $\mathbf{b}^\dagger(\vec{k}, \sigma)$ aufzulösen.

$$\int_{\mathbb{R}^3} d^3\vec{x} u_{\vec{k},+}^*(x) u_{\vec{k}',+}(x) = \frac{1}{2E(\vec{k})} \delta^{(3)}(\vec{k} - \vec{k}'), \quad (1.3.75)$$

$$\int_{\mathbb{R}^3} d^3\vec{x} u_{\vec{k},+}^*(x) u_{\vec{k}',+}^*(x) = \frac{1}{2E(\vec{k})} \exp(2iEt) \delta^{(3)}(\vec{k} + \vec{k}'). \quad (1.3.76)$$

Multiplication of (1.3.63) with $u_{\vec{k},+}(x)$ or $u_{\vec{k},+}^*(x)$ we find, using (1.3.73) and (1.3.74),

$$\begin{aligned} \mathbf{a}(\vec{k}, \sigma) &= \int_{\mathbb{R}^3} d^3\vec{x} u^\dagger(\vec{k}, \sigma) u_{\vec{k},+}^*(x) \psi(x), \\ \mathbf{b}(\vec{k}, \sigma) &= \int_{\mathbb{R}^3} d^3\vec{x} \psi^\dagger(x) v(\vec{k}, \sigma) u_{\vec{k},+}^*(x). \end{aligned} \quad (1.3.77)$$

With the anticommutation relations for the Dirac fields (1.3.60) and the orthogonality relations (1.3.73-1.3.74) from this we immediately obtain the anticommutation relations for the creation and annihilation operators,

$$\begin{aligned} \{\mathbf{a}(\vec{k}, \sigma), \mathbf{a}^\dagger(\vec{k}', \sigma')\} &= \{\mathbf{b}(\vec{k}, \sigma), \mathbf{b}^\dagger(\vec{k}', \sigma')\} = \delta^{(3)}(\vec{k} - \vec{k}') \delta_{\sigma\sigma'}, \\ \{\mathbf{a}(\vec{k}, \sigma), \mathbf{a}(\vec{k}', \sigma')\} &= \{\mathbf{b}(\vec{k}, \sigma), \mathbf{b}(\vec{k}', \sigma')\} = 0, \\ \{\mathbf{a}(\vec{k}, \sigma), \mathbf{b}(\vec{k}', \sigma')\} &= \{\mathbf{a}^\dagger(\vec{k}, \sigma), \mathbf{b}^\dagger(\vec{k}', \sigma')\} = 0. \end{aligned} \quad (1.3.78)$$

To evaluate the Hamilton operator we have to use the **normal-ordering prescription** as above for the scalar Klein-Gordon field. It is crucial that now we have used anticommutation relations and thus we have to define

$$:\mathbf{a}(\vec{k}, \sigma) \mathbf{a}^\dagger(\vec{k}', \sigma') := -\mathbf{a}^\dagger(\vec{k}', \sigma') \mathbf{a}(\vec{k}, \sigma), \quad (1.3.79)$$

i.e., the normal-ordered expression implies an additional sign of the permutation necessary to bring the operators from the given order to normal order.

According to (1.3.57) the Hamilton density for the Dirac field thus reads

$$\mathcal{H} =: \bar{\psi}(-i\gamma \cdot \vec{\nabla} + m)\psi :=: \bar{\psi}(i\gamma^0 \partial_t - i\vec{\gamma} + m)\psi(x) :=: \psi^\dagger i\partial_t \psi :. \quad (1.3.80)$$

Using the mode decomposition (1.3.63) and integrating over \vec{x} leads to the **positive semidefinite Hamilton operator**

$$\mathbf{H} = \int_V d^3\vec{x} \mathcal{H} = \int_{\mathbb{R}^3} d^3\vec{k} \sum_{\sigma} E(\vec{k}) [\mathbf{n}_a(\vec{k}, \sigma) + \mathbf{n}_b(\vec{k}, \sigma)]. \quad (1.3.81)$$

That is why the sign change (1.3.79) in the normal-ordering prescription for fermion-field operators is so important here, and the use of bosonic commutation relations in the canonical formalism would lead to a Hamilton operator that is not bounded from below and thus there would not exist a stable ground state ("the vacuum"). This is another manifestation of the general spin-statistics theorem, according to which fields representing particles with an odd (even) half-integer spin must be fermions (bosons).

For the charge operator according to (1.3.54) we find

$$\mathbf{Q} = \int_V d^3\vec{x} : \psi^\dagger \psi := \int_{\mathbb{R}^3} d^3\vec{k} \sum_{\sigma} [\mathbf{n}_a(\vec{k}, \sigma) - \mathbf{n}_b(\vec{k}, \sigma)]. \quad (1.3.82)$$

Here, the anticommutation relations for fermions lead to the fact that \mathbf{Q} is not positive definite as the hermitean expression within the normal-ordering symbol suggests, but the antiparticles (annihilated by the \mathbf{b} operators) carry the opposite charge of the particles (annihilated by the \mathbf{a} operators). Thus, as for charged scalar bosons, only the net-particle number, i.e., the difference between the number of particles and that of antiparticles is a conserved quantity. The **occupation-number operators** in (1.3.82) are defined by

$$\mathbf{n}_a(\vec{k}, \sigma) = \mathbf{a}^\dagger(\vec{k}, \sigma)\mathbf{a}(\vec{k}, \sigma), \quad \mathbf{n}_b(\vec{k}, \sigma) = \mathbf{b}^\dagger(\vec{k}, \sigma)\mathbf{b}(\vec{k}, \sigma) \quad (1.3.83)$$

definiert.

The energy-eigenvalue problem is again solved analogously to the harmonic oscillator. This task is even simpler than in the bosonic case since $\mathbf{a}^2(\vec{k}, \sigma) = \mathbf{b}^2(\vec{k}, \sigma) = 0$, i.e., the Fock basis is given by

$$\begin{aligned} |\{n_a(\vec{k}, \sigma)\}, \{n_b(\vec{k}, \sigma)\}\rangle &= \prod_{\vec{k}, \sigma} [\mathbf{a}^\dagger(\vec{k}, \sigma)]^{n_a(\vec{k}, \sigma)} [\mathbf{b}^\dagger(\vec{k}, \sigma)]^{n_b(\vec{k}, \sigma)} |\Omega\rangle \\ \text{with } n_a(\vec{k}, \sigma), n_b(\vec{k}, \sigma) &\in \{0, 1\}. \end{aligned} \quad (1.3.84)$$

Here $|\Omega\rangle$ denotes the vacuum state, where no particles are present and which is the **ground state** of the system. It is defined uniquely by

$$\forall \vec{k}, \sigma : \quad \mathbf{a}(\vec{k}, \sigma)|\Omega\rangle = \mathbf{b}(\vec{k}, \sigma)|\Omega\rangle = 0. \quad (1.3.85)$$

According to (1.3.84) in any Fock-basis state each single-particle mode can be occupied at most once. This proves that the anticommutation relations lead to **Pauli's exclusion principle**, as it should be the case for fermions.

1.3.3 Poincaré symmetry of the quantized Dirac theory

In this subsection we shall analyze the Poincaré-symmetry properties of quantized Dirac theory. As in Section 1.2 for the quantized Klein-Gordon fields we shall show that also the quantized Dirac field provides a unitary representation of the proper orthochronous Poincaré group. First we evaluate the canonical energy-momentum tensor. For the classical Dirac field it reads

$$\Theta^\mu{}_\nu = \frac{\partial \mathcal{L}}{\partial(\partial_\mu \psi_a)} \partial_\nu \psi_a - \mathcal{L} \delta^\mu{}_\nu = i \bar{\psi} \gamma^\mu \partial_\nu \psi - \mathcal{L} \delta^\mu{}_\nu. \quad (1.3.86)$$

For the energy-momentum operators we find, applying the normal-ordering description

$$\mathbf{P}_\nu = \int_{\mathbb{R}^3} d^3\vec{x} : \Theta^0{}_\nu := \int_{\mathbb{R}^3} d^3\vec{x} : \psi^\dagger(x) i \partial_\nu \psi(x) :, \quad (1.3.87)$$

where we have used $\bar{\psi} \gamma^0 = \psi^\dagger$.

The corresponding expressions for the rotation and boost generators (i.e., angular-momentum and center-momentum operators) we have to use the corresponding generators for the Dirac-spinor representation (1.3.39) and (1.3.28), respectively, i.e.,

$$\text{Drehungen: } \delta x^0 = 0, \quad \delta \vec{x} = -\delta \vec{\varphi} \times \vec{x}, \quad \delta \psi = i \delta \vec{\varphi} \cdot \vec{\Sigma} \psi, \quad (1.3.88)$$

$$\text{Boosts: } \delta x^0 = -\delta \eta \cdot \vec{x}, \quad \delta \vec{x} = -\delta \vec{\eta} t, \quad \delta \psi = -i \delta \vec{\eta} \cdot \vec{x} \psi. \quad (1.3.89)$$

Using the general formalism in Appendix A, we find after some algebra and applying again the normal-ordering prescription for the quantized quantities,

$$\vec{\mathbf{J}} = \int_{\mathbb{R}^3} d^3 \vec{x} : \psi^\dagger(x) [\vec{x} \times (-i \vec{\nabla}) + \vec{\Sigma}] \psi(x), \quad (1.3.90)$$

$$\vec{\mathbf{K}} = \int_{\mathbb{R}^3} d^3 \vec{x} : \psi^\dagger(x) [i \vec{x} \partial_0 + i t \vec{\nabla} + \vec{x}] \psi(x). \quad (1.3.91)$$

Using (1.3.59) for the canonical field momentum and the equal-time anticommutation rules (1.3.60) we find that the Dirac-field operators behave under Lorentz transformations as the corresponding classical fields, i.e., in a local way.

To prove this we first consider spatial and temporal translations, which should be given by the unitary operator

$$\mathbf{U}_T(a) = \exp(i a \cdot \mathbf{P}). \quad (1.3.92)$$

For an infinitesimal transformation we find

$$\psi'(x') = \mathbf{U}_T(\delta a) \psi(x') \mathbf{U}_T^\dagger(\delta a) = \psi(x') + i \delta a^\mu [\mathbf{P}_\mu, \psi(x')] + \mathcal{O}(\delta a^2). \quad (1.3.93)$$

Applying the general equation, valid for any set of three operators **A**, **B**, and **C**,

$$[\mathbf{AB}, \mathbf{C}] = \mathbf{A} \{\mathbf{B}, \mathbf{C}\} - \{\mathbf{A}, \mathbf{C}\} \mathbf{B}, \quad (1.3.94)$$

leads with help of (1.3.87) and the equal-time anticommutation relations (1.3.60) to

$$[\mathbf{P}_\mu, \psi(x')] = -i \partial_\mu \psi(x'). \quad (1.3.95)$$

From the transformation behavior of the unquantized Dirac field we expect that

$$x' = x - \delta a, \quad \psi(x') = \psi(x) = \psi(x' + \delta a) = \psi(x') + \delta a^\mu \partial_\mu \psi(x') \quad (1.3.96)$$

holds for the field operators too. Indeed, using (1.3.95) in (1.3.93) precisely shows that this is indeed the case.

The calculation for rotations and boosts works analogously. The unitary transformations read in this case⁵

$$\mathbf{U}_D(\vec{\varphi}) = \exp(-i \vec{\varphi} \cdot \vec{\mathbf{J}}), \quad \mathbf{U}_B(\vec{\eta}) = \exp(+i \vec{\eta} \cdot \vec{\mathbf{K}}), \quad (1.3.97)$$

and the commutator relations become (*check!*)

$$\begin{aligned} [\vec{\mathbf{J}}, \psi(x')] &= -[\vec{x}' \times (-i \vec{\nabla}) + \vec{\Sigma}] \psi(x'), \\ [\vec{\mathbf{K}}, \psi(x')] &= -[i \vec{x}' \partial_t + i t \vec{\nabla} - \vec{x}] \psi(x'), \end{aligned} \quad (1.3.98)$$

⁵The signs of the exponentials are just conventional.

which directly leads to the transformation behavior as expected from the classical fields,

$$\begin{aligned}\delta x^0 &= 0, & \delta \vec{x} &= -\delta \vec{\varphi} \times \vec{x}, & \psi'(x') &= (\mathbb{1} + \delta \vec{\varphi} \times \vec{\nabla} + i\delta \vec{\varphi} \cdot \vec{\Sigma}) \psi(x'), \\ \delta x^0 &= -\delta \vec{\eta} \cdot \vec{x}, & \delta \vec{x} &= -\delta \vec{\eta} x^0, & \psi'(x') &= (\mathbb{1} + \vec{x}' \partial_0 + x'^0 \vec{\nabla} - i\vec{x}') \psi(x').\end{aligned}\tag{1.3.99}$$

All this shows that the quantized Dirac-field theory indeed leads to a **local unitary representation of the proper orthochronous Poincaré group**. Since thus the field operators precisely behave under the transformations as their classical counterparts, i.e., they transform locally, we have again constructed a **local quantum field theory** as we have shown for Klein-Gordon fields in the last section. As we have seen above, the quantization as fermions has led to a positive semidefinite Hamilton operator and thus to the existence of a stable ground state, the vacuum. Local observables as the energy-momentum tensor or the conserved current (1.3.50), which are derived as **bilinear forms** of the Dirac-field operators, commute for space-time arguments that are spacelike separated. This immediately follows from (1.3.94) and the equal-time commutator relations of these quantities together with the local Lorentz-transformation properties of these operators. This particularly means that the theory obeys the relativistic constraints of causality.

To summarize, analogous to the quantized Klein-Gordon theory of the previous section also the quantized Dirac theory yields to a **local, microcausal quantum field theory with a positive semidefinite Hamiltonian** and thus allows for a proper physical interpretation in the sense of Born's probability interpretation of quantum theory. Also for Dirac fields, this goal is not possible within a naive single-particle interpretation of the "classical Dirac field", which thus has no direct physical interpretation.

1.3.4 The discrete symmetry transformations P , C and T

A glance at (1.3.28) and (1.3.39) shows that the Dirac representation of the proper orthochronous Lorentz group is **reducible** since the generators for boosts and rotations obviously are given by block-diagonal matrices, i.e., the two-component Weyl spinors, that build up the four-component Dirac spinor according to (1.3.46), transform within themselves. The same is true under space-time translations, and thus even as a representation of the proper orthochronous Poincaré group the representation is reducible. This is inherited of course by the quantized theory. As we shall see now, the representation becomes **irreducible** if extended by **discrete symmetry transformations** as space reflection and time reversal, i.e., when looking for representations of larger Poincaré groups. As we shall see, also another discrete symmetry transformation occurs, where all particles and antiparticles are interchanged, the so-called **charge-conjugation transformation**. As we shall see, the time-reversal transformation must be necessarily realized by antiunitary transformations in quantum-field theory.

Space reflections and parity

According to Wigner's theorem [Bar64], when looking for representations of **discrete symmetry transformations** one first has to check, whether the transformation should be realized as a unitary or an antiunitary transformation. This is most easily done by using the **Heisenberg algebra** of position and momentum operators. This is unproblematic in our case of massive or massless Dirac particles, but one should keep in mind that massless fields with a spin larger or equal to 1 (e.g., for photons) do not admit the definition of a position operator, fulfilling all Heisenberg-commutation relations.

A space reflection should act on the position and momentum operators as

$$\vec{x}' = \mathbf{U}(P)\vec{x}\mathbf{U}^\dagger(P) = -\vec{x}, \quad \vec{p}' = \mathbf{U}(P)\vec{p}\mathbf{U}^\dagger(P) = -\vec{p}.\tag{1.3.100}$$

The commutator relations transform according to

$$[\mathbf{x}'_i, \mathbf{p}'_j] = [-\mathbf{x}_i, -\mathbf{p}_j] = [\mathbf{x}_i, \mathbf{p}_j] \stackrel{\pm}{=} i\delta_{ij}. \quad (1.3.101)$$

On the other hand this must also follow from the canonical commutator relation for $\vec{\mathbf{x}}$ and $\vec{\mathbf{p}}$ by the direct similarity transformation with $\mathbf{U}(P)$:

$$[\mathbf{x}'_i, \mathbf{p}'_j] = \mathbf{U}(P)[\mathbf{x}_i, \mathbf{p}_j]\mathbf{U}^\dagger(P) = \mathbf{U}(P)i\delta_{ij}\mathbf{U}^\dagger(P) = \pm i\delta_{ij}, \quad (1.3.102)$$

where the upper sign is valid for a unitary, the lower for an antiunitary operator. Since the new position and momentum operators should fulfill the same Heisenberg-algebra properties as the original ones, we must necessarily assume that the space-reflection symmetry is realized as a **unitary operator**.

The **Dirac-field operator** should transform under space reflections as

$$\psi_P(t, \vec{x}) = \mathbf{U}(P)\psi(t, \vec{x})\mathbf{U}^\dagger(P) = \eta_P \hat{S}(P)\psi(t, -\vec{x}). \quad (1.3.103)$$

Here $\hat{S}(P)$ is a $\mathbb{C}^{4 \times 4}$ -matrix acting in spinor space that fulfills $\hat{S}^2(P) = \mathbb{1}$ and η_P an arbitrary phase factor. Since $\mathbf{U}(P)$ is unitary, also ψ_P must obey the Dirac equation, i.e., expressed in terms of the original field operator

$$\hat{S}^{-1}(P)(i\hat{d} - M)\hat{S}(P)\psi(t, -\vec{x}) = \hat{S}^{-1}(P)(i\gamma^0\partial_t - i\vec{\gamma} \cdot \vec{\nabla} - m)\hat{S}(P)\psi(t, -\vec{x}) \stackrel{!}{=} 0. \quad (1.3.104)$$

For ψ the Dirac equation holds, i.e.,

$$(i\hat{d} - m)\psi = (i\gamma^0\partial_t + i\vec{\gamma} \cdot \vec{\nabla} - m)\psi = 0. \quad (1.3.105)$$

From this (1.3.104) follows immediately if

$$\hat{S}^{-1}(P)\gamma^0\hat{S}(P) = \gamma^0, \quad \hat{S}^{-1}(P)\vec{\gamma}\hat{S}(P) = -\vec{\gamma} \quad \text{or} \quad \hat{S}^{-1}(P)\gamma^\mu\hat{S}(P) = P^\mu{}_\nu\gamma^\nu \quad (1.3.106)$$

holds. Here $(P^\mu{}_\nu) = \text{diag}(1, -1, -1, -1)$. It is obvious that due to the anticommutator relations of the Dirac matrices,

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}\mathbb{1}, \quad (1.3.107)$$

we can choose

$$\hat{S}(P) = \hat{S}^{-1}(P) = \gamma^0. \quad (1.3.108)$$

It is easy to see by direct calculation that this indeed fulfills (1.3.106).

Charge conjugation

The charge-conjugation transformation C by definition should interchange particles with antiparticles. Since ψ annihilates particles and creates antiparticles, this means that ψ_C should do the opposite, i.e., annihilate antiparticles and create particles. This obviously holds for the field operator $\bar{\psi}^t$, where the superscript t means transposition in spinor space.

The charge-conjugation transformation obviously commutes with position and momentum operators and thus from the Heisenberg commutation relations we can conclude that, analogously as shown above for the space reflection, it must be realized by a **unitary transformation**. Thus we have

$$\psi_C(t, \vec{x}) = \mathbf{U}(C)\psi(t, \vec{x})\mathbf{U}^\dagger(C) = \eta_C \hat{S}(C)\bar{\psi}^t(t, \vec{x}). \quad (1.3.109)$$

1.3 · Free Dirac fermions

Since $\mathbf{U}(C)$ is unitary also for ψ_C the Dirac equation must hold as for ψ , which means

$$\hat{S}^{-1}(C)(i\hat{\mathcal{D}} - m)\hat{S}(C)\bar{\psi}^t(t, \vec{x}) \stackrel{!}{=} 0. \quad (1.3.110)$$

On the other hand for the Dirac-adjoint operator we have the equation

$$\bar{\psi}(t, \vec{x})(i\overleftarrow{\mathcal{D}} + m) = 0, \quad (1.3.111)$$

and by transposing this equation in spinor space, we find

$$(i\hat{\mathcal{D}}^t + m)\bar{\psi}^t(t, x) = 0. \quad (1.3.112)$$

Comparing (1.3.110) with (1.3.112) leads to the condition

$$S^{-1}(C)\gamma^\mu \hat{S}(C) = -(\gamma^\mu)^t. \quad (1.3.113)$$

In our realization of the Dirac matrices (1.3.6) we have

$$(\gamma^\mu)^t = (-1)^\mu \gamma^\mu, \quad (1.3.114)$$

and as one easily proves by direct calculation that we can set

$$\hat{S}(C) = i\gamma^2\gamma^0, \quad \hat{S}^{-1}(C) = i\gamma^0\gamma^2 = -\hat{S}(C), \quad (1.3.115)$$

which fulfills the relations (1.3.113).

Time-reversal transformation

The time-reversal transformation should act on the position and momentum operators as

$$\mathbf{U}(T)\vec{x}\mathbf{U}^\dagger(T) = \vec{x}, \quad \mathbf{U}(T)\vec{p}\mathbf{U}^\dagger(T) = -\vec{p}. \quad (1.3.116)$$

An analogous calculation as performed for the parity operator leads to the conclusion that the **time-reversal transformation must be realized by an antiunitary operator**. Since an antiunitary operator leads to an adjunction of operators when acting on them by the corresponding similarity transformation, the time-reversal operator must act on the Dirac-field operator according to

$$\psi_T(t, \vec{x}) = \mathbf{U}(T)\psi(t, \vec{x})\mathbf{U}^\dagger(T) = \eta_T \hat{S}(T)\bar{\psi}^t(-t, \vec{x}). \quad (1.3.117)$$

From the Dirac equation for $\psi(t, \vec{x})$ and the antiunitarity of $\mathbf{U}(t)$ we find

$$(-i\hat{\mathcal{D}}^* - m)\psi_T(t, \vec{x}) = 0. \quad (1.3.118)$$

Using this in (1.3.117), leads to the condition

$$\hat{S}^{-1}(T)(i\hat{\mathcal{D}}^* + m)\hat{S}(T)\bar{\psi}^t(-t, \vec{x}) = 0. \quad (1.3.119)$$

Comparing this with (1.3.112) gives

$$\hat{S}^{-1}(T)(\gamma^0)^* \hat{S}(T) = -(\gamma^0)^t, \quad \hat{S}^{-1}(T)\vec{\gamma}^* \hat{S}(T) = \vec{\gamma}^t \Leftrightarrow \hat{S}^{-1}(T)(\gamma^\mu)^* \hat{S}(T) = T^\mu_\nu (\gamma^\mu)^t \quad (1.3.120)$$

with the time-reflection matrix $(T^\mu{}_\nu) = \text{diag}(-1, 1, 1, 1)$. In our representation (1.3.6) of the Dirac matrices γ^0 , γ^1 , and γ^3 are real and γ^2 purely imaginary. Together with (1.3.114) it follows from (1.3.120) that

$$\hat{S}^{-1}(T)\gamma^\mu\hat{S}(T) = -\gamma^\mu. \quad (1.3.121)$$

This means that we can choose

$$\hat{S}(T) = \hat{S}^{-1}(T) = \gamma^5 \quad (1.3.122)$$

with

$$\gamma^5 = \gamma_5 := i\gamma^0\gamma^1\gamma^2\gamma^3. \quad (1.3.123)$$

An alternative realization is found by using the charge-conjugation transformation (1.3.109)

$$\psi_T(t, \vec{x}) = \eta_T \eta_C^* \hat{S}(T) \hat{S}^{-1}(C) \psi_C(-t, \vec{x}). \quad (1.3.124)$$

Since ψ_C is related to ψ by a unitary transformation, we can write the time-reversal transformation also realize as

$$\psi_T(t, \vec{x}) = \eta'_T \hat{S}'(T) \psi_C(t, \vec{x}). \quad (1.3.125)$$

Obviously we have, up to an arbitrary phase

$$\hat{S}'(T) = \eta \hat{S}(T) \hat{S}^{-1}(C) = \eta \gamma_5 i \gamma^0 \gamma^2 = \eta \gamma^1 \gamma^3. \quad (1.3.126)$$

The standard choice for the phase is $\eta = i$, i.e.,

$$\hat{S}'(T) = i \gamma^1 \gamma^3 = \hat{S}'^{-1}(T). \quad (1.3.127)$$

Plugging (1.3.125) into the equation of motion (1.3.118) of the operator $\psi_T(t, \vec{x})$, by comparing with the Dirac equation we find the conditions

$$\hat{S}'^{-1}(T)(\gamma^0)^* \hat{S}'(T) = \gamma^0, \quad \hat{S}'^{-1}(T)\vec{\gamma}^* \hat{S}'(T) = -\vec{\gamma}. \quad (1.3.128)$$

In the Dirac representation as well as in the here used chiral representation of the Dirac matrices γ^0 , γ^1 , and γ^3 are real and γ^2 purely imaginary, and thus we can write (1.3.128) as

$$\hat{S}'^{-1}(T)\gamma^\mu\hat{S}'(T) = (-1)^\mu\gamma^\mu = (\gamma^\mu)^t. \quad (1.3.129)$$

By direct calculation one easily proves that (1.3.127) indeed fulfills this requirement. On the other hand, because of $[\hat{S}'(T)]^* = -\hat{S}'(T)$ we find for the conjugate complex of Eq. (1.3.128)

$$\hat{S}'^{-1}(T)\gamma^0\hat{S}'(T) = (\gamma^0)^*, \quad \hat{S}'^{-1}(T)\vec{\gamma}\hat{S}'(T) = -\vec{\gamma}^* \Rightarrow \hat{S}'^{-1}(T)\gamma^\mu\hat{S}'(T) = P^\mu{}_\nu(\gamma^\nu)^* \quad (1.3.130)$$

with the space-reflection matrix $(P^\mu{}_\nu) = \text{diag}(1, -1, -1, -1)$.

1.3.5 Sesquilinear forms of Dirac-field operators

For modelling **interactions** with Dirac-spinor fields the combinations $\bar{\psi}\Gamma\psi$ are important, where Γ are arbitrary $\mathbb{C}^{4 \times 4}$ matrices in Dirac-spinor space. Such sesquilinear forms can be used in the interaction part of the Lagrangian to build the coupling of Dirac fields with other particles. For this, also the relativistic invariance (i.e., invariance under proper orthochronous Poincaré transformations) of the corresponding action functional is crucial. Thus it is customary to find such matrices, Γ , that lead to

expressions with simple transformation properties under proper orthochronous Lorentz transformations.

E.g., choosing $\Gamma = \mathbb{1}$, leads to a **scalar field operator** because of (1.3.13), which shows that

$$\mathbf{S} = \bar{\psi}\psi \quad (1.3.131)$$

is a **scalar field**. Because of (1.3.108) it is also a scalar field under spatial reflections.

Analogously

$$\mathbf{V}^\mu = \bar{\psi}\gamma^\mu\psi \quad (1.3.132)$$

turns out to be a vector field under orthochronous Poincaré transformations and space reflections. To emphasize the transformation property under space reflections $\mathbf{V}^\mu \rightarrow P_{\mu\nu}\mathbf{V}^\mu$ one also calls such a vector a **polar vector**.

With the Dirac matrices one can form the

$$\gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3 = -\frac{i}{4!}\epsilon_{\mu\nu\rho\sigma}\gamma^0\gamma^1\gamma^2\gamma^3. \quad (1.3.133)$$

From the second form of this expression we can imagine that this has the properties of a scalar under orthochronous Lorentz transformations but flips its sign under space reflections, because $\det \mathcal{P} = -1$, and the Levi-Civita symbol $\epsilon_{\mu\nu\rho\sigma}$ is a fourth-rank pseudo tensor under improper Lorentz transformations. Indeed, one can easily show, using (1.3.103) and (1.3.108) that the expression

$$\mathbf{P} = \bar{\psi}\gamma^5\psi \quad (1.3.134)$$

is a **pseudoscalar field operator**.

In the same way one shows that

$$\mathbf{A}^\mu = \bar{\psi}\gamma^\mu\gamma^5\psi \quad (1.3.135)$$

is an **axial-vector field**, i.e., it transforms under proper orthochronous Lorentz transformations as a vector field, but flips its sign under space reflections,

$$\begin{pmatrix} \mathbf{A}^0(t, \vec{x}) \\ \vec{\mathbf{A}}(t, \vec{x}) \end{pmatrix} \xrightarrow{\mathcal{P}} \begin{pmatrix} -\mathbf{A}^0(t, -\vec{x}) \\ +\vec{\mathbf{A}}(t, -\vec{x}) \end{pmatrix}. \quad (1.3.136)$$

Finally

$$\mathbf{S}^{\mu\nu} = \bar{\psi}\sigma^{\mu\nu}\psi \quad \text{mit} \quad \sigma^{\mu\nu} = \frac{i}{4}[\gamma^\mu, \gamma^\nu] \quad (1.3.137)$$

is an **antisymmetric second-rank tensor field**.

Since the five matrices

$$\mathbb{1}_4, \quad \gamma^5, \quad \gamma^\mu, \quad \gamma^\mu\gamma^5, \quad \sigma^{\mu\nu} \quad (1.3.138)$$

are linearly independent in the space of $\mathbb{C}^{4 \times 4}$ matrices, and we have together $1 + 1 + 4 + 4 + 6 = 16$ matrices, any sesquilinear form of Dirac spinors can be composed of the above introduced field operators \mathbf{S} , \mathbf{V}^μ , \mathbf{A}^μ , and $\mathbf{T}^{\mu\nu}$ which in addition are also **self adjoint**.

Chapter 2

The real-time formulation of equilibrium quantum-field theory

2.1 The general Schwinger-Keldysh contour

In this section we briefly define the Schwinger-Keldysh time contour for the calculation of expectation values for general non-equilibrium situations as well as the extensions for the special case of thermal equilibrium in the grand-canonical ensemble. Of course, the general scheme contains also the vacuum quantum field theory as a special case.

2.1.1 States and observables in the Heisenberg picture

A quantum many-body system is generally described by a **space of states**, which is the projective space of a Hilbert space \mathcal{H} and an operator algebra which is generated by a complete set of **local field operators** $\{\phi_k\}_{k=1}^f$. In the previous chapter we have seen examples for the construction of the Hilbert space of such a kind of theory for free scalar (Klein-Gordon) bosons and spin-1/2 (Dirac) fermions. The Hilbert space is given as the **Fock space** of a system of non-interacting bosons or fermions of indetermined particle number, and we have constructed an explicit s(generalized) basis of symmetrized or antisymmetrized tensor products of single-particle momentum-spin eigenstates and the representation of the local quantum fields in terms of annihilation and creation operators of such states.

In the most general case the state of the system is determined by a positive **semidefinite selfadjoint operator** \mathbf{R} , the **Statistical Operator**. Observables are represented by **selfadjoint operators**, expressed as functions or functionals of the field operators. If \mathbf{O} is a selfadjoint operator, representing an observable (in the following we shall simply identify the observables with their operator representatives) and $|u_o\rangle \in \mathcal{H}$ is an eigenvector, that is normalized to unity or a generalized eigenvector that is “normalized to the δ distribution” of a non-degenerate eigenvalue of the observable \mathbf{O} , then the probability (or probability density) to find this eigenvalue o as result of an (ideal) measurement of the observable is given by

$$P_{\mathbf{R}}(o) = \langle u_o | \mathbf{R} | u_o \rangle. \quad (2.1.1)$$

A set of observables is called **compatible**, if the corresponding operators commute with each other and can thus take determined values if the system is prepared in a common eigenstate of these operators. Such a set of compatible observables is called **complete**, if all of the then existing common eigenspaces are one-dimensional. Then a system, being prepared such that all the values of these observables are determined precisely, is in the corresponding **pure state**, represented by the statistical op-

erator $\mathbf{R}_\psi = |\psi\rangle\langle\psi|$, where $|\psi\rangle$ is a normalized common eigenvector of the compatible and complete set of observables. Since then $|\psi\rangle$ is unique up to an arbitrary phase factor, the pure state is uniquely determined. In the following we shall assume that there exists a countable set of basis vectors defined by such a complete set of compatible observables, i.e., we have an eigenbasis of proper Hilbert-space vectors at hand. For the case of observables with (partially) continuous spectra, in the following the sums have to be substituted by the corresponding integrals.

Now we consider an observable O which is represented by a selfadjoint operator \mathbf{O} with its spectral decomposition

$$\mathbf{O} = \int do |o\rangle\langle o|. \quad (2.1.2)$$

The expectation value of the observable O is then given by

$$\langle O \rangle_{\mathbf{R}} = \int do o P_{\mathbf{R}}(o) = \int do o \langle o | \mathbf{R} | o \rangle = \int do \langle o | \mathbf{R} \mathbf{O} | o \rangle = \text{Tr}(\mathbf{R} \mathbf{O}) = \text{Tr}(\mathbf{O} \mathbf{R}). \quad (2.1.3)$$

In the last step we have used that within the trace operation the operators in a product can be interchanged, as can be shown by the following calculation with a complete orthonormal basis, $|u_k\rangle$

$$\begin{aligned} \text{Tr}(\mathbf{A} \mathbf{B}) &= \sum_j \langle u_j | \mathbf{A} \mathbf{B} | u_j \rangle = \sum_{jk} \langle u_j | \mathbf{A} | u_k \rangle \langle u_k | \mathbf{B} | u_j \rangle \\ &= \sum_{jk} \langle u_k | \mathbf{B} | u_j \rangle \langle u_j | \mathbf{A} | u_k \rangle = \sum_k \langle u_k | \mathbf{B} \mathbf{A} | u_k \rangle = \text{Tr}(\mathbf{B} \mathbf{A}). \end{aligned} \quad (2.1.4)$$

The dynamics of the system is determined by an observable which is bounded from below, represented by the **Hamilton operator** of the system. The time evolution is specified uniquely up to a time-dependent unitary transformation. By this freedom it is possible to choose the time evolution of the states and the operators representing observables with great flexibility without changing the physical content of the theory. Fixing this arbitrariness is called to choose the **picture of time evolution**.

For general considerations in quantum field theory the most convenient choice of the picture is the *Heisenberg picture* that we have already used in the previous chapter for the case of non-interacting particles (i.e., free fields), where the states are time independent while the observables evolve with the full Hamilton operator \mathbf{H} of the system.

This means that the fundamental field operators ϕ evolve according to the equation

$$\frac{d}{dt} \phi = \frac{1}{i} [\phi, \mathbf{H}]. \quad (2.1.5)$$

A general observable \mathbf{O} and the Hamilton operator \mathbf{H} are functions or functionals of the field operators and may depend explicitly on time,

$$\frac{d}{dt} \mathbf{O}[\phi, t] = \frac{1}{i} [\mathbf{O}[\phi, t], \mathbf{H}] + \partial_t \mathbf{O}[\phi, t]. \quad (2.1.6)$$

Here and in the following the partial time derivatives refer to the **explicit time dependence of an operator expression only**. The statistical operator, $\mathbf{R} = \mathbf{R}(\phi, t)$ does *not* represent an observable. In the Heisenberg picture its equation of motion is given by the **von Neumann equation**,

$$\frac{d}{dt} \mathbf{R} = \frac{1}{i} [\mathbf{H}, \mathbf{R}] + \partial_t \mathbf{R} = 0. \quad (2.1.7)$$

From this it follows, that a statistical operator describing **thermal equilibrium**, which must not be explicitly time dependent by definition, always must commute with the Hamiltonian \mathbf{H} . This of course holds true not only in the Heisenberg picture but in any picture of time evolution. Thus, it has to be a **function or functional of the conserved quantities of the system**.

2.1.2 The interaction picture

The main task of statistical physics is to describe the **dynamics of certain collective observables of a many-body system for a given initial state**. For an interacting field theory it is in general not possible to solve such a problem exactly, but (as in vacuum quantum field theory) one has to use **perturbation theory** or appropriate **resummations** to approximate the problem.

To derive the perturbative series we transform to the **interaction picture**. In this picture the field operators evolve with the “undisturbed” Hamiltonian $\mathbf{H}_I^{(0)}$ ¹:

$$\phi_I(t, \vec{x}) = \mathbf{A}_I(t, t_i) \phi_I(t_i, \vec{x}) \mathbf{A}_I^\dagger(t, t_i) \quad \text{with} \quad \mathbf{A}_I(t, t_i) = \mathcal{T}_c \exp \left[i \int_{t_i}^t dt' \mathbf{H}_I^{(0)}(t') \right] \quad (2.1.8)$$

and the statistical operator by the **interaction part** of the Hamiltonian

$$\begin{aligned} \mathbf{R}_I[\phi_I(t, \vec{x}), t] &= \mathbf{C}_I(t, t_i) \mathbf{R}_I[\phi_I(t, \vec{x}), t_i] \mathbf{C}_I^\dagger(t, t_i) \\ \text{with} \quad \mathbf{C}_I(t, t_i) &= \mathcal{T}_c \exp \left[-i \int_{t_i}^t dt' \mathbf{H}_I^{(i)}(t') \right]. \end{aligned} \quad (2.1.9)$$

The symbol \mathcal{T}_c stands for the *chronological time ordering* of the operators, i.e., if one expands the exponentials with respect to their arguments one has to order the operators with increasing time arguments from the right to the left. If the fields ϕ are fermionic it includes a sign change according to the signature of the permutation, which is necessary to bring the operators from the original time order into chronological order. The “unperturbed” and the “perturbation” Hamiltonian add necessarily to the full Hamiltonian in the interaction picture, i.e.,

$$\mathbf{H}_I = \mathbf{H}_I^{(0)} + \mathbf{H}_I^{(i)}. \quad (2.1.10)$$

Usually in quantum field theory one chooses $\mathbf{H}_I^{(0)}$ to be the Hamiltonian for free particles, which is a quadratic functional of the fields, and $\mathbf{H}_I^{(i)}$ as the remaining interaction parts which are a functional of degree 3 and higher. This choice admits the full solution of the field-operator equations of motion (2.1.8) as shown in the previous chapter for Klein-Gordon and Dirac fields.

Now we consider an arbitrary time-dependent operator $\mathbf{O}_I(t)$. Its expectation value can be calculated with help of the initial state $\mathbf{R}_I^{(0)} = \mathbf{R}[\phi_I(t_i, \vec{x})]$ by making use of (2.1.9) in Eq. (2.1.3),

$$\langle \mathbf{O}(t) \rangle_{\mathbf{R}} = \text{Tr}[\mathbf{R}_I(t) \mathbf{O}_I(t)] = \text{Tr}[\mathbf{R}_I^{(0)} \mathbf{C}_I^\dagger(t, t_i) \mathbf{O}_I(t) \mathbf{C}_I(t, t_i)]. \quad (2.1.11)$$

Here we have made use of the rule that we can commute operators within an operator product under the trace. Using (2.1.9) we can write

$$\langle \mathbf{O}(t) \rangle_{\mathbf{R}} = \text{Tr} \left[\mathbf{R}_I^{(0)} \mathcal{T}_a \left\{ \exp \left[i \int_{t_i}^t dt' \mathbf{H}_I^{(i)}(t') \right] \right\} \mathbf{O}_I(t) \mathcal{T}_c \left\{ \exp \left[-i \int_{t_i}^t dt' \mathbf{H}_I^{(i)}(t') \right] \right\} \right]. \quad (2.1.12)$$

¹Here and in the following we denote the interaction picture by a subscript I for operators and states. For details of how to derive these equations see [Hee02].

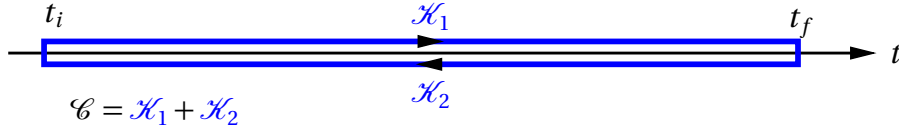


Figure 2.1: *The Schwinger-Keldysh contour. The two branches are denoted with \mathcal{K}_1 (chronological branch) and \mathcal{K}_2 (anti-chronological branch). The ordering symbol $\mathcal{T}_{\mathcal{C}}$ orders the operators with time arguments on the contour in the sense of the arrows from right to left. In the literature there are several conventions around. E.g. in the textbook [LP81] one finds the labels – and + instead of 1 and 2, respectively. In many papers the convention is the opposite. So use some care when studying the literature!*

Here \mathcal{T}_a is the antichronological time ordering symbol, which orders the operators from left to right with increasing time arguments (eventually including the usual sign changes for fermions). The change of order and of the sign in the exponential in the left factor comes from the Hermitean conjugation.

Now (2.1.12) can be compactified easily by introducing **the closed time contour** first defined by Schwinger [Sch61] and Keldysh [Kel64]. This contour is running from the initial time t_i to an arbitrary finite time t_f with $t_i < t < t_f$ and then back to t_i (see Fig. 2.1). Defining a contour ordering symbol $\mathcal{T}_{\mathcal{C}}$ such, that operators with time arguments on the contour are ordered from right to left in the sense of the contour we can write (2.1.12) as

$$\langle \mathbf{O}(t) \rangle_{\mathbf{R}} = \text{Tr} \left\{ \mathbf{R}_I^{(0)} \mathcal{T}_{\mathcal{C}} \left[\exp \left(-i \int_{\mathcal{C}} dt' \mathbf{H}_I^{(i)}(t') \right) \mathbf{O}_I(t) \right] \right\}. \quad (2.1.13)$$

Since the time evolution of the operators representing observables is due to the unperturbed Hamiltonian, the operator $\mathbf{O}_I(t)$ is known, and the initial state $\mathbf{R}_I^{(0)}$ at time t_i is given by the preparation of the physical situation in an experiment or by observation, we only need to calculate approximations for the contour-ordered exponential function, which can be done, for instance, in an analogous way as in usual perturbation theory.

One sees immediately, that (2.1.13) is independent of the final time t_f since the contributions of the time interval (t, t_f) from the two branches cancel. Further it is clear, that (2.1.13) can be generalized to operators with more than one time argument

$$\langle \mathcal{T}_{\mathcal{C}} \phi(x_1) \phi(x_2) \cdots \phi(x_n) \rangle_{\mathbf{R}} = \text{Tr} \left[\mathbf{R}_I^{(0)} \mathcal{T}_{\mathcal{C}} \left\{ \exp \left[-i \int_{\mathcal{C}} d\tau \mathbf{H}_I^{(i)}(\tau) \right] \phi_I(x_1) \cdots \phi_I(x_n) \right\} \right]. \quad (2.1.14)$$

We only must make sure that all time arguments are in the interval, $x_j^0 \in [t_i, t_f]$ for $j \in \{1, 2, \dots, n\}$.

2.1.3 The entropy principle

Up to now we did not specify how to choose the statistical operator. To establish rules for that, one has to add statistical concepts from outside of quantum theory itself. One possible rule has its origins in **statistical signal theory**. One defines the entropy as a measure of the missing information relative to a somehow defined complete knowledge of the system under the constraints of the given generally incomplete information [Jay57a, Jay57b, Kat67, Hob87]. In its quantum version the entropy of the system, described by a given statistical operator \mathbf{R} , this measure is given by the **von Neumann entropy**

$$S = -\langle \ln(\mathbf{R}) \rangle = -\text{Tr}[\mathbf{R} \ln(\mathbf{R})]. \quad (2.1.15)$$

If \mathbf{R} describes a pure state, i.e., is given by $\mathbf{R} = |\psi\rangle\langle\psi|$ with a normalized state ket $|\psi\rangle$, the entropy vanishes, as it should be, since in quantum mechanics the knowledge of the pure state of the system is the most complete knowledge we can have about it. So in this case there is no missing information, and that is indicated by $S = 0$.

In physics usually one has a certain incomplete knowledge about the system under consideration. The standard situation in statistical physics of many-body systems is, that we know the expectation values \mathcal{O}_i of a finite set $\{\mathbf{O}_i\}$ of some macroscopic (collective) observables. Then one defines the statistical operator \mathbf{R} by the demand, that the von Neumann entropy (2.1.15) should be maximal under the constraint, that the **expectation values** of the observables are these known values. This is also known as **Jaynes's principle of least prejudice** since with respect to the measure of the incompleteness of information about the system a maximized entropy guarantees not to pretend more knowledge about the system in the choice of the statistical operator, than there really exists by knowing the expectation values of the observables \mathbf{O}_i . Thus, we have to maximize

$$S[\mathbf{R}, \lambda_i] = \text{Tr} \left\{ -\mathbf{R} \left[\ln(\mathbf{R}) - \sum_i \lambda_i \mathbf{O}_i \right] \right\}, \quad (2.1.16)$$

where the λ_i are Lagrange parameters to be adjusted such, that the expectation values of the observables take the given numbers

$$\langle \mathbf{O}_i \rangle = \text{Tr}(\mathbf{O}_i \mathbf{R}) = \mathcal{O}_i. \quad (2.1.17)$$

The solution of the maximization problem reads

$$\mathbf{R} = \frac{1}{Z} \exp \left(- \sum_i \lambda_i \mathbf{O}_i \right) \quad \text{with} \quad Z = \text{Tr} \left[\exp \left(- \sum_i \lambda_i \mathbf{O}_i \right) \right]. \quad (2.1.18)$$

The **partition sum** Z appears in this equation in order to normalize the statistical operator to 1, i.e.,

$$\text{Tr} \mathbf{R} = 1. \quad (2.1.19)$$

We could have subsumed this as an additional constraint by choosing one of the \mathbf{O}_i to equal the identity operator $\mathbb{1}$. As we have already mentioned after Eq. (2.1.7) for a statistical operator describing thermal equilibrium the \mathbf{O}_i have to be conserved quantities.

2.1.4 Thermal equilibrium and thermodynamic potentials

Now we consider the case of **thermal equilibrium**, i.e., we investigate the **stationary state** of the many-body system. This means that the statistical operator is not explicitly time dependent, i.e.,

$$\frac{\partial \mathbf{R}}{\partial t} = 0. \quad (2.1.20)$$

Due to the von Neumann equation (2.1.7) this means that \mathbf{R} must commute with the Hamiltonian, i.e., it can only be a **function of the conserved quantities** of the system. For the simple case of an interacting gas consisting of charged Klein-Gordon particles, these conserved quantities are the total energy, total momentum, and total charge (or net-particle number, i.e., the number of particles minus the number of antiparticles, cf. (1.2.59)). Due to the maximum-entropy principle the only knowledge we may assume is then about the values of these conserved quantities. The statistical operator then reads

$$\mathbf{R} = \frac{1}{Z} \exp(-\beta u \cdot \mathbf{P} + \alpha Q), \quad (2.1.21)$$

where the **partition sum** is given by

$$Z = \text{Tr}[\exp(-\beta \mathbf{u} \cdot \mathbf{P} + \alpha \mathbf{Q})]. \quad (2.1.22)$$

Here we have written a somewhat more general statistical operator for the equilibrium than usually treated in the literature. We have written the Lagrange multipliers for the four momentum as $\beta \mathbf{u}$ with a scalar $\beta \in \mathbb{R}$ and a four vector $\mathbf{u} \in \mathbb{R}^4$ with $u^2 = 1$. We must take \mathbf{u} time like in order to have a Statistical operator for which the trace in (2.1.22) exists. The mean momentum and charge are then easily calculated as derivatives of the partition sum:

$$\langle P^\mu \rangle = -\frac{1}{\beta} \frac{\partial \Omega}{\partial u_\mu}, \quad \langle Q \rangle = \frac{\partial \Omega}{\partial \alpha} \quad (2.1.23)$$

with

$$\Omega = \ln Z. \quad (2.1.24)$$

Since the only vector available in the independent variables α , β , and u^μ is the latter quantity u^μ we must have

$$\langle P^\mu \rangle = U u^\mu, \quad (2.1.25)$$

where U is the total invariant mass of the system. Since u^μ is time-like, we also can make $u^\mu = (1, 0, 0, 0)$ by a Lorentz boost with three-velocity $\vec{v} = \vec{u}/u^0$. In this reference frame the many-particle system is at rest as a whole, since its average three-momentum vanishes. In this **rest frame of the heat bath** it has the total energy $\langle P^0 \rangle$, which is known in thermodynamics as the **internal energy**. That U is also the total mass of the system is Einstein's famous **energy-mass equivalence** in special relativity. By definition it is a scalar quantity. In the most general frame of reference, it is obviously given by

$$U = \mathbf{u} \cdot \langle \mathbf{P} \rangle = -\frac{\partial \Omega}{\partial \beta}. \quad (2.1.26)$$

To also interpret the other quantities we try to derive the relation of Ω to the usual thermodynamic quantities. The key to this derivation is the **first law of thermodynamics** in the form

$$dU = TdS - pdV + \mu d\langle Q \rangle. \quad (2.1.27)$$

Here, T is the temperature, S the entropy, p the pressure, V the volume, μ the chemical potential, and Q some conserved charge, as the average net-particle number $\langle N - \bar{N} \rangle$ in our case of charged bosons. In our quantum-field theoretical formalism the volume enters as an external parameter. This is formally achieved by considering a finite cubic box within a large volume and assuming some appropriate (e.g., periodic) boundary conditions (1.2.12). According to (2.1.21) the entropy is given by

$$S = -\text{Tr}(\mathbf{R} \ln \mathbf{R}) = \Omega + \beta U - \alpha \langle Q \rangle. \quad (2.1.28)$$

Here, all quantities have to be read as functions of the independent parameters, i.e., the Lagrange parameters of the entropy principle and the external parameters of the system, which in our case is only the volume V . From this we find

$$\begin{aligned} dS = dV & \left(\frac{\partial \Omega}{\partial V} + \beta \frac{\partial U}{\partial V} - \alpha \frac{\partial \langle Q \rangle}{\partial V} \right) \\ & + d\beta \left(\frac{\partial \Omega}{\partial \beta} + U + \frac{\partial U}{\partial \beta} \right) \\ & + d\alpha \left(\frac{\partial \Omega}{\partial \alpha} + \beta \frac{\partial U}{\partial \alpha} - \langle Q \rangle - \alpha \frac{\partial \langle Q \rangle}{\partial \alpha} \right). \end{aligned} \quad (2.1.29)$$

Now using (2.1.23) this simplifies to

$$dS = dV \frac{\partial \Omega}{\partial V} + \beta dU - \alpha d\langle Q \rangle. \quad (2.1.30)$$

Multiplying with $T = 1/\beta$ and solving for dU we get

$$dU = T dS - dV \frac{\partial(T\Omega)}{\partial V} + T \alpha d\langle Q \rangle. \quad (2.1.31)$$

A comparison with the first law (2.1.27) immediately leads to the identifications

$$T = \frac{1}{\beta}, \quad \mu = T\alpha, \quad p = \frac{\partial(T\Omega)}{\partial V}. \quad (2.1.32)$$

Now we can as well read all the thermodynamic quantities as functions of V , $T = 1/\beta$, and $\mu = \alpha/\beta$. Because of (2.1.23) we have

$$\left(\frac{\partial \Omega}{\partial T}\right)_{V,\mu} = -\frac{1}{T^2} \frac{\partial}{\partial \beta} \Omega(\beta, \alpha = \mu\beta) = \frac{1}{T^2} (U + \mu \langle Q \rangle), \quad (2.1.33)$$

and according to (2.1.28) the entropy is given by

$$S = \Omega + \frac{U}{T} - \frac{\mu}{T} \langle Q \rangle. \quad (2.1.34)$$

With (2.1.33) from this we immediately find

$$S = \left(\frac{\partial [T\Omega(T, \mu, V)]}{\partial T} \right)_{V,\mu}. \quad (2.1.35)$$

This leads us to the definition of the **Landau grand canonical potential**

$$\Phi(T, \mu, V) = -T\Omega(T, \mu, V). \quad (2.1.36)$$

From (2.1.34) we have

$$\Phi = -T\Omega = U - TS - \mu Q \quad (2.1.37)$$

and the total differential gives

$$d\Phi = -SdT + p dV + Qd\mu, \quad (2.1.38)$$

where we have made use of the first law of thermodynamics (2.1.31) again. The natural variables for the grand canonical potential thus are

$$\Phi = \Phi(T, \mu, V) \stackrel{2.1.38}{\Leftrightarrow} S = -\left(\frac{\partial \Phi}{\partial T}\right)_{\mu, V}, \quad p = -\left(\frac{\partial \Phi}{\partial V}\right)_{T, \mu}, \quad \langle Q \rangle = -\left(\frac{\partial \Phi}{\partial \mu}\right)_{T, V}. \quad (2.1.39)$$

As we shall see, the grand canonical potential is the most convenient thermodynamical quantity to evaluate in the quantum-field theoretical approach to equilibrium many-body theory: It is directly related with the partition sum via its definition (2.1.36) and Eq. (2.1.24). At the same time it admits a natural derivation of the physical renormalization conditions that render the quantum-field theoretical quantities finite. This is necessary since also quantum field theory at finite temperature and chemical potential is plagued by the same divergences as in the vacuum. The analogous quantity in the vacuum

is the **quantum effective action** (see, e.g., [Hee02]), and the trace of the partition sum also includes the vacuum vacuum state. Thus one must have at least the same infinities of the vacuum theory. Even for free particles one has to subtract the contributions from the vacuum-energy contribution of each field mode, which diverges when summed over all momenta. For the interacting field theory there are additional divergences from the loops in Feynman diagrams representing the corrections to the effective action within perturbation theory. We shall show later in these notes that these divergences from the vacuum contribution are the only divergences also at finite temperature and chemical potential, i.e., the theory is rendered finite by renormalizing the divergent vacuum parts of each diagram and subdiagram using the BPHZ renormalization formalism (for the vacuum case, see again [Hee02]).

2.2 Perturbation theory in thermal equilibrium

We begin our study of quantum many-body systems on hand of the most simple example of an interacting field theory with the goal to derive **diagram rules** for the perturbative evaluation of expectation values of observables for a system **in thermal equilibrium**, similar to the **Feynman-diagram technique**, used in “vacuum quantum field theory” to evaluate S -matrix elements for scattering cross sections. We shall study simple ϕ^4 theory as a toy model to establish these diagram rules for **thermal quantum field theory**.

2.2.1 The canonical statistical operator

Simple ϕ^4 theory is defined with as a model for self-interacting real scalar fields. In the **Heisenberg picture** the Lagrangian reads²

$$\mathcal{L}_H = \frac{1}{2}(\partial_\mu \phi_H)(\partial^\mu \phi_H) - \frac{m^2}{2}\phi_H^2 - \frac{\lambda}{4!}\phi_H^4. \quad (2.2.1)$$

We note that this model is renormalizable in the usual sense, i.e., any divergences coming up in the perturbative evaluation in higher orders of perturbation theory can be **renormalized** with counter terms in the Lagrangian that are of the same form as this original Lagrangian, i.e., with wave-function, mass, and coupling-constant renormalizations (see [Hee02] for a detailed treatment of perturbation theory in the vacuum). As we shall see in a later section, there appear no additional divergences in thermal field theory than in vacuum field theory, i.e., the thermal Feynman diagrams are renormalized with the same counter terms as vacuum theory, and thus the renormalized Lagrangian (or Hamiltonian) does not depend on temperature.

The canonical field momentum is

$$\Pi_H = \frac{\partial \mathcal{L}_H}{\partial \dot{\phi}_H} = \dot{\phi}_H, \quad (2.2.2)$$

and the Hamiltonian reads

$$\mathcal{H}_H = \Phi_H \Pi_H - \mathcal{L} = \frac{1}{2}\Pi_H^2 + (\vec{\nabla}\phi_H)^2 + \frac{m^2}{2}\phi_H^2 + \frac{\lambda}{4!}\phi_H^4. \quad (2.2.3)$$

Since the Lagrangian and thus also the Hamiltonian are not explicitly time dependent, according to Noether’s theorem the total energy

$$\mathbf{H}_H = \int_{\mathbb{R}^3} d^3\vec{x} \mathcal{H}_H \quad (2.2.4)$$

²To make the use of the different pictures of time evolution more clear in this section we label the operators in the Heisenberg picture with a subscript H and in the interaction picture with I.

is constant.

In the following we want to evaluate expectation values of arbitrary observables with respect to the **canonical statistical operator**

$$\mathbf{R}_H = \frac{1}{Z} \exp(-\beta \mathbf{H}_H) \quad \text{with} \quad Z = \text{Tr} \exp(-\beta \mathbf{H}_H). \quad (2.2.5)$$

Here, $\beta = 1/T$ is the inverse temperature which is assumed to be time independent, i.e., we describe a system in **global thermal equilibrium**. We also use the **restframe of the medium** as our frame of reference, setting $u = (1, 0, 0, 0)$ in (2.1.21).

As explained in Section 2.1.1, in the Heisenberg picture the field operators evolve in time by

$$\phi_H(t, \vec{x}) = \mathbf{A}_H(t, t_i) \phi_H(t_i, \vec{x}) \mathbf{A}_H^\dagger(t, t_i), \quad (2.2.6)$$

where the time-evolution operator obeys the differential equation and initial condition

$$\partial_t \mathbf{A}_H(t, t_i) = i \mathbf{H}_H \mathbf{A}_H(t, t_i), \quad \mathbf{A}_H(t_i, t_i) = \mathbb{1}. \quad (2.2.7)$$

Since the Hamiltonian does not depend on time the solution reads

$$\mathbf{A}_H(t, t_i) = \exp[i(t - t_i) \mathbf{H}_H]. \quad (2.2.8)$$

The time evolution operator is unitary as it should be, because \mathbf{H}_H is selfadjoint.

In the Heisenberg picture the statistical operator is time-independent, if it is not explicitly time dependent. For the following it is crucial that the equilibrium statistical operator (2.2.5) can be formally written as

$$\mathbf{R}_H = \frac{1}{Z} \mathbf{A}_H^\dagger(t_i - i\beta, t_i) \quad \text{with} \quad Z = \text{Tr} \exp(-\beta \mathbf{H}_H). \quad (2.2.9)$$

This corresponds to an inverse time evolution operator along the vertical contour in the complex time plane, running from t_i vertically down to $t_i - i\beta$.

The expectation value of an arbitrary observable is thus given by

$$\langle O(x) \rangle = \text{Tr}[\mathbf{R}_H \mathbf{O}_H(x)] = \frac{1}{Z} \text{Tr}[\mathbf{A}_H(t_i - i\beta, t_i) \mathbf{O}_H(x)]. \quad (2.2.10)$$

2.2.2 Thermal perturbation theory

In practice it is impossible to evaluate such expectation values exactly since the full time evolution of the field operators and thus the observables, built with field operators, cannot be solved explicitly. The same is true for the trace in (2.2.10).

What can be solved, is the equation of motion for the free field operator, and we can also evaluate expectation values with respect to the canonical Hamiltonian of the free field, i.e.,

$$\mathbf{R}_I^{(0)} = \frac{1}{Z_0} \exp(-\beta \mathbf{H}_I^0). \quad (2.2.11)$$

Here, the time evolution of field operators and observables, built as functions or functionals of field operators, is given with respect to the free Hamiltonian

$$\mathcal{H}_I^{(0)} = \frac{1}{2} (\partial_\mu \phi_I) (\partial^\mu \phi_I) - \frac{m^2}{2} \phi_I^2, \quad (2.2.12)$$

which leads to the equations of motion for the free fields, treated in chapter 1.2. Here the free Hamilton operator,

$$\mathbf{H}_I^{(0)} = \int_{\mathbb{R}^3} d^3\vec{x} \mathcal{H}_I^{(0)} \quad (2.2.13)$$

is time independent and thus the time evolution operator for field and observable operators reads

$$\mathbf{A}_I(t, t_i) = \exp[i(t - t_i)\mathbf{H}_I^{(0)}]. \quad (2.2.14)$$

The time evolution of the state, i.e., the statistical operator of the system in the interaction picture is

$$\mathbf{H}_I^{(i)}(t) = \frac{\lambda}{4!} \int_{\mathbb{R}^3} d^3\vec{x} \phi_I^4, \quad (2.2.15)$$

which is time dependent and thus the unitary time-evolution operator for the states, fulfilling the initial-value problem

$$\partial_t \mathbf{C}_I(t, t_i) = -i\mathbf{H}_I^{(i)}(t)\mathbf{C}_I(t, t_i), \quad \mathbf{C}_I(t_i, t_i) = \mathbb{1}, \quad (2.2.16)$$

is given by

$$\mathbf{C}_I(t, t_i) = \mathcal{T}_c \exp \left[-i \int_{t_i}^t dt' \mathbf{H}_I^{(i)}(t') \right]. \quad (2.2.17)$$

We assume that at the initial time t_i the operators in the Heisenberg and the interaction picture coincide. Especially for the equilibrium statistical operator we have

$$\mathbf{R}_H = \mathbf{R}_I(t_i) = \mathbf{C}_I^\dagger(t, t_i)\mathbf{R}_I(t)\mathbf{C}_I(t, t_i). \quad (2.2.18)$$

Thus the unitary transformation from the interaction to the Heisenberg picture reads

$$\mathbf{U}_{HI}(t, t_i) = \mathbf{C}_I^\dagger(t, t_i). \quad (2.2.19)$$

On the other hand we find the same transformation by investigating the time evolution of the field operators:

$$\phi_H(t, \vec{x}) = \mathbf{A}_H(t, t_i)\phi_I(t_i, \vec{x})\mathbf{A}_H^\dagger(t, t_i) = \mathbf{A}_H(t, t_i)\mathbf{A}_I^\dagger(t, t_i)\phi_I(t_i, \vec{x})\mathbf{A}_I(t, t_i)\mathbf{A}_H^\dagger(t, t_i). \quad (2.2.20)$$

From this we get

$$\mathbf{U}_{HI}(t, t_i) = \mathbf{A}_H(t, t_i)\mathbf{A}_I^\dagger(t, t_i). \quad (2.2.21)$$

Comparing (2.2.19) and (2.2.21) we see that this implies that

$$\mathbf{A}_H^\dagger(t, t_i) = \mathbf{A}_I^\dagger(t, t_i)\mathbf{C}_I(t, t_i). \quad (2.2.22)$$

To see that this is indeed true, we take the time derivative of the right-hand side of this equation:

$$\begin{aligned} \partial_t \left[\mathbf{A}_I^\dagger(t, t_i)\mathbf{C}_I(t, t_i) \right] &= -i\mathbf{A}_I^\dagger(t, t_i)\mathbf{H}_I^{(0)}(t)\mathbf{C}_I(t, t_i) - i\mathbf{A}_I^\dagger(t, t_i)\mathbf{H}_I^{(i)}(t)\mathbf{C}_I(t, t_i) \\ &= -i[\mathbf{H}_I^{(0)}(t) + \mathbf{H}_I^{(i)}(t)]\mathbf{A}_I^\dagger(t, t_i)\mathbf{C}_I(t, t_i) = -i\mathbf{H}_H\mathbf{A}_I^\dagger(t, t_i)\mathbf{C}_I(t, t_i). \end{aligned} \quad (2.2.23)$$

This means that the unitary operator on the right-hand side of (2.2.22) fulfills the equation of motion of $\mathbf{A}_H^\dagger(t, t_i)$. Since it also fulfills the same initial condition, $\mathbf{A}_H^\dagger(t_i, t_i) = \mathbb{1}$, it must indeed be that same operator as claimed in (2.2.22).

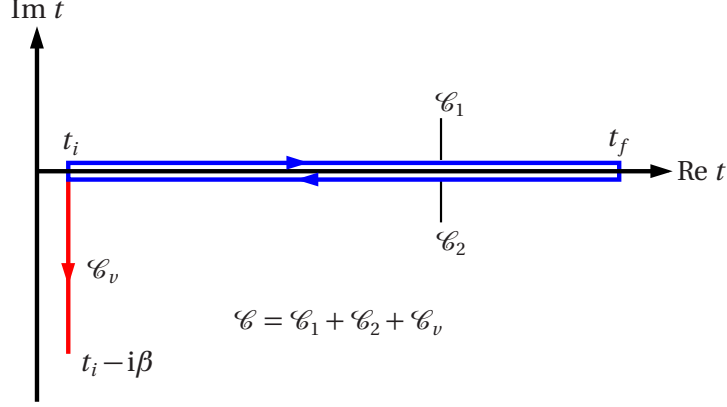


Figure 2.2: *The modified Schwinger-Keldysh contour for diagram rules applicable in thermal equilibrium.*

Using (2.2.9) we have

$$\mathbf{R}_H = \frac{1}{Z} \mathbf{A}_I^\dagger(t_i - i\beta, t_i) \mathbf{C}_I(t_i - i\beta, t_i) = \frac{1}{Z} \exp(-\beta \mathbf{H}_I^{(0)}) \mathcal{T}_{\mathcal{C}_v} \exp \left[-i \int_{\mathcal{C}_v} dt' \mathbf{H}_I^{(i)}(t') \right]. \quad (2.2.24)$$

Here, we have introduced the **vertical addition to the Schwinger-Keldysh contour**, cf. Fig. 2.2, which we shall find very convenient soon.

Thus the equilibrium expectation value of an observable is given by

$$\begin{aligned} \langle O(t) \rangle &= \text{Tr}[\mathbf{R}_H \mathbf{O}_H(x)] \\ &= \frac{1}{Z} \text{Tr} \left\{ \exp(-\beta \mathbf{H}_I^{(0)}) \mathcal{T}_{\mathcal{C}_v} \exp \left[-i \int_{\mathcal{C}_v} dt' \mathbf{H}_I^{(i)}(t') \right] \mathbf{C}_I^\dagger(t, t_i) \mathbf{O}_I(x) \mathbf{C}_I(t, t_i) \right\}. \end{aligned} \quad (2.2.25)$$

In the last step we have used (2.2.24) and the transformation operator (2.2.19) from the interaction to the Heisenberg picture.

Now, using the original real part of the Schwinger-Keldysh contour (cf. the blue paths running from t_i to t_f (\mathcal{C}_1) and back (\mathcal{C}_2) in Fig. 2.2, which together we call $\mathcal{C}_R = \mathcal{C}_1 + \mathcal{C}_2$), we can write

$$\mathbf{C}_I^\dagger(t, t_i) \mathbf{O}_I(x) \mathbf{C}_I(t, t_i) = \mathcal{T}_{\mathcal{C}_R} \exp \left[-i \int_{\mathcal{C}_R} dt' \mathbf{H}_I^{(i)}(t') \right] \mathbf{O}_I(t). \quad (2.2.26)$$

Here we have assumed $t_i \leq t \leq t_f$. This is not a real restriction since we always can put $t_i \rightarrow -\infty$ and $t_f \rightarrow \infty$ because the expectation values do not depend on t_i or t_f , which is clear from the first line of (2.2.25). Plugging (2.2.26) into (2.2.25) we can combine the contour ordered exponentials with respect to the vertical and the real part to the **full extended Schwinger-Keldysh contour**, leading to

$$\langle O(t) \rangle = \frac{1}{Z} \text{Tr} \left\{ \exp(-\beta \mathbf{H}_I^{(0)}) \mathcal{T}_{\mathcal{C}} \exp \left[-i \int_{\mathcal{C}} dt' \mathbf{H}_I^{(i)}(t') \right] \mathbf{O}_I(t) \right\}. \quad (2.2.27)$$

This is, up to a factor $Z^{(0)}$, indeed an expectation value of interaction-picture operators with respect to the free equilibrium statistical operator. Expansion of the \mathcal{C} -ordered exponential shall lead to the **perturbative expansion** of expectation values.

In the next Sect. we shall show that the perturbative evaluation of **contour-ordered Green's functions**

$$iG_{\mathcal{C}}^{(n)}(x_1, x_2, \dots, x_n) = \frac{1}{Z} \text{Tr} \left\{ \exp(-\beta \mathbf{H}_H) T_{\mathcal{C}} \phi_H(x_1) \phi_H(x_2) \cdots \phi_H(x_n) \right\} \quad (2.2.28)$$

for **time arguments along the real part of the contour** can be evaluated by making use of the real part of the contour only. In the same way as we have derived (2.2.27) we can write for (2.2.28)

$$iG_{\mathcal{C}}^{(n)}(x_1, x_2, \dots, x_n) = \frac{1}{Z} \text{Tr} \left\{ \exp(-\beta \mathbf{H}_I^{(0)}) T_{\mathcal{C}} \exp \left[-i \int_{\mathcal{C}} dt' \mathbf{H}_I^{(i)}(t') \right] \right. \\ \left. \times \phi_I(x_1) \phi_I(x_2) \cdots \phi_I(x_n) \right\} \quad (2.2.29)$$

2.2.3 The generating functional for Green's functions

It is a very convenient trick to use a **generating functional** for these Green's functions since it facilitates the derivation of the Feynman rules considerably. A more conventional way to come to the same rules is to first prove **Wick's theorem** which holds true for expectation values with respect to the free Hamiltonian in the same way as in the vacuum (see [Hee02] for a derivation). More generally it is true for any statistical operator which is given as the exponential of a one-particle operator, i.e., a quadratic functional of the field operators [Dan84]. The only difference is that for the contractions of field-operator pairs we have to use the free **one-particle contour Green's function**

$$i\Delta_{\mathcal{C}}(x_1, x_2) = \frac{1}{Z_0} \text{Tr} \left\{ \exp(-\beta \mathbf{H}_I^{(0)}) \mathcal{T}_{\mathcal{C}} \phi_I(x_1) \phi_I(x_2) \right\} =: \langle \mathcal{T}_{\mathcal{C}} \phi_I(x_1) \phi_I(x_2) \rangle^{(0)}. \quad (2.2.30)$$

We shall derive the Feynman rules by first introducing the **generating functional**

$$Z^{(0)}[J] = \frac{1}{Z_0} \text{Tr} \left\{ \exp(-\beta \mathbf{H}_I^{(0)}) \mathcal{T}_{\mathcal{C}} \exp \left[i \int_{\mathcal{C}} d^4x J(x) \phi_I(x) \right] \right\} \quad (2.2.31)$$

for **free Green's functions**. Here we have written $\int_{\mathcal{C}} d^4x := \int_{\mathcal{C}} dx^0 \int_{\mathbb{R}^3} d^3\vec{x}$. It is immediately clear that we get the n -point contour Green's function by functional derivatives of this functional,

$$iG_{\mathcal{C},0}^{(n)}(x_1, x_2, \dots, x_n) := \text{Tr} \left\{ \exp(-\beta \mathbf{H}_I^{(0)}) \mathcal{T}_{\mathcal{C}} \phi(x_1) \phi(x_2) \cdots \phi(x_n) \right\} \\ = \frac{\delta}{i\delta J(x_1)} \frac{\delta}{i\delta J(x_2)} \cdots \frac{\delta}{i\delta J(x_n)} Z^{(0)}[J] \Big|_{J=0}. \quad (2.2.32)$$

Obviously, by the same arguments, the generating functional for **exact Green's functions** is given by the analogous expression as (2.2.31) but with the full Hamiltonian and the Heisenberg-field operators,

$$Z'[J] = \frac{1}{Z} \text{Tr} \left\{ \exp(-\beta \mathbf{H}_H) \mathcal{T}_{\mathcal{C}} \exp \left[i \int_{\mathcal{C}} d^4x J(x) \phi_H(x) \right] \right\}. \quad (2.2.33)$$

Using (2.2.29) we can write this as

$$Z'[J] = \frac{1}{Z} \text{Tr} \left\{ \exp(-\beta \mathbf{H}_I^{(0)}) \mathcal{T}_{\mathcal{C}} \exp \left[-i \int_{\mathcal{C}} dt' \mathbf{H}_I^{(i)}(t') \right] \exp \left[i \int_{\mathcal{C}} d^4x J(x) \phi_I(x) \right] \right\}. \quad (2.2.34)$$

Now we use (2.2.15) and (2.2.32) to express the generating functional (2.2.33) for exact Green's functions in terms of that for perturbative Green's functions:

$$Z'[J] = \frac{Z_0}{Z} \exp \left[-\frac{i\lambda}{4!} \int_{\mathcal{C}} d^4x \frac{\delta^4}{\delta J(x)^4} \right] Z^{(0)}[J]. \quad (2.2.35)$$

Expanding the integro-differential exponential operator in its power series, we obtain the (formal) **Dyson series** for the generating functional, providing the perturbative expansion of the generating functional of exact Green's functions as a power series in the coupling constant, λ .

For convenience we can also define

$$Z[J] = \exp \left[-\frac{i\lambda}{4!} \int_{\mathcal{C}} d^4x \frac{\delta^4}{\delta J(x)^4} \right] Z^{(0)}[J]. \quad (2.2.36)$$

Because of (2.2.35) this implies

$$Z[J=0] = \frac{Z}{Z_0}, \quad (2.2.37)$$

and thus with this generating functional the Green's functions are given by

$$iG_{\mathcal{C}}^{(n)}(x_1, \dots, x_n) = \frac{1}{Z[J=0]} \left(\frac{\delta^n Z[J]}{i\delta J(x_1) i\delta J(x_2) \cdots i\delta J(x_n)} \right)_{J=0}. \quad (2.2.38)$$

To derive the Feynman rules, thus we first need to evaluate (2.2.32) To perform the trace, we use the occupation-number basis. We can use all formulae from Sect. 1.2, but since we here assumed a selfadjoint scalar field, describing uncharged particles, the mode decomposition reads

$$\phi_{\text{I}}(x) = \sum_{\vec{k}} \frac{1}{\sqrt{V}} \left[\mathbf{a}(\vec{k}) u_{\vec{k}}(x) + \mathbf{a}^\dagger(\vec{k}) u_{\vec{k}}^*(x) \right]. \quad (2.2.39)$$

Here we used the definition of the mode functions (1.2.24) and introduced a finite quantization volume V . According to (2.2.30) we have to evaluate the trace

$$\begin{aligned} Z_0 Z^{(0)}[J] &= \text{Tr} \left\{ \exp(-\beta \mathbf{H}_{\text{I}}^{(0)}) \mathcal{T}_{\mathcal{C}} \exp \left[i \int_{\mathcal{C}} d^4x J(x) \phi_{\text{I}}(x) \right] \right\} \\ &= \sum_{n(\vec{k})=0}^{\infty} \left\langle \{n(\vec{k})\} \left| \exp(-\beta \mathbf{H}_{\text{I}}^{(0)}) \mathcal{T}_{\mathcal{C}} \exp \left[i \int_{\mathcal{C}} d^4x J(x) \phi_{\text{I}}(x) \right] \right| \{n(\vec{k})\} \right\rangle. \end{aligned} \quad (2.2.40)$$

For the Hamiltonian we use the normal-ordered (renormalized) form (1.2.28), which for our neutral particles reads

$$\mathbf{H}_{\text{I}}^{(0)} = \sum_{\vec{k}} \mathbf{N}(\vec{k}) \omega_{\vec{k}}. \quad (2.2.41)$$

From this we find, letting the first exponential operator in (2.2.40) act to the left,

$$Z_0 Z^{(0)}[J] = \sum_{n(\vec{k})=0}^{\infty} \exp \left(-\beta \sum_{\vec{k}} n(\vec{k}) \omega_{\vec{k}} \right) \left\langle \{n(\vec{k})\} \left| \mathcal{T}_{\mathcal{C}} \exp \left[i \int_{\mathcal{C}} d^4x J(x) \phi_{\text{I}}(x) \right] \right| \{n(\vec{k})\} \right\rangle. \quad (2.2.42)$$

To evaluate the expectation value, we have to expand the exponential. This gives expectation values of contour-ordered field-operator products,

$$\begin{aligned}
 Z^{(n)}[J] &= \left\langle \mathcal{T}_{\mathcal{C}} \left\{ \prod_{a=1}^n J(x_a) \phi_{\mathbb{I}}(x_a) \right\}_{1\dots n} \right\rangle^{(0)} \\
 &= \frac{i^n}{n!} \sum_{n(\vec{k})=0}^{\infty} \exp \left[-\beta \sum_{\vec{k}} n(\vec{k}) \omega_{\vec{k}} \right] \\
 &\quad \times \left\langle \{n(\vec{k})\} \left| \mathcal{T}_{\mathcal{C}} \left\{ \prod_{a=1}^n J(x_a) \phi_{\mathbb{I}}(x_a) \right\}_{1\dots n} \right| \{n(\vec{k})\} \right\rangle,
 \end{aligned} \tag{2.2.43}$$

where we have introduced the short-hand notation

$$\{f(x_1, \dots, x_n)\}_{1\dots n} = \int_{\mathcal{C}} d^4x_1 \cdots \int_{\mathcal{C}} d^4x_n f(x_1, \dots, x_n), \tag{2.2.44}$$

where the temporal integrals run over the time contour and the spatial integrals over the cubic volume V .

Now we read the field operators in terms of the mode decomposition (2.2.39). Since the occupation-number states are orthogonal, and we have

$$\begin{aligned}
 \mathbf{a}^{\dagger}(\vec{p}) \left| \{n(\vec{k})\} \right\rangle &= \sqrt{n(\vec{p})+1} \left| \{n(\vec{k})\}_{\vec{k} \neq \vec{p}} \cup \{n(\vec{p}) \rightarrow n(\vec{p})+1\} \right\rangle, \\
 \mathbf{a}(\vec{p}) \left| \{n(\vec{k})\} \right\rangle &= \sqrt{n(\vec{p})} \left| \{n(\vec{k})\}_{\vec{k} \neq \vec{p}} \cup \{n(\vec{p}) \rightarrow n(\vec{p})-1\} \right\rangle,
 \end{aligned} \tag{2.2.45}$$

due to the trace all matrix elements in (2.2.43) are with respect to the same occupation-number basis state for the bra and the ket, only those contributions from the field-operator product which consists of the same number of annihilation operators \mathbf{a} and creation operators \mathbf{a}^{\dagger} . Because of the orthonormality of this basis we further have

$$\left\langle \{n'(\vec{k})\} \left| \{n(\vec{k})\} \right\rangle \right\rangle = \prod_{\vec{k}} \delta_{n'(\vec{k}), n(\vec{k})}, \tag{2.2.46}$$

and thus only those parts of the matrix elements which consist of the same number of annihilation and creation operators survive. This implies that only operator products with an even number, $n = 2j$, contribute, and these matrix elements are given by all sums over possible contractions, very similar as in the **Wick theorem** for vacuum expectation values (see [Hee02] for more details). The only difference is that here the contractions are defined by

$$\mathcal{T}_{\mathcal{C}} \phi_{\mathbb{I}}^{\bullet}(x_1) \phi_{\mathbb{I}}^{\bullet}(x_2) = \langle \mathcal{T}_{\mathcal{C}} \phi_{\mathbb{I}}(x_1) \phi_{\mathbb{I}}(x_2) \rangle^{(0)} = i \Delta_{\mathcal{C}}(x_1, x_2) \tag{2.2.47}$$

with the free contour-ordered propgator (2.2.30). Thus for an even number $n = 2j$ of field operators in (2.2.43) the sum over all contractions reduces just to the multiplication with the number of complete contractions³. Each contraction provides a factor $i^j [\{\Delta_{\mathcal{C}}(x_1, x_2) J(x_1) J(x_2)\}_{12}]^j$. This means that

$$Z_0^{(2j)}[J] = \frac{(-i)^j}{2^j \cdot j!} [\{\Delta_{\mathcal{C}}(x_1, x_2) J(x_1) J(x_2)\}_{12}]^j. \tag{2.2.48}$$

³This number is given as follows: there are $\binom{2j}{2} = 2j(2j-1)/2$ possibilities to choose the first pair out of the $(2j)$ field operators. Then there are $(2j-2)(2j-3)/2$ possibilities to choose the next pair out of the remaining $(2j-2)$ field operators, etc. This makes $(2j)!/2^j$ choices of j pairs, but we have to sum only once over each contraction, i.e., it does not matter in which order we have chosen the $j!$ pairs in one specific contraction. Thus the total combinatorial factor is finally $(2j)!/[2^j \cdot j!]$.

Summing these expressions over j we finally get

$$Z_0[J] = \exp \left[-\frac{i}{2} \{ \Delta_{\mathcal{C}}(x_1, x_2) J(x_1) J(x_2) \}_{12} \right]. \quad (2.2.49)$$

2.2.4 The free contour propagator

To complete the calculation of the generating functional for free Green's functions (2.2.49) we have to evaluate the free contour propagator. This is also a concrete example for the technique to calculate expectation values of contour-ordered field-operator products, we have looked at in the previous section.

First we derive some general properties about this propagator, which hold also true for the exact two-point Green's function (cf. (2.2.28) for $n = 2$). In both cases the derivation of these properties works in the same way, using the free Hamiltonian in the interaction picture or the full Hamiltonian in the Heisenberg picture respectively. Here, we write it down for the former case, i.e., the free propagator.

By definition according to (2.2.30) we have

$$i\Delta_{\mathcal{C}}(x_1, x_2) = \Theta_{\mathcal{C}}(t_1, t_2) i\Delta^{\gt}(x_1, x_2) + \Theta_{\mathcal{C}}(t_2, t_1) i\Delta^{\lt}(x_1, x_2), \quad (2.2.50)$$

where the **thermal Wightman functions** are defined by

$$i\Delta^{\gt}(x_1, x_2) = \langle \phi_{\mathbb{I}}(x_1) \phi_{\mathbb{I}}(x_2) \rangle^{(0)}, \quad (2.2.51)$$

$$i\Delta^{\lt}(x_1, x_2) = \langle \phi_{\mathbb{I}}(x_2) \phi_{\mathbb{I}}(x_1) \rangle^{(0)}. \quad (2.2.52)$$

The contour unit-step function is defined as

$$\Theta_{\mathcal{C}} : \mathcal{C} \times \mathcal{C} \rightarrow \mathbb{C}, \quad \Theta_{\mathcal{C}}(t_1, t_2) = \begin{cases} 1 & \text{for } t_1 \succ_{\mathcal{C}} t_2, \\ 1/2 & \text{for } t_1 = t_2, \\ 0 & \text{for } t_2 \prec_{\mathcal{C}} t_1. \end{cases} \quad (2.2.53)$$

The ordering symbols with \mathcal{C} as subscript denote the ordering of the times along the contour.

The functions (2.2.51) and (2.2.52) are to be read as functions with **complex time arguments**. In the following we shall also derive, in which domain of the complex time plane these functions are well defined. First of all we note that these functions are only functions of the difference of the space-time arguments, which is due to the translation invariance of the equilibrium state. To show this, we use the space-time translation operator (1.2.41) to write

$$i\Delta^{\gt}(x_1, x_2) = \left\langle \exp(ix_1 \cdot \mathbf{P}_{\mathbb{I}}^{(0)}) \phi_{\mathbb{I}}(0) \exp(-ix_1 \cdot \mathbf{P}_{\mathbb{I}}^{(0)}) \exp(ix_2 \cdot \mathbf{P}_{\mathbb{I}}^{(0)}) \phi_{\mathbb{I}}(0) \exp(-ix_2 \cdot \mathbf{P}_{\mathbb{I}}^{(0)}) \right\rangle^{(0)}. \quad (2.2.54)$$

Now, we can cyclically change the order of the operators under the trace and also use that the translation operator commutes with $\exp(-\beta \mathbf{H}_{\mathbb{I}}^{(0)})$ to get

$$i\Delta^{\gt}(x_1, x_2) = \left\langle \exp \left[i(x_1 - x_2) \cdot \mathbf{P}_{\mathbb{I}}^{(0)} \right] \phi_{\mathbb{I}}(0) \exp \left[-i(x_1 - x_2) \cdot \mathbf{P}_{\mathbb{I}}^{(0)} \right] \phi_{\mathbb{I}}(0) \right\rangle^{(0)}. \quad (2.2.55)$$

Using again (1.2.41-1.2.42) we see that this can be written as

$$i\Delta^{\gt}(x_1, x_2) = \langle \phi_{\mathbb{I}}(x_1 - x_2) \phi_{\mathbb{I}}(0) \rangle^{(0)} = i\Delta^{\gt}(x_1 - x_2, 0) =: i\Delta^{\gt}(x_1 - x_2). \quad (2.2.56)$$

For $\Delta^<$ in the very same way we obtain

$$\Delta^<(x_1, x_2) = \Delta^<(x_1 - x_2, 0) =: \Delta^<(x_1 - x_2). \quad (2.2.57)$$

Coming back to the question on the domain of definition concerning complex time arguments we use (2.2.56) and write out the corresponding expectation value (2.2.55) in terms of the trace again, leading to

$$i\Delta^>(x) = \langle \phi_I(x)\phi_I(0) \rangle^{(0)} = \frac{1}{Z_0} \text{Tr} \left\{ \exp \left[\mathbf{H}_I^{(0)}(-\beta + it) \right] \phi_I(0, \vec{x}) \exp(-i\mathbf{H}_I^{(0)}t) \phi_I(0) \right\}. \quad (2.2.58)$$

Now using the positive semidefiniteness of the Hamiltonian we see that the trace only exists if $\text{Im } t \in (-\beta, 0]$. From this form of writing the Wightman function we also find the **Kubo-Martin-Schwinger (KMS) relation**, which plays a very important role in the equilibrium case. For $\text{Im } t \in [0, \beta)$ we have

$$\begin{aligned} i\Delta^>(t - i\beta, \vec{x}) &= \frac{1}{Z_0} \text{Tr} \left\{ \exp(it\mathbf{H}_I^{(0)}) \phi_I(0, \vec{x}) \exp[-i\mathbf{H}_I^{(0)}(t - i\beta)] \phi_I(0) \right\} \\ &= \frac{1}{Z_0} \text{Tr} \left\{ \phi_I(x) \exp(-\beta\mathbf{H}_I^{(0)}) \phi_I(0) \right\} \\ &= \frac{1}{Z_0} \text{Tr} \left\{ \exp(-\beta\mathbf{H}_I^{(0)}) \phi_I(0) \phi_I(x) \right\} \\ &= i\Delta^<(x), \end{aligned} \quad (2.2.59)$$

which shows that $\Delta^<$ is defined in the strip $\text{Im } t \in [0, \beta)$ and that for such t

$$\Delta^>(t - i\beta, \vec{x}) = \Delta^<(x), \quad (2.2.60)$$

which is the KMS relation, holds. With (2.2.50) we have

$$\Delta_{\mathcal{C}}(x_1, x_2) = \Theta_{\mathcal{C}}(x_1, x_2) \Delta^>(x_1 - x_2) + \Theta_{\mathcal{C}}(x_2, x_1) \Delta^<(x_1 - x_2). \quad (2.2.61)$$

Since $\Delta^>$ is well defined for $\text{Im } t \in (-\beta, 0]$ and $\Delta^<$ for $\text{Im } t \in [0, \beta)$, $\Delta_{\mathcal{C}}$ is well defined for $\text{Im}(t_1 - t_2) \in (-\beta, \beta)$, i.e., for time arguments with $\text{Im } t_1, \text{Im } t_2 \in (-\beta, 0]$, as it should be for these time arguments on the Schwinger-Keldysh contour.

Because of the spatial and temporal translation invariance of the equilibrium state, for the Feynman rules it will turn out to be convenient to work in energy-momentum space, which is achieved by Fourier transformation, but this is not applicable for the contour ordered Green's function directly. Thus, one uses a **matrix notation** for the Green's functions, according to where the time arguments are located on the contour, i.e., one introduces

$$\Delta^{ij}(x_1, x_2) = \Delta_{\mathcal{C}}(x_1, x_2), \quad (2.2.62)$$

where on the left-hand side the superscripts run over the set $\{1, 2, v\}$, denoting where on the contour the time arguments are located (time-ordered part, anti-time-ordered part of the real-time contour, and the vertical addendum of the extended equilibrium Schwinger-Keldysh contour, respectively). Then these matrix propagators have all their time arguments defined as usual real numbers or along the vertical

part $t = t_i - i\tau$ with $\tau \in [0, \beta)$. Explicitly the definition (2.2.62) gives

$$\Delta^{11}(x_1, x_2) =: \Delta^{11}(x_1 - x_2) = \Theta(t_1 - t_2)\Delta^>(x_1 - x_2) + \Theta(t_2 - t_1)\Delta^<(x_1 - x_2), \quad (2.2.63)$$

$$\Delta^{12}(x_1, x_2) =: \Delta^{12}(x_1 - x_2) = \Delta^<(x_1 - x_2), \quad (2.2.64)$$

$$\Delta^{21}(x_1, x_2) =: \Delta^{21}(x_1 - x_2) = \Delta^>(x_1 - x_2), \quad (2.2.65)$$

$$\Delta^{22}(x_1, x_2) =: \Delta^{11}(x_1 - x_2) = \Theta(t_2 - t_1)\Delta^>(x_1 - x_2) + \Theta(t_1 - t_2)\Delta^<(x_1 - x_2), \quad (2.2.66)$$

$$\Delta^{1v}(x_1, x_2) = \Delta^{2v}(x_1, x_2) = \Delta^<(x_1 - x_2), \quad (2.2.67)$$

$$\Delta^{v1}(x_1, x_2) = \Delta^{v2}(x_1, x_2) = \Delta^>(x_1 - x_2), \quad (2.2.68)$$

$$\begin{aligned} \Delta^{vv}(x_1, x_2) &:= \Delta^{vv}(x_1 - x_2) \\ &= \Theta(\tau_1 - \tau_2)\Delta^>[-i(\tau_1 - \tau_2), \vec{x}_1 - \vec{x}_2] + \Theta(\tau_2 - \tau_1)\Delta^<[-i(\tau_1 - \tau_2), \vec{x}_1 - \vec{x}_2]. \end{aligned} \quad (2.2.69)$$

We note that only the mixed real-vertical matrix elements (2.2.66) and (2.2.67) depend on the initial time, t_i . To find the explicit expressions for these matrix Green's functions, we only need to calculate $\Delta^>(x)$, directly using its definition cf. (2.2.51). Then in our case of hermitean field operators we also know

$$\Delta^<(x) = \Delta^>(-x). \quad (2.2.70)$$

First we evaluate the **partition sum** of an ideal gas, which is the most simple example of this kind of calculations:

$$Z^{(0)} = \text{Tr} \exp(-\beta \mathbf{H}_I^{(0)}) = \sum_{n(\vec{k})=1}^{\infty} \langle \{n(\vec{k})\} | \exp(-\beta \mathbf{H}_I^{(0)}) | \{n(\vec{k})\} \rangle. \quad (2.2.71)$$

First we use (2.2.40) and the fact that our occupation-number basis vectors are eigenvectors of $\mathbf{H}_I^{(0)}$. This leads to

$$Z^{(0)} = \sum_{n(\vec{k})=0}^{\infty} \exp\left(-\beta \sum_{\vec{k}} n(\vec{k}) \omega_{\vec{k}}\right) = \prod_{\vec{k}} \sum_{n(\vec{k})=0}^{\infty} \exp[-\beta \omega_{\vec{k}} n(\vec{k})]. \quad (2.2.72)$$

The sums obviously are convergent geometric series, which yields

$$Z^{(0)} = \prod_{\vec{k}} \frac{1}{1 - \exp(-\beta \omega_{\vec{k}})}. \quad (2.2.73)$$

This infinite product we can translate into an infinite sum by taking the logarithm

$$\ln Z^{(0)} = - \sum_{\vec{k}} \ln [1 - \exp(-\beta \omega_{\vec{k}})]. \quad (2.2.74)$$

Here, we can also easily take the infinite-volume limit. In this limit the momenta become continuous, and we have to translate the sum into an integral. For the finite cubic volume, in a small momentum-space volume element $d^3\vec{k}$ there are obviously $d^3\vec{k} L^3 / (2\pi)^3$ single-particle modes since the discrete momentum values are $\vec{k} \in (2\pi/L)\mathbb{Z}$. Thus, the correct interpretation of the infinite-volume limit is achieved by making the volume very large (compared to β^3 as a typical volume scale of the thermalized system) and approximating the sum in (2.2.74) by the corresponding integral

$$\ln Z^{(0)} = -V \int_{\mathbb{R}^3} \frac{d^3\vec{k}}{(2\pi)^3} \ln [1 - \exp(-\beta \omega_{\vec{k}})]. \quad (2.2.75)$$

Further we need

$$\begin{aligned} iZ_0\Delta^>(x) &= \text{Tr} \left\{ \exp(-\beta\mathbf{H}_1^{(0)})\phi_1(x)\phi_1(0) \right\} \\ &= \sum_{n(\vec{k})=0}^{\infty} \exp\left(-\beta \sum_{\vec{k}} n(\vec{k})\omega_{\vec{k}}\right) \left\langle \{n(\vec{k})\} \left| \phi_1(x)\phi_1(0) \right| \{n(\vec{k})\} \right\rangle. \end{aligned} \quad (2.2.76)$$

To evaluate the matrix element we use the mode decomposition (2.2.39) and Eqs. (2.2.45) and (2.2.46). In the next equation we set $k_{1,2}^0 = \omega_{\vec{k}_{1,2}}$. Then for the matrix element in (2.2.76) we need

$$\begin{aligned} \left\langle \{n(\vec{k})\} \left| \frac{1}{V\sqrt{2k_1^0 2k_2^0}} \left[\mathbf{a}(\vec{k}_1)\exp(-ik_1x) + \mathbf{a}^\dagger(\vec{k}_1)\exp(ik_1x) \right] \left[\mathbf{a}(\vec{k}_2) + \mathbf{a}^\dagger(\vec{k}_2) \right] \right| \{n(\vec{k})\} \right\rangle \\ = \frac{1}{V2\omega_{\vec{k}_1}} \left\{ [1 + n(\vec{k}_1)]\exp(-ik_1 \cdot x) + n(\vec{k}_1)\exp(ik_1 \cdot x) \right\} \delta_{\vec{k}_1, \vec{k}_2}. \end{aligned} \quad (2.2.77)$$

This we have to multiply with the exponential in (2.2.76) and sum over \vec{k}_1 and \vec{k}_2 within the sum over the $n(\vec{k})$. After some algebra we get

$$\begin{aligned} iZ_0\Delta^>(x) &= \frac{1}{V} \sum_{\vec{k}_1} \left[\prod_{\vec{k} \neq \vec{k}_1} \exp[-\beta n(\vec{k})\omega_{\vec{k}}] \right] \\ &\times \sum_{n(\vec{k}_1)=0}^{\infty} \exp[-\beta n(\vec{k}_1)\omega_{\vec{k}_1}] \frac{1}{2\omega_{\vec{k}_1}} \left\{ [1 + n(\vec{k}_1)]\exp(-ik_1 \cdot x) + n(\vec{k}_1)\exp(ik_1 \cdot x) \right\}. \end{aligned} \quad (2.2.78)$$

For the product we can obviously write

$$\prod_{\vec{k} \neq \vec{k}_1} \exp[-\beta n(\vec{k})\omega_{\vec{k}}] = Z_0 \left\{ 1 - \exp(-\beta n(\vec{k}_1)) \right\}. \quad (2.2.79)$$

And for the sum over $n(\vec{k}_1)$ we need

$$\sum_{n=0}^{\infty} n \exp(-\alpha n) = -\frac{d}{d\alpha} \sum_{n=0}^{\infty} \exp(-\alpha n) = -\frac{d}{d\alpha} \left(\frac{1}{1 - \exp(-\alpha)} \right) = \frac{\exp(-\alpha)}{[1 - \exp(-\alpha)]^2}. \quad (2.2.80)$$

Plugging (2.2.79) and (2.2.80) with $\alpha = -\beta\omega_{\vec{k}_1}$ into (2.2.78) we finally get after some algebra

$$i\Delta^>(x) = \frac{1}{V} \sum_{\vec{k}_1} \frac{1}{2\omega_{\vec{k}_1}} \left\{ [1 + f_B(\omega_{\vec{k}_1})]\exp(-ik_1 \cdot x) + f_B(\omega_{\vec{k}_1})\exp(ik_1 \cdot x) \right\}_{k_1^0 = \omega_{\vec{k}_1}}. \quad (2.2.81)$$

In the infinite-volume limit this translates into the integral

$$i\Delta^>(x) = \int_{\mathbb{R}^3} \frac{d^3\vec{k}}{(2\pi)^3 2\omega_{\vec{k}}} \left\{ [1 + f_B(\omega_{\vec{k}})]\exp(-ik_1 \cdot x) + f_B(\omega_{\vec{k}})\exp(ik_1 \cdot x) \right\}_{k_1^0 = \omega_{\vec{k}}} \quad (2.2.82)$$

with the Bose-Einstein distribution function

$$f_B(k^0) = \frac{1}{\exp(\beta k^0) - 1}. \quad (2.2.83)$$

Now we can rewrite (2.2.82) to a four-dimensional integral making use of the **on-shell δ distribution**,

$$\delta(k^2 - m^2) = \frac{1}{2\omega_{\vec{k}}} \left[\delta(k^0 - \omega_{\vec{k}}) + \delta(k^0 + \omega_{\vec{k}}) \right], \quad (2.2.84)$$

and the property

$$f_B(-k^0) = -1 - f_B(k^0) \quad (2.2.85)$$

to give

$$i\Delta^>(x) = \int_{\mathbb{R}^4} \frac{d^4k}{(2\pi)^4} 2\pi\sigma(k^0)\delta(k^2 - m^2)[1 + f_B(k^0)]\exp(-ik \cdot x). \quad (2.2.86)$$

This is a Fourier representation for the function $\Delta^>$. The sign function in the energy domain is defined as usual in connection with Fourier transformations:

$$\sigma(k^0) = \begin{cases} -1 & \text{for } k^0 < 0, \\ 0 & \text{for } k^0 = 0, \\ 1 & \text{for } k^0 > 0. \end{cases} \quad (2.2.87)$$

In principle that is what we need in the practical use of the perturbative evaluation of n -point Green's functions, but as it will turn out later it is customary to regularize the on-shell δ distribution under the integral such that we obtain a regularized function $\Delta_\eta^>$ which still fulfills the KMS condition (2.2.60).

For this purpose, following [Mab97], we regularize the δ distributions in energy space and the Fourier transformed Heaviside unit-step functions in a specific way. For the unit-step function the regularization in the time domain reads

$$\Theta_\eta(t) = \Theta(t)\exp(-\eta|t|). \quad (2.2.88)$$

Here and in the following the regularization parameter $\eta > 0$. In the following we assume all calculations to be performed with a finite η in the limit $\eta \rightarrow 0^+$, where the limit has to be taken after all energy integrals are evaluated, i.e., as a weak limit in the sense of distribution theory. Physically the regularization of this kind has to be interpreted as a generalization of the theory of **asymptotic states** and evaluating transition rates in the corresponding S -matrix formalism in vacuum quantum field theory to the case of equilibrium many-body theory. We come back to this issue from time to time later.

With this regularization the Fourier transform of the unit-step function to the energy domain becomes

$$\check{\Theta}_\eta(p_0) = \int_0^\infty dt \exp[t(-\eta + ip_0)] = \frac{i}{p_0 + i\eta}. \quad (2.2.89)$$

The distribution $\delta(p_0 - \omega)$ for $\omega \in \mathbb{R}$ corresponds to $\exp(-i\omega t)/(2\pi)$ in the time domain. Thus the regularization for the δ distribution within our scheme reads

$$\begin{aligned} \delta_\eta(p_0 - \omega) &= \frac{1}{2\pi} \int_{\mathbb{R}} dt \exp[i(p_0 - \omega)t - \eta|t|] \\ &= \frac{i}{2\pi} \left[\frac{1}{p_0 - \omega + i\eta} - \frac{1}{p_0 - \omega - i\eta} \right] \\ &= \frac{1}{\pi} \frac{\eta}{(p_0 - \omega)^2 + \eta^2}. \end{aligned} \quad (2.2.90)$$

For the unit-step function in the energy domain we find

$$\Theta_\eta(p_0) = \int_{-\infty}^{p_0} dp_0 \delta_\eta(p_0) = \frac{1}{2} + \frac{1}{\pi} \arctan\left(\frac{p_0}{\eta}\right) \quad (2.2.91)$$

and for the sign function,

$$\sigma_\eta(p_0) = \Theta_\eta(p_0) - \Theta_\eta(-p_0) = \frac{2}{\pi} \arctan\left(\frac{p_0}{\eta}\right). \quad (2.2.92)$$

In the following we evaluate the so-called **Mills representation** of the propagator, i.e., the mixed time-momentum representation [Mil69]. From (2.2.82) we find

$$i\Delta_{\mathbf{M}}^{\geq}(t, \vec{k}) = \frac{1}{2\omega_{\vec{k}}} \left\{ [1 + f_{\mathbf{B}}(\omega_{\vec{k}})] \exp(-i\omega_{\vec{k}} t) + f_{\mathbf{B}}(\omega_{\vec{k}_1}) \exp(i\omega_{\vec{k}} t) \right\} \quad (2.2.93)$$

for the unregularized function. For the regularized one we have to substitute the combined expression $\sigma(k_0)\delta(k^2 - m^2)$ by

$$\delta_\eta^{(\sigma)}(k^2 - m^2) = \frac{i}{2\pi(2\omega_{\vec{k}})} \left[\frac{1}{k_0 - \omega_{\vec{k}} + i\eta} - \frac{1}{k_0 - \omega_{\vec{k}} - i\eta} - \frac{1}{k_0 + \omega_{\vec{k}} + i\eta} + \frac{1}{k_0 + \omega_{\vec{k}} - i\eta} \right] \quad (2.2.94)$$

in (2.2.86)⁴. The Mills representation of the regularized propagator is then given by

$$i\Delta_{\mathbf{M},\eta}^{\geq}(t, \vec{k}) = \int_{C_t} \frac{dk^0}{2\pi} 2\pi \delta_\eta^{(\sigma)}[(k^0)^2 - \omega_{\vec{k}}^2] [1 + f_{\mathbf{B}}(k^0)] \exp(-ik^0 t). \quad (2.2.95)$$

Here we can take t in the open strip $\text{Im } t \in (-\beta, 0)$ in the complex t plane. The original integration path along the real k^0 axis is closed with a large semi circle in the upper (lower) complex plane for $\text{Re } t < 0$ ($\text{Re } t > 0$), leading to the closed contours C_t in the complex k^0 plane shown in Fig. 2.3. For this choice of the contour the large semi circle does not contribute in the limit of its radius to infinity due to the exponential function. Since due to our regularization procedure the integrand is an analytic function, we can use the theorem of residues to evaluate the integral.

The only singularities of the integrand are the simple poles of $\delta_\eta^{(\sigma)}(k^2 - m^2)$ close to the real axis and the simple poles of $f_{\mathbf{B}}(k^0)$ at $i\omega_n$ where the **bosonic Matsubara frequencies** are given by $\omega_n = 2\pi n/\beta = 2\pi nT$ with $n \in \mathbb{Z}$. Note that the pole at $n = 0$ is compensated by the factor $\delta_\eta^{(\sigma)}(k^2 - m^2)$, so that there is no problem with this pole when integrating along the real axis (see Fig. 2.3).

For $\text{Re } t > 0$ we have to close the contour close to the real k^0 axis in the lower plane, and thus this contour is oriented clockwise. This gives

$$\begin{aligned} i\Delta_{\mathbf{M},\eta}^{\geq}(t, \vec{k}) &= \frac{1}{2\omega_{\vec{k}}} \left\{ [1 + f_{\mathbf{B}}(\omega_{\vec{k}} - i\eta)] \exp[-i(\omega_{\vec{k}} - i\eta)t] + f_{\mathbf{B}}(\omega_{\vec{k}} + i\eta) \exp[i(\omega_{\vec{k}} + i\eta)t] \right\} \\ &\quad - \frac{T}{2\omega_{\vec{k}}} \sum_{n=1}^{\infty} X_n \exp(-\omega_n t) \quad \text{if } \text{Re } t > 0, \quad \text{Im } t \in (-\beta, 0) \end{aligned} \quad (2.2.96)$$

with

$$\begin{aligned} X_n(\vec{k}) &= \frac{1}{i\omega_n - \omega_{\vec{k}} + i\eta} - \frac{1}{i\omega_n - \omega_{\vec{k}} - i\eta} + \frac{1}{i\omega_n + \omega_{\vec{k}} - i\eta} - \frac{1}{i\omega_n + \omega_{\vec{k}} + i\eta} \\ &= \frac{8\eta\omega_n\omega_{\vec{k}}}{[(i\omega_n - \omega_{\vec{k}})^2 + \eta^2][(i\omega_n + \omega_{\vec{k}})^2 + \eta^2]}. \end{aligned} \quad (2.2.97)$$

⁴It is important to note that we must not substitute the δ distribution and sign function by their regularized versions (2.2.90) and (2.2.92), because generally a product of distributions is not well-defined. Here, in the unregularized form the meaning of the product is clear, but it is not generally allowed to write such a product as the weak limit of the product of the corresponding regularized expressions.

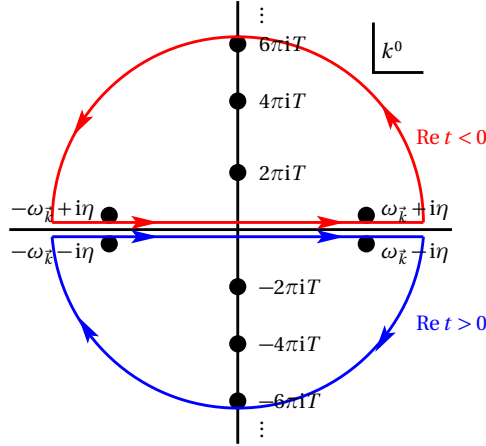


Figure 2.3: The integration contours in the complex k^0 plane for the evaluation of the regularized propagator (2.2.95).

For $\text{Re } t < 0$ we have to close the contour in the upper plane, which is counter clockwise, i.e., positively oriented. Picking up the corresponding residues in the upper k^0 half-plane, we find

$$\begin{aligned} i\Delta_{M,\eta}^>(t, \vec{k}) &= \frac{1}{2\omega_{\vec{k}}} \left\{ [1 + f_B(\omega_{\vec{k}} + i\eta)] \exp[-i(\omega_{\vec{k}} - i\eta)t] + f_B(\omega_{\vec{k}} - i\eta) \exp[i(\omega_{\vec{k}} + i\eta)t] \right\} \\ &\quad - \frac{T}{2\omega_{\vec{k}}} \sum_{n=1}^{\infty} X_n \exp(\omega_n t) \quad \text{if } \text{Re } t < 0, \quad \text{Im } t \in (-\beta, 0). \end{aligned} \quad (2.2.98)$$

This we can combine with (2.2.99) to the expression

$$\begin{aligned} i\Delta_{M,\eta}^>(t, \vec{k}) &= \frac{1}{2\omega_{\vec{k}}} \exp(-\eta\sigma t) \sum_{\varepsilon=\pm 1} [\Theta(\varepsilon) + f(\omega_{\vec{k}} - i\varepsilon\sigma\eta)] \exp(-i\varepsilon\omega_{\vec{k}}t) \\ &\quad - \frac{T}{2\omega_{\vec{k}}} \sum_{n=1}^{\infty} \exp(-\omega_n\sigma t) X_n \quad \text{with } \sigma = \sigma(\text{Re } t). \end{aligned} \quad (2.2.99)$$

Because of (2.2.70) we have for $\text{Im } t \in (0, \beta)$

$$\begin{aligned} i\Delta_{M,\eta}^<(t, \vec{k}) &= \Delta_{M,\eta}^>(-t, \vec{k}) = \frac{1}{2\omega_{\vec{k}}} \exp(-\eta\sigma t) \sum_{\varepsilon=\pm 1} [\Theta(-\varepsilon) + f(\omega_{\vec{k}} - i\varepsilon\sigma\eta)] \exp(-i\varepsilon\omega_{\vec{k}}t) \\ &\quad - \frac{T}{2\omega_{\vec{k}}} \sum_{n=1}^{\infty} \exp(-\omega_n\sigma t) X_n \quad \text{with } \sigma = \sigma(\text{Re } t). \end{aligned} \quad (2.2.100)$$

It is easy to see that the KMS condition (2.2.60) holds also for the regularized propagator,

$$\Delta_{M,\eta}^>(t - i\beta, \vec{k}) = \Delta_{M,\eta}^<(t, \vec{k}) \quad \text{for } \text{Im } t \in (0, \beta). \quad (2.2.101)$$

The Mills representation of the contour-ordered regularized free propagator then is given by

$$\begin{aligned}
 i\Delta_{M,\eta}^{(\varphi)}(t_1, t_2; \vec{k}) &= i\Theta_{\varphi}(t_1, t_2)\Delta_{\varphi,\eta}^{\gt}(t_1 - t_2; \vec{k}) + i\Theta_{\varphi}(t_2, t_1)\Delta_{\varphi}^{\lt}(t_1, t_2; \vec{k}) \\
 &= \frac{1}{2\omega_{\vec{k}}} \exp(-\eta\sigma t) \sum_{\varepsilon=\pm 1} [\Theta_{\varphi}(t_1, t_2)\Theta(\varepsilon) + \Theta_{\varphi}(t_2, t_1)\Theta(-\varepsilon)] \exp(-i\varepsilon\omega_{\vec{k}}t) \\
 &\quad + \frac{1}{2\omega_{\vec{k}}} \exp(-\eta\sigma t) \sum_{\varepsilon=\pm 1} f(\omega_{\vec{k}} - i\varepsilon\sigma\eta) \exp(-i\varepsilon\omega_{\vec{k}}t) \\
 &\quad - \frac{T}{2\omega_{\vec{k}}} \sum_{n=1}^{\infty} \exp(-\omega_n\sigma t) X_n \quad \text{with } \sigma = \sigma(\text{Re } t), \quad \text{Im } t \in (-\beta, \beta).
 \end{aligned} \tag{2.2.102}$$

Here \vec{k} is the momentum in the Fourier transform with respect to the “relative position”, $\vec{x}_1 - \vec{x}_2$.

Now we come back to the generating functional for free contour-ordered Green’s functions (2.2.49). Using the regularized propagator (2.2.102) shows that in the limit $t_i \rightarrow -\infty$ only the contributions from the pure real-time propagators $\Delta^{ij}(x_1 - x_2)$ (with $i, j \in \{1, 2\}$) and the pure imaginary-time (or Matsubara) propagators survive. The reason is that for any $\eta > 0$ both, $\Delta_{M,\eta}^{\gt}(x)$ and $\Delta_{M,\eta}^{\lt}(x)$ vanish for $\text{Re } t \rightarrow \pm\infty$. Now, cf. (2.2.63-2.2.69) the mixed real-imaginary-time propagators, $\Delta_{M,\eta}^{jv}(x_1 - x_2)$ and $\Delta_{M,\eta}^{vj}(x_1 - x_2)$, depend on t_i , and thus their contribution to the exponential in (2.2.49) vanish in the limit $t_i \rightarrow -\infty$. This means that the generating functional factorizes as follows:

$$\begin{aligned}
 Z_0[J] &= \exp\left(\frac{i}{2} \int_{\mathcal{C}_{\mathbb{R}}} d^4x \Delta_{\varphi}(x_1, x_2) J(x_1) J(x_2)\right) \exp\left(\frac{i}{2} \int_{\mathcal{C}_v} d^4x \Delta_{\varphi}(x_1, x_2) J(x_1) J(x_2)\right) \\
 &= Z_0^{(\mathbb{R})}[J] Z_0^{(v)}[J].
 \end{aligned} \tag{2.2.103}$$

Both expressions do not depend on t_i as to be expected for a translation-invariant state.

2.2.5 Feynman rules

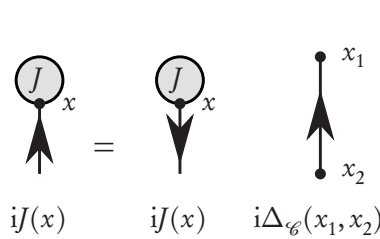


Figure 2.4: *Contour-Feynman diagram elements to evaluate the corrections to the generating functional.*

Now we can easily derive the Feynman rules to evaluate contour-ordered Green’s functions perturbatively. We start with the calculation of the corrections to the **partition function**. From (2.2.37) we know that

$$Z = Z_0 Z[J = 0]. \tag{2.2.104}$$

First we expand $Z[J]$ in powers of the coupling constant, λ , by expanding the operator-valued exponential in (2.2.36). Writing

$$\hat{V}(x) = \frac{\lambda}{4!} \frac{\delta^4}{\delta [iJ(x)]^4} \tag{2.2.105}$$

the expansion takes the form

$$Z[J] = \sum_{j=0}^{\infty} \frac{1}{j!} (-i)^j \prod_{k=1}^j \int_{\mathcal{C}} d^4x_k \hat{V}(x_k) Z_0[J]. \tag{2.2.106}$$

$$= -\frac{i\lambda}{4!} \frac{1}{2!} \left(\frac{1}{2}\right)^2 \int_{\mathcal{G}} d^4x [i\Delta_{\mathcal{G}}(x, x)]^2 \quad \underbrace{\times 4}_{\text{from 1st derivative wrt. } iJ(x)} \quad \underbrace{\times 3}_{\text{from 2nd derivative wrt. } iJ(x)} \quad \underbrace{\times 2}_{\text{from 3rd derivative wrt. } iJ(x)}$$

Figure 2.5: Diagrammatic evaluation of the first order correction to $Z[J = 0]$.

Then we also expand $Z_0[J]$

$$Z_0[J] = \exp\left(-\frac{i}{2} \{\Delta_{12} J_1 J_2\}_{12}\right) = \sum_{l=0}^{\infty} \frac{1}{l!} \left(-\frac{i}{2} \{\Delta_{12} J_1 J_2\}_{12}\right)^l. \quad (2.2.107)$$

Here we have written $\Delta_{ij} = \Delta_{\mathcal{G}}(x_i, x_j)$ for convenience. To evaluate the contribution of order λ^j to $Z[J = 0]$ we only have to derive the term with $l = 2j$ from the exponential series in (2.2.107). This is quite simple but a bit tedious to be done by hand. Thus we use **Feynman-diagram techniques**. For the terms in the series in (2.2.107) we use the diagrammatic elements with their meaning given in Fig. 2.4. We make the diagrammatic procedure clear on the example of the first-order correction to $Z[J = 0]$. This is depicted in (2.5). Each functional derivative in $\hat{V}(x)$ takes away one blob, symbolizing iJ . Since the terms in the expansion (2.2.107) are totally symmetric under the exchange of the iJ 's we have just to take the derivatives successively once and multiply with the number of J 's still left. At the end we have a closed diagram with one point x , over which one has to integrate. At j^{th} order there can be several such diagrams. We note that the first derivative with respect to J always cancels the factor $1/2^j$ in the series (C.74). Also the factor $1/l! = 1/(2j)!$ from the expansion of $Z_0[J]$ is cancelled from the successive derivatives of the corresponding power $l = 2j$ of $\{J_1 \Delta_{\mathcal{G},12} J_2\}_{12}$.

From these considerations we get the following Feynman rules to evaluate the j^{th} -order correction to $Z[J = 0]$.

- Draw j vertices with four legs. Each of those stand for a factor

$$= -\frac{i\lambda}{4!}. \quad (2.2.108)$$

Multiply the whole expression with a factor $1/j!$.

- connect each pair of legs with a propagator line standing for $i\Delta_{\mathcal{G}}(x_1, x_2)$ to obtain totally closed diagrams. Find all possible different topologies of this kind of diagrams. For each diagram multiply the expression with a factor counting the number of possible ways to do the connections of vertex points with propagator lines to obtain this topology. Sum all the so obtained expressions.
- integrate over all space-time points with an integral operator $\int_{\mathcal{G}} d^4x$.

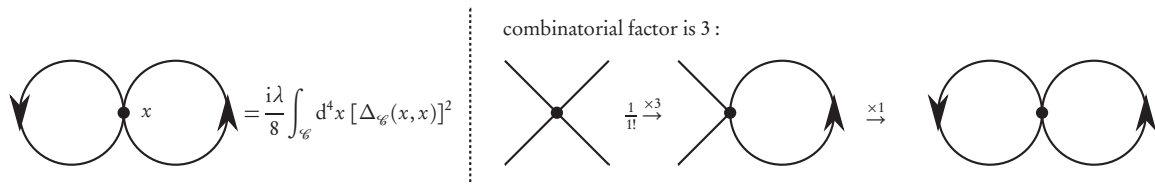


Figure 2.6: Example for the determination of the combinatorial factor for the closed “eight diagram”, which symbolizes the first-order correction to $Z[J = 0]$.

The reader should make himself or herself clear that these rules really describe taking the successive derivatives from the $\hat{V}(x_k)$

To explain how to obtain the 1st correction from these rules, where the most complicated task is to figure out the correct combinatorial factor, look at Fig. 2.6. Finally we note that we only need to take into account the **vertical imaginary-time part** in the integrals for the evaluation of these **closed diagrams without external points**. The reason is that the generating functional for free Green’s functions factorizes into a pure imaginary-time and a pure real-time functional (cf. (2.2.103)). Thus, when splitting the integrations in all the closed diagrams in its real- and an imaginary-time part, no diagram can contain the “mixed propagators” Δ^{vj} or Δ^{jv} and thus only diagrams with all vertices on the real axis or with all vertices on the vertical part of the time contour occur. Now the real part of the contour is closed by itself and thus the along the real-time contour vanish. Thus, we need to take into account only the integrations along the vertical part remain.

Of course, the expressions from the diagrams derived above are still not well defined, because in general the integrals do not exist. We come back to this issue in the next section, where we shall show on examples that the divergences are **renormalizable** for Dyson-renormalizable quantum field theories in the same sense as the corresponding vacuum quantum field theory is Dyson-renormalizable. Also the counter terms for the wave-function normalization, the mass, and the coupling constant necessary to render all Green’s functions finite at any order of perturbation theory are precisely the counter terms of vacuum quantum field theory, i.e., no temperature dependent counter terms are necessary, and the theory is well defined independently of the thermodynamic state of the system.

It is now clear that the same diagrammatic technique also applies to the evaluation of Green’s functions since they are also given by derivatives with respect to the external current, $J(x)$. The only difference is that, of course, over the external points is not integrated.

In general, at a given order of perturbation theory, the corrections to an n -point Green’s function will consist of sums over diagrams of different topology with j vertices. Together there are $j + n$ space-time points in such a diagram, but only over the inner vertex point one has to integrate. Usually each diagram can consist of several disconnected subdiagrams. It is the great advantage of the diagram technique that one can evaluate each connected piece separately.

Now, if we like to evaluate n -point functions with time arguments on the real part of the contour, any subdiagram that is connected to at least one external point can contain only space-time points with the time argument on the real part of the contour, as discussed for the closed diagrams without external points. Thus, for such diagrams we only need to work with the real-time Green’s functions Δ^{ij} with $i, j \in \{1, 2\}$. The closed diagrams are the corrections to $Z[J = 0]$, and we shall show later that they are precisely canceled to the given order of perturbation theory by the normalization factor $1/Z[J = 0]$ in (2.2.38).

Before, we shall derive the Feynman rules for real-time propagators in momentum space. To that end we go over to the **matrix formalism**, i.e., we work with the propagators Δ^{ij} , defined by (2.2.63)-

(2.2.66) and want to perturbatively evaluate the corresponding n -point Green's functions $G_n^{i_1, \dots, i_n}$. The superscripts run over $\{1, 2\}$ and note on which part of the Keldysh contour the time argument is located. These functions are all defined as functions along the usual real-time axis. Accordingly each inner vertex point and each external space-time point must be labeled with the corresponding index. Over the inner points we have to integrate over \mathbb{R}^4 and to sum over the corresponding index. There one has to take into account that the part of the time integration in the sense of the contour integral along the anti-time ordered branch, indicated by an index 2 is from $+\infty$ to $-\infty$ and thus one must flip the sign, i.e., each vertex with a time index 2 stands for $+i\lambda/4!$, while each vertex with a time index 1 for $-i\lambda/4!$.

The advantage of the matrix formalism is that the free propagator functions Δ^{ij} can be Fourier transformed also with respect to time. First, we give the non-regularized versions of these functions. From (2.2.86) we read immediately off that

$$i\tilde{\Delta}^{21}(k) = i\tilde{\Delta}^>(k) = 2\pi\sigma(k^0)\delta(k^2 - m^2)[1 + f_B(k^0)]. \quad (2.2.109)$$

The KMS relation (2.2.59) translates in Fourier space to

$$i\tilde{\Delta}^{12}(k) = i\exp(-k^0\beta)\tilde{\Delta}^{21}(k) = 2\pi\sigma(k^0)\delta(k^2 - m^2)f_B(k^0). \quad (2.2.110)$$

The thermal time-ordered Green's function is given from these thermal Wightman functions by (2.2.63). Now we can use the convolution rule for Fourier transformations. We define the convolution for two functions in the frequency domain by

$$[\tilde{f} * \tilde{g}](\omega) = \int_{\mathbb{R}} \frac{d\omega'}{2\pi} \tilde{f}(\omega - \omega') \tilde{g}(\omega'). \quad (2.2.111)$$

Expressing them in terms of their Fourier integrals we get

$$[\tilde{f} * \tilde{g}](\omega) = \int_{\mathbb{R}} \frac{d\omega'}{2\pi} \int_{\mathbb{R}} dt \int_{\mathbb{R}} dt' \exp[i(\omega - \omega')t + i\omega't'] f(t)g(t'). \quad (2.2.112)$$

Now performing the frequency integral gives a factor $2\pi\delta(t - t')$, and integration over t' thus finally gives

$$[\tilde{f} * \tilde{g}](\omega) = \int_{\mathbb{R}} dt \exp(i\omega t) f(t)g(t). \quad (2.2.113)$$

This means that a product of functions in the time domain corresponds to the convolution in the frequency domain. It also shows that the convolution operation is commutative, i.e.,

$$\tilde{f} * \tilde{g} = \tilde{g} * \tilde{f}. \quad (2.2.114)$$

Using (2.2.89) we find

$$\begin{aligned} i\tilde{\Delta}^{11}(k) &= i \int_{\mathbb{R}^4} d^4x [\Theta(t)\Delta^{21}(x) + \Theta(-t)\Delta^{12}(x)] \exp(-ik \cdot x) \\ &= - \int_{\mathbb{R}} \frac{dz}{2\pi} \left[\frac{\Delta^{21}(z, \vec{k})}{k^0 - z + i0^+} - \frac{\Delta^{12}(z, \vec{k})}{k^0 - z - i0^+} \right]. \end{aligned} \quad (2.2.115)$$

Using (2.2.109) and (2.2.110) and working out the integral, using the on-shell δ distribution yields after some algebra

$$i\tilde{\Delta}^{11}(k) = \frac{i}{k^2 - m^2 + i0^+} + 2\pi\delta(k^2 - m^2)f(|k^0|). \quad (2.2.116)$$

From this we immediately find the anti-timeordered propagator by noting that from the definition of the various propagators follows the relation

$$\Delta^{11} + \Delta^{22} = \Delta^{12} + \Delta^{21} \Rightarrow \Delta^{22} = \Delta^{12} + \Delta^{21} - \Delta^{11}. \quad (2.2.117)$$

After some algebra for the Fourier transform this can be brought into the form

$$i\tilde{\Delta}^{22}(k) = -\frac{i}{k^2 - m^2 - i0^+} + 2\pi\delta(k^2 - m^2)f(|k^0|). \quad (2.2.118)$$

This form of the propagators with a $f(|k^0|)$ has the advantage to make it easy to calculate the limit $T \rightarrow 0^+$, i.e., $\beta \rightarrow \infty$, which yields the limit $\mathbf{R} \rightarrow |\Omega\rangle\langle\Omega|$, i.e., it leads to **vacuum quantum field theory**.

We also bring the off-diagonal propagators into this form by using (2.2.85). This gives

$$\begin{aligned} i\Delta^{12}(k) &= 2\pi[\Theta(-k^0) + f(|k^0|)]\delta(k^2 - m^2), \\ i\Delta^{21}(k) &= 2\pi[\Theta(k^0) + f(|k^0|)]\delta(k^2 - m^2). \end{aligned} \quad (2.2.119)$$

We finally note that problems occur in the case, where in the perturbative evaluations of real-time Green's functions two or more free propagators with the same momentum argument are multiplied, because of corresponding powers of on-shell δ functions. In such cases we have to work with the regularized propagators. We shall show in a moment that with the above introduced regularization of the propagators these problems become well-defined distributions in the limit $\eta \rightarrow 0^+$.

The Feynman rules in space contour-time form can then easily translated into energy-momentum space form. To that end we first write them in terms of the matrix propagators $\Delta^{ij}(x_1, x_2) \equiv \Delta^{ij}(x_1 - x_2)$ and apply the convolution theorem for Fourier transforms this time in the space-time domain, i.e.,

$$[f * g](x) = \int_{\mathbb{R}^4} d^4x' f(x - x')g(x') \Leftrightarrow \widetilde{[f * g]}(k) = \tilde{f}(k)\tilde{g}(k). \quad (2.2.120)$$

It turns out that, as expected from translation invariance, the n -point functions contain an energy-momentum conserving factor $\delta^{(4)}(\sum k)$, i.e.,

$$G_n^{i_1, \dots, i_n}(k_1, \dots, k_n) = (2\pi)^4 \delta^{(4)}(k_1 + \dots + k_n) \tilde{G}_n^{i_1, \dots, i_n}(k_1, \dots, k_n). \quad (2.2.121)$$

The Feynman rules to evaluate the j^{th} -order correction \tilde{G}_n to the n -point real time function in momentum space then read

- draw j vertices and n external points and connect them in any possible way to diagrams which may be connected or disconnected but any connected subdiagram must contain at least one external point. Each space time point (inner vertex point or external point) is labeled with a contour index $i \in \{1, 2\}$.
- Calculate the combinatorial factor of the diagram as explained above for the space contour-time Feynman rules.
- the meaning of the diagram elements for ϕ^4 theory are as follows:

$$\begin{aligned} \text{Diagram 1: } \text{X-vertex with index } i &= (-1)^i \frac{i\lambda}{4!}, & \text{Diagram 2: } \text{Vertical line with indices } i \text{ and } j &= i\Delta^{ij}(k). \end{aligned} \quad (2.2.122)$$

It is important to note that the propagator lines carry an arrow indicating the flow of momentum and, concerning the contour indices have to be read against the direction of the arrow.

- Label the directed propagator lines with momenta such that at any vertex four-momentum conservation is fulfilled and integrate over any momentum left that is not a momentum labeling an external leg. Such momenta occur in diagrams with closed loops.

Obviously problems for such diagrams with the on-shell δ distributions only occur for **self-energy** insertions, i.e., insertions of diagrams in one propagator (two-point function) line. Formally such insertions can be resummed by defining the **self energy** by the **Dyson equation**,

$$G_2^{ij}(k) = \Delta^{ij}(k) - \Delta^{ik}(k) \eta_{kl} \Sigma^{lm}(k) \eta_{mn} G_2^{nj}(k), \quad (2.2.123)$$

where we have defined

$$(\eta_{ij}) = \text{diag}(1, -1) \quad (2.2.124)$$

to take into account the sign changes according to the integration over the backward (anti-time ordered) part of the contour. This can be written more conveniently in matrix notation,

$$\hat{G}_2 = \hat{\Delta} - \hat{\Delta} \hat{\eta} \hat{G}_2. \quad (2.2.125)$$

Obviously the self energy Σ^{ij} consists of all diagrams with two external legs stripped from the external propagators, which cannot be made disconnected by cutting only one propagator line. Such diagrams with an arbitrary number of external points with amputated legs in general are called **one-particle irreducible vertex functions**. We shall also discuss the appropriate generating functional below in Sect. 3.3. For such self-energy insertions one has to use the regularized propagators, as discussed after Eq. (2.2.87).

Now we shall investigate the very important **analyticity** structure of two-point functions in energy-momentum representation. We use the free propagator as an example. Besides the matrix elements of the matrix propagator also the **retarded and advanced** propagators are of great physical importance. As we shall see below, they appear in linear-response theory which is an important tool to derive physical properties of the many-body system in equilibrium, e.g., the dielectric function or the index of refraction of electromagnetic waves in a medium from many-body QED or other transport coefficients. The free retarded propagator is defined in the space-time representation by

$$i\Delta_{\text{ret}}(x) = \Theta(t) \langle [\phi_{\text{I}}(x), \phi_{\text{I}}(0)] \rangle^{(0)} = i[\Delta^{11}(x) - \Delta^{12}(x)]. \quad (2.2.126)$$

From (2.2.110) and (2.2.116) we obtain

$$\tilde{\Delta}_{\text{ret}}(k) = \frac{1}{k^2 - m^2 + i\sigma(k^0)0^+} = \frac{1}{(k^0 + i0^+)^2 - \omega_{\vec{k}}^2}. \quad (2.2.127)$$

In regularized form it reads

$$\tilde{\Delta}_{\text{ret},\eta}(k) = \frac{1}{2\omega_{\vec{k}}} \left[\frac{1}{k^0 - \omega_{\vec{k}} + i\eta} - \frac{1}{k^0 + \omega_{\vec{k}} + i\eta} \right]. \quad (2.2.128)$$

As it must be, the poles of this propagator are slightly shifted into the lower k^0 plane. On the other hand we can also directly use the definition (2.2.126) of the retarded propagator, applying once more

the convolution theorem of Fourier transforms:

$$\begin{aligned}\Delta_{\text{ret}}(x) &= \Theta(t)[\Delta^{21}(x) - \Delta^{12}(x)] \\ \Rightarrow \tilde{\Delta}_{\text{ret}}(k) &= [\tilde{\Theta} * (\tilde{\Delta}^{21} - \tilde{\Delta}^{12})](k) = \int_{\mathbb{R}} \frac{dz}{2\pi} \frac{A_0(z, \vec{k})}{k^0 - z + i\eta}.\end{aligned}\quad (2.2.129)$$

This is the **Kramers-Kronig relation**. For the so-called **spectral function** we have on the one hand from (2.2.129)

$$A_0(z, \vec{k}) = i[\tilde{\Delta}^{12}(k) - \tilde{\Delta}^{21}(k)]. \quad (2.2.130)$$

On the other hand we can use the relation

$$\text{Im} \frac{1}{z - k^0 + i\eta} = -\pi \delta_{\eta}(z - k^0) \quad (2.2.131)$$

to obtain the spectral function as

$$A_0(k) = -2 \text{Im} \tilde{\Delta}_{\text{ret}}(k), \quad (2.2.132)$$

which also holds true for the regularized functions.

The advanced Green's function is defined as

$$\begin{aligned}i\Delta_{\text{adv}}(x) &= -\Theta(-t) \langle [\phi_{\text{I}}(x), \phi_{\text{I}}(0)] \rangle \\ &= -i\Theta(-t)[\Delta^{21}(x) - \Delta^{12}(x)].\end{aligned}\quad (2.2.133)$$

Since the Fourier transform of $\Theta(-t)$ is $\tilde{\Theta}^*(p^0)$ and $i\Delta^{12}$ as well as $i\Delta^{21}$ are real functions, we immediately get

$$\tilde{\Delta}_{\text{adv}}(k) = \tilde{\Delta}_{\text{ret}}^*(k) = \frac{1}{(k^0 - i0^+)^2 - \omega_{\vec{k}}^2}, \quad (2.2.134)$$

and again the same relation holds true for the regularized functions (for which simply the 0^+ has to be substituted by a finite positive number η).

As we see, the retarded and advanced Green's function can be interpreted as limiting values of an analytic function in the complex k^0 plane which only has poles on the real axis, namely

$$\tilde{\Delta}_{\text{a}}(k) = \frac{1}{(k^0)^2 - \omega_{\vec{k}}^2}, \quad (2.2.135)$$

where $\omega_{\vec{k}} = \sqrt{m^2 + \vec{k}^2} > 0$. In terms of the retarded and advanced Green's functions we can write the diagonal propagator-matrix elements in the form

$$\Delta^{11}(k) = \Delta_{\text{ret}}(k) + \Delta^{12}(k). \quad (2.2.136)$$

Another important function is the **Feynman propagator**, which is defined as

$$\begin{aligned}\tilde{\Delta}_{\text{F}}(k) &= \tilde{\Delta}_{\text{a}}(k^0 + i\sigma(k^0)0^+, \vec{k}) \\ &= \frac{1}{k^2 - m^2 + i0^+} \\ &= \frac{1}{2\omega_{\vec{k}}} \left[\frac{1}{k^0 - \omega_{\vec{k}} + i0^+} - \frac{1}{k^0 + \omega_{\vec{k}} - i0^+} \right] \\ &= \Theta(k^0)\Delta_{\text{ret}}(k) + \Theta(-k^0)\Delta_{\text{adv}}(k).\end{aligned}\quad (2.2.137)$$

The latter form is the reason for calling this propagator the Feynman propagator: The modes with positive frequency propagate with the retarded propagator and those with negative frequency with the advanced one. In the case of vacuum (zero-temperature) quantum field theory this propagator is identical with the time-ordered propagator. It is important to keep in mind that this is *not* the case anymore at finite temperature.

The regularized form is again given by substituting the finite positive number η for 0^+ . With help of (2.2.126) and the corresponding relation between the advanced and anti-time ordered propagator we can write

$$\tilde{\Delta}^{11}(k) = \tilde{\Delta}_{\text{ret}}(k) + \tilde{\Delta}^{12}(k), \quad (2.2.138)$$

$$\tilde{\Delta}^{22}(k) = \Delta^{12}(k) - \tilde{\Delta}_{\text{adv}}(k) = -[\tilde{\Delta}^{11}(k)]^*. \quad (2.2.139)$$

The advantage of this way of writing the propagators is that we immediately know the regularized form. We just have to use (2.2.128) and (2.2.134) (with the substitution $0^+ \rightarrow \eta$) for the retarded and advanced propagator and (2.2.110) with $\sigma(k^0)\delta(k^2 - m^2) \rightarrow \delta_\eta^{(\sigma)}(k^2 - m^2)$ cf. (2.2.94). Now we can express the retarded Green's function as well with help of the Feynman propagator

$$\tilde{\Delta}_{\text{ret}}(k) = \Theta(k^0)\Delta_{\text{F}}(k) + \Theta(-k^0)\Delta_{\text{F}}^*(k). \quad (2.2.140)$$

Using this in (2.2.138) together with the property of the Bose-distribution function (2.2.85), we can finally cast the regularized matrix propagator into the form [Lv87, Gel99].

$$\hat{\Delta}_\eta(k) = \hat{U}(k^0)\hat{\Delta}_{\text{D},\eta}(k)\hat{U}_\eta(k^0) \quad (2.2.141)$$

with the matrices

$$\hat{U} = \begin{pmatrix} \sqrt{1 + f_{\text{B}}(|k^0|)} & \frac{\Theta(-k^0) + f_{\text{B}}(|k^0|)}{\sqrt{1 + f_{\text{B}}(|k^0|)}} \\ \frac{\Theta(k^0) + f_{\text{B}}(|k^0|)}{\sqrt{1 + f_{\text{B}}(|k^0|)}} & \sqrt{1 + f_{\text{B}}(|k^0|)} \end{pmatrix}, \quad \hat{\Delta}_{\text{D},\eta}(k) = \text{diag}[\tilde{\Delta}_{\text{F},\eta}(k), -\tilde{\Delta}_{\text{F},\eta}^*(k)]. \quad (2.2.142)$$

This is immediately verified by working out the matrix product (2.2.141), using the identity

$$\delta_\eta^{(\sigma)}(k^2 - m^2) = \frac{i}{2\pi}[\tilde{\Delta}_{\text{F},\eta}(k) - \tilde{\Delta}_{\text{F},\eta}^*(k)], \quad (2.2.143)$$

and comparing the matrix elements with their explicit expressions in the form (2.2.117)-(2.2.119). Further by direct calculation one finds

$$\hat{U}\hat{\eta}\hat{U} = \hat{\eta} \Rightarrow \hat{U}^{-1} = \hat{\eta}\hat{U}\hat{\eta}. \quad (2.2.144)$$

Now Dyson's equation (2.2.123) can be solved in terms of a geometric series

$$\hat{G}_2 = \hat{\Delta} + \hat{\Delta}\hat{\eta}\hat{\Sigma}\hat{\eta}\hat{\Delta} + \dots = \hat{\Delta} \sum_{n=0}^{\infty} (\hat{\eta}\hat{\Sigma}\hat{\eta}\hat{\Delta})^n. \quad (2.2.145)$$

Supposed that $\hat{\Sigma}$ has no δ - or pinch singularities itself, then it is easy to show that also \hat{G} or any finite partial sum truncated at a specific n can have such singularities since we simply can write

$$\hat{G}_2 = \hat{U}\hat{\Delta}_{\text{D}}\hat{U} \sum_{n=0}^{\infty} (\hat{\eta}\hat{U}\hat{\Sigma}_{\text{D}}\hat{U}\hat{\eta}\hat{U}\hat{\Delta}_{\text{D}}\hat{U})^n \stackrel{(2.2.144)}{=} \hat{U}\hat{\Delta}_{\text{D}} \sum_{n=0}^{\infty} (\hat{\eta}\hat{\Sigma}_{\text{D}}\hat{\eta}\hat{\Delta}_{\text{D}})^n \hat{U}. \quad (2.2.146)$$

Now, since the analytic properties of the free propagator-matrix elements follow simply from the time-ordering along the real-time contour in space-time representation, the same structure (2.2.142) holds for the exact two-point Green's function, \hat{G}_2 , with the same matrix \hat{U} , i.e., the matrix $\hat{\Sigma}_D$ must indeed also be diagonal, and thus the potentially dangerous products $\hat{\Delta}_F \hat{\Delta}_F^*$ never occur in (2.2.146), and this also holds true for any truncation of this series. Such products are dangerous, because the singularities at $k^0 = \omega_{\vec{k}}$ of the free propagators in the limit $\eta \rightarrow 0^+$ are then **pinched** from both sides of the real axis, and thus such products do not have a well-defined weak limit in the sense of distributions. But now, due to (2.2.146) in fact only products of the type $\hat{\Delta}_F^n$ or $(\hat{\Delta}_F^*)^n$ occur, and thus have a definite meaning as distributions in the limit $\eta \rightarrow 0^+$. They are defined by the corresponding contour integration in the complex k^0 plane via the residuum theorem of function theory and in the limit lead to Cauchy-principle values auf derivatives of the functions and derivatives of the on-shell δ functions.

That the self energy $\hat{\Sigma}(k)$ is indeed free of pinch singularities itself is shown by induction with respect of the perturbative order under consideration. Suppose the assertion where true up to order $\mathcal{O}(\lambda^n)$. Then any line within a proper subdiagram of a contribution to the self energy of order $\mathcal{O}(\lambda^{n+1})$ can only have self-energy insertions of lower order in the coupling and is thus free of pinch singularities by assumption. That the leading-order $\mathcal{O}(\lambda^1)$ self energy is free of singularities is clear since it is given by the simple tadpole diagram

$$-i\tilde{\Sigma}_1^{ii}(k) = l \text{ (tadpole diagram) } \Rightarrow \hat{\Sigma} = \text{diag}(\Sigma^{11}, -\Sigma^{11}) = \Sigma^{11} \hat{\eta}. \quad (2.2.147)$$

The latter equality we shall prove in the next section. It obviously has only diagonal elements and is independent of k , i.e., after renormalization it is just a **temperature dependent mass term**. Thus in leading order the self energy is non-singular and thus by induction this is the case for self-energy contributions at any order.

Another important feature of the above considerations is seen at this example of a constant self energy. If we plug this in into the infinite sum (2.2.145) we first have to use the regularized expressions for Δ_F and also the Bose-distribution functions contained in the matrix \hat{U} have to be taken as $f_B(|k^0|)$ and *not* as $f_B(\omega_{\vec{k}})$, which superficially is the same in the weak limit $\eta \rightarrow 0^+$, where the on-shell δ distribution in the free propagators render these prescriptions equivalent. However, precisely to resum the Dyson series, we have to use the regularized form of the propagators, and due to our analysis with the Mills representation, we have seen that there we must take the distribution functions as a function of k^0 and not $\omega_{\vec{k}}$. The limit $\eta \rightarrow 0^+$ has to be taken after the resummation. Now due to (2.2.144) the diagonal form of the leading-order self energy is also

$$\hat{\Sigma}_D = \hat{\Sigma}^{11} \hat{\eta}, \quad (2.2.148)$$

and thus after some algebra

$$\hat{G}_D^{(1)} = (\mathbb{1} - \hat{\Sigma}^{11} \hat{\Delta}_D \hat{\eta})^{-1} \hat{\Delta}_D = (\hat{\Delta}_D)_{m^2 \rightarrow m^2 + \hat{\Sigma}^{11}}, \quad (2.2.149)$$

as expected. This we have to multiply from both sides with the matrix, \hat{U} , and *only then* to take the weak limit $\eta \rightarrow 0^+$. This leads to the correct form for a mass insertion, i.e., the on-shell δ distributions refer to the shifted mass and thus also the Bose-distribution functions get their argument at $\omega_{\vec{k}}^* =$

$\sqrt{\vec{k}^2 + m^2 + \tilde{\Sigma}^{11}}$ as it must be. This example verifies the above abstractly proven fact that with this regularization prescription the update of the distribution functions are properly taken into account within the real-time diagram technique. There has been no need to take into account the contribution of the vertical part of the contour explicitly. As shown above, this is due to the analytic structure of the Green's functions in thermal equilibrium and thus also closely related to the KMS condition.

Finally we have to come back to the correction factors for the partition sum, i.e., the closed diagrams contributing to the perturbative evaluation of $Z[J = 0]$. The straight-forward way would be to just work on the vertical part of the contour only. This leads to the **imaginary-time or Matsubara Feynman rules** with discrete imaginary Matsubara frequencies instead of real continuous energies. This will be explained in more detail in Sect. 3.2 and Appendix B. Here one only has to take into account that any perturbative correction to a two-point function has exactly the analytic properties assumed to translate the Matsubara sums into integrals, and that the integration path for the last remaining momentum integral can be deformed to two contours close to the positive real k^0 axis as explained in Sect. 3.2.2. The analytic properties then show that this final momentum integral can be performed by knowing the corresponding real-time two-point function (more precisely it is sufficient to know the time-ordered two-point function only).

Formally any closed diagram can be taken as closing an arbitrary complicated truncated subdiagram with two external space-time points, which we denote with $-iA(x_1, x_2)$, with the propagator line $i\Delta$. The corresponding contribution to the correction factor reads, using the original form of the complete extended Schwinger"=Keldysh"=contour formlism

$$z = \int_{\mathcal{C}} d^4x_1 \int_{\mathcal{C}} d^4x_2 A_{\mathcal{C}}(x_1, x_2) \Delta_{\mathcal{C}}(x_2, x_1). \quad (2.2.150)$$

Defining first the two-point function

$$C_{\mathcal{C}}(x_1, x_3) = \int_{\mathcal{C}} A_{\mathcal{C}}(x_1, x_2) \Delta_{\mathcal{C}}(x_2, x_3) \quad (2.2.151)$$

leads to

$$z = \int_{\mathcal{C}} d^4x C_{\mathcal{C}}(x, x). \quad (2.2.152)$$

Now, it is easy to see that at least at any finite order of perturbation theory, all the two-point functions have the same analytical properties as the (free or full) propagator. From translation invariance it is clear that $C_{\mathcal{C}}(x_1, x_2) = C_{\mathcal{C}}(x_1 - x_2)$ and thus $C_{\mathcal{C}}(x, x) = C_{\mathcal{C}}(0)$ and finally

$$z = -i\beta V C_{\mathcal{C}}(0), \quad (2.2.153)$$

where $C_{\mathcal{C}}$ is the Matsubara-two-point function, which is defined solely on the vertical part of the contour. We also have used the finite-volume regularization of the spatial integral. Our goal is to express (2.2.153) in terms of the real-time two-point function along the Kedysh contour $\mathcal{C}_{\mathbb{R}}$. For this purpose we note that any two-point function obeys the general analytical properties as the perturbative propagator $\Delta_{\mathcal{C}}(x_1, x_2) =: \Delta_{\mathcal{C}}(x_1 - x_2)$ and the full propagator $G_{\mathcal{C}}^{(2)}(x_1, x_2) =: G_{\mathcal{C}}^{(2)}(x_1 - x_2)$, where we have used the translation invariance of the equilibrium state in both space and time. We have derived these properties above (Eq. (2.2.126) and the following paragraphs).

Due to the KMS condition its Fourier representation is given by

$$C_{\mathcal{C}}(-i\tau, \vec{x}) = \frac{1}{\beta} \sum_{n \in \mathbb{Z}} \int \frac{d^3\vec{k}}{(2\pi)^3} \exp(-i\omega_n \tau + i\vec{k} \cdot \vec{x}) \tilde{C}_{\mathcal{C}}(i\omega_n, \vec{k}) \quad (2.2.154)$$

with the Matsubara frequencies

$$\omega_n = \frac{2\pi n}{\beta} = 2\pi nT, \quad n \in \mathbb{Z}. \quad (2.2.155)$$

The Matsubara two-point function is immediately related to the corresponding real-time functions via

$$C_\gamma(-i\tau, \vec{x}) = C^>(-i\tau, \vec{x}), \quad \tau \in [0, \beta]. \quad (2.2.156)$$

In momentum space we can express the real-time functions with help of the spectral function

$$A_C(k) = i[\tilde{C}^>(k) - \tilde{C}^<(k)] = i\tilde{C}^<(k)[\exp(\beta k^0) - 1] = i\tilde{C}^>(k)[1 - \exp(-\beta k^0)], \quad (2.2.157)$$

where in the last steps we have used the Fourier-transformed KMS condition (2.2.59), which is valid for any two-point function as for the free propagator. We have also shown above that this quantity is real and thus related to the retarded two-point function by

$$A_C(k) = -2\text{Im} \tilde{C}_{\text{ret}}(k). \quad (2.2.158)$$

Further we have defined the analytic two-point function

$$\tilde{C}_a(k) = \int_{\mathbb{R}} \frac{dz}{2\pi} \frac{A_C(z, \vec{k})}{k^0 - z}. \quad (2.2.159)$$

For real k^0 the retarded and advanced two-point functions are given by

$$C_{\text{ret}}(k) = C_a(k^0 + i0^+, \vec{k}), \quad C_{\text{adv}}(k) = C_a(k^0 - i0^+, \vec{k}) = C_{\text{ret}}^*(k) \quad \text{for } k^0 \in \mathbb{R}. \quad (2.2.160)$$

Using the inverse Fourier transform of (2.2.154) and (2.2.156),

$$\tilde{C}_\gamma(i\omega_n, \vec{k}) = \int_0^\beta d\tau \int_{\mathbb{R}^3} d^3\vec{x} \exp(i\omega_n \tau - i\vec{k} \cdot \vec{x}) C^>(-i\tau, \vec{x}), \quad (2.2.161)$$

and

$$C^>(-i\tau, \vec{x}) = \int_{\mathbb{R}^4} \frac{d^4k}{(2\pi)^4} \tilde{C}^>(k) \exp(-\tau k^0 + i\vec{k} \cdot \vec{x}) \quad (2.2.162)$$

we finally obtain

$$\begin{aligned} \tilde{C}_\gamma(i\omega_n, \vec{k}) &= \int_{\mathbb{R}} \frac{dz}{2\pi} \frac{\tilde{C}^>(z, \vec{k})}{i\omega_n - z} [\exp(-\beta z) - 1] \\ &\stackrel{(2.2.157)}{=} - \int_{\mathbb{R}} \frac{dz}{2\pi} \frac{A_C(z, \vec{k})}{i\omega_n - z} \stackrel{2.2.159}{=} -C_a(i\omega_n, \vec{k}). \end{aligned} \quad (2.2.163)$$

Now we need

$$C_\gamma(0) = \frac{1}{\beta} \sum_{n \in \mathbb{Z}} \int_{\mathbb{R}^3} \frac{d^3\vec{k}}{(2\pi)^3} \tilde{C}_\gamma(i\omega_n, \vec{k}). \quad (2.2.164)$$

Using (B.1.6) and (2.2.163) together with (2.2.160) we get

$$\begin{aligned}
 C_{\mathcal{V}}(0) &= \frac{1}{2} \int_{\mathbb{R}^4} \frac{d^4 k}{(2\pi)^4 i} [1 + 2f_B(k^0)] [C_{\text{adv}}(k) - C_{\text{ret}}(k)] \\
 &= \frac{1}{2} \int_{\mathbb{R}^4} \frac{d^4 k}{(2\pi)^4} [1 + 2f_B(k^0)] A_C(k_0) \\
 &= \frac{1}{2} \int_{\mathbb{R}^4} \frac{d^4 k}{(2\pi)^4} [\tilde{C}^>(k) + \tilde{C}^<(k)] \\
 &= \frac{1}{2} \int_{\mathbb{R}^4} \frac{d^4 k}{(2\pi)^4} [\tilde{C}^{11}(k) + \tilde{C}^{22}(k)] = \int_{\mathbb{R}^4} \frac{d^4 k}{(2\pi)^4} \tilde{C}^{11}(k).
 \end{aligned} \tag{2.2.165}$$

Thus we find

$$z = -i\beta V \int_{\mathbb{R}^4} \frac{d^4 k}{(2\pi)^4} \tilde{C}^{11}(k). \tag{2.2.166}$$

2.2.6 Renormalization

We shall close our considerations on the operator techniques and real-time Feynman rules by giving two simple one-loop examples of ϕ^4 theory for calculations of loop integrals, showing that indeed only the **vacuum counter terms**, known from usual vacuum quantum field theory⁵, are needed to render the diagrams finite. The vacuum case is always given in the limit $T \rightarrow 0$, and the key is to carefully separate off the vacuum contributions to the thermal Feynmandiagrams and renormalize them in the usual way, using a customary regularization scheme (we shall use dimensional regularization as our standard method) or directly BPHZ renormalization, which is most appropriate in the real-time formalism, because the free propagator can be easily split into pure vacuum and temperature-dependent parts. According to Eqs. (2.2.116-2.2.119), the vacuum and temperature parts of the propagator-matrix elements are given by⁶

$$i\Delta_{\text{vac}}^{11}(k) = \frac{i}{k^2 - m^2 + i0^+}, \quad i\Delta_T^{11}(k) = 2\pi\delta(k^2 - m^2)f_B(|k^0|), \tag{2.2.167}$$

$$i\Delta_{\text{vac}}^{12}(k) = 2\pi\delta(k^2 - m^2)\Theta(-k^0), \quad i\Delta_T^{11}(k) = 2\pi\delta(k^2 - m^2)f_B(|k^0|), \tag{2.2.168}$$

$$i\Delta_{\text{vac}}^{21}(k) = 2\pi\delta(k^2 - m^2)\Theta(k^0), \quad i\Delta_T^{11}(k) = 2\pi\delta(k^2 - m^2)f_B(|k^0|), \tag{2.2.169}$$

$$i\Delta_{\text{vac}}^{22}(k) = -\frac{i}{k^2 - m^2 - i0^+}, \quad i\Delta_T^{22}(k) = 2\pi\delta(k^2 - m^2)f_B(|k^0|). \tag{2.2.170}$$

As the first (somewhat untypical) example we consider the **tadpole selfenergy**

$$-i\Sigma_1^{ii}(k) = l \text{ } \begin{array}{c} \text{---} k \\ \text{---} i \\ \text{---} k \end{array} \tag{2.2.171}$$

Using the Feynman rules and counting the combinatorial factor as explained above we get

$$\Sigma_1^{11}(k) = \frac{i\lambda}{2} \int_{\mathbb{R}^4} \frac{d^4 l}{(2\pi)^4} \Delta^{11}(l). \tag{2.2.172}$$

⁵For a detailed treatment of renormalization in vacuum quantum field theory, see [Hee02]

⁶From here on we leave out the tilde for the momentum-space propagators.

Here we see that indeed only the vacuum diagram is quadratically divergent. It is simply a temperature-independent infinite correction to m^2 . Choosing the so-called **on-shell renormalization scheme**, where the counter terms are chosen such that at any order of perturbation theory the renormalized mass in the vacuum is given by the mass parameter m , we simply subtract the vacuum contribution leading to

$$\Sigma_{1,\text{ren}}^{11}(k) = \frac{i\lambda}{2} \int_{\mathbb{R}^4} \frac{d^4l}{(2\pi)^4} \Delta_T^{11}(l) = \frac{\lambda}{2} \int_{\mathbb{R}^4} \frac{d^4l}{(2\pi)^4} 2\pi \delta(l^2 - m^2) f_B(|l^0|). \quad (2.2.173)$$

As expected from our general discussion above, there is no problem with the use of the unregularized propagator, and we can simply perform the k^0 integration to get rid of the δ distribution, leading to the obviously finite result

$$\Sigma_{1,\text{ren}}^{11}(k) = \frac{\lambda}{2} \int_{\mathbb{R}^3} \frac{d^3\vec{k}}{(2\pi)^3} \frac{1}{\omega_{\vec{k}}} f_B(\omega_{\vec{k}}). \quad (2.2.174)$$

This shows that in leading order the self energy leads to a **temperature dependent shift** of the particles' effective mass. It is a well-known phenomenon from condensed matter physics that often the physics of excitations due to finite temperature (and/or density) lead to a description of the fundamental excitations of the system as "particles" which share most properties of the original particles, building the constituents of the matter under consideration but with changed effective parameters (like here the mass). Such excitations are called **quasiparticles**. As we shall see later, often there also occur quasiparticles with totally different properties than the particles, building the elementary constituents of the matter. E.g., in a superconducting medium, electrons (which are fermions) close to the Fermi surface form quasi particles consisting of pairs of electrons, the so-called **Cooper pairs** with bosonic properties. It is clear that in the case of the tadpole diagram, the off-diagonal elements vanish, because it is effectively only a one-point function (which also leads to the fact that it is a four-momentum independent constant due to translation invariance of the equilibrium state). The general property (2.2.117) then leads to

$$\Sigma_{1,\text{ren}}^{22}(k) = -\Sigma_{1,\text{ren}}^{11}(k). \quad (2.2.175)$$

Chapter 3

Path-integral formulation

The path integral formulation of quantum field theory is convenient for general considerations especially in the context of gauge theories. Here we shall apply it first to the theory of many-body systems of **charged scalar bosons** in order to have a gentle introduction to the path-integral technique and to also treat an example with chemical potential, which is a true extension of the considerations on simple ϕ^4 theory of the previous chapter.

3.1 Definition of the path integral

To have a certain example at hand, we consider the quantized version of a complex field ϕ with the dynamics of the classical theory defined by the Lagrangian¹

$$\mathcal{L} = (\partial_\mu \phi^*)(\partial^\mu \phi) - m^2 \phi^* \phi - \frac{\lambda}{8} (\phi^* \phi)^2. \quad (3.1.1)$$

The canonically conjugated field momenta are given by

$$\Pi^* = \frac{\partial \mathcal{L}}{\partial \dot{\phi}^*} = \dot{\phi}, \quad \Pi = \frac{\partial \mathcal{L}}{\partial \dot{\phi}} = \dot{\phi}^*, \quad (3.1.2)$$

while the Hamilton density is

$$\mathcal{H} = \dot{\phi} \Pi^* + \dot{\phi}^* \Pi - \mathcal{L} = \Pi^* \Pi + (\text{grad } \phi^*)(\text{grad } \phi) + m^2 \phi^* \phi + \frac{\lambda}{8} (\phi^* \phi)^2. \quad (3.1.3)$$

This theory has not only the Poincaré symmetry of space-time but also a global U(1) symmetry $\phi \rightarrow \exp(-i\chi)\phi$, $\phi^* \rightarrow \exp(i\chi)\phi^*$ giving rise to the conserved Noether charge

$$Q = \int d^3 \vec{x} \phi^*(x) i \overleftrightarrow{\partial}_0 \phi(x). \quad (3.1.4)$$

¹It should be kept in mind that in the Lagrangian and the action principle ϕ and ϕ^* are independent field variables, rather than conjugate complex quantities. While in vacuum quantum field theory, for the *solutions of the field equations*, the star becomes the meaning of complex conjugation, this is not the case at finite chemical potential. As we shall see, in this case, we have to impose boundary conditions for the fields, integrated over in the path integral, which are not compatible with an interpretation of ϕ^* as the conjugate complex of ϕ .

As already in the previous chapter for free fields the canonical quantisation is done by making the fields to field operators which according to the spin-statistics theorem obey the bosonic canonical equal-time commutation relations

$$[\phi(t, \vec{x}), \phi(t, \vec{y})] = 0, \quad [\phi(t, \vec{x}), \Pi(t, \vec{y})] = i\delta(\vec{x} - \vec{y}). \quad (3.1.5)$$

The quantization of the Hamiltonian and the Noether charge (3.1.4) leads to characteristic operator-ordering problems. Also the products of local operator expressions are not well defined at all since we have to define the meaning of the product of generalised functions like the δ -distributions appearing in the commutator relations (3.1.5). Here we use the usual very naive physicists's rule of thumb to chose a convenient ordering of the operators to define formal operator expressions from the classical definitions, always keeping in mind, that we have to renormalize the physical quantities calculated from these expressions.

Since we like to apply the path integral formalism we use the **left ordering** in the canonical formulation, i.e., we always order the field momentum operators to the left of the field operators themselves. For the charge (3.1.4) this rule yields

$$\mathbf{Q} = i \int d^3\vec{x} (\Pi^\dagger \phi^\dagger - \Pi \phi). \quad (3.1.6)$$

This is a selfadjoint operator up to an indefinite field-independent constant. With help of (3.1.5) one proves immediately the commutation relations

$$[\mathbf{Q}, \phi(x)] = -\phi(x), \quad [\mathbf{Q}, \phi^\dagger(x)] = \phi^\dagger(x), \quad (3.1.7)$$

which tell us, that \mathbf{Q} is the generator of the underlying U(1) symmetry of the theory. This is the quantum analogue of Noether's theorem known from classical field theory: Each one-parameter symmetry group defines a conserved charge which in turn is the generator of this symmetry group.

Now we like to investigate the equilibrium state

$$\mathbf{R} = \frac{1}{Z} \exp(-\beta \mathbf{H} + \alpha \mathbf{Q}), \quad Z = \text{Tr}[\exp(-\beta \mathbf{H} + \alpha \mathbf{Q})]. \quad (3.1.8)$$

To define the path integral we introduce **eigenstates of the field operators** in the Heisenberg picture:

$$\phi(x)|\phi, \phi^*, t\rangle = \phi(x)|\phi, \phi^*, t\rangle, \quad \phi^\dagger(x)|\phi, \phi^*, t\rangle = \phi^*(x)|\phi, \phi^*, t\rangle. \quad (3.1.9)$$

These generalized eigenkets are time dependent since in the Heisenberg picture we have by definition

$$\phi(t, \vec{x}) = \exp(i\mathbf{H}t)\phi(0, \vec{x})\exp(-i\mathbf{H}t). \quad (3.1.10)$$

Here we have set the initial time to 0 and made use of the fact, that \mathbf{H} is a time-independent quantity. From this we get

$$|\phi, \phi^*, t\rangle = \exp(i\mathbf{H}t)|\phi, \phi^*, 0\rangle. \quad (3.1.11)$$

Due to (3.1.7) for $\alpha \in \mathbb{R}$ we also find the relations

$$\exp(-\alpha \mathbf{Q})\phi(x)\exp(\alpha \mathbf{Q}) = \exp(\alpha)\phi(x), \quad \exp(-\alpha \mathbf{Q})\phi^\dagger(x)\exp(\alpha \mathbf{Q}) = \exp(-\alpha)\phi^\dagger(x), \quad (3.1.12)$$

which means for the field-operator eigenstates

$$\exp(\alpha \mathbf{Q})|\phi, \phi^*\rangle = |\exp(\alpha)\phi, \exp(-\alpha)\phi^*\rangle. \quad (3.1.13)$$

3.1 · Definition of the path integral

We can also introduce the generalized eigenkets for the canonical field momenta. From the commutator relations (3.1.5) one obtains

$$\langle \phi, \phi^*, t=0 | \Pi, \Pi^*, t=0 \rangle = \exp \left(i \int d^3 \vec{x} [\Pi(0, \vec{x}) \phi(0, \vec{x}) + \Pi^*(0, \vec{x}) \phi^*(0, \vec{x})] \right). \quad (3.1.14)$$

We define the normalisation such that

$$\int D\phi D\phi^* |\phi, \phi^*, t\rangle \langle \phi, \phi^*, t| = \int \frac{D\Pi D\Pi^*}{(2\pi)^2} |\Pi, \Pi^*, t\rangle \langle \Pi, \Pi^*, t| = 1. \quad (3.1.15)$$

As usual, here the functional integrals have to be defined in terms of a discretised version of the space-time arguments and then one has to take the continuum limit.

Now for a time-dependent functional $F(t) = F[\phi, t]$ due to (3.1.15) we have

$$\langle F(t) \rangle = \frac{1}{Z} \text{Tr} \{ \exp(-\beta \mathbf{H} + \alpha \mathbf{Q}) F(t) \} \quad (3.1.16)$$

For the following we insert $\mathbb{1} = \exp(-i\mathbf{H}t) \exp(+i\mathbf{H}t)$ and, using $[\mathbf{Q}, \mathbf{H}] = 0$, we can write

$$\begin{aligned} \langle F(t) \rangle &= \frac{1}{Z} \text{Tr} \{ \exp(-i\mathbf{H}t) \exp(+i\mathbf{H}t) \exp(-\beta \mathbf{H} + \alpha \mathbf{Q}) F(t) \} \\ &= \frac{1}{Z} \text{Tr} \{ \exp(-i\mathbf{H}t) \exp(-\beta \mathbf{H} + \alpha \mathbf{Q}) \exp(+i\mathbf{H}t) F(t) \} \\ &= \frac{1}{Z} \text{Tr} \{ \exp(-\beta \mathbf{H} + \alpha \mathbf{Q}) \exp(+i\mathbf{H}t) F(t) \exp(-i\mathbf{H}t) \}. \end{aligned} \quad (3.1.17)$$

Now we use (3.1.15) to evaluate the trace with help of the eigenvectors $|\phi, \phi^*, 0\rangle$, setting the initial time $t_i = 0$ for convenience,

$$\langle F(t) \rangle = \frac{1}{Z} \int D\phi \int D\phi^* \langle \phi, \phi^*, 0 | \exp(-\beta \mathbf{H} + \alpha \mathbf{Q}) \exp(+i\mathbf{H}t) F(t) \exp(-i\mathbf{H}t) | \phi, \phi^*, 0 \rangle. \quad (3.1.18)$$

Now we have, because of $[\mathbf{H}, \mathbf{Q}] = 0$,

$$\begin{aligned} \langle \phi, \phi^*, 0 | \exp(-\beta \mathbf{H} + \alpha \mathbf{Q}) &= \langle \phi, \phi^*, 0 | \exp(\alpha \mathbf{Q}) \exp(-\beta \mathbf{H}) \\ &\stackrel{(3.1.13)}{=} \langle \exp(\alpha) \phi, \exp(-\alpha) \phi^*, 0 | \exp(-\beta \mathbf{H}) \\ &\stackrel{(3.1.11)}{=} \langle \exp(\alpha) \phi, \exp(-\alpha) \phi^*, -i\beta |. \end{aligned} \quad (3.1.19)$$

Plugging this in (3.1.18) we finally get

$$\langle F(t) \rangle = \frac{1}{Z} \int D\phi D\phi^* \langle \exp(\alpha) \phi, \exp(-\alpha) \phi^*, -i\beta | \exp(+i\mathbf{H}t) F(t) \exp(-i\mathbf{H}t) | \phi, \phi^*, 0 \rangle. \quad (3.1.20)$$

This is the typical situation for a path-integral formulation: We have to calculate a matrix element of an operator for the time evolution from $t = 0$ to $t = -i\beta$ with an insertion of time-evolution along the real-time axis and back. Thus, the original Schwinger-Keldysh contour (Fig. 2.1) is extended at the end by a **vertical part** running from 0 to $-i\beta$. Again the real part of the contour can be extended to run from $t = t_i$ to an arbitrary final time $t_f > t$ (see Fig. 2.2). It is clear, that the same holds true

for the initial time which can be chosen to be $t_i < 0$. As we have already seen in Sect. 2.2.103 for the equilibrium case it is convenient to extend the real part of the contour along the whole time axis, i.e., taking $t_i \rightarrow -\infty$. This freedom is due to the **time-translation invariance** of the equilibrium state. It should be kept in mind, that for a general non-equilibrium situation, it does not make sense to consider times smaller than the initial time, where the system has been prepared.

To derive a path-integral expression for (3.1.20) we take advantage of the fact that for our system, defined by the Lagrangian (3.1.1), the Hamiltonian (3.1.2) is of the form

$$\mathbf{H} = \mathbf{H}_1[\boldsymbol{\Pi}, \boldsymbol{\Pi}^\dagger] + \mathbf{H}_2[\boldsymbol{\Phi}, \boldsymbol{\Phi}^\dagger]. \quad (3.1.21)$$

Now, for any real or complex parameter $\Delta\tau$, we have

$$\exp[\Delta\tau(\mathbf{H}_1 + \mathbf{H}_2)] = \exp(\Delta\tau\mathbf{H}_1)\exp(\Delta\tau\mathbf{H}_2) + \mathcal{O}(\Delta\tau^2). \quad (3.1.22)$$

Using this decomposition in (3.1.20), where we introduce a lattice on the time contour according to Fig. 3.1, we can write

$$\begin{aligned} \langle \mathbf{F}(t) \rangle &= \int \mathcal{D}\phi_k^{j*} d\phi_k^j \int \frac{\mathcal{D}\Pi_k^{j*} \mathcal{D}\Pi_k^j}{(2\pi)^2} \\ &\times \langle \phi_{N_3}^3 | \exp[-i\Delta t_3 \mathbf{H}_1(t_{N_3}^3)] | \Pi_{N_3}^3 \rangle \langle \Pi_{N_3}^3 | \exp[-i\Delta t_3 \mathbf{H}_2(t_{N_3}^3)] | \phi_{N_3-1}^3 \rangle \\ &\times \langle \phi_{N_3-1}^3 | \exp[-i\Delta t_3 \mathbf{H}_1(t_{N_3-1}^3)] | \Pi_{N_3-1}^3 \rangle \langle \Pi_{N_3-1}^3 | \exp[-i\Delta t_3 \mathbf{H}_2(t_{N_3}^3)] | \phi_{N_3-2}^3 \rangle \dots \\ &\times \langle \phi_1^3 | \exp[-i\Delta t_3 \mathbf{H}_1(t_1^3)] | \Pi_1^3 \rangle \langle \Pi_1^3 | \exp[-i\Delta t_3 \mathbf{H}_2(t_{N_3}^3)] | \phi_0^3 \rangle \\ &\times \langle \phi_{N_2}^2 | \exp[-i\Delta t_2 \mathbf{H}_1(t_{N_2}^2)] | \Pi_{N_2}^2 \rangle \langle \Pi_{N_2}^2 | \exp[-i\Delta t_3 \mathbf{H}_2(t_{N_2}^2)] | \phi_{N_2-1}^2 \rangle \\ &\times \dots \\ &\times \langle \phi_1^2 | \exp[-i\Delta t_2 \mathbf{H}_1(t_1^2)] | \Pi_1^2 \rangle \langle \Pi_1^2 | \exp[-i\Delta t_3 \mathbf{H}_2(t_1^2)] | \phi_0^2 \rangle \\ &\times \langle \phi_0^2 | \mathbf{F}(t_i^2) | \phi_{N_1}^1 \rangle \\ &\times \langle \phi_{N_1}^1 | \exp[-i\Delta t_1 \mathbf{H}_1(t_{N_1}^1)] | \Pi_{N_1}^1 \rangle \langle \Pi_{N_1}^1 | \exp[-i\Delta t_1 \mathbf{H}_2(t_{N_1}^1)] | \phi_{N_1-1}^1 \rangle \\ &\times \dots \\ &\times \langle \phi_1^1 | \exp[-i\Delta t_1 \mathbf{H}_1(t_1^1)] | \Pi_1^1 \rangle \langle \Pi_1^1 | \exp[-i\Delta t_3 \mathbf{H}_2(t_1^1)] | \phi_0^1 \rangle \end{aligned} \quad (3.1.23)$$

The inserted projectors $|\Pi\rangle \langle \Pi|$ and $|\phi\rangle \langle \phi|$ have to be understood to be taken always at the appropriate time arguments. At the boundaries of the contour we have $t_i^1 = t_i^3 = t_{N_2}^2$ and $t_i^2 = t_{N_1}^1$. Further we have to imply boundary conditions for the outermost bra and ket (the so called *KMS-condition*, named after Kubo, Martin, and Schwinger): $\phi_{N_3}^3 = \exp(-\alpha)\phi_0^1$ and $(\phi_{N_3}^3)^* = \exp(+\alpha)(\phi_0^1)^*$. There are no boundary conditions for the canonical field momenta.

Now from (3.1.21) and (3.1.14) we find the following expressions for the matrix elements appearing in (3.1.23):

$$\begin{aligned} \langle \phi_k^j | \exp(-i\Delta t_j \mathbf{H}_1) | \Pi_k \rangle &= \exp \left[-i\Delta t_j H_1(\Pi_k, \Pi_k^*) + i \int d^3 \vec{x} (\phi_k \Pi_k + \text{cc}) \right], \\ \langle \Pi_k | \exp(-i\Delta t_j \mathbf{H}_2) | \phi_{k-1} \rangle &= \exp \left[-i\Delta t_j H_2(\phi_{k-1}, \phi_{k-1}^*) - i \int d^3 \vec{x} (\phi_{k-1} \Pi_k + \text{cc}) \right]. \end{aligned} \quad (3.1.24)$$

3.1 · Definition of the path integral

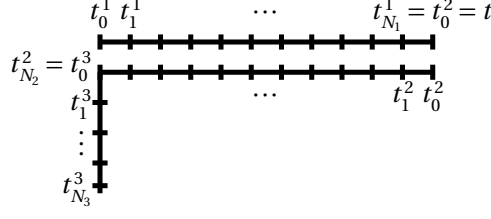


Figure 3.1: *The time lattice for the extended Schwinger-Keldysh contour.*

Plugging this in (3.1.23) and reading the expression as the lattice version of a path integral one obtains in the continuum limit $N_j \rightarrow \infty$ ($j \in \{1, 2, 3\}$):

$$\langle \mathbf{F}(t) \rangle = \frac{1}{Z} \int_{\text{KMS}} \text{D}\phi \text{D}\phi^* \int \frac{\text{D}\Pi \text{D}\Pi^*}{(2\pi)^2} \exp \left[-i \int_{\mathcal{C}} d^4x \left(\mathcal{H} - \Pi \dot{\phi} - \Pi^* \dot{\phi}^* \right) \right] F(t), \quad (3.1.25)$$

where “KMS” at the path integral sign reminds us that we have to impose the boundary conditions

$$\phi(-i\beta, \vec{x}) = \exp(-\alpha) \phi(0, \vec{x}), \quad \phi^*(-i\beta, \vec{x}) = \exp(\alpha) \phi^*(0, \vec{x}). \quad (3.1.26)$$

We have to integrate also with respect to $\phi(0, \vec{x})$ and $\phi^*(0, \vec{x})$ because of the trace in (3.1.17). As our derivation clearly shows, there are no boundary conditions for the functional integration over the canonical field momenta.

Finally we note that a path-integral with a functional of multiple time arguments along the contour gives an expectation value of **contour-time ordered operator products**, i.e.,

$$\begin{aligned} \langle \mathcal{T}_{\mathcal{C}} \mathbf{F}_1(t_1) \cdots \mathbf{F}_n(t_n) \rangle &= \frac{1}{Z} \int_{\text{KMS}} \text{D}\phi \text{D}\phi^* \frac{\text{D}\Pi \text{D}\Pi^*}{(2\pi)^2} \\ &\times \exp \left[-i \int_{\mathcal{C}} d^4x \left(\mathcal{H} - \Pi \dot{\phi} - \Pi^* \dot{\phi}^* \right) \right] F_1(t_1) \cdots F_n(t_n). \end{aligned} \quad (3.1.27)$$

Now we can use the fact, that the Hamiltonian (3.1.3) is quadratic in the field momenta Π and Π^* with field-independent coefficients. Thus we can evaluate the functional integration with respect to the field momenta in (3.1.25) exactly. The result is the stationary point of the exponential times an indefinite factor. Thus, we can write

$$\langle \mathbf{F}(t) \rangle = \frac{1}{Z'} \int_{\text{KMS}} \text{D}\phi \text{D}\phi^* \exp \{ i S_{\mathcal{C}}[\phi, \phi^*] \} F(t) \quad \text{with} \quad S_{\mathcal{C}}[\phi, \phi^*] = \int_{\mathcal{C}} d^4x \mathcal{L}. \quad (3.1.28)$$

In the following we shall use the abbreviation

$$\{f_{1\dots n}\}_{1\dots n} = \int_{\mathcal{C}} d^4x_1 \cdots d^4x_n f(x_1, \dots, x_n) \quad (3.1.29)$$

for the integration of a function with multiple space-time arguments. The time argument is always running along the time contour.

The new partition sum Z' has to be chosen such, that $\langle \mathbb{1} \rangle = 1$, yielding

$$Z' = \int_{\text{KMS}} \text{D}\phi \text{D}\phi^* \exp [i \{ \mathcal{L}_1 \}_1]. \quad (3.1.30)$$

Generalizing (3.1.28) to the expectation value of local field operators at different times we find immediately

$$\langle \mathcal{T}_\epsilon \phi(x_1) \cdots \phi(x_n) \rangle = \frac{1}{Z'} \int_{\text{KMS}} \text{D}\phi \text{D}\phi^* \phi(x_1) \cdots \phi(x_n) \exp[i\{\mathcal{L}_1\}_1]. \quad (3.1.31)$$

The generating functional for expectation values of contour-ordered operator products is defined as

$$Z[j, j^*] = \int_{\text{KMS}} \text{D}\phi \text{D}\phi^* \exp[i\{\mathcal{L}_1 + j_1^* \phi_1 + j_1 \phi_1^*\}_1] \quad (3.1.32)$$

3.1.1 Two-point functions along the real-time contour

First we study the general case of a non-equilibrium situation and thus restrict ourselves to the real-time branch of the contour. In the next section we shall treat the equilibrium case and the analytic continuation necessary to go over from the real- to the imaginary-time formalism.

We define a two-point function on the Schwinger-Keldysh contour (see Fig. 2.1) as

$$iF(x, y) = \langle \mathcal{T}_\epsilon \mathbf{A}(x) \mathbf{B}(y) \rangle. \quad (3.1.33)$$

Herein \mathbf{A} and \mathbf{B} are arbitrary bosonic local field operators².

Further we like to use Fourier transformations which are only available if we use real times, not contour times. Thus, we introduce a matrix Green's function formalism as follows:

$$\hat{F}(x, y) = \begin{pmatrix} F^{11}(x, y) & F^{12}(x, y) \\ F^{21}(x, y) & F^{22}(x, y) \end{pmatrix} = -i \begin{pmatrix} \langle \mathcal{T}_\epsilon \mathbf{A}(x) \mathbf{B}(y) \rangle & \langle \mathbf{B}(y) \mathbf{A}(x) \rangle \\ \langle \mathbf{A}(x) \mathbf{B}(y) \rangle & \langle \mathcal{T}_\epsilon \mathbf{A}(y) \mathbf{B}(x) \rangle \end{pmatrix}. \quad (3.1.34)$$

Since the off-diagonal elements of this matrix are expectation values of fixed operator products and the time evolution is unitary, they are analytic functions for $t \in \mathbb{R}$. The four matrix elements obviously are not independent of each other but fulfil the relation

$$F^{11} + F^{22} = F^{12} + F^{21}. \quad (3.1.35)$$

With help of the contour unit-step function (2.2.53) we can write the contour Green's function as

$$F(x, y) = \Theta_\epsilon(x_0, y_0) F^{21}(x, y) + \Theta_\epsilon(y_0, x_0) F^{12}(x, y). \quad (3.1.36)$$

Sometimes the introduction of the retarded and advanced two-point functions is useful. Both have real time arguments (not contour time arguments):

$$\begin{aligned} F_R(x, y) &= F^{11}(x, y) - F^{12}(x, y) = \Theta(x_0 - y_0)[F^{21}(x, y) - F^{12}(x, y)], \\ F_A(x, y) &= F^{11}(x, y) - F^{21}(x, y) = -\Theta(y_0 - x_0)[F^{21}(x, y) - F^{12}(x, y)]. \end{aligned} \quad (3.1.37)$$

For the matrix elements (3.1.34) we can introduce the **Wigner transform**

$$\tilde{F}^{ij}(X, p) = \int d^4\xi F^{ij}(X + \xi/2, X - \xi/2) \exp(ip\xi), \quad i, j \in \{1, 2\}. \quad (3.1.38)$$

If the state is translation invariant then obviously \tilde{F} depends on p only. This is the case for the vacuum state and thermal equilibrium.

²For the fermionic case one has to introduce the usual sign convention when interchanging operators to bring them in the order assigned by the various time ordering symbols.

3.1 · Definition of the path integral

For the special case $\mathbf{B} = \mathbf{A}^\dagger$ we find from (3.1.36)

$$\begin{aligned} i\tilde{F}^{\pm\mp}(X, p) &\in \mathbb{R}, \\ [i\tilde{F}^{\pm\pm}(X, p)]^* &= i\tilde{F}^{\mp\mp}(X, p), \\ [\tilde{F}_R(X, p)]^* &= \tilde{F}_A(X, p). \end{aligned} \quad (3.1.39)$$

From (3.1.37) we get

$$\tilde{F}_R(X, p) = [\tilde{\Theta} * \underbrace{(\tilde{F}^{21} - \tilde{F}^{12})}_{-iF_S}](X, p), \quad (3.1.40)$$

where the p_0 -convolution of Wigner functions is defined as

$$[\tilde{\Theta} * f](X, p) = \int \frac{dp_0}{2\pi} \tilde{\Theta}(p_0 - p'_0) f(X, p'_0, \vec{p}). \quad (3.1.41)$$

Since

$$\Theta(t) = \int \frac{dp_0}{2\pi} \frac{i}{p_0 + i0^+} \exp(-ip_0 t) \quad (3.1.42)$$

(3.1.40) reads

$$\tilde{F}_R(X, p) = \int \frac{dp'_0}{2\pi} \frac{\tilde{F}_S(X, p')}{p_0 + i0^+ - p'_0}, \quad \vec{p}' = \vec{p}. \quad (3.1.43)$$

From

$$\frac{1}{p_0 - p'_0 + i0^+} = \mathcal{P} \frac{1}{p_0 - p'_0} - i\pi \delta(p_0 - p'_0) \quad (3.1.44)$$

we find the expression

$$\tilde{F}_S(X, p) = -2\text{Im} \tilde{F}_R(X, p) \quad (3.1.45)$$

for the spectral function and the **Kramers-Kronig relation**

$$\text{Re} \tilde{F}_R(X, p) = -\mathcal{P} \int \frac{dp'_0}{\pi} \frac{\text{Im} \tilde{F}_R(X, p')}{p_0 - p'_0}. \quad (3.1.46)$$

It is important to note that in the special case $\mathbf{B} = \mathbf{A}^\dagger$ (particularly for the two-point Green's function, where $\mathbf{A} = \phi$ and $\mathbf{B} = \phi^\dagger$) we have the additional properties

$$\begin{aligned} [iF^{21}(x, y)]^* &= iF^{21}(y, x), & [iF^{12}(x, y)]^* &= iF^{12}(y, x), \\ [iF^{11}(x, y)]^* &= iF^{22}(y, x), & [iF^{22}(x, y)]^* &= iF^{11}(y, x), \\ [F_R(x, y)]^* &= F_A(y, x). \end{aligned} \quad (3.1.47)$$

3.1.2 The two-point Green's function in equilibrium

In thermodynamic equilibrium due to translation invariance the two-point matrix Green's functions depend on the relative coordinate $\xi = x_1 - x_2$ only. Also the Green's functions have additional properties due to the KMS condition on the fields. In the following we note only the time arguments of the Green's function, which makes the notation more convenient. In this chapter we discuss the **Green's function** for scalar fields, which is defined by setting $\mathbf{A}(x) = \phi(x)$ and $\mathbf{B}(x) = \phi^\dagger(x)$ in (3.1.34):

$$iG(x, y) = \langle \mathcal{T}_\epsilon \phi(x) \phi^\dagger(y) \rangle. \quad (3.1.48)$$

In terms of the path integral the 21-two-point function is defined by

$$\begin{aligned}
 iZ[0]G^{21}(\xi) &= \int_{\text{KMS}} D\phi D\phi^* \phi(\xi^+) \phi^*(0^-) \exp(iS[\phi, \phi^*]) \\
 &= \int_{\text{KMS}} D\phi D\phi^* \exp(-\mu\beta) \phi(\xi) \phi^*(-i\beta) \exp(iS[\phi]) \\
 &= iZ[0]G^{12}(\xi + i\beta) \exp(-\mu\beta).
 \end{aligned} \tag{3.1.49}$$

Here the time argument of ξ is located at the real part of the contour. Thus, we have the analytic continuation of G^{12} to imaginary time arguments, and it fulfills

$$G^{21}(\xi - i\beta) = \exp(-\mu\beta) G^{12}(\xi) \quad \text{for } -\beta < \text{Im } \xi < 0. \tag{3.1.50}$$

The Fourier transform of this KMS-condition reads

$$\tilde{G}^{21}(p) = \exp[\beta(p_0 - \mu)] \tilde{G}^{12}(p). \tag{3.1.51}$$

From (3.1.45) follows

$$G_S(p) = A(p) = -2 \text{Im } \tilde{G}_R(p), \tag{3.1.52}$$

$$i\tilde{G}^{12}(p) = A(p) f_B(p_0 - \mu), \tag{3.1.53}$$

$$i\tilde{G}^{21}(p) = A(p) [1 + f_B(p_0 - \mu)], \tag{3.1.54}$$

where we have introduced the **Bose-Einstein distribution function**

$$f_B(x) = \frac{1}{\exp(\beta x) - 1}. \tag{3.1.55}$$

With the spectral representation (3.1.43) we have

$$\tilde{G}_R(p) = \int \frac{dp'_0}{2\pi} \frac{A(p'_0, \vec{p})}{p_0 - p'_0 + i0^+}. \tag{3.1.56}$$

With (3.1.37) and (3.1.39) we find the following expression for the contour Green's function

$$iG_{\mathcal{C}}(x', x) = \int \frac{d^4 p}{(2\pi)^4} A(p) \exp[-ip(x' - x)] [\Theta_{\mathcal{C}}(t', t) + f_B(p_0 - \mu)], \tag{3.1.57}$$

where we have used the contour unit-step function (2.2.53) for compact notation.

3.1.3 The free equilibrium propagator

The Feynman rules for perturbation theory at finite temperatures can be derived in the same way as the Feynman rules for vacuum physics. The only difference is, that the propagators are replaced by the real-time propagators or the imaginary-time propagators. Here we use the path integral formalism. The generating functional for the free theory reads

$$Z_0[j, j^*] = N \int_{\text{KMS}} D\phi D\phi^* \exp[-i \{ \phi_1^*(\square + m^2) \phi_1 \}_1 + i \{ j_1^* \phi_1 + j_1 \phi_1^* \}_1]. \tag{3.1.58}$$

3.1 · Definition of the path integral

Since the path integral is Gaussian, it can be calculated exactly. One needs to find the stationary point of the exponential, which is given by the Klein-Gordon equations of motion with the auxiliary fields j and j^* as sources,

$$\begin{aligned} -(\square + m^2)\phi_j &= -j, & -(\square + m^2)\phi_j^* &= -j^*, \\ \phi_j(-i\beta, \vec{x}) &= \exp(-\alpha)\phi_j(0, \vec{x}), & \phi_j^*(-i\beta, \vec{x}) &= \exp(\alpha)\phi_j^*(0, \vec{x}) \end{aligned} \quad (3.1.59)$$

where the second line gives the KMS conditions on the fields. Using the invariance of the path integral measure under field translations it turns out immediately, that (3.1.58) is given by

$$Z_0[j, j^*] = \exp \left[-i \int_{\mathcal{C}} d^4x j^*(x) \phi_j(x) \right]. \quad (3.1.60)$$

The solutions ϕ_j and ϕ_j^* of (3.1.59) are given with help of the free contour Green's function

$$\phi_j(x) = - \int d^4x' \Delta_{\mathcal{C}}(x, x') j(x'). \quad (3.1.61)$$

Due to the translation invariance of the equilibrium state, in both time and space, the contour Green's function is a function of the coordinate difference only, i.e., $\Delta_{\mathcal{C}}(x, x') = \Delta_{\mathcal{C}}(x - x')$.

itself is uniquely determined by the equation of motion

$$-(\square + m^2)\Delta_{\mathcal{C}}(x) = \delta_{\mathcal{C}}(x). \quad (3.1.62)$$

Since this is the Green's function for the field ϕ_j , it must fulfill the corresponding boundary condition, cf. Eq. (3.1.59),

$$\Delta_{\mathcal{C}}(t - i\beta, \vec{x}) = \exp(-\alpha)\Delta_{\mathcal{C}}(t, \vec{x}). \quad (3.1.63)$$

The contour δ -distribution is defined as usual by

$$\int_{\mathcal{C}} dt' f(t') \delta_{\mathcal{C}}(t - t') = f(t), \quad (3.1.64)$$

where f is an arbitrary test function defined along the time contour \mathcal{C} .

It is more easy to find the retarded Green's function and use the general equations (3.1.52-3.1.54) for the other real-time functions. Since $\Delta_R(x) \propto \Theta(t)$ we find the solution for (3.1.62) with this boundary condition to be

$$\tilde{\Delta}_R(p) = \frac{1}{p^2 - m^2 + i0^+ \text{sign}(p_0)}. \quad (3.1.65)$$

So the spectral function is given by

$$A_0(p) = -2 \text{Im} \tilde{\Delta}_R(p) = 2\pi \text{sign}(p_0) \delta(p^2 - m^2). \quad (3.1.66)$$

Using (3.1.52-3.1.54) this leads to the following expressions for the free real-time propagators

$$\begin{aligned} \Delta^{11}(p) &= \frac{1}{p^2 - m^2 + i0^+ \sigma(p_0)} - 2\pi i \delta(p^2 - m^2) \sigma(p_0) f_B(p_0 - \mu), \\ \Delta^{12}(p) &= -2\pi i \delta(p^2 - m^2) \sigma(p_0) f_B(p_0 - \mu), \\ \Delta^{21}(p) &= -2\pi i \delta(p^2 - m^2) \sigma(p_0) [1 + f_B(p_0 - \mu)], \\ \Delta^{22}(p) &= -\frac{1}{p^2 - m^2 - i0^+ \sigma(p_0)} - 2\pi i \delta(p^2 - m^2) \sigma(p_0) f_B(p_0 - \mu). \end{aligned} \quad (3.1.67)$$

Using (3.1.61) in (3.1.60) we get the solution for the generating functional for the free-field case

$$Z_0[j, j^*] = \exp[-i\{\Delta_{\mathcal{G}}(x_1 - x_2)j_1^*j_2\}_{12}]. \quad (3.1.68)$$

The generating functional for the interacting fields can be expressed with help of the free functional

$$Z[j, j^*] = \left\{ \exp\left(iS_I \left[\frac{\delta}{i\delta j(x_1)}, \frac{\delta}{i\delta j^*(x_1)} \right] \right) Z_0[j, j^*] \right\}_1. \quad (3.1.69)$$

The perturbation series is obtained by expanding the exponential functional derivation operator in powers of S_I .

As we have seen in Sect. 2.2.4, that then one has to regularize the δ -distribution in the “causally correct way”, namely

$$\delta(x) = \text{w-lim}_{\epsilon \rightarrow 0^+} \delta_\epsilon(x) = \text{w-lim}_{\epsilon \rightarrow 0^+} \frac{1}{2\pi i} \left(\frac{1}{x - i\epsilon} - \frac{1}{x + i\epsilon} \right) = \frac{1}{\pi} \frac{\epsilon}{x^2 + \epsilon^2}. \quad (3.1.70)$$

For more details, also see [Gel96, LM96, Mab97, Gel99].

Further when using the regularized δ distributions, it is important to write $f_B(p_0 - \mu)$ and *not* $f_B(\omega_{\vec{p}} - \mu)$ in (3.1.67). From our derivation of the equilibrium Feynman rules in Sect. 2.2.5 we know that then we do not need to bother with possible contributions from the vertical part of the contour, which was due to the factorization (2.2.103) of the generating functional for Green’s functions along the full contour in pure real-time and imaginary-time generating functionals.

3.2 Thermodynamics of ideal Bose gases

The only place we really need the imaginary time formalism is when we want to calculate thermodynamic bulk quantities. We show now how to do this with help of analytic continuations of the real-time quantities. We shall also use the ideal gas as an example to further develop some techniques to evaluate path integrals and give some low- and high-temperature expansions of the partition sum, which also introduces interesting calculational techniques, that are also useful for other calculations in thermal quantum field theory.

3.2.1 Path-integral evaluation of the partition sum

In order to obtain the correct T - and μ -dependent factors to calculate the partition sum of the non-interacting charged scalar bosons we have to go back to the Hamiltonian path integral

$$Z(\beta, \mu) = N \int_{\text{KMS}} D\phi D\phi^* \int D\Pi D\Pi^* \exp[-i\{\mathcal{H}_1 - \Pi_1 \dot{\phi}_1 - \Pi_1^* \dot{\phi}_1^*\}_{\mathcal{G}_V 1}]. \quad (3.2.1)$$

We need to calculate only along the vertical part of the contour since the contributions from the two real-time branches cancel, since the real-time contour is closed for itself.

While the time-domain is the bounded imaginary interval $(0, -i\beta)$ to regularize the path integral in the infrared domain at first we have to restrict the spatial coordinates to a finite volume which we chose as a cube of length L . We imply periodic boundary conditions. Taking the thermodynamic limit $L \rightarrow \infty$ for the **densities** the dependence on the boundary conditions drops out.

The β - and μ -dependence comes from the KMS-conditions on the fields, which, cf. (3.1.59), read now

$$\phi(\tau = \beta, \vec{x}) = \phi(\tau = 0, \vec{x}) \exp(-\beta\mu), \quad \phi^*(\beta, \vec{x}) = \phi^*(0, \vec{x}) \exp(\beta\mu). \quad (3.2.2)$$

Since this affects only the time argument of the fields we need to discretise only this variable to keep track of the right normalisation factors of the Gaussian path integrals³. We substitute $t = -i\tau$ in (3.2.1) and divide the τ -interval $(0, \beta)$ in n equidistant parts. With $\epsilon = \beta/n$ the τ -discretised version reads:

$$\begin{aligned} Z_0(\beta, \mu) = N \lim_{n \rightarrow \infty} \int \mathcal{D}\phi_k^* \mathcal{D}\phi_k \int \mathcal{D}\Pi_k^* \mathcal{D}\Pi_k \\ \exp \left[-\epsilon \sum_{k=1}^n \int d^3\vec{x} \left(\Pi_k^* \Pi_k + (\nabla\phi_k^*)(\nabla\phi_k) + m^2\phi_k^* \phi_k \right. \right. \\ \left. \left. - i\Pi_k \frac{\phi_k - \phi_{k-1}}{\epsilon} - i\Pi_k^* \frac{\phi_k^* - \phi_{k-1}^*}{\epsilon} \right) \right], \end{aligned} \quad (3.2.3)$$

where we write Z_0 for the partition sum of the ideal gas, N denoting the indefinite β - and μ -independent overall normalisation factor. We write ϕ_k for $\phi(k\epsilon, \vec{x})$ etc. The periodic KMS boundary conditions (3.2.2) are realized by

$$\phi_n = \phi_0 \exp(-\beta\mu), \quad \phi_n^* = \phi_0^* \exp(+\beta\mu). \quad (3.2.4)$$

Next we evaluate the integral over the canonical field momenta,

$$\begin{aligned} Z_0(\beta, \mu) = N' \lim_{n \rightarrow \infty} \frac{1}{\epsilon^n} \int_{\text{KMS}} \mathcal{D}\phi_k^* \mathcal{D}\phi_k \\ \times \exp \left[-\epsilon \sum_{k=1}^n \int d^3\vec{x} \frac{|\phi_k - \phi_{k-1}|^2}{\epsilon^2} + m^2\phi_k^* \phi_k + (\nabla\phi_k^*)(\nabla\phi_k) \right], \end{aligned} \quad (3.2.5)$$

where N' is an indefinite factor that is *independent of β and μ* . In the continuum limit this goes of course over to the Lagrangian version of the path integral but with the special normalisation of the path integral contained in ϵ , which uniquely determines the β and μ dependence. If we define this continuum limit we can include the correct normalization factor of the discretised form (3.2.4) in the path integral measure $\tilde{\mathcal{D}}\phi^* \tilde{\mathcal{D}}\phi$ and write (3.2.5)

$$Z_0(\beta, \mu) = N' \int_{\text{KMS}} \tilde{\mathcal{D}}\phi^* \tilde{\mathcal{D}}\phi \exp \left[-\int_0^\beta d\tau \int d^{2\omega-1}\vec{x} \mathcal{L}_E \right] \quad (3.2.6)$$

Here we have explicitly written the time-integral in the parameterisation with the real euclidian time variable τ . The euclidian version of the free Lagrangian reads:

$$\mathcal{L}_E = (\partial_\tau \phi^*)(\partial_\tau \phi) + (\nabla\phi^*)(\nabla\phi) + m^2\phi^* \phi \quad (3.2.7)$$

which by definition is obtained from the negative Minkowski metric by substituting $x^0 \rightarrow -i\tau$. So we obtain a positive definite euclidian metric.

To calculate (3.2.6) we Fourier transform the fields to spatial momentum space but keep the time variable (this is the Mills representation). Due to our finite volume and periodic boundary conditions this reads

$$\phi(x) = \frac{1}{V} \sum_{\vec{p}} \phi(\tau, \vec{p}) \exp(i\vec{p}\vec{x}), \quad \phi^*(x) = \frac{1}{V} \sum_{\vec{p}} \phi^*(\tau, \vec{p}) \exp(-i\vec{p}\vec{x}). \quad (3.2.8)$$

³Of course also here this factor is determined only up to an indefinite constant, independent of β and μ .

Herein we have set $V = l^3$. The sums run over the momenta $\vec{p} = (2\pi/l)(n_1, n_2, n_3)$ with $n_k \in \mathbb{Z}$. In the thermodynamic limit we can substitute

$$\sum_{\vec{p}} \rightarrow \frac{V}{(2\pi)^3} \int d^3\vec{p}. \quad (3.2.9)$$

In the Mills representation the euclidian action reads

$$S_E = \int_0^\beta d\tau \frac{1}{V} \sum_{\vec{p}} [(\partial_\tau \phi^*)(\partial_\tau \phi) + \omega^2 \phi^* \phi] \quad \text{with} \quad \omega^2 = \vec{p}^2 + m^2. \quad (3.2.10)$$

Now we look for the stationary point of the action functional for fixed \vec{p}

$$S_E(\vec{p}) = \int_i^\beta d\tau [(\partial_\tau \phi^*)(\partial_\tau \phi) + \omega^2 \phi^* \phi] \quad (3.2.11)$$

with the boundary conditions given by the KMS condition of the path integral:

$$\left. \frac{\delta S_E}{\delta \phi} \right|_{\phi=\phi_{\text{cl}}} = \left. \frac{\delta S_E}{\delta \phi^*} \right|_{\phi=\phi_{\text{cl}}} = 0, \quad (3.2.12)$$

$$\phi(0, \vec{p}) = \phi_0, \quad \phi(\beta, \vec{p}) = \exp(-\beta\mu)\phi_0, \quad \phi^*(0) = \phi_0^*, \quad \phi^*(\beta) = \exp(\beta\mu)\phi_0^*.$$

The solutions of these classical imaginary-time harmonic oscillator equations are given by

$$\begin{aligned} \phi_{\text{cl}}(\tau) &= \phi_0 \left[\cosh(\omega\tau) + \frac{[\exp(-\beta\mu) - \cosh(\omega\beta)]}{\sinh(\omega\beta)} \right], \\ \phi_{\text{cl}}^*(\tau) &= \phi_0^* \left[\cosh(\omega\tau) + \frac{[\exp(\beta\mu) - \cosh(\omega\beta)]}{\sinh(\omega\beta)} \right]. \end{aligned} \quad (3.2.13)$$

Then we can write the general field within the path integral as

$$\phi = \phi_{\text{cl}} + \phi' \quad \text{with} \quad \phi'(\tau=0) = \phi'(\tau=\beta) = 0. \quad (3.2.14)$$

From the homogeneity of the boundary conditions for ϕ' we obtain immediately

$$S_E[\phi, \vec{p}] = S_E[\phi_{\text{cl}}] + S_E[\phi']. \quad (3.2.15)$$

Substitution of (3.2.13) yields

$$S_E[\phi_{\text{cl}}, \vec{p}] = 2\omega\phi_0^*\phi_0 \frac{\sinh[\beta(\mu - \omega)/2] \sinh[\beta(\mu + \omega)/2]}{\cosh(\beta\omega/2) \sinh(\beta\omega/2)} \quad (3.2.16)$$

For the partition sum we get

$$\begin{aligned} Z(\beta, \mu) &= N \prod_{\vec{p}} \int d(\phi_0^*/\sqrt{V}) d(\phi_0/\sqrt{V}) \exp[S_E[\phi_{\text{cl}}]] \times \\ &\quad \times \underbrace{\int_{\phi(\tau=0)=0}^{\phi(\tau=\beta)=0} D(\phi^*/\sqrt{V}) D(\phi/\sqrt{V}) \exp[S_E[\phi]]}_{Z_{\text{hom}}}. \end{aligned} \quad (3.2.17)$$

Here we have scaled the path-integral measure by a factor $1/V$. To calculate Z_{hom} , the partition sum for fields with homogeneous boundary conditions, we have to go back to the time-discretised version of the path integral (3.2.5) again since it depends on β , and we want to calculate the corresponding factors correctly. Due to our homogeneous boundary conditions we can write

$$S_E^{\text{lat}} = -\phi^{*t} \frac{\hat{M}}{\epsilon} \phi \quad (3.2.18)$$

where $\phi = (\phi_1, \dots, \phi_{n-1})^t$ is the momentum dependent vector at the time-lattice points. The matrix is given by

$$\hat{M} = \begin{pmatrix} 2 + \omega^2 \epsilon^2 & -1 & 0 & \dots & 0 \\ -1 & 2 + \omega^2 \epsilon^2 & -1 & \dots & 0 \\ 0 & -1 & 2 + \omega^2 \epsilon^2 & -1 & \dots \\ 0 & 0 & -1 & \dots & \ddots \end{pmatrix}. \quad (3.2.19)$$

Now we need the determinant of this matrix because of the formula

$$\int d^n z^* d^n z \exp(-az^\dagger \hat{A} z) = \frac{2\pi i}{a^n \det \hat{A}}. \quad (3.2.20)$$

For the determinant we find the recursion formula

$$D_{n-1} = \det \hat{M} = (2 + \omega^2 \epsilon^2) D_{n-2} - D_{n-3}, \quad D_0 = 1, \quad D_{-1} = 0. \quad (3.2.21)$$

It is easily solved by writing it in the form

$$\begin{pmatrix} D_n \\ D_{n-1} \end{pmatrix} = \underbrace{\begin{pmatrix} 2 \cosh u & -1 \\ 1 & 0 \end{pmatrix}}_{\hat{A}} \begin{pmatrix} D_{n-1} \\ D_{n-2} \end{pmatrix} \quad \text{with} \quad 2 \cosh u = 2 + \omega^2 \epsilon^2. \quad (3.2.22)$$

By iteration this leads to

$$\begin{pmatrix} D_n \\ D_{n-1} \end{pmatrix} = \hat{A}^n \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \quad (3.2.23)$$

We diagonalise the matrix \hat{A} and transform back to the original basis which finally gives

$$D_{n-1} = \frac{2n^2}{\omega\beta} \frac{\sinh \left[n \operatorname{arcosh} \left(1 + \frac{\omega^2}{2n^2} \right) \right]}{\sqrt{4n^2 + \omega^2 \beta^2}}. \quad (3.2.24)$$

For the continuum limit we need this expression only in leading order for large n :

$$D_{n-1} \underset{n \rightarrow \infty}{\cong} \frac{n}{\beta} \frac{\sinh(\omega\beta)}{\omega} = \frac{1}{\epsilon} \frac{\sinh(\omega\beta)}{\omega}. \quad (3.2.25)$$

Putting this into the time-lattice (3.2.5) version of (3.2.17) yields by using (3.2.25)

$$Z_{\text{hom}}(\vec{p}) = N \prod_{\vec{p}} \frac{\omega}{\sinh(\omega\beta)}. \quad (3.2.26)$$

Note, that the factor $1/\epsilon^n$ from the integration over the canonical field momenta has cancelled. The final result for (3.2.17) now reads

$$Z(\beta, \mu; \vec{p}) = N \prod_{\vec{p}} \frac{1}{\cosh(\beta\omega) - \cosh(\beta\mu)}. \quad (3.2.27)$$

To evaluate this we take the logarithm and make use of (3.2.9). Thereby we have to take care of the zero mode $\vec{p} = 0$, i.e., $\omega = m$ because due to $d^3\vec{p} = \omega\sqrt{\omega^2 - m^2} d\omega d(\cos\theta) d\phi$ it is cancelled when going over to the integral. Some algebraic manipulations finally yield

$$\begin{aligned} \Omega_\infty(\beta, \mu) = & -V \int \frac{d^3\vec{p}}{(2\pi)^3} \{ \beta\omega + \ln[1 - \exp[-\beta(\omega + \mu)]] + \ln[1 - \exp[-\beta(\omega - \mu)]] \} - \\ & - \ln[1 - \exp(-\beta(m - \mu))] - \ln[1 - \exp(-\beta(m + \mu))]. \end{aligned} \quad (3.2.28)$$

This expression is divergent, because of the term $\beta\omega$ in the integrand. Using (2.1.35) to calculate the entropy this divergent contribution cancels. Using the entropy to define the potential Ω we see, that it is cancelled by the renormalisation of the pure vacuum **zero-point energy**. Had we made use of the operator formalism this would have been cured by using the **normal ordering** for field operators. On the other hand the normal ordering becomes problematic in the context of gauge theories. The result of this procedure leads finally to

$$\begin{aligned} \Omega_0(\beta, \mu) = & -V \int \frac{d^3\vec{p}}{(2\pi)^3} \{ \ln[1 - \exp[-\beta(\omega + \mu)]] + \ln[1 - \exp[-\beta(\omega - \mu)]] \} - \\ & - \ln[1 - \exp(-\beta(m - \mu))] - \ln[1 - \exp(-\beta(m + \mu))]. \end{aligned} \quad (3.2.29)$$

Now it is easy to take the thermodynamic limit. It is clear that this expression only makes sense if $m \pm \mu > 0$, i.e., $-m < \mu < m$. For such μ we find in the thermodynamic limit, $V \rightarrow \infty$

$$\begin{aligned} \frac{1}{V} \Omega_0(\beta, \mu) \underset{V \rightarrow \infty}{\cong} & - \int \frac{d^3\vec{p}}{(2\pi)^3} \{ \ln[1 - \exp[-\beta(\omega + \mu)]] + \ln[1 - \exp[-\beta(\omega - \mu)]] \} \\ & := \frac{1}{V} \Omega_0^*(\beta, \mu). \end{aligned} \quad (3.2.30)$$

The star denotes the fact, that this is only the expression for the occupation of states different from the ground state. It is again clear, that this expression makes only sense if $|\mu| < m$. As we have seen, in this case the fraction of the particles in the ground state is as “infinitesimal” as those of any other state and the substitution of the momentum-sum by the integral is justified.

This changes if for a given temperature the charge density of the gas becomes so high, that it cannot be reached with $|\mu| < m$. Then a “macroscopic” number of particles is in the ground state, which phenomenon is known as **Bose-Einstein condensation**. Then we have to let $\mu \rightarrow \pm m$ in the thermodynamic limit. But for this limit the contribution from the zero mode in (3.2.28) diverges if it is taken for fixed V . In the integral (3.2.30) this singularity does not provide any trouble since it is integrable.

This discussion shows, that at presence of a Bose-Einstein condensate we have to take the limit $\mu \rightarrow \pm m$ together with the thermodynamic limit $V \rightarrow \infty$. For definiteness we discuss the limit $\mu \rightarrow +m$. The treatment of the “charge conjugated” state $\mu \rightarrow -m$ is analogous. At finite V we have to choose $\mu < m$ and for $\mu \rightarrow m$ the contribution of

$$\Omega_{\text{cond}}(\beta, \mu) = -\ln[1 - \exp(-\beta(m - \mu))] \quad (3.2.31)$$

cannot be neglected. Now the physical sense of this contribution is, that the fraction of the charge density in the condensate has to be fixed when taking the thermodynamic limit. For finite volume we have

$$q_{\text{cond}}(\beta, \mu) = \frac{1}{V} [\partial_{\alpha} \Omega_{\text{cond}}(\beta, \mu = \alpha/\beta)]_{\alpha=\beta\mu} = \frac{1}{V} \frac{1}{\exp[\beta(m-\mu)] - 1} \stackrel{!}{=} q_0 > 0. \quad (3.2.32)$$

This means that we have to take the thermodynamic limit by letting the volume

$$V(\beta, \mu) = \frac{1}{q_0} \frac{1}{\exp[\beta(m-\mu)] - 1} \quad (3.2.33)$$

and make $\mu \rightarrow m$. The condensate delivers a contribution to the energy and entropy density given by

$$\begin{aligned} \epsilon_0 &= \lim_{\mu \rightarrow m-0} \frac{1}{V(\beta, \mu)} [\partial_{\beta} \Omega_{\text{cond}}(\beta, \alpha/\beta)]_{\alpha=\beta\mu} = q_0 m, \\ s_0 &= \lim_{\mu \rightarrow m-0} \frac{1}{V(\beta, \mu)} T \Omega_{\text{cond}}(1/T, \mu) = 0. \end{aligned} \quad (3.2.34)$$

In this case the “particles” with positive charge quantum number build the condensate. For the other possible limit $\mu \rightarrow -m$, the condensate is built by the negatively charged “anti-particles”.

$$q_0 < 0, \quad \epsilon_0 = |q_0| m, \quad s_0 = 0. \quad (3.2.35)$$

We close this section by noting, that we can also take into account adiabatic changes of the volume V . In the thermodynamic limit all extensive quantities become proportional to the volume and thus we can write for the first fundamental law of thermodynamics

$$dU = T dS + \mu dQ - \frac{T\Omega}{V} dV. \quad (3.2.36)$$

The physical meaning of Ω is thus given by

$$\Omega = \frac{PV}{T}, \quad (3.2.37)$$

where P is the pressure of the gas.

The result for the thermodynamic quantities of the ideal Bose gas of charged particles finally summarizes as follows:

$$\begin{aligned} \Phi(T, \mu) &= VT \int \frac{d^3 \vec{p}}{(2\pi)^3} \left\{ \ln \left[1 - \exp\left(-\frac{\omega - \mu}{T}\right) \right] \right. \\ &\quad \left. + \ln \left[1 - \exp\left(-\frac{\omega + \mu}{T}\right) \right] \right\} + \Omega_{\text{cond}}(T, \mu), \end{aligned} \quad (3.2.38)$$

$$U(T, \mu) = V \int \frac{d^3 \vec{p}}{(2\pi)^3} \omega [f_{\text{B}}(\omega - \mu) + f_{\text{B}}(\omega + \mu)] + Q_0 m, \quad (3.2.39)$$

$$Q(T, \mu) = V \int \frac{d^3 \vec{p}}{(2\pi)^3} [f_{\text{B}}(\omega - \mu) - f_{\text{B}}(\omega + \mu)] + Q_0, \quad (3.2.40)$$

$$\begin{aligned} S(T, \mu) &= - \left(\frac{\partial \Phi}{\partial T} \right)_{V, T} = V \int \frac{d^3 \vec{p}}{(2\pi)^3} \left\{ [1 + f_{\text{B}}(\omega - \mu)] \ln [1 + f_{\text{B}}(\omega - \mu)] \right. \\ &\quad \left. - f_{\text{B}}(\omega - \mu) \ln f_{\text{B}}(\omega - \mu) + (\mu \rightarrow -\mu) \right\}. \end{aligned} \quad (3.2.41)$$

Here, one has to keep in mind that in the thermodynamic limit, if there is a condensate, we have to make $\mu \rightarrow m$ in the sense detailed above.

To derive the expression for the entropy we have used the identities

$$\ln[1 - \exp(-\omega'/T)] = -\frac{\omega'}{T} - \ln f_B(\omega') = -\ln[1 + f_B(\omega')]. \quad (3.2.42)$$

3.2.2 The partition sum as functional determinant and the heat-kernel method

We have seen in the previous section, that the β -dependent factor from the integration over the field momenta, can only be cancelled if one goes over to the modified path integral measure for the partition sum

$$Z(\beta, \mu) = N' \int_{\text{KMS}} \tilde{D}\phi^* \tilde{D}\phi \exp[-S_E[\phi^*, \phi]], \quad (3.2.43)$$

which is defined by the path integral's time-lattice version (3.2.5).

On the other hand, we have found a rather simple result and we now like to find an expression for the functional determinant such that we can directly use the continuum limit.

Instead of using the modified measure in (3.2.43) for the Lagrangian description of the path integral we can go back to the usual one and introduce a β -dependent indefinite normalisation constant.

We demonstrate this on the simple example of a noninteracting neutral scalar field. The introduction of a chemical potential for charged fields does not change the argument, since the indefinite factor depends only on β and not on μ . We come back to this case in the next section.

The Euclidian Lagrangian reads

$$\mathcal{L}_E = \frac{1}{2}(\partial_\mu^E \phi)(\partial_\mu^E \phi) + \frac{m^2}{2}\phi^2 \quad (3.2.44)$$

with $\phi \in \mathbb{R}$. We write the partition sum in the following form

$$Z_0(\beta) = N(\beta) \int_{\text{KMS}} D\phi \exp\left[-\int_0^\beta d\tau \int_V d^3\vec{x} \mathcal{L}_E\right]. \quad (3.2.45)$$

The KMS condition here is the simple periodic one without a chemical potential, which we cannot introduce in this case, because there is no conserved charge. Thus, we directly use the formal equation

$$\begin{aligned} \ln N(\beta) \int_{\text{KMS}} D\phi \exp\left[-\frac{1}{2} \int d^4x' \int d^4x \phi(x') D^{-1}(x, x') \phi(x)\right] &= \ln \frac{N(\beta)}{\sqrt{\text{Det} D^{-1}}} \\ &= -\frac{1}{2} \text{Tr} \ln(D^{-1}/M^2). \end{aligned} \quad (3.2.46)$$

Here M is a constant with dimension mass or energy to render the argument of the logarithm dimensionless. Further we have to read the inverse propagator as the operator

$$D^{-1} = (\square_E - m^2). \quad (3.2.47)$$

So far (3.2.46) is only a formal functional extension of the discretized Euclidean path integral, treated in Sect. 3.2.1 in the sense of a continuum limit. In the evaluation of Gaussian path integrals in their form with a discretized space-time lattice, one naturally arrives at **determinants** which arise from the

discretized version of the differential operators appearing in the Lagrangian that is quadratic in the integration-field variables. This arises from the most simple multidimensional real Gaussian integral

$$\int_{\mathbb{R}^N} d^N \vec{x} \exp\left(-\frac{1}{2} \vec{x}^t \hat{A} \vec{x}\right) = \sqrt{\frac{(2\pi)^N}{\det \hat{A}}}. \quad (3.2.48)$$

Here, \hat{A} is a positive definite symmetric matrix. The proof of this formula is simple: The matrix \hat{A} can always be diagonalized by an orthogonal transformation: $\hat{A}' = \hat{O} \hat{A} \hat{O}^t = \text{diag}(\lambda_1, \dots, \lambda_N)$ with eigenvalues $\lambda_j > 0$ for $j \in \{1, \dots, N\}$ and $\hat{O}^t = \hat{O}^{-1}$. Then introducing new integration variables $\vec{x}' = \hat{O}^t \vec{x}$, $d^N \vec{x} = |\det \hat{O}| d^N \vec{x}' = d^N \vec{x}'$ leads to

$$\int_{\mathbb{R}^N} d^N \vec{x} \exp\left(\frac{1}{2} \vec{x}^t \hat{A} \vec{x}\right) = \int_{\mathbb{R}^N} d^N \vec{x}' \exp\left(\frac{1}{2} \sum_{j=1}^N \lambda_j x_j'^2\right) = \sqrt{\frac{(2\pi)^N}{\prod_{j=1}^N \lambda_j}}. \quad (3.2.49)$$

Further $\det \hat{A}' = \prod_{j=1}^N \lambda_j = \det(\hat{O} \hat{A} \hat{O}^t) = \det \hat{A}$, so that (3.2.49) implies (3.2.48). It is clear that in this most simple case, where $\lambda_j > 0$ for all $j \in \{1, 2, \dots, N\}$ we can also write

$$\int_{\mathbb{R}^N} d^N \vec{x} \exp\left(\frac{1}{2} \vec{x}^t \hat{A} \vec{x}\right) = (2\pi)^{N/2} \exp\left(-\frac{1}{2} \sum_{j=1}^N \ln \lambda_j\right) = (2\pi)^{N/2} \exp\left(-\frac{1}{2} \text{tr} \ln \hat{A}\right). \quad (3.2.50)$$

The difficulty now arises when taking the continuum limit of the multidimensional integral. There we silently assume that the corresponding limit of the determinant exists, but in fact usually it is not convergent and we have to **regularize and renormalize** the result, implementing the definite physical meaning of the calculated quantity by specifying appropriate **renormalization conditions**.

The D'Alembert operator in (3.2.47) is to be understood in the Euclidean sense, defined in the space of real scalar functions subject to the periodic KMS-boundary condition

$$\phi(\beta, \vec{x}) = \phi(0, \vec{x}). \quad (3.2.51)$$

To give the functional trace in (3.2.46) a definite meaning, we introduce the **heat-kernel technique**, which bases on the idea to read the operator $\mathbf{H} = (-\square_E + m^2)/M^2$ as a Hamilton operator in a Hilbert space for a particle in four spatial dimensions as in usual quantum mechanics, where the wave functions in position representation fulfill the KMS-boundary condition (3.2.51). Then the Euclidean time-evolution Green's function, introducing ϑ as an additional formal time parameter reads

$$U(\vartheta; x, x') = \langle x | \exp(-\mathbf{H}\vartheta) | x' \rangle. \quad (3.2.52)$$

This leads to the definition of the **heat kernel**⁴

$$H(\vartheta) = \text{Tr} \mathbf{U} = \int_{\mathcal{V}} d^4 x U(\vartheta; x, x). \quad (3.2.54)$$

⁴The name "heat kernel" originates from the fact that the Green's function (3.2.52) obviously obeys a differential equation similar to the heat-conduction equation in four spatial dimensions with ϑ as the time variable:

$$\partial_\vartheta U(\vartheta; x, x') = -\langle x | \exp(-\mathbf{H}\vartheta) \mathbf{H} | x' \rangle = \frac{\Delta_{E,x} - m^2}{M^2} U(\vartheta; x, x'). \quad (3.2.53)$$

Then formally we have

$$\tilde{H}(\alpha) = \int_0^\infty d\vartheta \vartheta^{-1+\alpha} H(\vartheta) = \Gamma(\alpha) \int_{\mathcal{V}} d^4x \langle x | \mathbf{H}^{-\alpha} | x \rangle. \quad (3.2.55)$$

Usually, for a positive definite Hermitian operator \mathbf{H} , the integral is convergent for $\alpha > 0$, but the right-hand side can be read as the analytic continuation to the whole complex α -plane except the simple poles of the Γ function at $\alpha \in \{0, -1, -2, \dots\}$.

For our case of evaluating functional determinants, we use the Laurent expansion of (3.2.55) around the pole at $\alpha = 0$. This gives

$$\tilde{H}(\alpha) = \beta V \left(\frac{1}{\alpha} - \gamma_E \right) - \int_{\mathcal{V}} d^4x \langle x | \ln \mathbf{H} | x \rangle + \mathcal{O}(\alpha) \quad (3.2.56)$$

with the Euler-Mascheroni constant $\gamma_E \approx 0.577$. We have used the regularization of the integration of the spatial part of x as to be restricted to a large but finite spatial volume, V . Thus, up to divergent constants, the $\tilde{H}(\alpha)$ gives the desired functional trace of $\ln \mathbf{H}$ as needed in (3.2.46).

For our case of a free scalar gas we can simply insert the “momentum eigenstates” to evaluate the proper-time-evolution propagator (3.2.52):

$$\begin{aligned} U(\vartheta; x, x') &= \langle x | \exp(-\vartheta \mathbf{H}) | x' \rangle = T \sum_{\omega_n} \int_{\mathbb{R}^3} d^4p \langle x | \exp(-\vartheta \mathbf{H}) | p \rangle \langle p | x' \rangle \\ &= T \sum_{\omega_n} \int_{\mathbb{R}^3} \frac{d^3 \vec{p}}{(2\pi)^3} \exp \left[-\frac{p_E^2 + m^2}{M^2} \vartheta \right] \exp[-i p_E \cdot (x - x')_E]. \end{aligned} \quad (3.2.57)$$

Here we have used that our “Hamiltonian” reads

$$\mathbf{H} = \frac{\mathbf{p}_E^2 + m^2}{M^2} \quad \text{with} \quad p^0 = \omega_n = 2\pi nT, \quad n \in \mathbb{Z}. \quad (3.2.58)$$

The p^0 component runs over the Bose-Matsubara frequencies due to the corresponding periodic KMS boundary conditions, while the spatial components are defined on \mathbb{R}^3 .

The heat kernel (3.2.54) is easily evaluated since

$$U(\vartheta; x, x) = T \sum_{\omega_n} \int_{\mathbb{R}^3} \frac{d^3 \vec{p}}{(2\pi)^3} \exp \left[-\frac{p_E^2 + m^2}{M^2} \vartheta \right] = \frac{T M^3}{8\pi^{3/2} \vartheta^{3/2}} \sum_{\omega_n} \exp \left(-\vartheta \frac{\omega_n^2 + m^2}{M^2} \right), \quad (3.2.59)$$

which is independent of x because of the translation invariance of the equilibrium state. The space-time integral thus becomes a trivial factor $\beta V = V/T$ (regularized again in the sense of the finite-volume result in the thermodynamic limit), and the heat kernel thus reads

$$\tilde{H}(\alpha) = \frac{M^3 V}{8\pi^{3/2}} \sum_{\omega_n} \left(\frac{m^2 + \omega_n^2}{M^2} \right)^{3/2-\alpha} \Gamma \left(-\frac{3}{2} + \alpha \right). \quad (3.2.60)$$

To evaluate the sum over the Matsubara frequencies we use (B.1.7) with

$$b(z) = \left(\frac{m^2 - z^2}{M^2} \right)^\epsilon = \exp \left[\epsilon \ln \left(\frac{m^2 - z^2}{M^2} \right) \right] \quad \text{with} \quad \epsilon = \frac{3}{2} - \alpha. \quad (3.2.61)$$

Here the power has to be understood as defined by the principal value for the logarithm, defined to be positive real for $m^2 - z^2 > 0$. Now it is more convenient to use the summation formula in the form (B.1.6), for which we need

$$b(p_0 + i0^+) - b(p_0 - i0^+) = -2i \left(\frac{p_0^2 - m^2}{M^2} \right)^\epsilon \sin[\pi \epsilon \operatorname{sign} p_0] \Theta(p_0^2 - m^2). \quad (3.2.62)$$

Since the integrand in (B.1.7) is symmetric we finally get

$$\tilde{H}(\alpha) = -\frac{V\beta M^3}{8\pi^{5/2}} \sin\left[\pi\left(\frac{3}{2} - \alpha\right)\right] \Gamma\left(-\frac{3}{2} + \alpha\right) \int_m^\infty dp_0 [1 + 2f_B(p_0)] \left(\frac{p_0^2 - m^2}{M^2}\right)^{3/2-\alpha}. \quad (3.2.63)$$

Now, the part including the Bose-distribution function is finite for $\alpha \rightarrow 0$ and thus we get

$$\operatorname{Tr} \ln \left(\frac{-\square_E + m^2}{M^2} \right)_T = -\frac{\beta V}{3\pi^2} \int_m^\infty dp_0 (p_0^2 - m^2)^{3/2} f_B(p_0). \quad (3.2.64)$$

For the “vacuum part” of (3.2.63) we have to keep $\alpha > 5/2$ in order get a convergent integral over p_0 :

$$\begin{aligned} \tilde{H}_{\text{vac}}(\alpha) &= -\frac{V\beta M^3}{16\pi^{5/2}} \sin\left[\pi\left(\frac{3}{2} - \alpha\right)\right] \Gamma\left(-\frac{3}{2} + \alpha\right) \int_m^\infty dp_0 \left(\frac{p_0^2 - m^2}{M^2}\right)^{3/2-\alpha} \\ &= -\frac{\beta V m^4}{32\pi^3} \sin\left[\pi\left(\frac{3}{2} - \alpha\right)\right] \left(\frac{M}{m}\right)^{2\alpha} \Gamma\left(\frac{5}{2} - \alpha\right) \Gamma\left(-\frac{3}{2} + \alpha\right) \Gamma(-2 + \alpha) \\ &= \frac{\beta V m^4}{64\pi^2} \left[\frac{2}{\alpha} + 3 - 2\gamma_E - 2 \ln\left(\frac{m^2}{M^2}\right) \right] + \mathcal{O}(\alpha). \end{aligned} \quad (3.2.65)$$

In the last step we have used the Laurent expansion around $\alpha = 0$, thus arriving at the desired analytic continuation. Finally we obtain for the **renormalized** grand-canonical potential

$$\Phi_{\text{vac,ren}} = \frac{T}{2} \operatorname{Tr} \ln \left(\frac{D^{-1}}{M^2} \right) \Big|_{T \rightarrow 0} = \frac{V m^4}{128\pi^2} \left[A + 2 \ln\left(\frac{m^2}{M^2}\right) \right], \quad (3.2.66)$$

where A is an arbitrary **temperature-independent constant**, which is physically irrelevant since an additive temperature-independent constant has the meaning of the vacuum contribution to the total energy and is thus unobservable within special relativity. This of course is also true for the logarithmic term in (3.2.66).

The part of (3.2.63) which contains the Bose distribution is finite for $\alpha = 0$ and needs no renormalization, and this is the only contribution to the grand-canonical potential that is relevant as a thermodynamic quantity. To see that this contribution,

$$\Phi_{\text{therm}} = -\frac{V}{6\pi^2} \int_m^\infty dp_0 (p_0^2 - m^2)^{3/2} f_B(p_0), \quad (3.2.67)$$

coincides with half of (3.2.38) for $\mu = 0$ and $\Omega_{\text{cond}} = 0$ we note that through integration by parts, using

$$f_B(p_0) = T \partial_{p_0} \ln[1 - \exp(-\beta p_0)], \quad (3.2.68)$$

we find

$$\Phi_{\text{therm}} = \frac{TV}{2\pi^2} \int_m^\infty dp_0 p_0 \sqrt{p_0^2 - m^2} \ln[1 - \exp(-\beta p_0)]. \quad (3.2.69)$$

This can of course be rewritten in terms of $|\vec{p}| = \sqrt{p_0^2 - m^2}$ and using $d^3\vec{p} = 4\pi d|\vec{p}|p^2$ for functions depending only on $|\vec{p}|$ but not on the angles of spherical coordinates:

$$\Phi_{\text{therm}} = TV \int_{\mathbb{R}^3} \frac{d^3\vec{p}}{(2\pi)^3} \ln[1 - \exp(-\beta\omega)] \quad \text{with} \quad \omega = \sqrt{\vec{p}^2 + m^2}. \quad (3.2.70)$$

This is indeed of the form (3.2.38) since

$$\Omega_{\text{therm}} = -\beta\Phi_{\text{therm}} = -V \int_{\mathbb{R}^3} \frac{d^3\vec{p}}{(2\pi)^3} \ln[1 - \exp(-\beta\omega)]. \quad (3.2.71)$$

The internal energy is given by

$$U_{\text{ren}} = -\frac{\partial\Omega_{\text{ren}}}{\partial\beta} = V \int_{\mathbb{R}^3} \frac{d^3\vec{p}}{(2\pi)^3} \omega f_{\text{B}}(\omega). \quad (3.2.72)$$

3.2.3 Functional treatment of Bose-Einstein condensation

Another application for the functional methods worked out so far is an alternative treatment of the Bose-Einstein condensation, which we have already found in Sect. 3.2. Here we follow [Kap81, KG06] with the simplification of implementing the chemical potential as a boundary (KMS) condition in the path integral rather than using the “grand-canonical Hamiltonian” $\mathbf{K} = \mathbf{H} - \mu\mathbf{Q}$, where \mathbf{Q} is the operator of the conserved charge from the U(1) symmetry of the charged boson field. Again we start from the Lagrangian of a free charged scalar field,

$$\mathcal{L} = (\partial_\mu\phi^*)(\partial^\mu\phi) - m^2\phi^*\phi. \quad (3.2.73)$$

The great simplification of our method to implement the chemical potential as a boundary condition in the path integral compared to the method with the introduction of the “grand-canonical Hamiltonian” and using the $\mu = 0$ -KMS condition (see [Kap81, KG06]) is that we can use the naive Lagrangian version path integral, as has been shown in great detail in Sect. 3.2.1.

Since we are interested in the grand-canonical potential only, we calculate only the partition sum using the vertical part of the contour only. As in the previous section we have

$$Z = \int_{\text{KMS}} D\phi D\phi^* \exp[-S_{\text{E}}[\phi, \phi^*]] \quad (3.2.74)$$

with

$$S_{\text{E}}[\phi, \phi^*] = \int_0^\beta d\tau \int_{\mathbb{R}^3} d^3\vec{x} [(\partial_\mu^{\text{E}}\phi^*)(\partial_\mu^{\text{E}}\phi) + m^2\phi^*\phi]. \quad (3.2.75)$$

The main difference is in the KMS-boundary conditions for the fields, which according to (3.1.26) read

$$\phi(\tau = \beta, \vec{x}) = \exp(-\beta\mu)\phi(0, \vec{x}), \quad \phi^*(\tau = \beta, \vec{x}) = \exp(-\beta\mu)\phi^*(0, \vec{x}). \quad (3.2.76)$$

Now we expand the action functional (3.2.75) around a stationary point, i.e., a classical solution φ of the imaginary-time solutions

$$(-\square_{\text{E}} + m^2)\varphi = (-\square_{\text{E}} + m^2)\varphi^* = 0. \quad (3.2.77)$$

which of course also have to fulfill the boundary conditions (3.2.76). Since we consider thermal equilibrium, we are only interested in spatially homogeneous solutions of this kind, i.e.,

$$\partial_\tau^2 \varphi(\tau) = m^2 \varphi, \quad \partial_\tau^2 \varphi^*(\tau) = m^2 \varphi^*, \quad (3.2.78)$$

The solutions, fulfilling the KMS conditions (3.2.76) are obviously

$$\begin{aligned} \varphi(\tau) &= \begin{cases} \varphi_0 \exp(-\mu\tau) & \text{if } \mu = m, \\ 0 & \text{otherwise} \end{cases} \\ \varphi^*(\tau) &= \begin{cases} \varphi_0^* \exp(\mu\tau) & \text{if } \mu = m, \\ 0 & \text{otherwise.} \end{cases} \end{aligned} \quad (3.2.79)$$

As we shall see, in the first case we have **Bose-Einstein condensation** as explained in Sect. 3.2.1. Without loss of generality we can choose $\varphi_0 = \varphi_0^* \in \mathbb{R}$, because otherwise we can redefine the phase of the field with an appropriate phase factor, which is physically irrelevant due to the invariance of the action with respect to such phase redefinitions, which are the group theoretical reason for the conservation of the charge according to Noether's theorem. The value φ_0 of the “condensate” has to be seen as an external parameter in the grand-canonical potential. Its value is determined by the equilibrium condition that this potential has to take a minimum under variation of such external parameters, while the thermodynamic variables, V , T , and μ are kept fixed. So we have to evaluate the partition sum, before we can find this value. Writing

$$\phi = \varphi + \phi', \quad \phi^* = \varphi^* + \phi'^* \quad (3.2.80)$$

and using the invariance of the path-integral measure under field translations we arrive at

$$\begin{aligned} Z &= \int_{\text{KMS}} \mathcal{D}\phi' \mathcal{D}\phi'^* \exp[-S_E[\varphi + \phi', \varphi_0^* + \phi'^*]] \\ &= \exp[\beta V(\mu^2 - m^2)\varphi_0^2] \int_{\text{KMS}} \mathcal{D}\phi' \mathcal{D}\phi'^* \exp(-S_E[\phi', \phi'^*]) \\ &= \exp[\beta V(\mu^2 - m^2)\varphi_0^2] \left[\det \left(\frac{-\square_E + m^2}{M^2} \right) \right]^{-1}. \end{aligned} \quad (3.2.81)$$

Note that this is not a contradiction since, of course, the path integral is independent of the labeling of the integration-field variables. We only have used the simplification that we have defined φ to be a spatially homogeneous solution of the classical Euclidean equations of motion. According to (3.2.79) $(m^2 - \mu^2)\varphi_0^2 = 0$ for this solution. This is equivalent to the stationarity of the grand canonical potential

$$\Phi = -T \ln Z = V(m^2 - \mu^2)\varphi_0^2 + \Phi'. \quad (3.2.82)$$

Since Φ' is independent of φ_0 , for $|\mu| < m$, we must have $\varphi_0 = 0$ in order to minimize Φ with respect to variations of φ_0 . For $\mu = m$ the value of φ_0 is indetermined from the stationarity condition of Φ , and we have Bose-Einstein condensation as we already know from the discussion in Sect. 3.2.1. To derive this result within our functional scheme, we first have to evaluate

$$\Phi' = T \text{Tr} \ln \left(\frac{-\square_E + m^2}{M^2} \right). \quad (3.2.83)$$

For the evaluation of the functional trace we use the very same heat-kernel regularization as in the previous section. The calculation evolves in the same way as there. The only difference is that we have

to take care of the changed KMS boundary conditions for the field. Here the Fourier expansion reads

$$\phi' = T \sum_{\omega_n} \int_{\mathbb{R}^3} \frac{d^3 \vec{p}}{(2\pi)^3} \tilde{\phi}(p) \exp[-i(\omega_n - i\mu)\tau] \exp(i\vec{p} \cdot \vec{x}). \quad (3.2.84)$$

Thus our calculation of the heat kernel for the uncharged scalar bosons of the previous Section can directly be used. The only change is that we have to substitute $\omega_n \rightarrow \omega_n - i\mu$ in (3.2.60):

$$\tilde{H}(\alpha) = \frac{M^3 V}{8\pi^{3/2}} \Gamma\left(-\frac{3}{2} + \alpha\right) \sum_{\omega_n} \left(\frac{m^2 + (\omega_n - i\mu)^2}{M^2} \right)^{3/2 - \alpha}. \quad (3.2.85)$$

The function to be used for the evaluation of the Matsubara sum with help of (B.1.7) thus now reads

$$h(p_0) = \left(\frac{m^2 - (p_0 + \mu)^2}{M^2} \right)^\epsilon = \exp\left[\epsilon \ln\left(\frac{m^2 - (p_0 + \mu)^2}{M^2} \right) \right] \quad \text{with} \quad \epsilon = \frac{3}{2} - \alpha. \quad (3.2.86)$$

We use again (B.1.6). The only difference in our evaluation compared to the one for the neutral scalar particles is that the integral is no longer symmetric with respect to p_0 . So we have two contributions from the branch cut of the logarithm in (3.2.87). The first one along the positive real axis is due to the particle contributions and reads after some algebra

$$\begin{aligned} \tilde{H}_+(\alpha) &= \frac{M^3 \beta V}{16\pi^{3/2}} \Gamma(-\epsilon) \int_{m-\mu}^{\infty} \frac{dp_0}{2\pi i} [1 + 2f_B(p_0)] [h(p_0 + i0^+) - h(p_0 - i0^+)] \\ &= -\frac{M^3 \beta V}{16\pi^{5/2}} \sin(\pi\epsilon) \Gamma(-\epsilon) \int_m^{\infty} dp_0 [1 + 2f_B(p_0 - \mu)] \left(\frac{p_0^2 - m^2}{M^2} \right)^\epsilon. \end{aligned} \quad (3.2.87)$$

The contribution along the negative real axis comes from the antiparticles and is given by

$$\tilde{H}_-(\alpha) = -\frac{M^3 \beta V}{16\pi^{5/2}} \sin(\pi\epsilon) \Gamma(-\epsilon) \int_m^{\infty} dp_0 [1 + 2f_B(p_0 + \mu)] \left(\frac{p_0^2 - m^2}{M^2} \right)^\epsilon \quad (3.2.88)$$

Again, the contributions from the integrals (3.2.87) and (3.2.88) that do not involve Bose-distribution factors are divergent and independent of T and μ , i.e., vacuum contributions that are regularized by the heat-kernel method. They can be treated as above for the neutral scalar bosons, leading to the same result,

$$\begin{aligned} \tilde{H}_{\text{vac}}(\alpha) &= -\frac{V \beta M^3}{8\pi^{5/2}} \sin\left[\pi\left(\frac{3}{2} - \alpha\right)\right] \Gamma\left(-\frac{3}{2} + \alpha\right) \int_m^{\infty} dp_0 \left(\frac{p_0^2 - m^2}{M^2} \right)^{3/2 - \alpha} \\ &= \frac{\beta V m^4}{64\pi^2} \left[\frac{2}{\alpha} + 3 - 2\gamma_E - 2\ln\left(\frac{m^2}{M^2}\right) \right] + \mathcal{O}(\alpha), \end{aligned} \quad (3.2.89)$$

where A is an arbitrary **temperature-independent constant**, which is physically irrelevant since an additive temperature-independent constant has the meaning of the vacuum contribution to the total energy and is thus unobservable within special relativity. This of course is also true for the logarithmic term.

For the finite part we can set $\alpha = 0$ in (3.2.87) and (3.2.88) to get

$$\tilde{H}_{\text{therm}}(0) = \frac{\beta V}{6\pi^2} \int_m^{\infty} dp_0 (p_0^2 - m^2)^{3/2} [f_B(p_0 - \mu) + f_B(p_0 + \mu)]. \quad (3.2.90)$$

First of all we note that this equation makes only sense for $|\mu| \leq m$. Then we find

$$\begin{aligned}
 \Phi_{\text{therm}} &= -T \ln Z = (m^2 - \mu^2) \varphi_0^2 V - T \tilde{H}_T(0) \\
 &= (m^2 - \mu^2) \varphi_0^2 V - \frac{V}{6\pi^2} \int_m^\infty dp_0 (p_0^2 - m^2)^{3/2} [f_B(p_0 - \mu) + f_B(p_0 + \mu)] \\
 &= (m^2 - \mu^2) \varphi_0^2 V + TV \int_{\mathbb{R}^3} \frac{d^3 \vec{p}}{(2\pi)^3} \ln \left[1 - \exp\left(-\frac{\omega - \mu}{T}\right) \right] \\
 &\quad + TV \int_{\mathbb{R}^3} \frac{d^3 \vec{p}}{(2\pi)^3} \ln \left[1 - \exp\left(-\frac{p_0 + \mu}{T}\right) \right],
 \end{aligned} \tag{3.2.91}$$

where in the last step we have integrated by parts, using

$$f_B(p_0 \pm \mu) = T \frac{\partial}{\partial p_0} \ln \left[1 - \exp\left(-\frac{p_0 \pm \mu}{T}\right) \right]. \tag{3.2.92}$$

We also have substituted $p_0 = \sqrt{P^2 + m^2} = \omega$ and $d^3 \vec{p} = 4\pi dP P^2 = 4\pi dp_0 p_0 \sqrt{p_0^2 - m^2}$ for integrands that depend only on P but not the angles in polar coordinates for \vec{p} .

As stressed above, in (3.2.91) we first interpret φ_0 as a parameter, to be chosen such that $\Phi_{\text{ren}} = \min$ for fixed thermodynamic variables, V , T , and μ . For $|\mu| < m$, we have to set $\varphi_0 = 0$ in order to minimize Φ_{ren} . For $|\mu| = m$ this criterion does not determine φ_0 since then it does not appear in (3.2.91) anymore, and Φ_{ren} does not change under variations of φ_0 . To make sense of this we evaluate the **net charge**, which according to (2.1.39) is given by

$$\begin{aligned}
 \langle Q \rangle &= - \left(\frac{\partial \Phi}{\partial \mu} \right)_{T,V} \\
 &= 2\mu \varphi_0^2 V + V \int_{\mathbb{R}^3} \frac{d^3 \vec{p}}{(2\pi)^3} [f_B(p_0 - \mu) - f_B(p_0 + \mu)] \\
 &:= \langle Q \rangle_{\text{cond}} + \langle Q \rangle_{\text{exc}}.
 \end{aligned} \tag{3.2.93}$$

Now the relation of φ_0 to **Bose-Einstein condensation** becomes clear: Let us discuss the case $\langle Q \rangle > 0$, i.e., $0 \leq \mu \leq m$. The integral part $\langle Q \rangle_{\text{exc}}$ is monotonously rising with T at fixed μ and with μ at fixed T . So if for some T we have $\langle Q \rangle_{\text{exc}} < \langle Q \rangle$ even for $\mu = m$, then we have to set $\mu = m$, and φ_0 is determined by

$$\varphi_0^2 = \frac{\langle Q \rangle - \langle Q \rangle_{\text{exc}, T, \mu=m}}{2mV} = \frac{Q_{\text{cond}}}{2mV} > 0. \tag{3.2.94}$$

Otherwise, i.e., if for the given T the integral contribution $\langle Q \rangle_{\text{exc}} > \langle Q \rangle \geq 0$ we have to choose $0 \leq \mu < m$ and then necessarily $\varphi_0 = 0$ in order to minimize Φ_{ren} . For $\langle Q \rangle < 0$ the same arguments go through with $\mu = -m$ and

$$\varphi_0^2 = -\frac{Q_{\text{cond}}}{2mV} > 0. \tag{3.2.95}$$

To find the mean total energy we rather go back to (2.1.26) using

$$\Omega(\beta, \alpha) = \ln Z = -\beta \Phi(T = 1/\beta, \mu = \alpha/\beta). \tag{3.2.96}$$

Taking the derivative and then setting $(\mu^2 - m^2) \varphi_0^2 = 0$, which holds for situations with or without a condensate, we obtain

$$U = - \left(\frac{\partial \Omega}{\partial \beta} \right)_{V, \alpha} = 2\mu^2 \varphi_0^2 V + V \int_{\mathbb{R}^3} \frac{d^3 \vec{p}}{(2\pi)^3} \omega [f_B(\omega - \mu) + f_B(\omega + \mu)]. \tag{3.2.97}$$

For $|\mu| < m$ we have to set $\varphi_0 = 0$, and the condensate contribution vanishes as it must be. For $|\mu| = m$, according to (3.2.94) we have a contribution $U_{\text{cond}} = |Q_{\text{cond}}|m$ to the total energy. This again shows the particle nature of the condensate: Each particle in the condensate is at rest, i.e., its momentum vanishes, and thus contributes with its rest energy $E(\vec{p} = 0) = m$ to the total energy of the system.

For $T \rightarrow 0^+$, all particles (or antiparticles) are in the condensate, forming a coherent state with a macroscopic mean particle number all occupying the same single-particle momentum eigenstate for $\vec{p} = 0$.

3.3 Interacting field theory

In this section, we shall derive the perturbative expansion for Green's functions with help of the path integral. Of course, we will find the same results as in Sect. 2.2, but from a different perspective and with some calculational advances.

3.3.1 Generating functionals

In this section we restrict ourselves to one of the most simple interacting quantum field theories, namely ϕ^4 -theory of a neutral scalar field. All the techniques developed on hand of this example can be easily generalized to more realistic cases. We postpone the treatment of interacting gauge theories to the next chapter, where we shall treat quantum electrodynamics at finite temperature and also nonabelian gauge theories. We follow [Wei96, Hee02], where the same ideas are developed for the S -matrix theory of vacuum quantum-field theory. All arguments are easily generalized to the many-body path integrals for equilibrium theory since the only difference are the boundary conditions for the integration over the fields, i.e., instead of homogeneous boundary conditions in the vacuum theory we have to use the KMS conditions (3.2.2). We also can start with the Lagrangian form of the path integral since there are no derivative couplings. We shall also use the naive path-integral, keeping in mind the prescription of the relevant β dependence of the normalization factor, derived using the lattice version of the path integral in Sect. 3.2.1.

The Lagrangian for ϕ^4 theory reads

$$\mathcal{L} = \frac{1}{2}(\partial_\mu \phi)(\partial^\mu \phi) - \frac{m^2}{2}\phi^2 - \frac{\lambda}{4!}\phi^4. \quad (3.3.1)$$

For the following it is convenient to explicitly reintroduce Planck's elementary action \hbar (we still use units with $c = 1$). Then the generating functional for Green's functions (3.1.32) is given by

$$Z[j] = N(\beta) \int_{\text{KMS}} \mathcal{D}\phi \exp \left[\frac{i}{\hbar} (S[\phi] + \{j_1 \phi_1\}_1) \right]. \quad (3.3.2)$$

This is the generating functional for Green's functions in the sense that

$$iG_{\mathcal{G}}^{(n)}(x_1, \dots, x_n) = \langle \mathcal{T}_{\mathcal{G}} \phi(x_1) \cdots \phi(x_n) \rangle = \frac{\hbar^n}{i^n Z[j=0]} \frac{\delta^n Z[j]}{\delta j(x_1) \cdots \delta j(x_n)} \Big|_{j=0}. \quad (3.3.3)$$

For the following it is also convenient to introduce Green's functions where the external source, j , is kept:

$$iG_{\mathcal{G}}^{(n)}(x_1, \dots, x_n) = \frac{\hbar^n}{i^n Z[j]} \frac{\delta^n Z[j]}{\delta j(x_1) \cdots \delta j(x_n)}. \quad (3.3.4)$$

In terms of Feynman diagrams for contour Green's functions these are all diagrams with connected and disconnected parts, but each connected part of any diagram is attached to at least one external point, because the factor $1/Z(j)$ cancels all closed diagrams, which factor out any derivative. This we shall prove with help of the path-integral formalism in a moment.

It is also immediately clear that we can define a generating functional for **connected Green's functions** by writing $Z[j]$ in terms of the products of connected diagrams. We arrange the corresponding sum by the number N of connected parts, including a formal contribution with $N = 0$ standing simply for 1. Now we only want to count each topology of connected parts once. Suppose the j^{th} connected diagram out of the N connected parts contains n_j vertices. From the expansion of the exponential in the interaction-picture time-evolution operator of the states, leading to the Dyson series (2.2.106) we get a factor $1/(n_1 + \dots + n_N)!$. Then there is a compensating factor $(n_1 + \dots + n_N)!$ from the permutations of all vertices, but we have to count all permutations that just describe the interchange the vertices of among the N connected components only once, giving a factor $1/N!$. So, if $iW[j]/\hbar$ is the sum of all connected diagrams, all diagrams of $Z[j]$ is given by

$$Z[j] = \sum_{N=0}^{\infty} \frac{1}{N!} (iW[j]/\hbar)^N = \exp\left(\frac{i}{\hbar} W[j]\right). \quad (3.3.5)$$

We have introduced the factor \hbar for convenience of power counting, as we shall see in a moment. The generating functional for **connected Green's functions** is given by

$$W[j] = -i \ln Z[j]. \quad (3.3.6)$$

For an inductive proof on the level of the Green's functions themselves, see [Hee02].

3.3.2 Loop expansion and effective action

Our next goal is the derivation of the Dyson-Wick series for the generating functional. To that end we split the action in a “free and an interaction part”,

$$\mathcal{L}_0 = \frac{1}{2} (\partial_\mu \phi)(\partial^\mu \phi) - \frac{m^2}{2} \phi^2, \quad \mathcal{L}_1 = \frac{M^2 - m^2}{2} \phi^2 - \frac{\lambda}{4!} \phi^4. \quad (3.3.7)$$

The perturbative expansion is formally in powers of the interaction part of the Lagrangian. Another useful expansion scheme is the expansion as a formal series in powers of \hbar rather than powers of λ . As we shall see, this is particularly convenient within the path-integral approach since it can be done as a formal **saddle-point expansion**. To that end we first define the generating functional for **free Green's functions** by

$$Z_0[j] = N \int_{\text{KMS}} D\phi \exp\left[\frac{i}{\hbar} \int_{\mathcal{C}} d^4x [\mathcal{L}_0(x) + j(x)\phi(x)]\right]. \quad (3.3.8)$$

Here N is a j -independent normalization factor, which does not play any physics relevant role. Now we define the field φ as the stationary point of the action, including the external source, j :

$$-(\square + M^2)\varphi = -j \Rightarrow \varphi(x) = - \int_{\mathcal{C}} d^4x' \Delta_{\mathcal{C}}(x, x') j(x'). \quad (3.3.9)$$

Now we expand the classical action around this solution, after some algebra leading to

$$\begin{aligned} S_0[\varphi + \phi', j] &= \int_{\mathcal{C}} d^4x \left[-\frac{1}{2} j(x)\varphi(x) + \frac{1}{2} (\partial_\mu \phi')(\partial^\mu \phi') - \frac{M^2}{2} \phi'^2 \right] \\ &= -\frac{1}{2} \int_{\mathcal{C}} d^4x \int_{\mathcal{C}} d^4x' \Delta_{\mathcal{C}}(x, x') j(x) j(x') + S_0[\phi']. \end{aligned} \quad (3.3.10)$$

Due to the translation invariance of the path-integral measure, $D\phi = D(\phi + \phi') = D\phi'$, we thus find

$$Z_0[j] = \exp \left[-\frac{i}{2\hbar} \int_{\mathcal{C}} d^4x \int_{\mathcal{C}} d^4x' \Delta_{\mathcal{C}}(x, x') j(x) j(x') \right] N \int_{\text{KMS}} D\phi' \exp \left(\frac{i}{\hbar} S_0[\phi'] \right). \quad (3.3.11)$$

This leads to

$$Z_0[j] = Z_0(M) \exp \left[-\frac{i}{2\hbar} \int_{\mathcal{C}} d^4x \int_{\mathcal{C}} d^4x' \Delta_{\mathcal{C}}(x, x') j(x) j(x') \right], \quad (3.3.12)$$

where $Z_0(M)$ is the partition sum for a free Bose gas for uncharged scalar particles with mass M , which is determined up to divergent factor from due to the “vacuum energy”, which is physically irrelevant. We have calculated it in Sect. 3.2.2 with help of the heat-kernel method. For our purpose to derive the perturbative expansion, i.e., the Feynman rules, the only relevant notion is that up to this factor, indeed $Z_0[j]$ is indeed identical with the result (2.2.49) obtained in a much more involved way in Sect. 2.2.3 within the operator formalism. The derivation of the Feynman rules has been given already there. For now we just need the full generating functional for Green’s functions in terms of this formal expansion. It is given by (2.2.106), taking care of the \hbar factors,

$$Z[j] = \exp \left(-\frac{i\lambda}{\hbar} \int_{\mathcal{C}} d^4x \hbar^4 \frac{\delta^4}{\delta j(x)^4} \right) Z_0[j]. \quad (3.3.13)$$

This means that in the Feynman diagrams each vertex point contributes effectively a factor \hbar^{-1} and each internal or external line a factor $\hbar \Delta_{\mathcal{C}}$, because each vertex is represented by four derivatives with respect to j and thus involves two factors $\propto \Delta_{\mathcal{C}}/\hbar$. Together with \hbar^4 this makes two propagator and an \hbar^2 factor. Each diagram (connected or disconnected) thus is of $\mathcal{O}(\hbar^{I-V})$. Now for a connected closed diagram (including those containing the external sources, j) in the momentum-space version one has I momenta running in internal lines, but at each vertex (including the one-point vertex standing for an external source) there is momentum conservation, and the total momentum flux is 0, thus one has $V - 1$ constraints on the momenta, and thus there are $L = I - V + 1$ loops in a connected diagram. Thus any connected diagram, contributing to $iW[j]/\hbar$ is of order $\mathcal{O}(\hbar^{L-1})$. Particularly the connected diagrams with no loops, i.e., the **tree-level diagrams** are of order $\mathcal{O}(1/\hbar)$, providing the leading-order $\mathcal{O}(1)$ of the \hbar expansion of W .

Next we can give a very elegant functional derivation for the **effective action**, which is defined as the **generating functional for one-particle irreducible diagrams** [Col85, Wei96]. In diagrammatic language each connected diagram, contributing to a connected n -point Green’s function, can be built using truncated diagrams (i.e., diagrams stripped off their external legs) that do not become disconnected by cutting just one of the remaining (necessarily internal) line, i.e., the **amputated 1PI diagrams**, which define the **proper vertex functions**, connected with *exact* propagators as internal lines and as external lines redressing the amputated external lines. In other words, we can express each connected Green’s function as formal tree-level diagrams, using the proper vertex functions with the internal and external legs expressing exact propagators.

Now it is easy to derive this generating functional from a formal consideration, using the just derived result of the fact that the loop expansion is a formal expansion in powers of \hbar . Suppose our generating functional for n -point proper vertex functions is given by $\Gamma[\phi]$, i.e., the proper vertex functions are given by

$$\Gamma^{(n)}(x_1, \dots, x_n) = \frac{\delta^n \Gamma}{\delta \phi_1 \dots \delta \phi_n}, \quad (3.3.14)$$

then the tree-level approximation is given by the $\mathcal{O}(\hbar^{-1})$ contribution to $iW_\Gamma[j]/\hbar$, where

$$Z_\Gamma[j] = \exp\left(\frac{i}{\hbar} W_\Gamma[j]\right) = \int_{\text{KMS}} \mathcal{D}\phi \exp\left[\frac{i}{\hbar} (\Gamma[\phi] + \{j_1\phi_1\}_1)\right]. \quad (3.3.15)$$

Now the tree-level contribution is given by the stationary point of the bracket in the exponential, i.e., for the solution of the equation

$$\frac{\delta\Gamma[\varphi_j]}{\delta\varphi_j(x)} = -j(x). \quad (3.3.16)$$

Thus the tree-level contribution to W_Γ is W , and thus we have

$$W[j] = \Gamma[\varphi_j] + \{j_1\varphi_j(x_1)\}_1. \quad (3.3.17)$$

Taking the derivative with respect to j of this equation, using (3.3.16) one finds

$$\varphi_j(x) := \frac{\delta W[j]}{\delta j(x)}. \quad (3.3.18)$$

It is clear, that only the 1PI connected parts of diagrams have to be renormalized, because two renormalized parts, connected only by a propagator line, will cause no further divergences. Thus, when the effective action is renormalized, all the proper vertex functions and thus all connected and disconnected Green's functions are well defined.

For the evaluation of the effective action, it is more customary to reorganize the loop expansion, using the so-called **background-field formulation** [Jac74], which also proves very useful for models with local Abelian or non-Abelian gauge symmetry like QED or standard model of elementary particles [Abb81, Abb82, AGS83].

To that end we substitute $\phi = \varphi_0 + \phi'$ in (3.3.2) with a background field φ_0 . Since the path-integral measure is invariant under such field translations we can write

$$\begin{aligned} Z[j] &= N(\beta) \int_{\text{KMS}} \mathcal{D}\phi' \exp\left\{\frac{i}{\hbar} [S[\varphi_0 + \phi'] + \{j_1(\varphi_{01} + \phi'_{01})\}_1]\right\} \\ &= \exp\left\{\frac{i}{\hbar} [S[\varphi_0] + \{\varphi_{01}j_1\}_1]\right\} Z_1, \end{aligned} \quad (3.3.19)$$

where

$$Z_1[j] = N(\beta) \int_{\text{KMS}} \mathcal{D}\phi \exp\left\{\frac{i}{\hbar} [S[\phi + \varphi_0] - S[\varphi_0] + \{\phi_{01}j_1\}_1]\right\}. \quad (3.3.20)$$

For convenience we write ϕ instead of ϕ' under the path integral again. From (3.3.19) and (3.3.20) we have

$$W[j] = -i\hbar \ln Z[j] = S[\varphi_0] + \{\varphi_{01}j_1\}_1 + W_1[j] \quad \text{with} \quad W_1[j] = -i\hbar \ln Z_1[j]. \quad (3.3.21)$$

Now we interpret j as a functional of φ_0 and write all functionals as functionals of φ_0 . Then, for the “mean field” for the Legendre transformation to the effective action (3.3.17) we find

$$\varphi_1 = \frac{\delta W[j]}{\delta j_1} = \varphi_{01} + \left\{ \left[\frac{\delta S[\varphi_0]}{\delta \varphi_{02}} + \frac{\delta W_1[\varphi_0]}{\delta \varphi_{02}} + j_{02} \right] \frac{\delta \varphi_{02}}{\delta j_1} \right\}_2. \quad (3.3.22)$$

Now, in order that $\varphi = \varphi_0$, we have to demand that

$$\frac{\delta S[\varphi_0]}{\delta \varphi_{01}} + \frac{\delta W_1[\varphi_0]}{\delta \varphi_{01}} + j_{01} = 0, \quad (3.3.23)$$

and then, according to (3.3.17) the effective action reads

$$\Gamma[\varphi] = S[\varphi] + W_1[\varphi]. \quad (3.3.24)$$

To find an appropriate perturbative scheme to evaluate the effective action, we thus need to calculate $W_1[\varphi]$. To that end we use (3.3.23) in (3.3.20) to eliminate j in favor of φ . This yields the functional integro-differential equation,

$$Z_1 = \exp\left(\frac{i}{\hbar} W_1\right) = N(\beta) \int_{\text{KMS}} D\phi \exp\left\{\frac{i}{\hbar} \left[\tilde{S}[\phi, \varphi] - \left\{ \phi_1 \frac{\delta W_1}{\delta \varphi_1} \right\}_1 \right]\right\}. \quad (3.3.25)$$

with

$$\tilde{S}[\phi, \varphi] = S[\phi + \varphi] - S[\varphi] - \left\{ \varphi_1 \frac{\delta S[\varphi]}{\delta \varphi_1} \right\}_1. \quad (3.3.26)$$

Now we introduce the new generating functional

$$\tilde{Z}[\varphi, K] = N(\beta) \int_{\text{KMS}} D\phi \exp\left\{\frac{i}{\hbar} \left[\tilde{S}[\phi, \varphi] + \{ \phi_1 K_1 \}_1 \right]\right\}. \quad (3.3.27)$$

Then, obviously

$$W_1[\varphi] = -i\hbar \ln \tilde{Z}[\varphi, K] \Big|_{K=-\delta W_1/\delta \varphi}. \quad (3.3.28)$$

Now we can expand $\tilde{Z}[\varphi, K]$ perturbatively in powers of \hbar with the usual techniques. Then the one-particle irreducible graphs for the theory with the action $\tilde{S}[\phi, \varphi]$ are given for that K , for which $\delta \tilde{Z}/\delta K = 0$. Now we can prove that the solution is indeed

$$K = -\frac{\delta W_1}{\delta \varphi} \Rightarrow \frac{\delta \tilde{Z}[\varphi, K]}{\delta K} = 0. \quad (3.3.29)$$

This implies that we can perform the usual perturbative calculations with the action $\tilde{S}[\phi, \varphi]$, defined by (3.3.26) although in practice this is only possible for a constant background field φ , but this is already an important case to study **phase transitions in thermal equilibrium**.

To prove (3.3.29), we have to show

$$\frac{\delta \tilde{Z}[\varphi, K]}{\delta K_1} \Big|_{K=-\delta W_1/\delta \varphi} = N(\beta) \int_{\text{KMS}} D\phi \phi_1 \exp\left\{\frac{i}{\hbar} \left[\tilde{S}[\phi, \varphi] - \left\{ \phi_1 \frac{\delta W_1(\varphi)}{\delta \varphi_1} \right\}_1 \right]\right\} = 0. \quad (3.3.30)$$

To this end we differentiate (3.3.25) wrt. to φ :

$$\begin{aligned} -i\hbar \frac{\delta Z_1}{\delta \varphi_1} &= N(\beta) \int_{\text{KMS}} D\phi \left[\frac{\delta \tilde{S}[\phi, \varphi]}{\delta \varphi_1} - \left\{ \phi_2 \frac{\delta^2 W_1(\varphi)}{\delta \varphi_1 \delta \varphi_2} \right\}_2 \right] \\ &\quad \times \exp\left\{\frac{i}{\hbar} \left[\tilde{S}[\phi, \varphi] - \left\{ \phi_1 \frac{\delta W_1(\varphi)}{\delta \varphi_1} \right\}_1 \right]\right\}. \end{aligned} \quad (3.3.31)$$

Now we evaluate this path integral for the first term from \tilde{S} ,

$$\begin{aligned}
 & \int_{\text{KMS}} \text{D}\phi \frac{\delta S[\phi + \varphi]}{\delta \varphi_1} \exp \left\{ \frac{i}{\hbar} \left[\tilde{S}[\phi, \varphi] - \left\{ \phi_1 \frac{\delta W_1(\varphi)}{\delta \varphi_1} \right\}_1 \right] \right\} \\
 &= -i\hbar \int_{\text{KMS}} \frac{\delta}{\delta \phi_1} \exp \left\{ \frac{i}{\hbar} \left[\tilde{S}[\phi, \varphi] - \left\{ \phi_1 \frac{\delta W_1(\varphi)}{\delta \varphi_1} \right\}_1 \right] \right\} \\
 &+ \int_{\text{KMS}} \text{D}\phi \left[\frac{\delta S[\varphi]}{\delta \varphi_1} + \frac{\delta W_1[\varphi]}{\delta \varphi} \right] \exp \left\{ \frac{i}{\hbar} \left[\tilde{S}[\phi, \varphi] - \left\{ \phi_1 \frac{\delta W_1(\varphi)}{\delta \varphi_1} \right\}_1 \right] \right\}.
 \end{aligned} \tag{3.3.32}$$

The first path integral over a total functional derivatives vanishes due to the periodic KMS conditions. Inserting the rest into (3.3.31) gives

$$\begin{aligned}
 -i\hbar \frac{\delta Z_1}{\delta \varphi_1} = \frac{\delta W_1}{\delta \varphi_1} Z_1 = N(\beta) \int_{\text{KMS}} \text{D}\phi \left[\frac{\delta W_1[\varphi]}{\delta \varphi_1} - \left\{ \phi_2 \frac{\delta^2}{\delta \varphi_1 \delta \varphi_2} \right\}_2 (S[\varphi] + W_1[\varphi]) \right] \\
 \exp \left\{ \frac{i}{\hbar} \left[\tilde{S}[\phi, \varphi] - \left\{ \phi_1 \frac{\delta W_1[\varphi]}{\delta \varphi_1} \right\}_1 \right] \right\}.
 \end{aligned} \tag{3.3.33}$$

Since the first term in the bracket under the path integral in the upper line does not depend on ϕ , we can take it out of the path integral, and the resulting term is just the left-hand side of the equation. This means we have

$$\begin{aligned}
 0 = N(\beta) \int_{\mathcal{C}} d^4 x_2 \frac{\delta^2}{\delta \varphi_1 \delta \varphi_2} [S[\varphi] + W_1[\varphi]] \\
 \times \int_{\text{KMS}} \text{D}\phi \phi_2 \exp \left\{ \frac{i}{\hbar} \left[\tilde{S}[\phi, \varphi] - \left\{ \phi_1 \frac{\delta W_1[\varphi]}{\delta \varphi_1} \right\}_1 \right] \right\}.
 \end{aligned} \tag{3.3.34}$$

The second functional derivative above is just the inverse propagator, and thus convoluting with the propagator proves (3.3.30).

This means, to evaluate the effective action $\Gamma[\varphi]$, we just have to evaluate the effective action for the theory defined by the classical action $\tilde{S}[\phi, \varphi]$, which in turn is defined by (3.3.26) with an arbitrary external field φ for vanishing expectation value of the “quantum field”, i.e., $\langle \phi \rangle = 0$. In general this is not possible in practice.

3.3.3 Perturbative evaluation of the effective potential and renormalization

However, we can perform the evaluation for $\varphi = \text{const}$. The corresponding function is called the **effective potential**. We start with deriving the Feynman rules. According to (3.3.26) we have to evaluate the Lagrangian for \tilde{S} :

$$\tilde{\mathcal{L}}(\phi, \varphi) = \frac{1}{2} (\partial_\mu \phi) (\partial^\mu \phi) - \left(\frac{m^2}{2} + \frac{\lambda}{2} \varphi^2 \right) \phi^2 - \frac{\lambda}{3!} \varphi \phi^3 - \frac{\lambda}{4!} \phi^4. \tag{3.3.35}$$

Since we assume $\varphi = \text{const}$ we have again a translation-invariant situation, and we can use the Feynman rules in momentum space. The propagator to be used is the usual free propagator but with a φ -dependent squared mass, given by $\mu^2(\varphi) = m^2 + \lambda \varphi^2$, which we assume to be larger than 0 for our

calculations. The Keldysh matrix elements for the real-time propagator are then given by (2.2.116-2.2.119)

$$\begin{aligned}
 i\mathcal{D}^{11}(p, \mu) &= \frac{i}{p^2 - \mu^2 + i\epsilon} + 2\pi\delta(p^2 - \mu^2)f_B(|p^0|), \\
 i\mathcal{D}^{12}(p, \mu) &= 2\pi[\Theta(-p^0) + f_B(|p^0|)]\delta(p^2 - \mu^2), \\
 i\mathcal{D}^{21}(p, \mu) &= 2\pi[\Theta(p^0) + f_B(|p^0|)]\delta(p^2 - \mu^2), \\
 i\mathcal{D}^{22}(p, \mu) &= -\frac{i}{p^2 - \mu^2 - i\epsilon} + 2\pi\delta(p^2 - \mu^2)f_B(|p^0|).
 \end{aligned} \tag{3.3.36}$$

We have written the propagators in the form, where they appear in terms of a vacuum and finite-temperature part, which is very convenient for the evaluation of the Feynman integral, because it admits an easy separation of temperature-independent vacuum parts and temperature-dependent in-medium parts. This is one of the advantages of the use of the real-time formalism also in equilibrium many-body quantum-field theory. This separation in vacuum and in-medium parts is particularly important to renormalize (divergent) loop integrals with vacuum counter terms. As we shall see in the following on this concrete example, the counter terms are defined entirely by the pure vacuum parts, i.e., after having subtracted all subdivergences of a diagram with multiple loops, the remaining overall divergence is in the temperature-independent part of the diagram. This is due to the on-shell δ distributions and the exponential decay of $f_B(|p^0|)$ for $p^0 \rightarrow \infty$.

The perturbative (tree-level) vertex functions are determined by the interaction Lagrangian, i.e., the last two terms in (3.3.35) that are cubic and quartic in the “quantum field”, ϕ . We thus have the following perturbative Feynman rules

$$\begin{array}{c} j \quad p \quad k \\ \bullet \longleftarrow \bullet \\ \bullet \quad \bullet \end{array} = i\mathcal{D}^{jk}(p, \mu), \tag{3.3.37}$$

$$\begin{array}{c} \otimes \\ \varphi \\ | \\ \bullet \\ / \quad \backslash \\ j \end{array} = i(-1)^j \frac{\lambda}{3!} \varphi, \tag{3.3.38}$$

$$\begin{array}{c} \diagup \quad \diagdown \\ \bullet \\ \diagdown \quad \diagup \end{array} = i(-1)^j \frac{\lambda}{4!}. \tag{3.3.39}$$

To set up the correct **renormalization** scheme, we note that the effective action $\Gamma[\tilde{\Phi}]$ is an even functional in $\tilde{\Phi}(x)$, i.e., $\Gamma[-\tilde{\Phi}] = \Gamma[\tilde{\Phi}]$, which means that only the n -point functions with even n are non-zero. when evaluating the effective potential with the just given Feynman rules for $\Phi = \varphi = \text{const}$, also the φ legs count to n .

Now we determine the superficial degree of divergence. For a diagram with E external lines (not counting lines symbolizing the constant mean field φ) and V_1 vertices of the type (3.3.38) and V_2 vertices of the type (3.3.39) we have $4V_1 + 3V_2$ four-momenta in the diagram. There are $V_1 + V_2 - 1$ constraints from the energy-momentum conservation at each vertex, which holds because for a constant mean field the situation is translation invariant. The -1 accounts for overall energy-momentum conservation. There

are $I = (3V_1 + 4V_2 - E)/2$ internal lines, which implies that there must always be an even number of V_1 -type vertices since E is even, and I must be an integer number. The superficial degree of divergence in four space-time dimensions is given by $D = 4L - 2I$, where L is the number of loops in the diagram, each which contributes an integral over the four-momentum running around the loop. Each propagator with momentum p , symbolized by the internal lines, goes like $1/p^2$ and thus diminishes the degree of divergence by this power. The number of loops is given by $L = I - (V_1 + V_2 - 1) = V_1/2 + V_2 + 1$, because there are $V_1 + V_2$ constraints on the four momenta due to energy-momentum conservation at each vertex, while overall energy-momentum conservation is already fulfilled by definition. Thus the superficial degree of divergence of a given diagram is

$$D = 4L - 2I = 2V_1 + 4V_2 + 4 - (3V_1 + 4V_2 - E) = 4 - V_1 - E. \quad (3.3.40)$$

According to the BPHZ theorem (see, e.g., [Hee02]) after subtracting the divergences of sub-diagrams recursively or by applying Zimmermann's forest formula, only diagrams with $D \geq 4$ are divergent. Thus only diagrams with $E \in \{0, \dots, 4\}$ can be divergent. So let's consider these cases

- $E = 0$, which are the closed diagrams symbolizing corrections to the effective potential, i.e., to the grand-canonical thermal potential Φ . Here only diagrams with $V_1 \in \{0, 2, 4\}$ are overall divergent.
- $E = 1$, the tadpole graphs and $E = 2$, the self-energy graphs. Only diagrams with $V_1 \in \{0, 2\}$ are divergent.
- $E = 3$ and $E = 4$, the contributions to the inverse propagator (i.e., the self-energy). Only diagrams with $V_2 = 0$ are overall divergent.

Now each vertex V_1 contains a factor φ , which shows that only n -point vertex functions with $n \in \{0, 2, 4\}$ are overall divergent, and this implies that the theory is renormalizable with the corresponding vacuum counterterms (vacuum energy, wave-function and mass as well as coupling-constant counterterms). The counter-term Lagrangian thus reads

$$\delta \mathcal{L} = \delta \Lambda + \frac{\delta Z}{2} (\partial_\mu \phi)(\partial^\mu \phi) - \frac{\delta m^2}{2} \phi^2 - \frac{\delta Z_m (m^2 - M^2)}{2} \phi^2 - \frac{\delta Z_\lambda}{4!} \lambda \phi^4. \quad (3.3.41)$$

We thus can renormalize the theory at a point $m^2 = M^2 > 0$ for the effective mass, where $\varphi = 0$ is the stable solution for the vacuum by imposing the **mass-independent renormalization conditions** [Kug77, Kug97]

$$\Gamma[\varphi = 0, m = M]|_{T=0} = 0 \Rightarrow \delta \Lambda_1, \quad (3.3.42)$$

$$\partial_{m^2} \Gamma[\varphi = 0, m = M]|_{T=0} = 0 \Rightarrow \delta \Lambda_2, \quad (3.3.43)$$

$$\partial_{m^2}^2 \Gamma[\varphi = 0, m = M]|_{T=0} = 0 \Rightarrow \delta \Lambda_3, \quad (3.3.44)$$

$$\Gamma^{(2)}[\varphi = 0, m = M, p = 0]|_{T=0} = -M^2 \Rightarrow \delta m, \quad (3.3.45)$$

$$\partial_{m^2} \Gamma^{(2)}[\varphi = 0, m, p = 0]|_{m=M, T=0} = -1 \Rightarrow \delta Z_m, \quad (3.3.46)$$

$$\Gamma^{(4)}[\varphi = 0, m = M, p_1 = p_2 = p_3 = 0]|_{T=0} = -\lambda \Rightarrow \delta Z_\lambda. \quad (3.3.47)$$

Here “mass independent” refers to the fact that all counter terms are defined for the theory with $m = M$.

To give the counter terms explicitly, we have to regularize the divergent diagrams (and sub-diagrams). Since we use the heat-kernel method to evaluate the effective potential, we should also use the corresponding regularization for evaluating the loop corrections to the self energy $\Sigma = -[\Gamma^{(2)} - \mathcal{D}^{-1}]$ and the proper vertex function $\Gamma^{(4)}$ at $m = M$ and $\varphi = 0$. Since these functions are given as functional derivatives with respect to the fully space-time dependent mean fields $\tilde{\Phi}$ this regularization is achieved with **Schwinger's proper-time method**. Since we only need the case $T = 0$ to get the counter terms that are defined entirely in the vacuum theory, it is sufficient to work with the usual time-ordered propagators and vertices only. The idea is to write

$$D(p, M) = \frac{1}{p^2 - M^2 + i\eta} = -i \int_0^\infty d\vartheta \exp[i\vartheta(p^2 - m^2 + i\eta)] \quad (3.3.48)$$

and to introduce the regularization in the same way as in Sect. 3.2.2 when we evaluated the functional determinant

$$D_\epsilon(p, M) = i \int_0^\infty d\vartheta (iM^2\vartheta)^\epsilon \exp[i\vartheta(p^2 - m^2 + i\eta)] = D(p, M) \left(\frac{M^2}{m^2 - p^2 - i\eta} \right)^\epsilon \Gamma(1 + \epsilon). \quad (3.3.49)$$

For sufficiently large ϵ with this expression for the propagator all loop integrals become finite. Of course, at the end of the calculation, when the counterterms are appropriately chosen to fulfill the MIR conditions (3.3.41-3.3.47), we have to let $\epsilon \rightarrow 0$ again.

The trick of the proper-time method is however to integrate over the loop momenta first and then over the “proper-time parameters” ϑ .

To evaluate the effective action and the counter-terms, however, it is sufficient to first evaluate $\Gamma[\varphi]$ with this regularization and then to use appropriate derivatives with respect to φ^4 , because the counter terms are all evaluated at external momenta $p_j = 0$, and this just

$$\Gamma^{(n)}(p_1 = \dots = p_{n-1} = 0) = \frac{1}{n!} \frac{\partial^n}{\partial \varphi^n} \Gamma[\varphi]. \quad (3.3.50)$$

For the counter terms we have to set $m^2 = M^2 > 0$ and $\varphi = 0$ after performing the derivatives.

For the one-loop approximation we thus can use (3.2.66) but with $m^2 \rightarrow \mu^2 = m^2 + \lambda\varphi^2/2$ and $A = -2/\alpha - 3 + \gamma_E$ to get the regularized vacuum part of the effective potential

$$\begin{aligned} V_{\text{reg, vac}}(\varphi, m, M) &= -\frac{T}{V} \Gamma_{\text{reg, vac}}(\varphi) = -\mathcal{L}(\varphi) + \frac{T}{2V} \text{Tr} \ln \left(\frac{\mathcal{D}^{-1}(\varphi)}{M^2} \right) \\ &= \frac{m^2}{2} \varphi^2 + \frac{\lambda}{4!} \varphi^4 \\ &\quad + \frac{1}{128\pi^2} \left(m^2 + \frac{\lambda}{2} \varphi^2 \right)^2 \left[-\frac{2}{\alpha} - 3 + 2\gamma_E + 2 \ln \left(\frac{m^2 + \lambda\varphi^2/2}{M^2} \right) \right]. \end{aligned} \quad (3.3.51)$$

The renormalization conditions (3.3.42-3.3.44) immediately give

$$\begin{aligned} \delta\Lambda &= V(\varphi = 0, M, M) + (m^2 - M^2) \partial_{m^2} V(0, m, M) \Big|_{m=M} + \frac{(m^2 - M^2)^2}{2} \partial_{m^2}^2 V(0, m, M) \Big|_{m=M} \\ &= \frac{2(\gamma_E - 1)m^2 - 4m^2M^2 + M^4}{128\pi^2}. \end{aligned} \quad (3.3.52)$$

The regularized two-point function at $m^2 = M^2$, $\varphi = 0$ is given by

$$\Gamma_{\text{reg,vac}}^{(2)}(p=0, m=M, \varphi=0) = -V''_{\text{reg,vac}}(\varphi)|_{\varphi=0, m^2=M^2} = -M^2 + \frac{\lambda M^2}{32\pi^2} \left(\frac{1}{\alpha} + 1 - \gamma_E \right). \quad (3.3.53)$$

From (3.3.45) this gives

$$\delta m^2 = \frac{\lambda M^2}{32\pi^2} \left(\frac{1}{\alpha} + 1 - \gamma_E \right). \quad (3.3.54)$$

Further we find

$$\partial_{M^2} \Gamma_{\text{reg,vac}}^{(2)}(\varphi=0, M, p=0) = -1 + \frac{\lambda}{32\pi^2} \left(\frac{1}{\alpha} + 1 - \gamma_E \right) \Rightarrow \delta Z_m = \frac{\lambda}{32\pi^2} \left(\frac{1}{\alpha} + 1 - \gamma_E \right). \quad (3.3.55)$$

Finally we get

$$\begin{aligned} \Gamma_{\text{reg,vac}}^{(4)}(\varphi=0, m=M, p_1=p_2=p_3=0) &= -\frac{d^4}{d\varphi^4} V(\varphi)|_{\varphi=0} = -\lambda + \frac{3\lambda^2}{32\pi^2} \left(\frac{1}{\epsilon} - \gamma_E \right) \\ &\Rightarrow \delta \lambda = \frac{3\lambda^2}{32\pi^2} \left(\frac{1}{\alpha} - \gamma_E \right). \end{aligned} \quad (3.3.56)$$

The renormalized vacuum part of the potential thus reads

$$\begin{aligned} V_{\text{vac,ren}}(\varphi, m, M) &= \frac{m^2 \phi^2}{2} + \frac{\lambda}{4!} \phi^4 - \frac{3m^4 - 4m^2 M^2 + M^4 + \lambda m^2 \varphi^2 + 3\lambda^2 \varphi^2/4}{128\pi^2} \\ &\quad + \frac{(m^2 + \lambda \varphi^2/2)^2}{64\pi^2} \ln \left(1 + \frac{\lambda \varphi^2}{2M^2} \right). \end{aligned} \quad (3.3.57)$$

As we know already from Sect. 3.2.2 there is no divergence in the temperature-dependent part of the effective potential. We can simply copy (3.2.67) with substituting $m^2 \rightarrow m^2 + \lambda \varphi^2/2$:

$$V_{\text{ren}}(\varphi, m, M) = V_{\text{vac,ren}}(\varphi, m, M) - \frac{1}{6\pi^2} \int_{m^2 + \lambda \varphi^2/2}^{\infty} dp_0 \left[p_0^2 - m^2 - \frac{\lambda}{2} \varphi^2 \right]^{3/2} f_B(p_0). \quad (3.3.58)$$

The mean field φ_0 is then given by finding a minimum of this effective potential. We note that, of course, the effective action in this perturbative approach is only well defined for mean fields such that $m^2 + \lambda \varphi^2/2 \geq 0$. As to be expected the perturbative expansion can only be defined for excitations not too far from a minimum of the effective potential, which defines the mean field present in the corresponding “vacuum state”. We shall investigate this problem in detail in the next chapter, where we investigate the **Baym functional**, which allows to formulate **self-consistent** resummations of the perturbation series for the propagator which at the same time obey **conservation laws** and are **thermodynamically consistent**. Here, “thermodynamical consistency” means that the definitions of the bulk quantities like internal energy, pressure, entropy, etc. from the partition function coincides with the definition of the same quantities from the self-consistently calculated one-particle Green’s function, i.e., the propagator with self-consistently resummed self-energies.

3.4 Fermions

The path-integral formalism for fermions is not very different from that of bosons. Nevertheless we need **eigenstates of fermion operators** which are defined as the generalized eigenvectors of field operators, as for bosons. To be consistent the anticommutator relations of the field operators, their eigenvalues have to be anticommuting. Thus, we need a new sort of algebraic objects, the so called **Grassmann**

numbers and a formal calculus, i.e., differentiation and integration with respect to those algebraic objects that allow for manipulations of path integrals and (functional) derivatives which are similar to the bosonic case. In the following subsection we start with the treatment of **Dirac fermions** as true particles obeying Fermi-Dirac statistics. Later, we shall also treat abelian and non-abelian gauge theories, where the **Faddeev-Popov ghost fields** are introduced as unphysical Grassmann valued fields obeying Bose-Einstein boundary conditions. As we shall see there they do not give rise to physically observable field degrees of freedom or particles but just compensate the unphysical field degrees of freedom of the gauge bosons, leading to a consistent description of “matter fields” with vector bosons.

3.4.1 Path integrals for Dirac fermions

For simplicity we start with free Dirac fermions, which have been treated in the operator formalism in Sect. 1.3. We start from the canonical formalism, i.e., with the real-time Lagrangean

$$\mathcal{L} = \bar{\psi}(i\mathcal{D} - m)\psi. \quad (3.4.1)$$

The canonically conjugated field momentum is

$$\Pi = \frac{\partial \mathcal{L}}{\partial \dot{\psi}} = i\bar{\psi}\gamma^0 = i\bar{\psi}^\dagger. \quad (3.4.2)$$

As we know from our discussion of Poincaré symmetry within the canonical quantization formalism in Sect. 1.3.3, we have to quantize these fields with **canonical equal-time anticommutation rules**,

$$\begin{aligned} \{\psi_\alpha(t, \vec{x}), \psi_\beta(t, \vec{y})\} &= \{\Pi_\alpha(t, \vec{x}), \Pi_\beta(t, \vec{y})\} = 0, \\ \{\psi_\alpha(t, \vec{x}), \Pi_\beta(t, \vec{y})\} &= i\{\psi_\alpha(t, \vec{x}), \psi_\beta^\dagger(t, \vec{y})\} = i\delta^{(3)}(\vec{x} - \vec{y})\delta_{\alpha\beta}, \end{aligned} \quad (3.4.3)$$

where $\alpha, \beta \in \{1, \dots, 4\}$ denote Dirac-spinor indices. In the following we shall work with ψ and $\psi^\dagger = -i\Pi$ for convenience.

For the thermal path integral along the extended Schwinger-Keldysh contour we have to discretize the space-time variables. We also put the particles in a finite cubic volume $V = L^3$ with periodic boundary conditions for the fields as we did for bosons, and we shall denote the discretized spatial and Dirac indices by one common index k . The corresponding equal-time anticommutators of course read

$$\{\psi_\alpha(t), \psi_\beta(t)\} = 0, \quad \{\psi_\alpha(t), \psi_\beta^\dagger(t)\} = \delta_{\alpha\beta}. \quad (3.4.4)$$

A complete set of compatible observables are the Hermitean occupation-number operators,

$$\mathbf{N}_\alpha(t) = \psi_\alpha^\dagger(t)\psi_\alpha(t). \quad (3.4.5)$$

Since $\psi_\alpha^2 = 0$, there exists a **vacuum state**

$$\forall \alpha: \quad \psi_\alpha |0\rangle = 0, \quad (3.4.6)$$

Ignoring the time argument for a while, working at a fixed time argument t , further we have

$$\mathbf{N}_\alpha^2 = \psi_\alpha^\dagger [\{\psi_\alpha, \psi_\alpha^\dagger\} - \psi_\alpha^\dagger \psi_\alpha] \psi_\alpha = \psi_\alpha^\dagger \psi_\alpha = \mathbf{N}_\alpha, \quad (3.4.7)$$

where we have used (3.4.4) and $\psi_\alpha^2 = 0$. (3.4.7) implies that the possible eigenvalues of \mathbf{N}_α are 0 or 1. From the anticommutators (3.4.4) further we obtain the **occupation-number basis**

$$|\{n_\alpha\}\rangle = \prod_\alpha \psi_\alpha^{n_\alpha} |0\rangle, \quad n_\alpha \in \{0, 1\}. \quad (3.4.8)$$

They form a complete set of orthonormal states.

For the path-integral representation we rather need a kind of **coherent states**, i.e., generalized eigenkets of the field operators and eigenbras of the canonical momenta. To establish the corresponding formalism we work in a state space for a particle at only one space-time Dirac-index lattice site. As we shall see, the generalization to the above considered case with multiple lattice sites is straight forward. So dropping the fixed index α for convenience. Then we have a situation that is similar to creation and annihilation operators of a simple harmonic oscillator but with anticommutation relations rather than commutation relations, i.e.,

$$\{\psi, \psi\} = 0, \quad \{\psi, \psi^\dagger\} = 1. \quad (3.4.9)$$

The corresponding Hilbert space is obviously just two-dimensional with the occupation-number basis $|0\rangle$ and $|1\rangle = \psi^\dagger |0\rangle$. Now we like to define formal field-operator eigenkets fulfilling

$$\psi |\eta\rangle = \eta |\eta\rangle \quad (3.4.10)$$

and momentum-operator eigenbras fulfilling

$$\langle \eta^* | \mathbf{\Pi} = \langle \eta^* | i\psi^\dagger = \langle \eta^* | i\eta^*. \quad (3.4.11)$$

From this we find

$$\psi^2 = 0 \Rightarrow \eta^2 = 0, \quad (\psi^\dagger)^2 = 0 \Rightarrow (\eta^*)^2 = 0. \quad (3.4.12)$$

Now we must have

$$|\eta\rangle = a |0\rangle + b |1\rangle \Rightarrow \psi |\eta\rangle = |0\rangle. \quad (3.4.13)$$

This means we have to set $a = 1$ and $b = -\eta$, i.e.,

$$|\eta\rangle = |0\rangle - \eta |1\rangle. \quad (3.4.14)$$

because then we have

$$\psi |\eta\rangle = -\psi \eta |1\rangle + \eta \psi \psi^\dagger |0\rangle = \eta |0\rangle = \eta(|0\rangle - \eta |1\rangle) = \eta |\eta\rangle. \quad (3.4.15)$$

Note that here we have assumed that the fermion-field operator *anticommutes* with the eigenvalue, η . We shall see that this is a convenient convention. It is clear that we can write

$$|\eta\rangle = \exp(-\eta \psi^\dagger) |0\rangle, \quad (3.4.16)$$

because

$$\exp(-\eta \psi^\dagger) = \sum_{j=0}^{\infty} \frac{(-\eta \psi^\dagger)^j}{j!} = 1 - \eta \psi^\dagger. \quad (3.4.17)$$

The series stops after $j = 1$, because $(\eta \psi^\dagger)^2 = \eta \psi^\dagger \eta \psi^\dagger = -\eta^2 (\psi^\dagger)^2 = 0$.

By formal adjungation of (3.4.17) we get

$$\langle \eta^* | = \langle 0 | \exp(-\psi \eta^*) = \langle 0 | (1 - \psi \eta^*) = \langle 0 | - \langle 1 | \eta^*. \quad (3.4.18)$$

Indeed we have

$$\langle \eta^* | \psi^\dagger = -\langle 1 | \eta^* \psi^\dagger = +\langle 1 | \psi^\dagger \eta^* = \langle 0 | \eta^* = (\langle 0 | - \langle 1 | \eta^*) \eta^* = \langle \eta^* | \eta^*. \quad (3.4.19)$$

From (3.4.15) and (3.4.19) it follows

$$\langle \eta^* | \eta \rangle = (\langle 0 | - \langle 1 | \eta^*) (|0\rangle - \eta |1\rangle) = 1 + \eta^* \eta = \exp(\eta^* \eta) = \exp(-\eta \eta^*), \quad (3.4.20)$$

where Finally we have assumed that also the field eigenvalues η and η^* anticommute. In this way we have established a so-called **Grassmann algebra**. Together with the complex numbers they build a four-dimensional algebra. The most general function that can be built as formal polynomials of Grassmann and ordinary complex numbers obviously is

$$f(\eta^*, \eta) = f_0 + f_1 \eta^* + f_2 \eta + f_{12} \eta^* \eta, \quad f_0, f_1, f_2, f_{12} \in \mathbb{C}. \quad (3.4.21)$$

As the next step we want to establish rules for **integration with respect to Grassmann numbers**. The purpose is to get a partion of the identity operator. First we evaluate

$$\begin{aligned} \exp(\eta \eta^*) | \eta \rangle \langle \eta^* | &= (1 + \eta \eta^*) (|0\rangle - \eta |1\rangle) (\langle 0 | - \eta^* \langle 1 |) \\ &= (1 + \eta \eta^*) (|0\rangle \langle 0 | - \eta |1\rangle \langle 0 | - \eta^* |0\rangle \langle 1 | + \eta \eta^* |1\rangle \langle 1 |) \\ &= |0\rangle \langle 0 | - \eta |1\rangle \langle 0 | - \eta^* |0\rangle \langle 1 | + \eta \eta^* |1\rangle \langle 1 | + \eta \eta^* |0\rangle \langle 0 |. \end{aligned} \quad (3.4.22)$$

We shall show now that we can establish algebraic rules for integration that are very similar to the integration with respect to usual real or complex numbers by defining

$$\int d\eta = \int d\eta^* = 0, \quad \int d\eta \eta = \int d\eta^* \eta^* = 1, \quad \int d\eta \eta^* = \int d\eta^* \eta = 0. \quad (3.4.23)$$

Also all Grassmann valued quantities, including the “differentials” should anticommute. Further we define

$$\int d\eta^* d\eta = \int d\eta \int d\eta^* = - \int d\eta d\eta^*. \quad (3.4.24)$$

Integration (3.4.22) thus gives

$$\int d\eta^* d\eta \exp(\eta \eta^*) | \eta \rangle \langle \eta^* | = |0\rangle \langle 0 | + |1\rangle \langle 1 | = \mathbb{1}, \quad (3.4.25)$$

which is precisely the “completeness relation” for fermionic coherent states, we wished to establish.

Next we want to calculate the trace of operators representing observables. Observables are all built by an **even number of fermion operators** such that $\mathbf{A} \eta = \eta \mathbf{A}$ etc. We first write down the trace with help of the usual occupation-number eigenbasis and then introduce completeness relations of the form (3.4.25):

$$\text{Tr } \mathbf{A} = \sum_{n=0}^1 \langle n | \mathbf{A} | n \rangle = \sum_{n=0}^1 \int d\eta^* d\eta \int d\eta' d\eta'^* \exp(\eta \eta^* + \eta' \eta'^*) \langle n | \eta \rangle \langle \eta^* | \mathbf{A} | \eta' \rangle \langle \eta'^* | n \rangle. \quad (3.4.26)$$

Here we could lump the exponentials together, because its arguments consist of an even number of Grassmann variables, and thus these arguments commute. Now we want to get rid of the occupation-number states. First of all we can commute the last factor with the operator matrix element since the

latter obviously consists of an even number of Grassmann variables. However, we have to commute $\langle n | \eta \rangle$ with $\langle \eta'^* | n \rangle$, which has to be handled with care. To that end we use (3.4.14) and (3.4.18):

$$\langle n | \eta \rangle = \delta_{0n} - \eta \delta_{1n}, \quad \langle \eta'^* | n \rangle = \delta_{0n} - \eta'^* \delta_{1n}. \quad (3.4.27)$$

Thus we get

$$\langle n | \eta \rangle \langle \eta'^* | n \rangle = \delta_{0n} + \eta \eta'^* \delta_{1n} \quad (3.4.28)$$

but

$$\langle \eta'^* | n \rangle \langle n | \eta \rangle = \delta_{0n} + \eta'^* \eta \delta_{1n} = \delta_{0n} - \eta \eta'^* \delta_{1n}. \quad (3.4.29)$$

Thus, we have

$$\langle n | \eta \rangle \langle \eta'^* | n \rangle = \langle -\eta'^* | n \rangle \langle n | \eta \rangle, \quad (3.4.30)$$

where we have lumped the additional minus sign arbitrarily to the bra-coherent state. Summing over n thus leads to

$$\begin{aligned} \text{Tr } \mathbf{A} &= \int d\eta'^* d\eta' \exp(\eta' \eta'^*) \int \exp(\eta \eta^*) \langle -\eta'^* | \eta \rangle \langle \eta^* | \mathbf{A} | \eta' \rangle \\ &\stackrel{(3.4.25)}{=} \int d\eta'^* d\eta' \exp(\eta' \eta'^*) \langle -\eta'^* | \mathbf{A} | \eta' \rangle. \end{aligned} \quad (3.4.31)$$

As we shall now see, the most important feature is the minus sign in the bra of the matrix element. Now it is immediately clear that all these considerations hold true for the case with more than one lattice site, i.e., for a discretized field operator we simply have

$$\text{Tr } \mathbf{A} = \int d^N \eta^* d^N \eta \exp\left(\sum_{\alpha} \eta_{\alpha} \eta_{\alpha}^*\right) \langle -\eta^* | \mathbf{A} | \eta' \rangle, \quad \int d^N \eta^* d^N \eta := \int \prod_{\alpha=1}^N (d\eta_{\alpha}^* d\eta_{\alpha}). \quad (3.4.32)$$

Now we apply this to the **partition sum for Dirac fermions**. We immediately include a **chemical potential** for the conserved charge, i.e., the discretized form of (1.3.82)

$$\mathbf{Q}(t) = \sum_{\alpha} \psi_{\alpha}^{\dagger} \psi, \quad (3.4.33)$$

where we have silently omitted the normal-ordering prescription since for our path-integral formalism we want to establish Weyl ordering, i.e. we like to have all conjugated field momenta (or ψ^{\dagger} for that matter) to the left of all field operators ψ . Thus our partition sum reads

$$Z = \text{Tr} \exp(-\beta \mathbf{H} + \alpha \mathbf{Q}), \quad (3.4.34)$$

as for the bosonic case, but now we use our path-integral description of traces over observable operators built with Dirac-field operators (3.4.32). The evaluation goes quite in parallel with the bosonic case. In order to have a conveniently defined real-time path integral, we'll use the implementation of a finite chemical potential in terms of boundary conditions for the fields as for the charged bosons. From the commutation relations we find

$$\exp(-\alpha \mathbf{Q}) \psi_{\beta} \exp(\alpha \mathbf{Q}) = \exp(\alpha) \psi_{\beta}, \quad \exp(\alpha \mathbf{Q}) \psi_{\beta}^{\dagger} (-\alpha \mathbf{Q}) = \exp(+\alpha) \psi_{\beta}^{\dagger}. \quad (3.4.35)$$

This implies

$$\langle -\eta^* | \exp(\alpha \mathbf{Q}) = \langle -\eta^* \exp \alpha |. \quad (3.4.36)$$

Thus, for the partition sum we can write

$$\mathrm{Tr} \exp(-\beta \mathbf{H} + \alpha \mathbf{Q}) = \int d^n \eta^* d^n \eta \exp\left(\sum_{\beta} \eta_{\beta} \eta_{\beta}^*\right) \langle -\exp \alpha \eta^* | \exp(-\beta \mathbf{H}) | \eta \rangle. \quad (3.4.37)$$

Now introducing the extended real-time contour the very same calculation as in the bosonic case in Sect. 3.1 leads to

$$\mathrm{Tr} \exp(-\beta \mathbf{H} + \alpha \mathbf{Q}) = N \int_{\mathrm{KMS}} D\bar{\psi} D\psi \exp(iS_{\mathcal{E}}[\bar{\psi}, \psi]), \quad (3.4.38)$$

where we have relabeled the Grassmann fields from η to ψ and from η^* to $\bar{\psi}$. The **KMS boundary conditions for fermions** read, because of (3.4.36),

$$\bar{\psi}(-i\beta, \vec{x}) = -\exp(\mu\beta) \bar{\psi}(0, \vec{x}). \quad (3.4.39)$$

From the commutation relations (3.4.35) this implies

$$\psi(-i\beta, \vec{x}) = -\exp(-\mu\beta) \psi(0, \vec{x}). \quad (3.4.40)$$

Here we have written $\alpha = \mu\beta$ again.

To evaluate the partition sum it is again enough to consider the imaginary-time part of the Schwinger-Keldysh path, and the calculation is very similar to the bosonic case. There are only two differences: First of all we have quasi-antiperiodic boundary conditions for fermions rather than quasi-periodic boundary conditions for bosons. Second we have to evaluate the **Gaussian integral over Grassmann numbers**. We start with the one-dimensional case

$$\int d\eta^* d\eta \exp(-\lambda \eta^* \eta) = \int d\eta^* d\eta (1 - \lambda \eta^* \eta) = \int d\eta^* d\eta (-\lambda \eta^* \eta) = +\lambda. \quad (3.4.41)$$

Now in the n -dimensional case with a hermitean complex matrix from this we immediately have

$$\int d^n \eta^* d^n \eta \exp\left(-\sum_{ij=1}^n A_{ij} \eta_i^* \eta_j\right) = \det \hat{A}. \quad (3.4.42)$$

This is proven as for bosons, using the fact that a hermitean matrix, \hat{A} , can be diagonalized with an $\mathrm{SO}(n)$ matrix. We only need the substitution rule for our Grassmann integrations. First of all for a general function it is clear that one only needs to consider

$$f(\eta_{\alpha}, \eta_{\alpha}^*) = \dots + f_{1\dots n} \prod_{\alpha=1}^n \eta_{\alpha} \eta_{\alpha}^*. \quad (3.4.43)$$

Then the integral reads

$$\int d^n \eta^* d^n \eta f(\eta_{\alpha}, \eta_{\alpha}^*) = f_{1\dots n}. \quad (3.4.44)$$

Now we consider the substitution

$$\eta'_{\alpha} = \sum_{\beta} M_{\alpha\beta} \eta_{\beta}, \quad \eta_{\alpha}^* = \sum_{\beta} N_{\alpha\beta} \eta_{\beta}^*. \quad (3.4.45)$$

Then

$$\prod_{\alpha=1}^n \eta'_\alpha = \prod_{\alpha=1}^n \sum_{\beta} M_{\alpha\beta} \eta_\beta. \quad (3.4.46)$$

The only non-vanishing contribution is the one, where all indices β are different, i.e.,

$$\prod_{\alpha=1}^n \eta'_\alpha = \prod \beta = 1^n \eta_\beta \sum_{P \in \mathcal{S}_n} \sigma(P) \prod_{\alpha=1}^n M_{\alpha P(\alpha)} = \prod_{\beta=1}^n \eta_\beta \det \hat{M}. \quad (3.4.47)$$

From this we get

$$f(\eta'_a, \eta'^*_a) = \dots + f_{1\dots n} \prod_{\alpha=1}^n \eta'_\alpha \eta'^*_\alpha = \dots f_{1\dots n} \det(\hat{M}\hat{N}) \prod_{\alpha} \eta_\alpha \eta^*_\alpha \quad (3.4.48)$$

Thus in order to have

$$f_{1\dots n} = \int d^n \eta'^* d^n \eta' f(\eta'_a, \eta'^*_a) = \int d^n \eta^* d^n \eta f(\eta'_a, \eta'^*_a) \quad (3.4.49)$$

as for usual integral we have to define

$$\int d^n \eta'^* d^n \eta' = \int d^n \eta^* d^n \eta \frac{1}{\det(\hat{M}\hat{N})}. \quad (3.4.50)$$

In the substitution rule thus the determinant of the transformation appears in the denominator instead of the numerator for usual numbers. Thus we can keep in mind that concerning Gaussian integrals and the substitution rule in the Grassmann integrals the determinants appear on the opposite place compared to the rules for normal integrals.

For the proof for the Gaussian integral we need

$$\sum_{\alpha\beta} A_{\alpha\beta} \eta'_\alpha \eta'_\beta = \sum_{\alpha,\dots,\delta} A_{\alpha\beta} U_{\alpha\gamma}^* \eta_\gamma^* U_{\beta\delta} \eta_\delta = \sum_{\alpha} \lambda_{\alpha} \eta_\alpha^* \eta_\alpha. \quad (3.4.51)$$

There we have assumed that

$$\hat{U}^\dagger \hat{A} \hat{U} = \text{diag}(\lambda_1, \dots, \lambda_n). \quad (3.4.52)$$

Thus we only have to apply the substitution rule (3.4.50) for $\hat{M} = \hat{U}^{\dagger T}$ and $\hat{N} = \hat{U}$. Then we have $\det \hat{M}\hat{N} = \det \hat{U}^\dagger \det \hat{U} = 1$, and this proves (3.4.42).

We only have to think about the Euclidean form of the action. This we most achieve most easily using

$$iS_E = \int_{\mathcal{V}} d^4x \bar{\psi} (i\not{\partial} - m) \psi = -i \int_0^\beta d\tau \int_V d^3\vec{x} \bar{\psi} (-\gamma^0 \partial_\tau - i\vec{\gamma} \vec{\nabla} - m) \psi. \quad (3.4.53)$$

Setting

$$\gamma_0^{(E)} = \gamma^0, \quad \gamma_j^{(E)} = -i\gamma^j, \quad (3.4.54)$$

we find

$$S_E = \int_0^\beta d\tau \int_V d^3\vec{x} \bar{\psi} (\gamma_\mu^{(E)} \partial_\mu^{(E)} + m) \psi = \int_0^\beta d\tau \int_V d^3\vec{x} \bar{\psi} (\not{\partial}^{(E)} + m) \psi. \quad (3.4.55)$$

We note that the Euclidean Dirac matrices are all hermitean and build the Clifford algebra of Euclidean space with a positive metric,

$$\{\gamma_\mu^{(E)}, \gamma_\nu^{(E)}\} = \delta_{\mu\nu}. \quad (3.4.56)$$

3.4.2 Partion sum for non-interacting Dirac fermions

The partition sum then reads

$$Z = N \int_{\text{KMS}} \overline{D\psi} D\psi \exp(-S_E). \quad (3.4.57)$$

Since this is a Gaussian integral over Grassmann numbers we can immediately give the result, using (3.4.42):

$$Z = N \text{Det}(\not{d}^{(E)} + m). \quad (3.4.58)$$

Here, the determinant is in the numerator. Otherwise the calculation is pretty similar to the Bosonic case. The only difference are the quasi-antiperiodic boundary conditions (3.4.39) and (3.4.40). We can take the determinant with respect to the Dirac-spinor space first, leading to

$$\det_{\text{spin}}(\not{d}^{(E)} + m) = (-\square_E + m^2)^2. \quad (3.4.59)$$

The partition sum thus is

$$Z = N [\text{Det}_x(-\square_E + m^2)]^2. \quad (3.4.60)$$

The grand-canonical potential thus is

$$\Phi = -T \ln Z = -2T \text{Tr}_x \ln \left(\frac{-\square_E + m^2}{M^2} \right), \quad (3.4.61)$$

where we have written the indetermined constant in terms of a mass-scaling parameter M in order to make the argument of the logarithm dimensionless. The **degeneracy factor** 2 stems from the $2s + 1$ spin-degrees of freedom, where for the here considered Dirac fermions $s = 1/2$.

The evaluation of the functional trace also parallels the bosonic case. Again, we use the heat-kernel method. Again we can immediately use (3.2.85) but we have to take into account the fermionic KMS conditions (3.4.39) and (3.4.40). This leads to the summation over different Matsubara frequencies,

$$\psi(\tau, \vec{x}) = T \sum_{\tilde{\omega}_n} \int_{\mathbb{R}} \frac{d^3 \vec{p}}{(2\pi)^3} \tilde{\psi}(p) \exp(i\vec{p} \cdot \vec{x}) \exp(-p_0 \tau) \Big|_{p_0 = i\tilde{\omega}_n + \mu}, \quad (3.4.62)$$

where the **fermionic Matsubara frequencies** are given by

$$\tilde{\omega}_n = (2n + 1)\pi T, \quad n \in \mathbb{Z}. \quad (3.4.63)$$

They lead to the additional sign in the fermionic KMS conditions in comparison to the bosonic case. The heat kernel for the functional determinant (3.4.61) thus reads

$$\tilde{H}(\alpha) = \frac{M^3 V}{8\pi^{3/2}} \Gamma(-\epsilon) \sum_{\tilde{\omega}_n} \left(\frac{m^2 + (\tilde{\omega}_n - i\mu)^2}{m^2} \right)^\epsilon \quad \text{with} \quad \epsilon = \frac{3}{2} - \alpha. \quad (3.4.64)$$

This means we can also reuse (3.2.86) to evaluate the fermionic Matsubara sum with help of (B.2.4). Instead of (3.2.87) and (3.2.88) we finally have

$$\begin{aligned} \tilde{H}_+(\alpha) &= -\frac{M^3 \beta V}{16\pi^{5/2}} \sin(\pi\epsilon) \Gamma(-\epsilon) \int_m^\infty dp_0 [1 - 2f_F(p_0 - \mu)] \left(\frac{p_0^2 - m^2}{M^2} \right)^\epsilon, \\ \tilde{H}_-(\alpha) &= -\frac{M^3 \beta V}{16\pi^{5/2}} \sin(\pi\epsilon) \Gamma(-\epsilon) \int_m^\infty dp_0 [1 - 2f_F(p_0 + \mu)] \left(\frac{p_0^2 - m^2}{M^2} \right)^\epsilon. \end{aligned} \quad (3.4.65)$$

The T and μ independent **divergent vacuum part** is identical as for bosons, except for the sign and the spin-degeneracy factor, which we write as $2s + 1$ to make its origin explicit:

$$\begin{aligned}\Phi_{\text{vac,reg}} &= -(2s + 1)[\tilde{H}_+(\alpha \rightarrow 0) - \tilde{H}_-(\alpha \rightarrow 0)] \\ &= \frac{(2s + 1)V m^4}{64\pi^2} \left[\frac{2}{\alpha} + 3 - 2\gamma_E - 2 \ln \left(\frac{m^2}{M^2} \right) \right] + \mathcal{O}(\alpha).\end{aligned}\quad (3.4.66)$$

For the thermal part we can again set $\alpha = 0$. Here, the sign in (3.4.61) is cancelled by the sign in front of the Fermi-Dirac distribution in (3.4.65). Thus we find in close analogy to (3.2.91)

$$\begin{aligned}\Phi_{\text{therm}} &= -(2s + 1)TV \int_{\mathbb{R}^3} \frac{d^3\vec{p}}{(2\pi)^3} \ln \left[1 + \exp \left(-\frac{\omega - \mu}{T} \right) \right] \\ &\quad - (2s + 1)TV \int_{\mathbb{R}^3} \frac{d^3\vec{p}}{(2\pi)^3} \ln \left[1 + \exp \left(-\frac{\omega + \mu}{T} \right) \right],\end{aligned}\quad (3.4.67)$$

where $\omega = \sqrt{\vec{p}^2 + m^2}$. The finally occurring extra sign originates from the additional sign in

$$f_F = -T \partial_{p_0} \ln [1 + \exp(-\beta p_0)], \quad (3.4.68)$$

which has to be used when integrating by parts as in the bosonic case in the step from (3.2.90) to (3.2.91). As in the bosonic case the upper line is the contribution from the particles, the upper from the antiparticles. We note that there is no restriction to the chemical potential anymore, and thus there is no need for a condensation mechanism as for bosons for $T \rightarrow 0^+$.

To derive the other thermodynamical quantities it is again more convenient to use

$$\Omega_{\text{therm}}(\beta, \alpha) = \ln Z = -\beta \Phi_{\text{therm}}(T = 1/\beta, \mu = T\alpha). \quad (3.4.69)$$

Then we have (cf. (2.1.23), (2.1.26), and (2.1.39))

$$U = -\left(\frac{\partial \Omega}{\partial \beta} \right)_{V, \alpha} = (2s + 1)V \int_{\mathbb{R}^3} \frac{d^3\vec{p}}{(2\pi)^3} \omega [f_F(p_0 - \mu) + f_F(p_0 + \mu)], \quad (3.4.70)$$

$$\langle Q \rangle = \left(\frac{\partial \Omega}{\partial \alpha} \right)_{V, \beta} = (2s + 1)V \int_{\mathbb{R}^3} \frac{d^3\vec{p}}{(2\pi)^3} [f_F(p_0 - \mu) - f_F(p_0 + \mu)] \quad (3.4.71)$$

$$\begin{aligned}S &= -\left(\frac{\partial \Phi}{\partial T} \right)_{V, \mu} = -(2s + 1)V \int_{\mathbb{R}^3} \frac{d^3\vec{p}}{(2\pi)^3} \{ [1 - f_F(\omega - \mu)] \ln [1 - f_F(\omega - \mu)] \\ &\quad + f_F(\omega - \mu) \ln [f_F(\omega - \mu)] + (\mu \rightarrow -\mu) \}.\end{aligned}\quad (3.4.72)$$

3.4.3 The free propagator

As an example for the derivation of the free real-time propagator, using the opposite way than that used for bosons, namely starting from the Matsubara propagator, we calculate the free propagator for Dirac fermions. Here and in the following the γ^μ are the usual Minkowski space Clifford-algebra elements:

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}. \quad (3.4.73)$$

The easiest way to find the real-time propagators is to start with the Matsubara propagator which is defined in terms of real-time quantities by

$$\Delta_{\text{FM}}^{-1}(i\tilde{\omega}_n + \mu, \vec{p}) = -(\not{p} - m)|_{p_0=i\tilde{\omega}_n+\mu}, \quad (3.4.74)$$

where we used the momentum representation. Here the $\tilde{\omega}_n$ are the Fermion Matsubara frequencies as defined in (3.4.63). Inverting the matrix yields

$$\Delta_{\text{FM}}(i\omega_n + \mu, \vec{p}) = - \left. \frac{\not{p} + m}{p^2 - m^2} \right|_{p_0 = i\omega_n + \mu}. \quad (3.4.75)$$

The first step to find the real-time matrix propagator by analytic continuation is to transform to the Mills representation, which is defined by

$$\Delta_{\text{FM}}(\tau, \vec{p}) = - \frac{1}{\beta} \sum_{n=-\infty}^{\infty} \frac{\not{p} + m}{p_0^2 - \omega^2} \exp(-p_0 \tau) \Big|_{p_0 = i\omega_n + \mu} \quad \text{with } \omega = \sqrt{\vec{p}^2 + m^2}. \quad (3.4.76)$$

Now we can use (B.2.3) and the residuum theorem as in Sect. B.1.3. Finally we get

$$\begin{aligned} \Delta_{\text{FM}}(\tau, \vec{p}) &= \frac{1}{2\omega} [1 - f_{\text{F}}(\omega - \mu)] (\gamma^0 \omega - \vec{p} \vec{\gamma} + m) \exp(-\omega \tau) \\ &\quad - \frac{1}{2\omega} f_{\text{F}}(\omega + \mu) (-\gamma^0 \omega - \vec{p} \vec{\gamma} + m) \exp(\omega \tau) \end{aligned} \quad (3.4.77)$$

As discussed in Sect. B.1.2 the analytic continuation to complex τ gives $-i\Delta_{\text{FM}}^{21}(t, \vec{p})$ for $\tau = it$. The Fourier transformation wrt. t yields after some algebra

$$i\Delta_{\text{F}}^{21}(p) = 2\pi [1 - f_{\text{F}}(p_0 - \mu)] \sigma(p_0) (\not{p} + m) \delta(p^2 - m^2). \quad (3.4.78)$$

Using the path integral and the KMS conditions (3.4.39) and (3.4.40) we find the KMS condition for the off-diagonal real-time Green's functions:

$$\Delta_{\text{F}}^{21}(x) = -\exp(-\mu\beta) \Delta^{12}(x_0 + i\beta, \vec{x}) \Leftrightarrow \Delta^{12}(p) = -\exp[-\beta(p_0 - \mu)] \Delta^{21}(p). \quad (3.4.79)$$

With the identity $1 - f_{\text{F}}(-z) = f_{\text{F}}(z)$ from (3.4.78) we get

$$i\Delta_{\text{F}}^{12}(p) = -2\pi f_{\text{F}}(p_0 - \mu) \sigma(p_0) (\not{p} + m) \delta(p^2 - m^2). \quad (3.4.80)$$

For practical calculations it is more convenient to rewrite the propagator in a form, where it splits into a vacuum and an in-medium part explicitly. That can be done by using the identity

$$f_{\text{F}}(-x) = 1 - f_{\text{F}}(x). \quad (3.4.81)$$

Then, introducing the functions

$$n_{\text{F}}^{\pm}(p_0) = f_{\text{F}}(|p_0| \pm \mu), \quad (3.4.82)$$

we find after some simple algebraic manipulations

$$\begin{aligned} i\Delta_{\text{F}}^{21}(p) &= 2\pi \{ \Theta(p_0) [1 - n_{\text{F}}^-(p_0)] - \Theta(-p_0) n_{\text{F}}^+(p_0) \} (\not{p} + m) \delta(p^2 - m^2), \\ i\Delta_{\text{F}}^{12}(p) &= 2\pi \{ \Theta(-p_0) [1 - n_{\text{F}}^+(p_0)] - \Theta(p_0) n_{\text{F}}^-(p_0) \} (\not{p} + m) \delta(p^2 - m^2). \end{aligned} \quad (3.4.83)$$

One should note that n_{F}^- refers to particles n_{F}^+ to antiparticles.

As a consistency check we calculate the retarded Green's function from the dispersion relation

$$\begin{aligned} \Delta_{\text{FR}}(p) &= \int \frac{dz}{2\pi} \frac{A_{\text{F}}(z, \vec{p})}{p_0 + i0^+ - z}, \\ A_{\text{F}}(p) &= i[\Delta_{\text{F}}^{21}(p) - \Delta_{\text{F}}^{12}(p)] = 2\pi \sigma(p_0) (\not{p} + m) \delta(p^2 - m^2). \end{aligned} \quad (3.4.84)$$

Indeed we find the correct result

$$\Delta_{\text{FR}}(p) = \frac{\not{p} + m}{p_0^2 - \omega^2 + i0^+ \sigma(p_0)}. \quad (3.4.85)$$

From the general relations (3.1.37) we find also the diagonal-matrix elements of the real-time propagators:

$$\begin{aligned} \Delta_{\text{F}}^{11}(p) &= \Delta_{\text{FR}}(p) + \Delta_{\text{F}}^{12}(p) \\ &= \left\{ \frac{1}{p^2 - m^2 + i0^+} + 2\pi i [\Theta(p_0)n_{\text{F}}^-(p_0) + \Theta(-p_0)n_{\text{F}}^+(p_0)] \delta(p^2 - m^2) \right\} (\not{p} + m), \\ \Delta_{\text{F}}^{22}(p) &= \Delta_{\text{F}}^{21}(p) - \Delta_{\text{FR}}(p) \\ &= \left\{ -\frac{1}{p^2 - m^2 - i0^+} + 2\pi i [\Theta(p_0)n_{\text{F}}^-(p_0) + \Theta(-p_0)n_{\text{F}}^+(p_0)] \delta(p^2 - m^2) \right\} (\not{p} + m). \end{aligned} \quad (3.4.86)$$

3.5 Gauge models

The single-most important type of quantum-field theoretical models in physics are **gauge models**, which have a local gauge symmetry. In this section, we shall investigate first the case of QED and give a path-integral derivation of Planck's radiation Law, i.e., the partition function of **free photons**.

3.5.1 The electromagnetic field

The most simple example for a gauge theory is **Maxwell's electrodynamics**. One can show, using the representation theory of the homogeneous orthochronous Poincaré group, that a massless vector field necessarily must be treated as a gauge-field theory if one likes to use local vector fields A^μ as their representatives [Hee02]. Here, we use the shorter way of "quantizing" the classical electromagnetic field, starting from its Lagrange density,

$$\mathcal{L}_\gamma = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} \quad \text{with} \quad F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu. \quad (3.5.1)$$

As we have emphasized before, for a complete quantization via path integrals, we have to go through the **Hamiltonian** formulation. There we are confronted with the problem of gauge invariance already at the classical level, because the canonical field momenta are given by

$$\Pi_\mu = \frac{\partial \mathcal{L}}{\partial(\partial_0 A^\mu)} = F^0{}_\mu. \quad (3.5.2)$$

Now $\Pi_0 = 0$. This means that A^0 is not a dynamical degree of freedom in the usual sense. Also the manifest covariant structure of the model is lost, because Π_μ is *not* a four vector, but this is the case in the canonical formalism anyway. The reason for the problem of $\Pi_0 = 0$ is **gauge invariance**, because for any scalar field χ the Lagrange density (3.5.1) is invariant under the **local gauge transformation**

$$A'_\mu = A_\mu - \partial_\mu \chi. \quad (3.5.3)$$

We thus can choose A_μ such that

$$A_0 = 0. \quad (3.5.4)$$

In this way we eliminate the nondynamical field-degree of freedom from the Lagrangian. The disadvantage of this **choice of gauge** is that then manifest Lorenz invariance is lost even at the Lagrangian level. We shall, however proceed in this noncovariant way for a while and restore Lorentz invariance later within the path-integral formalism.

The gauge condition (3.5.3) does not fix the gauge completely since we still have the freedom to use a time-independent field $\chi(x) = \tilde{\chi}(\vec{x})$ in the gauge transformation (3.5.3) without violating (3.5.4) for the transformed vector potential if this constraint is fulfilled for the original one. To fix the gauge completely, we can thus choose another arbitrary constraint. We know from classical electromagnetism that a free electromagnetic field has a complete set of plain-wave solutions that are transverse with respect to the propagation direction, given by the wave vector \vec{k} . It is thus most convenient to use the **Coulomb-gauge condition**

$$\partial_\mu A^\mu \stackrel{(3.5.4)}{=} \vec{\nabla} \cdot \vec{A} = 0 \quad (3.5.5)$$

in addition to (3.5.4). For a plain-wave solution this means that $\vec{k} \cdot \vec{A} = 0$, i.e., encodes the transversality of the electromagnetic waves into the vector potential of the electromagnetic field.

Now we want to work within a framework with only two gauge-field degrees of freedom. Obviously from (3.5.5) we can write

$$A^3(x) = \tilde{A}^3[A^1, A^2, x] := - \int_{-\infty}^{x^3} dz' [\partial_1 A^1(t, x^1, x^2, z') + \partial_2 A^2(t, x^1, x^2, z')]. \quad (3.5.6)$$

Further we have

$$\begin{aligned} \Pi_3 &= F^0_3 \stackrel{(3.5.4)}{=} \partial_t A_3 = -\partial_t A^3 = E^3[\Pi_1, \Pi_2] \\ &= - \int_{-\infty}^{x^3} dz' [\partial_1 \Pi^1(t, x^1, x^2, z') + \partial_2 \Pi^2(t, x^1, x^2, z')], \end{aligned} \quad (3.5.7)$$

where we have written E^3 for the three-component of the electric field. In the following we write A^3 and $\Pi_3 = E^3$, understanding the functionals (3.5.6) and (3.5.7).

It is easy to show that all the constraints are compatible with the equations of motion from Hamilton's principle with the Lagrange density (3.5.1)

$$\square A_\mu - \partial_\mu \partial_\nu A^\nu = 0 \quad (3.5.8)$$

which are just Maxwell's equations of motion for the free electromagnetic field.

The Hamilton density is then defined as

$$\mathcal{H}(\Pi_1, \Pi_2, A^1, A^2) = \Pi_\mu \partial_t A^\mu - \mathcal{L} = \frac{1}{2}(\vec{E}^2 + \vec{B}^2) \quad \text{with} \quad B^c = \epsilon^{abc} \partial_a A^b. \quad (3.5.9)$$

This is the well-known (gauge invariant) energy density of the electromagnetic field. Note, however, that here we understand \mathcal{H} as the functional of $E^1 = \Pi_1$, $E^2 = \Pi_2$, A^1 , and A^2 with A^3 and E^3 given by (3.5.6) and (3.5.7) respectively.

Now we can write the **Hamiltonian version** of the path integral. According to the spin-statistics theorem, a spin-one field describes necessarily bosons, and we have to use usual c-number fields for the gauge fields A^1 and A^2 and their conjugate momenta and apply the KMS conditions for bosons. Since

there is no conserved quantity for free photons, we have to write down the partition function for $\mu = 0$. Thus we find for the partition sum

$$Z(\beta) = N \int_{\text{KMS}} \mathcal{D}\Phi^1 \mathcal{D}\Phi^2 \int \mathcal{D}\Pi^1 \mathcal{D}\Pi^2 \exp \left[i \left\{ (\Pi_1 \partial_t A^1 + \Pi_2 \partial_t A^2 - \mathcal{H}) \right\}_{\mathcal{C}_V} \right]. \quad (3.5.10)$$

The direct evaluation of this path integral is, however, not so straight forward, because of the non-local nature of the Hamilton density (3.5.9) with (3.5.6) and (3.5.7) for A^3 and Π_3 . To be able to apply the techniques of the previous sections 3.2 and 3.4 we have to rewrite the path integral as one over a local Hamilton density. Particularly we would like apply the “short cut” to evaluate the partition function with help of the functional determinant over the propagator of the fields as detailed in sect. 3.2.2 and thus like to be able to evaluate the path integrals over the momenta.

Our next goal is thus to reformulate (3.5.10) in terms of a **local Hamilton density**. First we reintroduce the field A^3 satisfying the constraint (3.5.9) with help of the functional δ distribution

$$\delta(\Pi_3 - E^3[\Pi_1, \Pi_2]) = \delta(\vec{\nabla} \cdot \vec{A}) \det \left(\frac{\delta \vec{\nabla} \cdot \vec{A}}{\delta A^3} \right) = \delta(\vec{\nabla} \cdot \vec{\Pi}) \det(\partial_3). \quad (3.5.11)$$

This gives

$$Z(\beta) = N \int_{\text{KMS}} \mathcal{D}A^1 \mathcal{D}A^2 \int \mathcal{D}\Pi_1 \mathcal{D}\Pi_2 \mathcal{D}\Pi_3 \delta(\vec{\nabla} \cdot \vec{\Pi}) \det(\partial_3) \times \delta(\partial_j \Pi_j) \exp \left[i \left\{ \Pi_1 \partial_t A^1 + \Pi_2 \partial_t A^2 - \mathcal{H} \right\}_{\mathcal{C}_V} \right]. \quad (3.5.12)$$

The functional δ distribution we can express as a functional Fourier transform

$$\delta(\vec{\nabla} \cdot \vec{\Pi}) = N \int_{\text{KMS}} \mathcal{D}A^0 \exp \left(\left\{ i A^0 \vec{\nabla} \cdot \vec{\Pi} \right\}_{\mathcal{C}_V} \right). \quad (3.5.13)$$

After an integration by parts and introducing another functional δ distribution to also reintroduce an integral over an auxilliary field A^3 this gives

$$Z(\beta) = N \int_{\text{KMS}} \mathcal{D}^4 A^\mu \int \mathcal{D}^3 \Pi_j \det(\partial_3) \delta(A^3) \times \exp \left[i \left\{ \Pi_j \partial_t A^j - (\partial_j A^0) \Pi_j - \frac{1}{2} \Pi_j \Pi_j - \frac{1}{2} \vec{B}^2 \right\}_{\mathcal{C}_V} \right]. \quad (3.5.14)$$

Now one can do the momentum integrals, which finally leads back to the Lagrangian version of the path integral with

$$Z(\beta) = N'(\beta) \int_{\text{KMS}} \mathcal{D}^4 A^\mu \det(\partial_3) \delta(A^3) \exp \left[i S_{\gamma, \mathcal{C}_V}[A] \right]. \quad (3.5.15)$$

Here, $S_{\gamma, \mathcal{C}_V}$ is the action functional along the vertical part of the contour with the Lagrange density (3.5.1), and the $N'(\beta)$ is our formal notation for the correctly normalized integral measures $\mathcal{D}^4 A^\mu$ as described in detail in Sect. 3.2.2.

Now we still are not able to evaluate the partition sum because of the remaining functional δ distribution in the path integral (3.5.15). To cure this, we use the fact that (3.5.15) is a gauge-invariant expression since we have completely fixed the gauge from the very beginning. Thus, if we write

$$A_\chi^\mu = A^\mu - \partial^\mu \chi \quad (3.5.16)$$

with an arbitrary scalar function χ (3.5.15) cannot change. Thus, because of $D^4 A^\mu = D^4 A_\chi^\mu$ we have

$$Z(\beta) = N'(\beta) \int_{\text{KMS}} D^4 A_\chi^\mu \det(\partial_3) \delta(A_\chi^3 - \partial^3 \chi) \exp[iS_{\gamma, \mathcal{G}_V}[A_\chi]] \quad (3.5.17)$$

Since this is independent of χ we can take an arbitrary functional of $\partial^3 \chi$ and weight the path integral over it without changing $Z(\beta)$ by more than another indefinite temperature independent factor, which we lump into $N'(\beta)$. In order to have a well-defined propagator in the corresponding effective action, we use a weighting factor

$$\exp\left[-\frac{i}{2} \left\{ \Lambda^2 (A_\chi^3)^2 \right\}\right] \quad (3.5.18)$$

(with Λ an arbitrary scale factor of mass dimension 1) and integrate over $\partial^3 \chi$, which gives

$$Z(\beta) = N'(\beta) \int_{\text{KMS}} D^4 A^\mu \det(\partial_3) \exp[iS_{\text{GF}, \mathcal{G}_V}[A]] \quad (3.5.19)$$

with the gauge-fixed action functional

$$S_{\text{GF}, \mathcal{G}_V}[A] = \left\{ -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} - \frac{\Lambda^2}{2} (A^3)^2 \right\}_{\mathcal{G}_V}. \quad (3.5.20)$$

Here the functional determinant $\det(\partial_3)$ is independent of all fields and can thus be taken out of the path integral. From the above calculation it follows that this determinant has to be also understood in the sense of a bosonic functional determinant, and thus we can formally write it as a path integral over two **bosonic** field-degrees of freedom. However, since the determinant must be in the **numerator** we need **Grassmann fields** for this purpose. This technique is borrowed from the analogous analysis by **Faddeev and Popov** for the non-Abelian case. The corresponding Grassmann fields are thus called **Faddeev-Popov ghosts**. Also Feynman has given such an idea before Faddeev and Popov for the Abelian case, and thus for QED the ghosts are sometimes called **Feynman ghosts**. Thus our final path-integral expression for the path integral reads

$$Z(\beta) = N'(\beta) \int_{\text{KMS}} D^4 A^\mu \int_{\text{KMS}} D\eta D\bar{\eta} \exp[iS_{\text{FP}, \mathcal{G}_V}[A, \bar{\eta}, \eta]] \quad (3.5.21)$$

with $S_{\text{FP}, \mathcal{G}_V}[A, \bar{\eta}, \eta] + \{\Lambda \bar{\eta} \partial_3 \eta\}_{\mathcal{G}_V}$.

We have written the action for the Faddeev-Popov ghosts with the same scale parameter as we have introduced above. In principle we could have introduced another arbitrary parameter of mass dimension 1, but this would only lead to an additional temperature independent factor for $Z(\beta)$, which does not lead to any changes in the physical meaning of the partition function. Now we have achieved our goal to write the partition sum for the electromagnetic field in terms of a path integral over a local action functional.

As the derivation shows, we can use **any gauge-fixing condition**

$$g[A, x] = 0 \quad (3.5.22)$$

we like without changing the result, e.g. the Lorenz-gauge condition⁵

$$g_L[A, x] = \frac{1}{\sqrt{\xi}} \partial_\mu A^\mu. \quad (3.5.23)$$

⁵Contrary to many older textbooks we name this gauge constraint after the Danish physicist Ludvig Lorenz, who found this auxilliary condition long before the Dutch physicist Hendrik A. Lorentz and also long before the discovery of the special theory of relativity [JO01].

The reason for this is that we just rewrite the gauge independent partition function, as given by the path integral (3.5.10) with another gauge constraint (3.5.23). The final expression for the Faddeev-Popov action then reads

$$S_{\text{FP}, \mathcal{G}_V}^{(g)}[A, \bar{\eta}, \eta] = \left\{ -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} - \frac{1}{2} g^2[A, x] + \bar{\eta} \hat{F}[g] \eta \right\}_{\mathcal{G}_V} \quad (3.5.24)$$

with $\hat{F}[g] = \left(\frac{\delta g[A_\chi, x]}{\delta \chi} \right)_{\chi=0}$.

For the Lorenz-gauge constraint (3.5.23) we get

$$\hat{F}[g_L] = -\frac{1}{\sqrt{\xi}} \square. \quad (3.5.25)$$

Now it is easy to calculate the partition function, using the short cut explained in sect. 3.2.2. Our original version of the path integral (3.5.21) within this interpretation is given by the **spatial axial gauge**, defined by the constraining functional

$$g_{\text{spatial}}[A, x] = \Lambda A^3 \Rightarrow \hat{F}[g_{\text{spatial}}] = \Lambda \partial_3. \quad (3.5.26)$$

Using this gauge-fixing prescription, the inverse photon propagator in momentum space is given by

$$(\Delta^{-1})_{\text{spatial}}^{\mu\nu}(k) = -g^{\mu\nu} k^2 + k^\mu k^\nu - \Lambda^2 \delta_3^\mu \delta_3^\nu. \quad (3.5.27)$$

The determinant over the tensor indices is given by

$$\det(\Delta^{-1}) = -\Lambda^2 (k^3)^2 (k^2)^2. \quad (3.5.28)$$

in an analogous way as in sect. 3.2.2 for the neutral scalar field, from this expression we find for the contribution of the path integral over the gauge fields to our grand canonical potential

$$\ln Z_\gamma(\beta) = -\text{Tr} \ln(\square/M^2) - \text{Tr} \ln(\Lambda \partial_3/M^2). \quad (3.5.29)$$

The path integral over the Faddeev-popov ghosts also gives a bosonic determinant but *with the opposite sign* because the integration is taken over Grassmann fields. That we have the trace over the bosonic Matsubara frequencies is however due to our above derivation:

$$\ln Z_{\text{FP}} = +\text{Tr} \ln(\Lambda \partial_3/M^2), \quad (3.5.30)$$

and the grand potential becomes, again as shown in sect. 3.2.2

$$\Phi = -T \ln Z(\beta) = T \text{Tr} \ln(\beta^2 \square) = 2TV \int \frac{d^3 \vec{k}}{(2\pi)^3} \ln[1 - \exp(-\beta |\vec{k}|)]. \quad (3.5.31)$$

This is the expected result: We get the partition function for a noninteracting Bose gas with two internal degrees of freedom per particle. For the photon these are the two *physical* spatially transverse polarization states (e.g., left- and right-circular polarized waves, corresponding to helicity states with $\lambda \in \{-1, 1\}$). Here also the less formal reason of the Faddeev-Popov ghosts' nature becomes clear. They are precisely present in the path integral to cancel the two **unphysical field degrees of freedom** contained in the vector field A^μ .

To check explicitly that the same result also is found with the manifestly covariant Lorenz-gauge fixing functional (3.5.25), we note that in this case the determinant of the inverse gauge-field propagator is given by

$$\det(\Delta^{-1}) = -\frac{1}{\xi}(k^2)^2. \quad (3.5.32)$$

The contribution from the gauge fields to the grand-canonical potential in this case thus is

$$\ln Z_\gamma(\beta) = -2 \text{Tr} \ln(\beta^2 \square) + \ln(\sqrt{\xi}), \quad (3.5.33)$$

and the Faddeev-Popov ghosts contribute

$$\ln Z_{\text{FP}}(\beta) = + \text{Tr} \ln(\beta^2 \square) - \ln(\sqrt{\xi}) \quad (3.5.34)$$

This finally leads again to

$$\ln Z(\beta) = - \text{Tr} \ln(\beta^2 \square) = -2V \int \frac{d^3 \vec{k}}{(2\pi)^3} \ln[1 - \exp(-\beta|\vec{k}|)]. \quad (3.5.35)$$

Chapter 4

Self-consistent Φ -derivable approximations

In this chapter we discuss an important technique to evaluate physical quantities in a certain class of self-consistent approximations that are derivable from a functional principle due to Luttinger and Ward [LW60], Baym and Kadanoff [BK61, Bay62], and (in the relativistic context) Cornwall, Jackiw and Tomboulis [CJT74]. These approximation schemes are known under the names “ Φ -derivable approximations”, the CJT formalism and the 2PI formalism. The latter name originates from the fact that the diagrams, defining the corresponding action as a functional of the **mean field** (as in the usual action functional, leading to 1PI diagrams) and the **full propagator (two-point function)**. The equations of motion are given by the stationarity of this generalized action functional under independent variations of both the mean fields and the exact propagators, leading to a self-consistent set of equations for the mean field and the self-energy in terms of the fully dressed Green’s function. As we shall show, this kind of approximations fulfill a set of important constraints like the obedience of conservation laws from underlying symmetry principles and thermodynamic consistency, i.e., the bulk properties of the medium can be derived from both the (approximate) partition sum, defined by the functional with the mean field an propagator given as the solution of the equations of motion, and directly from the corresponding expressions of the Green’s function the Green’s function. As has been shown by Baym [Bay62], only such self-consistent approximations of this kind fulfill all these constraints that are derivable from an appropriate functional $\Gamma[\varphi, D]$.

4.1 Necessity of resummations

The most simple example to demonstrate the necessity of resummations is the self-energy or the partition sum of a massless-boson gas in ϕ^4 theory. The Lagrangian reads

$$\mathcal{L} = \frac{1}{2}(\partial_\mu \phi)(\partial^\mu \phi) - \frac{\lambda}{4!}\phi^4. \quad (4.1.1)$$

In leading order the self-energy is given by the tadpole diagram. Using the real-time formalism this is a pure temperature-dependent constant mass term contributing to the diagonal matrix elements of the inverse Keldysh propagator:

$$\Pi_1^{11} = -\Pi_1^{22} = \frac{i\lambda}{2} \int \frac{d^4 l}{(2\pi)^4} D^{11}(l). \quad (4.1.2)$$

The vacuum part is, of course, quadratically divergent. Using the “physical renormalization scheme”, we can subtract this vacuum distribution completely and lump it into the mass-counter term.

This is allowed, because there is no vacuum divergence involved in this diagram. The remaining thermal part is given by

$$\Pi_{1,\text{ren}}^{11} = \frac{\lambda}{2} \int \frac{d^4 l}{(2\pi)^4} 2\pi \delta(l^2) f_B(|l_0|) = \frac{\lambda}{24} T^2. \quad (4.1.3)$$

Already the contribution at the two-loop level given by the following diagram



$$(4.1.4)$$

shows an infrared divergence in the contribution of the one-loop correction to the four-point vertex. Here, also the regularization of the apparent pinch singularities, as discussed in Sect. 2.2.5, has to be applied. As we have seen there, a resummation of the constant self-energy insertion leads to a propagator with a mass given by this tadpole-self-energy insertion.

Thus we can evaluate the one-loop diagram, using this dressed propagator. Due to the now finite thermal mass, no infrared singularities occur anymore. However, we cannot simply subtract the “vacuum part” anymore since the mass is now a temperature-dependent in-medium contribution. We have to subtract the UV divergent vacuum parts of the diagram, which can be found by evaluating the vacuum part for an arbitrary mass M^2 . It is given by the quadratically divergent contribution

$$\Pi_{1,\text{vac}}^{11} = \frac{i\lambda}{2} \int \frac{d^4 l}{(2\pi)^4} \frac{1}{l^2 - M^2 + i0^+}. \quad (4.1.5)$$

Here, it is most convenient to use dimensional regularization, i.e., to perform the integral in $4 - 2\epsilon$ space-time dimensions. For the standard formulae see [Hee02]. The result is

$$\Pi_{1,\text{vac}}^{11} = -\frac{\lambda}{32\pi^2} M^2 \left[\frac{1}{\epsilon} - \gamma_E + \ln \left(\frac{M^2}{4\pi\mu^2} \right) \right]. \quad (4.1.6)$$

Here, μ is the renormalization scale of dimensional regularization. For $M^2 \rightarrow 0$ this contribution vanishes, and thus does not need to be renormalized. Taking the derivative with respect to M^2 leads to the UV- and IR-divergent sub-diagram in (4.1.4), i.e., the one-loop correction to the four-point vertex for 0 momenta:

$$\partial_{M^2} \Pi_{1,\text{vac}}^{11} = -\frac{\lambda}{32\pi^2} \left[\frac{1}{\epsilon} - \gamma_E + \ln \left(\frac{M^2}{4\pi\mu^2} \right) \right]. \quad (4.1.7)$$

Using the “modified minimal-subtraction scheme”, we renormalize this UV subdivergence by just setting

$$(\partial_{M^2} \Pi_{1,\text{vac}}^{11})_{\text{ren}} = -\frac{\lambda}{32\pi^2} \ln \left(\frac{M^2}{4\pi\mu^2} \right). \quad (4.1.8)$$

Integrating this again with respect to M^2 , demanding that the expression should vanish for $M^2 \rightarrow 0$ leads to

$$(\Pi_{1,\text{vac}}^{11})_{\text{ren}} = \frac{\lambda}{32\pi^2} M^2 \left[1 - \ln \left(\frac{M^2}{4\pi\mu^2} \right) \right]. \quad (4.1.9)$$

Now we can set $M^2 = \lambda T^2/24$. This is a contribution at order λ^2 at the two-loop level.

The temperature-dependent part is given by the analogous expression (4.1.3) with finite mass

$$\Pi_{1,T}^{11} = \frac{\lambda}{2} \int \frac{d^4 l}{(2\pi)^4} 2\pi \delta(l^2 - M^2) f_B(|l_0|) = \frac{\lambda}{4\pi^2} \int_0^L dL \frac{L^2}{\sqrt{M^2 + L^2}} f_B(\sqrt{M^2 + L^2}). \quad (4.1.10)$$

We want to derive a series expansion in powers of $M^2 = \lambda T^2/24$. Using the Matsubara-summation formula (B.1.9), we find

$$T \sum_{\omega_n} \frac{1}{E^2 + \omega_n^2} = \frac{1}{2E} [1 + 2f_B(E)] \quad (4.1.11)$$

or

$$\frac{1}{E} f_B(E) = \frac{T}{E^2} - \frac{1}{2E} + 2T \sum_{n=1}^{\infty} \frac{1}{E^2 + \omega_n^2}. \quad (4.1.12)$$

Plugging this into (4.1.10), defining $E = \sqrt{L^2 + m^2}$ and introducing a regularizing factor $(\mu/L)^\epsilon$ leads to

$$\Pi_{1,T}^{(\epsilon)} = \frac{\lambda}{4\pi^2} \int_0^\infty dL L^2 \left(\frac{\mu}{L}\right)^{2\epsilon} \left[\frac{T}{E^2} - \frac{1}{2E} + 2T \sum_{n=1}^{\infty} \frac{1}{E^2 + (2\pi n T)^2} \right]. \quad (4.1.13)$$

To obtain a formal series in powers of M/T we have to evaluate the first term and then Laurent expand around $\epsilon = 0$. This is the infrared-sensitive part of the integral, leading to

$$\Pi_{1,T}^{(\text{IR})} := \frac{\lambda}{4\pi^2} \int_0^\infty dL L^2 \left(\frac{\mu}{L}\right)^{2\epsilon} \frac{1}{L^2 + M^2} = -\frac{\lambda M T}{8\pi} + \mathcal{O}(\epsilon). \quad (4.1.14)$$

This is already the surprising contribution we are after. Although one might expect that the expansion should go with even powers of M , here we get a contribution with power M . Since in our context $M^2 = \lambda T/24$, we find a contribution of order $\lambda^{3/2}$ in the expansion of the thermal self-energy with respect to powers in the coupling λ which shows that $\lambda = 0$ is not an analytical point if the self-energy is interpreted as function of λ .

The second term gives a contribution

$$\Pi_{1,T}^{(1)} := -\frac{\lambda}{8\pi^2} \int_0^\infty dL \frac{L^2}{\sqrt{L^2 + M^2}} \left(\frac{\mu}{L}\right)^{2\epsilon} = \frac{\lambda M^2}{32\pi^2} \left[\frac{1}{\epsilon} - 1 + \ln\left(\frac{4\mu^2}{M^2}\right) \right] + \mathcal{O}(\epsilon). \quad (4.1.15)$$

The rest we can treat as a formal expansion in powers of M since the non-zero-Matsubara frequencies in the denominator prevent any infrared singularities. Thus we write

$$\frac{1}{E^2 + \omega_n^2} = \frac{1}{L^2 + \omega_n^2} \sum_{k=0}^{\infty} (-1)^k \left(\frac{M^2}{L^2 + \omega_n^2}\right)^k. \quad (4.1.16)$$

In the integral the only UV divergent pieces are those for $k = 0$ and $k = 1$. For $k = 0$ we find

$$\Pi_{1,T}^{(\text{rest}, k=0)} := \frac{\lambda^2}{2\pi} T \sum_{n=1}^{\infty} \int_0^\infty dL L^2 \left(\frac{\mu}{L}\right)^{2\epsilon} \frac{1}{L^2 + \omega_n^2} = \frac{\lambda T^2}{24} + \mathcal{O}(\epsilon). \quad (4.1.17)$$

This shows that after summation over n no UV divergence remains.

For $k = 1$ we find

$$\begin{aligned} \Pi_{1,T}^{(\text{rest}, k=1)} &:= -\frac{\lambda^2 M^2 T}{2\pi} \sum_{n=1}^{\infty} \int_0^\infty dL \frac{L^2}{(L^2 + \omega_n^2)^2} \left(\frac{\mu}{L}\right)^{2\epsilon} \\ &= \frac{\lambda M^2}{32\pi^2} \left[-\frac{1}{\epsilon} + 2 - 2\gamma_E - \ln\left(\frac{\mu^2}{(2\pi T)^2}\right) \right] + \mathcal{O}(\epsilon). \end{aligned} \quad (4.1.18)$$

All other contributions from (4.1.16) to the integral (4.1.13) are UV finite and after some algebra lead to

$$\Pi_{1,T}^{(\text{rest}, k \geq 2)} = \frac{\lambda T^2}{4\sqrt{\pi}} \sum_{k=2}^{\infty} \frac{(-1)^k}{k!} \left(\frac{M}{2\pi T} \right)^{2k} \Gamma\left(k - \frac{1}{2}\right) \zeta(2k - 1). \quad (4.1.19)$$

Adding up all contributions (4.1.14-4.1.19) leads to the UV- and IR-convergent expression

$$\begin{aligned} \Pi_{1,T} &= \frac{\lambda T^2}{24} - \frac{\lambda T^2}{8\pi} \frac{M}{T} + \frac{\lambda M^2}{32\pi^2} \left[1 - 2\gamma_E - 2 \ln\left(\frac{M}{4\pi T}\right) \right] \\ &+ \frac{\lambda T^2}{4\sqrt{\pi}} \sum_{k=2}^{\infty} \frac{(-1)^k}{k!} \left(\frac{M}{2\pi T} \right)^{2k} \Gamma\left(k - \frac{1}{2}\right) \zeta(2k - 1). \end{aligned} \quad (4.1.20)$$

With $M^2 = \lambda T^2/24$ we see that due to the $\lambda^{3/2}$ and the $\ln \lambda$ contribution, the self-energy is not an analytic function around $\lambda = 0$.

This implies that a resummation of the kind employed here is in order: The propagator should be dressed with the thermal self-energy contributions in order to lead to the parametrically correct power expansion in λ (including non-integer powers and logarithmic contributions). This further suggests that the use of (approximate) **self-consistent** propagators might be in order. Here, first one has to ensure that any double counting is avoided. If we use a self-consistently dressed propagator, we must only use **skeleton diagrams** for the self-energies, which are expressed not in terms of the perturbative (free) propagator but in terms of the self-consistent one. Another important point is to obey **conservation laws** for energy, momentum, and various charges (if applicable). Last but not least, one would like to ensure **thermodynamical consistency**, i.e., the approximation should be defined in terms of an effective action with the meaning of the grand-canonical thermal potential as the action functional defined above, so that all bulk thermodynamical properties like energy and particle densities, pressure, entropy, etc. obey the usual thermodynamical rules and that the particle density obtained from the one-body Green's function coincides with the definition from the grand-canonical potential. It has been shown by Baym and Kadanoff that such self-consistent approximations are exactly those given by the so-called Φ -derivable approximations [LW60, BK61, Bay62] which are known in the relativistic many-body-theory community also under the names 2PI or CJT (after Cornwall, Jackiw, and Tomboulis [CJT74]). In the following Section we shall derive these approximations following the modern path-integral treatment in ([CJT74]) and then give proofs for the above mentioned properties concerning the validity of conservation laws and thermodynamic consistencies. Then we also prove the renormalizability of Φ -derivable approximations and discuss some problems concerning symmetries.

4.2 Φ -derivable approximations

Following ([CJT74]) we use the path-integral formalism to define the Φ -derivable approximations, leading to self-consistent equations of motion for the mean fields and self-energy in terms of the full propagator. The idea is very similar to the techniques presented in Section 3.3.2 to derive the loop-expansion of the usual effective action, which is the generating functional for one-particle irreducible (1PI) amputated vertex function.

The new idea compared to these 1PI techniques is the introduction of an additional **bilocal source** into the partition sum,

$$Z[J, K] = \int_{\text{KMS}} \mathcal{D}\phi \exp\left(iS[\phi] + i \{J_1 \phi_1\}_1 + \frac{i}{2} \{K_{12} \phi_1 \phi_2\} \right). \quad (4.2.1)$$

Then $W[J, K] = -i \ln Z[J, K]$ is, read as a functional of the local source J with a fixed bilocal source K , the generating functional for connected Green's function for an action given by

$$S_K[\phi] = S[\phi] + \frac{1}{2} \{K_{12} \phi_1 \phi_2\}_{12}. \quad (4.2.2)$$

Particularly the mean field and connected Green's function at presence of both local and bilocal sources is given by

$$\varphi_1 = \frac{\delta W}{\delta J_1} = \langle \phi_1 \rangle_{J, K}, \quad G_{12} = -\frac{\delta^2 W}{\delta J_1 \delta J_2} = i(\varphi_1 \varphi_2 - \langle \mathcal{T}_\phi \phi_1 \phi_2 \rangle). \quad (4.2.3)$$

Using the path-integral representation for Z (4.2.1) leads to

$$\frac{\delta W}{\delta K_{12}} = \frac{1}{2} (\varphi_1 \varphi_2 + i G_{12}). \quad (4.2.4)$$

The **2PI-action functional** is then defined as the functional double-Legendre transform of W ,

$$\Gamma[\varphi, G] = W[J, K] - \{\varphi_1 J_1\}_1 - \frac{1}{2} \{K_{12}(\varphi_1 \varphi_2 + i G_{12})\}. \quad (4.2.5)$$

Upon variation with respect to the external sources J and K , using (4.2.3) and (4.2.4) to define φ and G as functionals of J and K leads indeed to the conclusion that the natural variables for Γ are indeed φ and G and that

$$\frac{\delta \Gamma}{\delta \varphi_1} = -J_1, \quad \frac{\delta \Gamma}{\delta G_{12}} = -\frac{i}{2} K_{12}. \quad (4.2.6)$$

Following the same strategy as with the 1PI-action functional, we substitute $\phi = \phi' + \varphi$ in (4.2.1). Due to the translation invariance of the path integral measure we get

$$Z[J, K] = \exp\left(iS[\varphi] + i\{J_1 \varphi_1\}_1 + \frac{i}{2} \{K_{12} \varphi_1 \varphi_2\}_{12}\right) Z_1[J', K], \quad (4.2.7)$$

where the new functional Z_1 is defined by

$$Z_1[j, K] = \int_{\text{KMS}} D\phi' \exp\left(\frac{i}{2} \{(\mathcal{D}_{12}^{-1} + K_{12}) \phi'_1 \phi'_2\}_{12} + i\tilde{S}_I[\phi', \varphi] + i\{j_1 \phi'_1\}\right). \quad (4.2.8)$$

In (4.2.7) we have further introduced the abbreviations

$$\mathcal{D}_{12}^{-1} = \frac{\delta^2 S[\varphi]}{\delta \varphi_1 \delta \varphi_2} = \left(-\Delta_1 - m^2 - \frac{\lambda}{2} \varphi_1^2\right) \delta^{(4)}(x_1 - x - 2), \quad (4.2.9)$$

$$\tilde{S}_I[\phi', \varphi] = S[\varphi] - \left\{ \frac{\delta S[\varphi]}{\delta \varphi_1} \phi'_1 \right\}_1 - \frac{1}{2} \{ \mathcal{D}_{12}^{-1} \phi'_1 \phi'_2 \}_{12}, \quad (4.2.10)$$

$$J'_1 = \frac{\delta S[\varphi]}{\delta \varphi_1} + J_1 + \{K_{12} \varphi_2\}_2. \quad (4.2.11)$$

Now we want to prove that the expectation value of ϕ' of the quantum-field theory defined by the action functional $Z_1[j, K]$ must vanish if we demand that

$$\varphi_1 = \frac{\delta W}{\delta J_1} \quad (4.2.12)$$

should hold. To that end we take the functional derivative of (4.2.7) with respect to J . Here it is important that J'_1 is a functional of J, K and φ , but φ is still to be taken as an independent background field. This leads to

$$\begin{aligned} \frac{\delta Z[J, K]}{\delta J_1} &= i\varphi_1 Z + \left. \frac{\delta Z_1[j, K]}{\delta j_1} \right|_{j_1=J'_1} \exp\left(iS[\varphi] + i\{J_1\varphi_1\}_1 + \frac{i}{2}\{K_{12}\varphi_1\varphi_2\}_{12}\right) \\ &= i\varphi_1 Z + i\langle\phi'_1\rangle_{J'_1} Z. \end{aligned} \quad (4.2.13)$$

Now, if we demand that (4.2.12) holds, we must indeed have

$$\langle\phi'_1\rangle_{J'_1} = 0. \quad (4.2.14)$$

Thus we can find approximations for $\Gamma[\varphi, G]$ by evaluating $Z_1[j, K]$ for such a j that $\delta Z_1/\delta j_j = 0$ in the sense of a loop expansion. Now we use the techniques explained in Sect. 3.2.2 to write

$$Z_1[j, K] = \exp(iW_1[j, K]) = \exp\left[\frac{1}{2}\text{Tr}\ln(iGM^2) + i\Gamma_2[\varphi, G]\right], \quad (4.2.15)$$

where M^2 is an arbitrary constant, which is irrelevant for the derivation of the equations of motion and can be used to define the normalization of the partition sum in the vacuum. The functional Γ_2 consists of all two-loop diagrams with vertices defined by $\tilde{S}[\varphi, \phi']$ and the propagator G given by

$$G_{12}^{-1} = \mathcal{D}_{12}^{-1} + K_{12}. \quad (4.2.16)$$

This determines K as a functional of G and φ , while j is already determined as a functional of these quantities through the demand (4.2.14). Putting this result into (4.2.5) using (4.2.7) leads to

$$\Gamma[\varphi, G] = S[\varphi] - \frac{i}{2}\text{Tr}\ln(iGM^2) + \frac{i}{2}\{\mathcal{D}_{12}^{-1}(G_{12} - \mathcal{D}_{12})\}_{12} + \Gamma_2[\varphi, G]. \quad (4.2.17)$$

Now we are interested in the theory at vanishing of the original sources J and K . According to (4.2.6) this determines the equations of motion through the **Baym variational principle**

$$\frac{\delta\Gamma}{\delta\varphi} = 0, \quad \frac{\delta\Gamma}{\delta G} = 0. \quad (4.2.18)$$

Using (4.2.17), the second equation becomes

$$\mathcal{D}_{12}^{-1} - G_{12}^{-1} := \Sigma_{12} = 2i\frac{\delta\Gamma_2}{\delta G_{12}}. \quad (4.2.19)$$

This gives a self-consistent equation for the self-energy, relative to the free propagator \mathcal{D}_{12} (which depends on the mean field $\varphi!$), given as a set of diagrams with **lines representing exact propagators** and vertices determined from $\tilde{S}[\varphi, \phi']$.

Diagrammatically taking the derivative of $i\Gamma_2$ with respect to iG means to open each propagator line of a diagram and summing the result, leaving behind a truncated self-energy diagram. This must not only be one-particle irreducible, i.e., cutting through the diagram separating the external points must hit more than one propagator but also there must not be any self-energy insertions in the internal lines of the diagram, because the lines already represent the full propagator. In other words, Γ_2 as a functional of G must be the generating functional for **1PI truncated self-energy skeleton diagrams**. For $i\Gamma_2$ this

means all diagrams must not get disconnected by cutting one or two lines, i.e., it should be **two-particle irreducible (2PI)**.

Thus, $i\Gamma_2$ is diagrammatically represented by all closed diagrams without external points with propagator lines representing the full propagator, G , and with perturbative point vertices from the classical action $\tilde{S}_\gamma(\varphi, \phi')$, where φ is the external background field, represented by a “needle” and external truncated lines representing the quantum fields, ϕ' , attached to the corresponding space-time vertex point. The equation for the mean field is given by the first equation in (4.2.18):

$$-\left(\square_1 + m^2 + \frac{i\lambda}{2}\varphi_1^2 G_{11}\right)\varphi_1 - \frac{\lambda}{3!}\varphi_1^3 + \frac{\delta\Gamma_2}{\delta\varphi_1} = 0. \quad (4.2.20)$$

As an illustration we give the Γ functional for ϕ^4 theory up to the order λ^2 :

$$i\Gamma[\varphi, G] = iS[\varphi] - \frac{1}{2} \left\{ \mathcal{D}_{12}^{-1}(G_{12} - \mathcal{D}_{12}) \right\}_{12} + \frac{1}{2} \text{Tr} \ln(M^2 iG) \quad (4.2.21)$$

$$+ \text{diagram 1} + \text{diagram 2} + \text{diagram 3} + \mathcal{O}(\lambda^3).$$

Here the last row gives the diagrammatic representation of Γ_2 up to $\mathcal{O}(\lambda^2)$.

4.3 Renormalization of Φ -derivable approximations

To illustrate the renormalization technique applicable for self-consistent Φ -derivable approximations [HK02a, HK02b] in this Section we first treat the model first to order λ at vanishing mean field ($m^2 > 0$) and for the case $\varphi = \text{const}$ and $m^2 < 0$. Then we also discuss the somewhat more complicated case up to order λ^2 . We work in the real-time formalism.

4.3.1 Order λ , $m^2 > 0$

We begin our discussion with the most simple case of ϕ^4 theory up to order λ in the 2PI functional $\Gamma[\varphi, G]$. As we shall see, already this approximation is not trivial, but gives rise to a self-consistently determined temperature-dependent correction to the particle mass, which includes the non-trivial contribution to order $\lambda^{3/2}$ discussed in Sect. 4.1 but in fact resums infinitely many perturbative diagrams. We start with the most simple case of an unbroken field-reflection symmetry, i.e., the symmetry of the action under the transformation $\phi \rightarrow \varphi$, assuming $m^2 > 0$ and the solution $\varphi = 0$. Then $\mathcal{D} = D$ is the usual free propagator, and the self-energy is given by the tadpole diagram with the full propagator. Due to translation invariance this is a constant temperature-dependent correction to the effective squared mass of the particles. It is diagonal in the Keldysh-matrix formalism with

$$\Sigma^{11} = -\Sigma^{22} = \frac{i\lambda}{2}. \quad (4.3.1)$$

Since this is effectively only a one-point function and the equilibrium state is translation invariant in space and time, it is also a constant. This means that in this case the full propagator has the same form as the free propagator but with the **temperature dependent mass**

$$M^2 = m^2 + \Sigma^{11}. \quad (4.3.2)$$

Thus we have

$$G^{11}(p) = \frac{1}{p^2 - M^2 + i0^+} - 2\pi i \delta(p^2 - M^2) f_B(|p_0|). \quad (4.3.3)$$

From the diagram rules we find for the dimensionally regularized tadpole self-energy

$$\Sigma^{11} = \frac{i\lambda}{2} \int_{\mathbb{R}^{2\omega}} \frac{d^{2\omega} l}{(2\pi)^4} \frac{\mu^{2\epsilon}}{l^2 - M^2 + i0^+} + \frac{\lambda}{2} \int_{\mathbb{R}^3} \frac{d^3 \vec{l}}{(2\pi)^3} \frac{1}{\omega_M} f_B(\omega_M). \quad (4.3.4)$$

We have written $d = 2\omega = 4 - 2\epsilon$ and $\omega_M = \sqrt{\vec{l}^2 + M^2}$. Of course, we have regularized only the divergent part,

$$\Sigma_{\text{div}}^{11} = -\frac{\lambda M^2}{32\pi^2} \left[\frac{1}{\epsilon} - \gamma_E + 1 + \ln\left(\frac{\mu^2}{M^2}\right) + \mathcal{O}(\epsilon) \right]. \quad (4.3.5)$$

Here, we cannot simply subtract the divergent part $\propto 1/\epsilon$, because M^2 is temperature dependent. We can, however demand that for $T = 0$ the physical mass should be given by $M_{T=0} = m$, i.e., we have to subtract the **mass counter term**

$$\delta m^2 = -\frac{\lambda m^2}{32\pi^2} \left[\frac{1}{\epsilon} - \gamma_E + 1 + \ln\left(\frac{\mu^2}{m^2}\right) + \mathcal{O}(\epsilon) \right], \quad (4.3.6)$$

but this is insufficient to render the tadpole finite:

$$\Sigma_{\text{div}}^{11} - \delta m^2 = -\frac{\lambda \Sigma^{11}}{32\pi^2 \epsilon} + \text{finite terms}. \quad (4.3.7)$$

To show that also the remaining divergence can be subtracted with vacuum counter terms we remember that from a perturbative perspective we resum infinitely many diagrams, also containing one looking like (4.1.4), and this contains a logarithmically diverging vacuum-subdiagram contributing to the four-point function. This piece can thus be renormalized by an appropriate part of the coupling-constant counter term.

To extract this piece we split the full Green's function in our present approximation at finite temperature in the vacuum piece and the rest:

$$\begin{aligned} G(p) &= \frac{1}{p^2 - m^2 + i0^+} + \left(\frac{1}{p^2 - M^2 + i0^+} - \frac{1}{p^2 - m^2 + i0^+} \right) - 2\pi i \delta(p^2 - M^2) f_B(p_0) \\ &= \frac{1}{p^2 - m^2 + i0^+} + \frac{\Sigma^{11}}{(p^2 - m^2 + i0^+)^2} + \mathcal{O}\left(\frac{1}{(p^2 - m^2 + i0^+)^3}\right) \\ &\quad - 2\pi i \delta(p^2 - M^2) f_B(p_0). \end{aligned} \quad (4.3.8)$$

Plugging this into (4.3.4), we see that despite the pure vacuum piece, which we have already renormalized, the remaining divergent part is due to a logarithmically divergent one-loop contribution to the four-point function in the vacuum:

$$i \begin{array}{c} \textcircled{\Sigma^{11}} \\ \downarrow \uparrow \\ \times \\ \swarrow \searrow \end{array} = \Sigma_2^{11} = \frac{\lambda \Sigma^{11}}{2} \int_{\mathbb{R}^{2\omega}} \frac{d^{2\omega} l}{(2\pi)^4} \frac{\mu^{2\epsilon}}{(l^2 + m^2 + i0^+)^2} = -\frac{\lambda \Sigma^{11}}{32\pi^2} \left[\frac{1}{\epsilon} - \gamma_E + \ln\left(\frac{\mu^2}{m^2}\right) \right]. \quad (4.3.9)$$

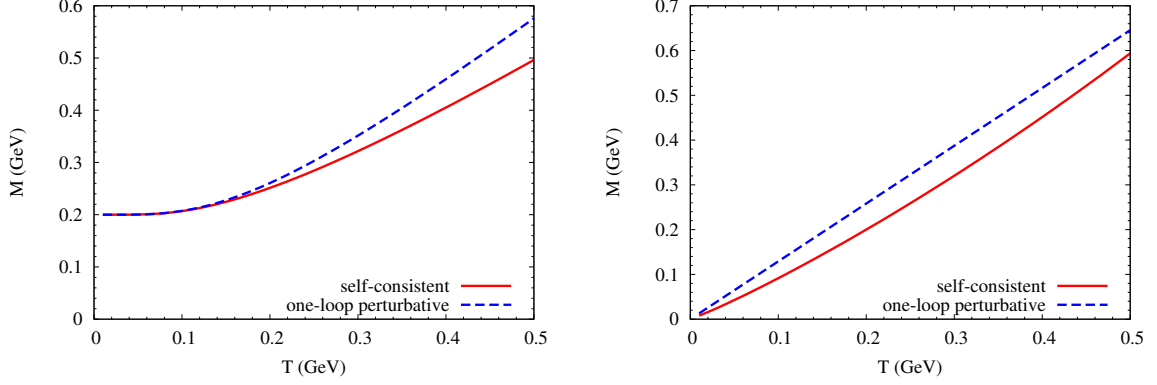


Figure 4.1: *Left panel: The numerical solution of Eq. (4.3.10). We show the self-consistent result (solid red line) in comparison to the perturbative one-loop result. As parameters we have chosen $m = 0.2$ GeV and $\lambda = 40$; right panel: the same but for $m = 0$, $\lambda = 0$, $\Lambda = 0.1$ GeV.*

Taking as a renormalization condition that in the vacuum the four-point coupling is given by λ at vanishing four-momenta, we have to subtract also this contribution from (4.3.5). Also adding the finite piece with the explicit temperature dependence, we finally get the **gap equation**

$$M^2 = m^2 + \frac{\lambda}{32\pi^2} \left[M^2 \ln \left(\frac{M^2}{m^2} \right) + m^2 - M^2 \right] + \frac{\lambda}{4\pi^2} \int_0^\infty dL \frac{L^2}{\omega_M} f_B(\omega_M). \quad (4.3.10)$$

This equation is easily solved numerically by fixed-point iteration (see left panel in Fig. 4.1).

4.3.2 Order λ , $m^2 = 0$

Now we investigate the same case as in the previous section but with $m^2 = 0$, considering solutions of the self-consistent equations with vanishing mean field, $\varphi = 0$. The whole calculation is analogous as for $m^2 > 0$. The only difference is that for $T = 0$ the vacuum-tadpole diagram vanishes in dimensional regularization automatically. Thus we only have to renormalize the logarithmic divergence from the four-point function, but at $m = 0$ we cannot subtract at vanishing four-momenta on the external legs. Instead in the vacuum we subtract the vacuum-four-point function at the symmetric space-like point $s = t = u = -\Lambda^2$, where s , t , and u denote the usual Mandelstam variables for four-point scattering. The corresponding renormalized gap equation then reads

$$M^2 = \Sigma^{11} = \frac{\lambda}{32\pi^2} M^2 \left[1 + \ln \left(\frac{M^2}{\Lambda^2} \right) \right] + \frac{\lambda}{4\pi^2} \int_0^\infty dL \frac{L}{\omega_M} f_B(\omega_M). \quad (4.3.11)$$

Again this equation can be solved numerically by iteration. The result is shown in the right panel of Fig. 4.1.

4.4 Symmetry analysis of the 1PI and 2PI action functionals

4.5 Linear $O(N)$ - σ model

Part II

Nonequilibrium Theory

Chapter 5

Classical transport theory

As a preparation for the quite abstract treatment of the **non-equilibrium quantum field theory**, in this chapter we give a self-contained overview about **classical transport theory**. We start with the derivation of the **non-relativistic Boltzmann equation for a dilute gas of interacting particles** and further approximations like **ideal and viscous hydrodynamics** with applications to the basic phenomena of electromagnetic plasmas. Finally we discuss the basic properties of relativistic transport theory. We follow in this chapter mainly [LP81] and [dvv80]. As we shall see, our derivation is not completely classical, but we have to refer to some basic quantum-theoretical input at characteristic places of our treatment of many-body theory.

5.1 Hamiltonian dynamics and Liouville's theorem

Classical statistical physics deals with the treatment of systems of many point particles. Here we constrain ourselves to the most simple example for such a system that can be described by the **Hamilton function**

$$H = \sum_{j=1}^N \frac{\vec{p}_j^2}{2m} + \frac{1}{2} \sum_{j=1}^N \sum_{k \neq j}^N V(|\vec{x}_j - \vec{x}_k|), \quad (5.1.1)$$

i.e., the particles are interacting via forces between particle pairs that have a **central potential**. We also assume that this potential is **short-ranged**, i.e., that $V(r)$ is a function, rapidly going to 0 for $r \rightarrow \infty$. As will become clear later, **long-range potentials** like the Coulomb potential require special treatment in many-body theory.

With this Hamilton function we aim to describe a gas within a cubic box of length L as a system of interacting classical point particles. Of course, since in this case the number of particles is in the order of Avogadro's number, i.e., $N \simeq 10^{24}$, we have no chance to solve the equations of motion in phase space, which are given by Hamilton's canonical equations,

$$\dot{\vec{x}}_j = \frac{\partial H}{\partial \vec{p}_j} = \frac{\vec{p}_j}{m}, \quad \dot{\vec{p}}_j = -\frac{\partial H}{\partial \vec{x}_j} = -\sum_{k \neq j} \frac{\vec{x}_j - \vec{x}_k}{|\vec{x}_j - \vec{x}_k|^3} V'(|\vec{x}_j - \vec{x}_k|). \quad (5.1.2)$$

On the other hand, such a detailed description of the gas is not even sensible. What we like to describe are **macroscopic observables** like the gas's density and flow as a function of time and position for some given initial condition of such parameters. Transport theory aims to derive equations for such macroscopic observables.

The idea for this treatment goes back to **Bernoulli, Maxwell, and Boltzmann**. The basic ansatz is to describe the behavior of the many-body system by **statistical phase-space distribution functions**. Formally the picture behind this is to define an **ensemble** of many realizations of the many-body system by preparing each of this realizations in a way, such that the microscopic initial conditions (fixing \vec{x}_j and \vec{p}_j at the initial time) fitting some given macroscopic parameters like the density and flow of the gas.

For a complete description of this kind, one would have to give some distribution of the $6N$ phase-space variables $(\vec{x}_1, \vec{p}_1; \vec{x}_2, \vec{p}_2; \dots; \vec{x}_N, \vec{p}_N) = (\tau_1, \dots, \tau_N)$ at an initial time and calculate the time evolution of this distribution from the Hamiltonian dynamics¹. This, of course is as impossible as the microscopic approach, because it is equivalent to it. In order to solve this problem, one would have to solve the Hamiltonian equations of motion (5.1.2) for many different initial conditions to define the ensemble and then calculating the **N -body phase-space distribution function**

$$f^{(N)}(t, \tau_1, \dots, \tau_N) = \left\langle \delta^{(6N)}(\tau_1 - \tilde{\tau}_1(t), \dots, \tau_N - \tilde{\tau}_N(t)) \right\rangle, \quad (5.1.3)$$

where the average is over the ensemble defined by the initial conditions. The $\tilde{\tau}_j(t)$ is the solution of the Hamiltonian equations of motion for the N particles in phase space with initial conditions $\tilde{\tau}_j(t = t_0) = \tilde{\tau}_{j0}$, which are given in a statistical sense by the corresponding initial distribution

$$f^{(N)}(t = t_0, \tau_1, \dots, \tau_N) = f_0^{(N)}(\tau_1, \dots, \tau_N). \quad (5.1.4)$$

As a probability distribution (5.1.3) fulfills

$$\int_{\Gamma} d^6 \tau_1 \cdots d^6 \tau_N f^{(N)}(t, \tau_1, \dots, \tau_N) = \int_{\Gamma} d^6 \tau_1 \cdots d^6 \tau_N f^{(N)}(t, \tau_1, \dots, \tau_N) = 1. \quad (5.1.5)$$

Here Γ denotes the integration domain over the box volume V for each particle's position vector and \mathbb{R}^3 for each particle's momentum vector.

On the other hand for each initial condition the Hamilton equations of motion lead to a unique solution in phase phase space at any later time t . Thus the phase-space distribution must be given from the initial distribution via this **flux in phase space**:

$$f^{(N)}(t, \tau_1, \dots, \tau_N) = f_0^{(N)} \left[\tilde{\tau}_1^{(0)}(t; \tau_1, \dots, \tau_N), \dots, \tilde{\tau}_N^{(0)}(t; \tau_1, \dots, \tau_N) \right]. \quad (5.1.6)$$

Here $\tilde{\tau}_j^{(0)}(t; \tau_1, \dots, \tau_N)$ are those initial conditions for the N particles leading to a configuration of this system at time t given by the phase-space point (τ_1, \dots, τ_N) .

We shall now prove that this dynamics of the N -particle distribution function is consistent with the normalization condition (5.1.5). Indeed, taking the time derivative of (5.1.5) taking into account that the phase-space points move with time according to the Hamiltonian dynamics leads to

$$\int_{\Gamma} d^6 \tau_1 \cdots d^6 \tau_N \left[\partial_t f^{(N)}(t, \tau_1, \dots, \tau_N) + \sum_{j=1}^N \frac{\partial}{\partial \tau_j} [\dot{\tau}_j f^{(N)}(t, \tau_1, \dots, \tau_N)] \right] = 0. \quad (5.1.7)$$

but now we have

$$\sum_{j=1}^N \frac{\partial}{\partial \tau_j} (\dot{\tau}_j f^{(N)}) = \sum_{j=1}^N \left[\frac{\partial}{\partial \vec{x}_j} \left(\frac{\partial H}{\partial \vec{p}_j} f^{(N)} \right) - \frac{\partial}{\partial \vec{p}_j} \left(\frac{\partial H}{\partial \vec{x}_j} f^{(N)} \right) \right] = \{H, f^{(N)}\}_{\text{pb}}, \quad (5.1.8)$$

¹Here we have introduced the abbreviation $\tau_j = (\vec{x}_j, \vec{p}_j)$ for the six components of position and momentum vectors of the j^{th} particle.

where we have used the definition **Poisson bracket** of two phase-space functions A and B :

$$\{A, B\}_{\text{pb}} = \sum_{j=1}^N \left(\frac{\partial A}{\partial \vec{x}_j} \cdot \frac{\partial B}{\partial \vec{p}_j} - \frac{\partial A}{\partial \vec{p}_j} \cdot \frac{\partial B}{\partial \vec{x}_j} \right). \quad (5.1.9)$$

This means that

$$\int_{\Gamma} d^6\tau_1 \cdots d^6\tau_N \left[\partial_t f^{(N)} + \{H, f^{(N)}\}_{\text{pb}} \right] = 0. \quad (5.1.10)$$

Now, for a classical system of particles, we also assume that there are no particles destroyed or created in the dynamics. This means that the fraction of particles contained in a phase-space element at initial time will not change when this phase-space element is moving according to the equations of motion. This means that the phase-space distribution function must fulfill even the stronger local condition,

$$\partial_t f^{(N)}(t, \tau_1, \dots, \tau_N) + \sum_{j=1}^N \frac{\partial}{\partial \tau_j} [\dot{\tau}_j f^{(N)}(t, \tau_1, \dots, \tau_N)] = \partial_t f^{(N)} + \{H, f^{(N)}\}_{\text{pb}} = 0. \quad (5.1.11)$$

This continuity equation of the flow in phase space for a closed system of classical particles is known as **Liouville's theorem**.

5.2 The BBGKY Hierarchy

Of course, a solution of the full Liouville equation of motion for the N -body phase-space distribution function (5.1.11) is as demanding as to solve the complete set of Hamilton's equations of motion of the N -particle system itself. The aim thus must be to find approximate equations for the **reduced distribution functions**

$$f^{(k)}(t, \tau_1, \dots, \tau_k) = \int d^6\tau_{k+1} \cdots d^6\tau_N f^{(N)}(t, \tau_1, \dots, \tau_N). \quad (5.2.1)$$

We note that, since the particles are assumed all to be of the same kind, they are indistinguishable, the full N -body distribution function is symmetric under arbitrary changes of the order of phase-space arguments, and thus the choice of the first $N - k$ phase-space variables in the above integral is just convenient. We are particularly interested in an equation for the **one-body phase-space distribution**, $f^{(1)}(t, \tau_1)$ which describes the probability distribution to find a particle in a neighborhood of the one-particle phase-space position τ_1 .

To find an equation of motion for $f^{(1)}$, we have to integrate the Liouville equation (5.1.11) over τ_2, \dots, τ_N . Writing out the Poisson bracket and bringing the terms with the interactions to the right-hand side of the equation, we find

$$\partial_t f_1^{(1)} + \frac{\vec{p}_1}{m} \cdot \frac{\partial f_1^{(1)}}{\partial \vec{x}_1} = (N-1) \int d^6\tau_2 \frac{\partial f_{12}^{(2)}}{\partial \vec{p}_1} \cdot \frac{\partial V_{12}}{\partial \vec{x}_1} \simeq N \int d^6\tau_2 \frac{\partial f_{12}^{(2)}}{\partial \vec{p}_1} \cdot \frac{\partial V_{12}}{\partial \vec{x}_1}, \quad (5.2.2)$$

where we have used the abbreviations $V_{12} := V(|\vec{x}_1 - \vec{x}_2|)$ and $f^{(2)}(t, \tau_1, \tau_2) = f_{12}^{(2)}$. On the left-hand side we have used Gauss's theorem to the integrals over the total divergences with respect to \vec{x}_j and \vec{p}_j and assumed that the distribution functions vanish at the boundary of the corresponding one-body phase space. On the right-hand side we have used the approximation that $N \gg 1$ and have set the factor to N instead of $(N - 1)$.

The general structure of the equations for the reduced phase-space distributions $f^{(k)}$ is already clear from this calculation for $f^{(1)}$: The equation for $f^{(k)}$ will always depend on the next distribution $f^{(k+1)}$. Thus, one finds a hierarchy of coupled integro-differential equations for all $f^{(k)}$ with $k \in \{1, \dots, N\}$. These equations are known as the **BBGKY hierarchy**, named after the physicists Bogolyubov, Born, Green, Kirkwood, and Yvon. It is clear that again this set of equations leads to a full description of the N -body Hamiltonian dynamics since so far we haven't made any approximations. The aim now must be to truncate the hierarchy by making assumptions on $f^{(2)}$ to find a closed equation for $f^{(1)}$. To that end we look at the equation for $f^{(2)}$,

$$\begin{aligned} \partial_t f_{12}^{(2)} + \frac{\partial f_{12}^{(2)}}{\partial \vec{x}_1} \frac{\vec{p}_1}{m} + \frac{\partial f_{12}^{(2)}}{\partial \vec{x}_2} \frac{\vec{p}_2}{m} - \frac{\partial V_{12}}{\partial \vec{x}_1} \frac{\partial f_{12}^{(2)}}{\partial \vec{p}_1} - \frac{\partial V_{12}}{\partial \vec{x}_2} \frac{\partial f_{12}^{(2)}}{\partial \vec{p}_2} \\ \simeq N \int d^6 \tau_3 \left(\frac{\partial f_{123}^{(3)}}{\partial \vec{p}_1} \frac{\partial V_{13}}{\partial \vec{x}_1} + \frac{\partial f_{123}^{(3)}}{\partial \vec{p}_2} \frac{\partial V_{23}}{\partial \vec{x}_2} \right), \end{aligned} \quad (5.2.3)$$

where again we have set the factor $(N-2)$ on the right-hand side of the equation to N due to $N \gg 1$.

5.3 The Boltzmann equation for a dilute gas

In this Section we shall derive the famous **Boltzmann transport equation** for the one-body phase-space distribution for a **dilute gas**. To that end we make the following assumptions to truncate the BBGKY hierarchy:

1. The interaction potential is only relevant for a finite range d , i.e., the forces $-\partial_{\vec{x}_i} V(|\vec{x}_1 - \vec{x}_2|)$ can be neglected for inter-particle distances $r_{12} = |\vec{x}_1 - \vec{x}_2| > d$.
2. The mean distance $\bar{r} := \langle r_{12} \rangle$ of two particles is large compared to the range of the potential, i.e., $\bar{r} \gg d$.

To truncate the BBGKY hierarchy on the level of the one-particle phase-space distribution, we have to first consider the equation (5.2.3) for the two-particle distribution. The idea has to make an assumption such as to express $f^{(2)}$ approximately with $f^{(1)}$. This is achieved by making a formal expansion of the integrals on the right-hand side of Eqs. (5.2.2) and (5.2.3) with respect to the small quantity $d/\bar{r} \ll 1$. For the first term on the right-hand side of the equation, we need to consider only the small sphere $|\vec{x}_3| \lesssim d$ in the integral over position space, and within this small volume we can approximate the interaction force by

$$\frac{\partial V_{13}}{\partial \vec{x}_1} \simeq \frac{\partial V(|\vec{x}_1|)}{\partial \vec{x}_1} \quad (5.3.1)$$

and thus take this factor out of the integral. This leads to

$$N \int d^3 \vec{x}_3 d^3 \vec{p}_3 \frac{\partial f_{123}^{(3)}}{\partial \vec{p}_1} \frac{\partial V_{13}}{\partial \vec{x}_1} \simeq N \frac{\partial V(|\vec{x}_1|)}{\partial \vec{x}_1} \frac{\partial f_{12}^{(2)}}{\partial \vec{p}_1} \frac{d^3}{V}, \quad (5.3.2)$$

where V is the total volume of the container of the gas. Further $V \simeq N\bar{r}^3$ and thus

$$N \int d^3 \vec{x}_3 d^3 \vec{p}_3 \frac{\partial f_{123}^{(3)}}{\partial \vec{p}_1} \frac{\partial V_{13}}{\partial \vec{x}_1} \simeq \frac{\partial V(|\vec{x}_1|)}{\partial \vec{x}_1} \frac{\partial f_{12}^{(2)}}{\partial \vec{p}_1} \frac{d^3}{\bar{r}^3}. \quad (5.3.3)$$

The same kind of approximations we can also apply to the second term on the right-hand side of (5.2.3). These estimates show that the right-hand side of (5.2.3) is parametrically smaller than the left-hand side by a factor $d^3/\bar{r}^3 \ll 1$. Thus we can neglect this right-hand side completely, which leads to the approximate validity of the Liouville equation for the two-body distribution function,

$$\partial_t f_{12}^{(2)} + \frac{\partial f_{12}^{(2)}}{\partial \vec{r}_1} \frac{\vec{p}_1}{m} + \frac{\partial f_{12}^{(2)}}{\partial \vec{r}_2} \frac{\vec{p}_2}{m} - \frac{\partial V_{12}}{\partial \vec{x}_1} \frac{\partial f_{12}^{(2)}}{\partial \vec{p}_1} - \frac{\partial V_{12}}{\partial \vec{x}_2} \frac{\partial f_{12}^{(2)}}{\partial \vec{p}_2} = 0. \quad (5.3.4)$$

This we can also write as

$$\frac{d}{dt} f_{12}^{(2)} = \partial_t f_{12}^{(2)} + \{f_{12}^{(2)}, H^{(2)}\}_{\text{pb}} = 0, \quad (5.3.5)$$

where the two-body Hamilton function is given by

$$H^{(2)} = \frac{\vec{p}_1^2 + \vec{p}_2^2}{2m} + V_{12}. \quad (5.3.6)$$

The physical interpretation of (5.3.4) is now clear: (5.3.5) tells us that in leading order of the expansion in terms of the “gas parameter” $(d/\bar{r})^3$ the two-body phase-space distribution is time independent along the phase-space flow of these two interacting particles. This is, because the range of the interaction, d , of the two particles with a third particle is much smaller than the mean distance between the particles. So the mean time between two collisions is very large compared to the duration of the collision itself, and thus in leading order of $(d/\bar{r})^3$, the change of $f^{(2)}$ due to three-particle collisions can be neglected and thus the **three-body collision integral** on the right-hand side of (5.2.3) can be neglected.

Let us come back to the equation for $f^{(1)}$ (5.2.2). To close this equation, we have to express the collision term on the right-hand side in terms of $f^{(1)}$. To that end we consider a time t_0 at which any two particles, described by the two-body distribution $f^{(2)}$ have a large distance from each other compared to the range of the potential, d . Then we can make the second assumption due to Boltzmann that these two particles are stochastically independent of each other, i.e., that $f^{(2)}(t_0, \tau_1, \tau_2) = f^{(1)}(t_0, \tau_1) f^{(1)}(t_0, \tau_2)$. Now according to (5.1.6) we have

$$\begin{aligned} f^{(2)}(t, \tau_1, \tau_2) &= f_{12}^{(2)}[t_0, \hat{\tau}_1^{(0)}(t, \tau_1, \tau_2), \hat{\tau}_2^{(0)}(t, \tau_1, \tau_2)] \\ &= f^{(1)}[t_0, \hat{\tau}_1^{(0)}(t, \tau_1, \tau_2)] f^{(1)}[t_0, \hat{\tau}_2^{(0)}(t, \tau_1, \tau_2)] := f_{1^0}^{(1)} f_{2^0}^{(1)}, \end{aligned} \quad (5.3.7)$$

where the flow in two-body phase space can be evaluated with the two-body Hamiltonian (5.3.6), because of our above discussed approximations, leading to (5.3.5). This is known as **Boltzmann’s hypothesis of molecular chaos**.

We note that at this point we have tacitly assumed that time is a directed quantity in the sense of the **causality principle**.

According to (5.3.4) and (5.3.7) we have

$$\frac{d}{dt} (f_{1^0}^{(1)} f_{2^0}^{(1)}) = \left[\frac{\vec{p}_1}{m} \frac{\partial}{\partial \vec{x}_1} + \frac{\vec{p}_2}{m} \frac{\partial}{\partial \vec{x}_2} - \frac{\partial V_{12}}{\partial \vec{x}_1} \frac{\partial}{\partial \vec{p}_1} - \frac{\partial V_{12}}{\partial \vec{x}_2} \frac{\partial}{\partial \vec{p}_2} \right] f_{1^0}^{(1)} f_{2^0}^{(1)} = 0. \quad (5.3.8)$$

This we solve for the expression with $\partial/\partial \vec{p}_1$ and substitute this into (5.2.2). Since the contributions with the derivatives with respect to \vec{x}_2 and \vec{p}_2 can be written as total divergences, the corresponding integrals vanish, and we find the following approximation for the collision term²

$$\frac{1}{N} C[f] := N \int d^3 \vec{x}_2 d^3 \vec{p}_2 \left[\frac{\vec{p}_1}{m} \frac{\partial}{\partial \vec{x}_1} + \frac{\vec{p}_2}{m} \frac{\partial}{\partial \vec{x}_2} \right] f_{1^0}^{(1)} f_{2^0}^{(1)}. \quad (5.3.9)$$

²The factor $1/N$ in the definition of the collision term will become clear in a moment.

Due to the spatial translation invariance of the two-particle Hamiltonian (5.3.6) the expression $f_{10}^{(1)} f_{20}^{(2)}$ can only depend on the relative coordinates $\vec{r} = \vec{x}_1 - \vec{x}_2$, and thus we have

$$\frac{1}{N} C[f] = N \int d^3 \vec{x}_2 d^3 \vec{p}_2 \vec{v}_{\text{rel}} \frac{\partial}{\partial \vec{r}} f_{10}^{(1)} f_{20}^{(1)} \quad (5.3.10)$$

with the relative velocity

$$\vec{v}_{\text{rel}} = \frac{\vec{p}_1 - \vec{p}_2}{m} \quad (5.3.11)$$

of the two particles. Now we introduce cylinder coordinates (ρ, φ, z) for \vec{r} with the z axis pointing into the direction of \vec{v}_{rel} . Then the integral (5.3.10) simplifies to

$$\frac{1}{N} C[f] = N \int d^3 \vec{x}_2 d^3 \vec{p}_2 \vec{v}_{\text{rel},z} \frac{\partial}{\partial z} f_{10}^{(1)} f_{20}^{(1)} = \int d^3 \vec{p}_2 d\rho d\varphi \rho v_{\text{rel}} [f_{10}^{(1)} f_{20}^{(1)}]_{z \rightarrow -\infty}^{z \rightarrow \infty}, \quad (5.3.12)$$

where we have symbolically written $z \rightarrow \pm\infty$ that the component of the relative coordinate in direction of \vec{v}_{rel} of the two particles at time t is large compared to the interaction range, d . Thus “ $z \rightarrow -\infty$ ” describes the case that at time t the particles still move towards each other, and thus they have been even farther away from each other at time t_0 . This implies that no collision between these two particles has occurred between t_0 and t , and this implies that $\vec{p}_1^{(0)} = \vec{p}_1$ and $\vec{p}_2^{(0)} = \vec{p}_2$ since the momenta of the particles are conserved, if there is no interaction, i.e., collision between them. The case $z \rightarrow \infty$, however describes the situation that at time t the particles are moving away from each other, and thus there must have been a collision of the two particles on each other. So at time t_0 the two particles must have had momenta \vec{p}'_1 and \vec{p}'_2 such that due to the collision they have momenta \vec{p}_1 and \vec{p}_2 at time t . The area element $\rho d\rho d\varphi$ perpendicular to \vec{v}_{rel} has the meaning of a classical differential cross section for elastic two-body collisions, where the one term (“ $z \rightarrow -\infty$ ”) has the meaning of a scattering of two particles with momenta \vec{p}'_1, \vec{p}'_2 into momenta \vec{p}_1, \vec{p}_2 and the other (“ $z \rightarrow \infty$ ”) has the meaning of scattering two particles with momenta \vec{p}'_1, \vec{p}'_2 to other momenta \vec{p}'_1, \vec{p}'_2 . This leads to gain and loss of particles with momentum \vec{p}_1 due to elastic two-particle collisions, respectively. As soon as the particles move away from each other after a collision, they become free again, i.e., total kinetic energy and momentum are conserved during a collision process:

$$\vec{p}_1 + \vec{p}_2 = \vec{p}'_1 + \vec{p}'_2, \quad \frac{\vec{p}_1^2}{2m} + \frac{\vec{p}_2^2}{2m} = \frac{\vec{p}'_1^2}{2m} + \frac{\vec{p}'_2^2}{2m}. \quad (5.3.13)$$

Now $v_{\text{rel}} \rho d\rho d\varphi = v_{\text{rel}} d\sigma$ is the transition probability per unit time and per projectile and target particle w_{fi} , for a collision scattering a two particles from an initial momentum state i to a final momentum state f . In this way we finally get for the collision term

$$\begin{aligned} \frac{1}{N} C[f] = N \int d^3 \vec{p}_2 \int d^3 \vec{p}'_1 \int d^3 \vec{p}'_2 [& w(\vec{p}_1, \vec{p}_2 \leftarrow \vec{p}'_1, \vec{p}'_2) f^{(1)}(t, \vec{x}_1, \vec{p}'_1) f^{(1)}(t, \vec{x}_1, \vec{p}'_2) \\ & - w(\vec{p}'_1, \vec{p}'_2 \leftarrow \vec{p}_1, \vec{p}_2) f^{(1)}(t, \vec{x}_1, \vec{p}_1) f^{(1)}(t, \vec{x}_1, \vec{p}_2)]. \end{aligned} \quad (5.3.14)$$

Here we also have neglected the small variation of the positions, neglecting the finite range of the potential against the large inter-particle distances and assumed a local collision at the position \vec{x}_1 of the particle under consideration in $f^{(1)}(t, \tau_1)$.

Now we write (5.2.2) in a more custom form by multiplying the whole equation by N , expressing everything in terms of the **single-particle phase-space number density** $f(t, \tau_1) = N f^{(1)}(t, \tau_1)$. It has the

meaning that at time t the phase-space element $d^6\tau_1$ contains on average $dN = d^6\tau_1 f(t, \tau_1)$ particles, where the average is taken as an ensemble average in the sense described in the previous section. This leads to the final form of the **Boltzmann transport equation**:

$$\begin{aligned} \left[\frac{\partial}{\partial t} + \frac{\vec{p}_1}{m} \frac{\partial}{\partial \vec{x}_1} \right] f(t, \vec{x}_1, \vec{p}_1) = & \int d^3\vec{p}_2 \int d^3\vec{p}'_1 \int d^3\vec{p}'_2 \\ & \times \left[w(\vec{p}_1, \vec{p}_2 \leftarrow \vec{p}'_1, \vec{p}'_2) f(t, \vec{x}_1, \vec{p}'_1) f(t, \vec{x}_1, \vec{p}'_2) \right. \\ & \left. - w(\vec{p}'_1, \vec{p}'_2 \leftarrow \vec{p}_1, \vec{p}_2) f(t, \vec{x}_1, \vec{p}_1) f(t, \vec{x}_1, \vec{p}_2) \right]. \end{aligned} \quad (5.3.15)$$

The physical interpretation of the collision integral on the right-hand side is now very simple: It describes the rate of elastic two-body collisions which either scatter one of the two particles from one arbitrary momentum into the momentum \vec{p}_1 (**gain term**) or kick a particle with momentum \vec{p}_1 out of this momentum state (**loss term**).

We can simplify the collision integral further by using the fact that the Hamilton operator (5.4.1) is symmetric under time reversal, $T(\vec{x}_i, \vec{p}_i) = (\vec{x}_i, -\vec{p}_i)$, as well as under spatial reflection, $P(\vec{x}_i, \vec{p}_i) = (-\vec{x}_i, -\vec{p}_i)$, transformations. This implies the corresponding symmetries for the scattering rates, i.e.,

$$\begin{aligned} w(\vec{p}_1, \vec{p}_2 \leftarrow \vec{p}'_1, \vec{p}'_2) &= w(-\vec{p}'_1, -\vec{p}'_2 \leftarrow -\vec{p}_1, -\vec{p}_2) \quad (\text{time-reversal symmetry}), \\ w(\vec{p}_1, \vec{p}_2 \leftarrow \vec{p}'_1, \vec{p}'_2) &= w(-\vec{p}_1, -\vec{p}_2 \leftarrow -\vec{p}'_1, -\vec{p}'_2) \quad (\text{space-reflection symmetry}). \end{aligned} \quad (5.3.16)$$

In the first equation we have taken into account that the time-reversal transformation not only flips the momenta but also initial and final states of the particles. Using also space-reflection symmetry, we finally get

$$w(\vec{p}_1, \vec{p}_2 \leftarrow \vec{p}'_1, \vec{p}'_2) = w(\vec{p}'_1, \vec{p}'_2 \leftarrow \vec{p}_1, \vec{p}_2). \quad (5.3.17)$$

This relation is usually known as the **detailed-balance principles**, because it states that the collision rates for a transition $f \rightarrow i$ equal the one for the opposite transition $i \rightarrow f$. As we shall see in the next Section, this relation leads to a universal **equilibrium distribution**, i.e., under the here considered circumstances the **Maxwell-Boltzmann distribution** for an ideal gas. Using (5.3.17) in (5.3.15) the Boltzmann equation simplifies to

$$\begin{aligned} \left[\frac{\partial}{\partial t} + \frac{\vec{p}_1}{m} \frac{\partial}{\partial \vec{x}_1} \right] f(t, \vec{x}_1, \vec{p}_1) = & \int d^3\vec{p}_2 \int d^3\vec{p}'_1 \int d^3\vec{p}'_2 w(\vec{p}'_1, \vec{p}'_2 \leftarrow \vec{p}_1, \vec{p}_2) \\ & \times \left[f(t, \vec{x}_1, \vec{p}'_1) f(t, \vec{x}_1, \vec{p}'_2) - f(t, \vec{x}_1, \vec{p}_2) f(t, \vec{x}_1, \vec{p}_1) \right]. \end{aligned} \quad (5.3.18)$$

We close this Section with the important remark that this form of the Boltzmann equation also holds without the assumption of time-reversal and space-reflection symmetry of the Hamiltonian. For that we have to use a quantum theoretical argument [LP81]. In quantum theoretical scattering theory the transition rates w_{fi} are given in terms of the **scattering-matrix elements** by

$$w_{fi} = |S_{fi}|^2, \quad (5.3.19)$$

where the scattering operator describes the **unitary quantum-theoretical time evolution** from an asymptotically free initial state to a asymptotically free final state in the interaction picture. To simplify the further line of arguments, we assume that the particles are constrained to a large cubic box, assuming periodic boundary conditions for the corresponding wave functions. Then the possible momenta become discrete, and the **unitarity condition for the scattering operator**,

$$\mathbf{S}^\dagger \mathbf{S} = \mathbf{S} \mathbf{S}^\dagger = \mathbb{1} \quad (5.3.20)$$

translates into the form

$$\sum_f S_{fi}^* S_{fi} = \sum_i S_{fi} S_{fi}^* \Rightarrow \sum_f w_{fi} = \sum_i w_{fi} \quad (5.3.21)$$

for the matrix elements with respect to momentum space. In the limit of an infinite volume, the sums become integrals in the usual way, and the relation reads

$$\int d^3 \vec{p}'_1 d^3 \vec{p}'_2 w(\vec{p}_1, \vec{p}_2 \leftarrow \vec{p}'_1, \vec{p}'_2) = \int d^3 \vec{p}'_1 d^3 \vec{p}'_2 w(\vec{p}'_1, \vec{p}'_2 \leftarrow \vec{p}_1, \vec{p}_2). \quad (5.3.22)$$

This is known as the **weak principle of detailed balance**. In the original form of the Boltzmann equation (5.3.15) the integral with respect to \vec{p}'_1 and \vec{p}'_2 only affects the transition rate w , and we can thus apply (5.3.22) directly to bring the Boltzmann equation into the simpler form (5.3.18). Thus, the universality of the equilibrium distribution follows already from the weaker form (5.3.22) which is a direct consequence of the unitarity of quantum theoretical time evolution and not on the strong principle of detailed balance which needs the assumption of the symmetry of the interaction under the combined time-reversal and space-reflection transformation. As is well known, the weak interaction violates this PT symmetry.

5.4 The entropy and the H -Theorem

Even to define entropy in a classical way, the cleanest way is to consider quantum theory. To this end, again we assume a cubic volume of length L and periodic boundary conditions for the wave functions of the particles, which we also assume to be indistinguishable. Then the momentum eigenvalues for a single particle within this box are³

$$\vec{p} = \frac{2\pi\hbar}{L} \vec{n}, \quad \vec{n} \in \mathbb{Z}. \quad (5.4.1)$$

Now we consider classical phase space as separated into phase-space cells $\Delta^6 \tau$ which are microscopically large, i.e., as containing many states. Here $\Delta^3 \vec{x}$ can be seen as a box in position space of the type just considered above. On the other hand the phase-space cell is considered macroscopically small, i.e., we assume that the single-particle phase-space distribution $f(t, \tau)$ does not change considerably over each of these phase-space cells. Then according of (5.4.1) each of these phase-space cells corresponds to

$$G_j = \frac{\Delta^6 \tau_j}{(2\pi\hbar)^3} \quad (5.4.2)$$

quantum states. For a dilute gas, i.e., if the number N_j of particles contained in the phase-space element $\Delta^6 \tau_j$ is on average small compared to the number of quantum states, G_j , we can neglect the degeneracy according to quantum (Bose-Einstein or Fermi-Dirac) statistics. Then the statistical weight of the corresponding phase-space distribution is estimated as

$$\Delta\Gamma_j = \frac{1}{N_j!} G_j^{N_j}. \quad (5.4.3)$$

The factorial in the denominator takes into account the indistinguishability of particles, i.e., it does not matter which individual particle of the N_j particles populates one of the G_j quantum states. So any

³Here we explicitly introduce Planck's constant \hbar , which is important in the argument.

distribution of the N_j particles which differs from one such states only by permutation of all particles must be considered as the same N_j -particle state, and this is taken into account by the factorial in the denominator.

Following Boltzmann and Planck the **entropy** of the system for a given distribution of the N particles in phase space, given by the numbers N_j of particles in the phase-space cells $\Delta^6\tau_j$, is defined as

$$S = \sum_j \ln \Delta\Gamma_j = \sum_j [N_j \ln G_j - \ln(N_j!)] \simeq \sum_j [N_j \ln G_j - N_j(\ln N_j - 1)]. \quad (5.4.4)$$

In the last step we have used **Stirling's approximation**, $\ln(N!) \simeq_{N \rightarrow \infty} N(\ln N - 1)$. Now we introduce the average number of particles per quantum state

$$n_j = \frac{N_j}{G_j}. \quad (5.4.5)$$

Then we can write (5.4.4) as

$$S = \sum_j N_j \ln \left(\frac{eG_j}{N_j} \right) = \sum_j n_j G_j \ln \left(\frac{e}{N_j} \right) = \sum_j \frac{\Delta^6\tau_j}{(2\pi\hbar)^3} n_j \ln \left(\frac{e}{n_j} \right). \quad (5.4.6)$$

Now in the limit of macroscopically small phase-space cells we can write

$$n_j = \frac{(2\pi\hbar)^3 N_j}{\Delta^6\tau_j} \simeq (2\pi\hbar)^3 f(t, \vec{x}). \quad (5.4.7)$$

Thus the entropy of a dilute gas is given in terms of phase-space by the semiclassical expression

$$S(t) = - \int d^3\vec{x} d^3\vec{p} f(t, \vec{x}, \vec{p}) \{ \ln[(2\pi\hbar)^3 f(t, \vec{x}, \vec{p})] - 1 \}. \quad (5.4.8)$$

The above consideration shows that for a detailed foundation of classical statistical mechanics one needs quantum-theoretical arguments in order to give a proper definition of entropy in terms of the phase-space distribution function. The reason is that in classical physics there is no “natural measure” for the size of phase-space cells, i.e., one cannot unambiguously count the number of microscopic states leading to a given macroscopic distribution of particles in phase space. As we have shown above, this problem is quite simply solved by using basic concepts of quantum theory. The factor $(2\pi\hbar)^3$ in the logarithm in (5.4.8) is important in order to make this argument dimensionless as it must be.

Now we want to prove **Boltzmann's H theorem**⁴, which is a very important general result of kinetic theory and thermodynamics. Often one reads the statement that this theorem, which states that the entropy of a system cannot decrease as a function of time. As we have seen above, this is not entirely true, since the derivation of the Boltzmann equation, which we shall use to prove this statement, included the assumption of a direction of time as defined by causality. The H theorem thus only proves that the so-called “thermodynamical arrow of time”, defined as the time direction, in which the entropy grows, is the same as the “causal arrow of time”, i.e., the time direction defined by causality, which is a more or less explicitly stated assumption behind all physical theories.

⁴Here H stands for the Greek letter Eta, which was Boltzmann's label for the entropy.

To derive the H theorem we take the time derivative of (5.4.8),

$$\dot{S}(t) = - \int d^3 \vec{x} d^3 \vec{p} \frac{\partial f(t, \vec{x}, \vec{p})}{\partial t} \ln[f(t, \vec{x}, \vec{p})(2\pi \hbar)^3]. \quad (5.4.9)$$

Using the Boltzmann equation (5.3.18) to substitute ∂_t , taking into account that the term containing the spatial derivatives is a total divergence and thus vanishes upon integration over space, leads to

$$\dot{S}(t) = - \int d^3 \vec{x} d^3 \vec{p} C[f; t, \vec{x}, \vec{p}] \ln[f(t, \vec{x}, \vec{p})(2\pi \hbar)^3]. \quad (5.4.10)$$

Since we need expressions of this times frequently, we define the **collision functional**

$$\text{Coll}[\phi; t, \vec{x}_1] := \int d1 C[f; 1] \phi_1 = \int d1 d2 d1' d2' w(1'2' \leftarrow 12) \phi_1 (f_{1'} f_{2'} - f_1 f_2) \quad (5.4.11)$$

for an arbitrary one-particle phase-space function with the abbreviations $d1 = d^3 \vec{p}_1$, $\phi_1 = \phi(t_1, \vec{x}_1, \vec{p}_1)$, etc. In the second term we can interchange the momentum-integration variables (12) and (1'2') and use (5.3.17). Then we find

$$\text{Coll}[\phi; \vec{x}_1, \vec{p}_1] = \int d2 d1' d2' w(1'2' \leftarrow 12) (\phi_1 - \phi_{1'}) f_{1'} f_{2'}. \quad (5.4.12)$$

On the other hand we deal with identical particles, we can interchange in this equation the momentum pairs (11') and (22') without changing the result. Thus adding the corresponding expression and dividing by 2 leads to the following symmetric form for the collision functional:

$$\text{Coll}[\phi] = \frac{1}{2} \int d2 d1' d2' w(1'2' \leftarrow 12) (\phi_1 + \phi_2 - \phi_{1'} - \phi_{2'}) f_{1'} f_{2'}. \quad (5.4.13)$$

Setting $\phi = \ln[f(2\pi \hbar)^3]$, according to (5.4.10) we get

$$\dot{S} = \frac{1}{2} \int d1 d2 d1' d2' d^3 \vec{x}_1 w(1'2' \leftarrow 12) f_{1'} f_{2'} \ln \left(\frac{f_{1'} f_{2'}}{f_1 f_2} \right). \quad (5.4.14)$$

This we can write in the form

$$\dot{S} = \frac{1}{2} \int d1 d2 d1' d2' d^3 \vec{x} w(1'2' \leftarrow 12) f_1 f_2 \frac{f_{1'} f_{2'}}{f_1 f_2} \ln \left(\frac{f_{1'} f_{2'}}{f_1 f_2} \right). \quad (5.4.15)$$

Setting $\phi = 1$ in (5.4.13) leads to

$$\frac{1}{2} \int d^3 \vec{p} C[f; t, \vec{x}, \vec{p}] = 0. \quad (5.4.16)$$

Adding this to (5.4.15) we find

$$\dot{S} = \frac{1}{2} \int d1 d2 d1' d2' d^3 \vec{x} w(1'2' \leftarrow 12) f_1 f_2 \left\{ \frac{f_{1'} f_{2'}}{f_1 f_2} \left[\ln \left(\frac{f_{1'} f_{2'}}{f_1 f_2} \right) - 1 \right] + 1 \right\}. \quad (5.4.17)$$

Now we investigate the real function $f(\alpha) = 1 + \alpha(\ln \alpha - 1)$ for $\alpha > 0$. Obviously $f(1) = 0$, and we have $f'(\alpha) = \ln \alpha$ and $f''(\alpha) = 1/\alpha$, which implies that at $\alpha = 1$ the function has its only minimum, and this shows that $f(\alpha) \geq 0$ and $f(\alpha) = 0 \Leftrightarrow \alpha = 1$.

From this from (5.4.17) we can indeed conclude that the total entropy is never decreasing,

$$\dot{S} \geq 0, \quad \dot{S} = 0 \Leftrightarrow f_{1'} f_{2'} = f_1 f_2. \quad (5.4.18)$$

5.5 Local equilibrium

Now we look for (approximate) solutions of the Boltzmann equation (5.3.18), which are of general meaning for kinetic theory. We shall also see, how classical continuum-mechanical descriptions like the **Euler equation for ideal fluids** and the **Navier-Stokes equations for viscous fluids** can be derived from the underlying microscopic dynamics.

For that purpose we first look for distributions which lead to **adiabatic motion** of the fluid, i.e., which fulfill $\dot{S} = 0$. As we have just derived in the previous Section, this implies (5.4.18). Writing the distribution function as

$$f(t, \vec{x}, \vec{p}) = \exp[\phi(t, \vec{x}, \vec{p})], \quad (5.5.1)$$

this equation reads

$$\phi_{1'} + \phi_{2'} = \phi_1 + \phi_2, \quad (5.5.2)$$

which should hold for all scattering processes $1'2' \leftarrow 12$, under the constraint of energy and momentum conservation,

$$\vec{p}_1 + \vec{p}_2 = \vec{p}_{1'} + \vec{p}_{2'}, \quad \frac{\vec{p}_1^2}{2m} + \frac{\vec{p}_2^2}{2m} = \frac{\vec{p}_{1'}^2}{2m} + \frac{\vec{p}_{2'}^2}{2m}. \quad (5.5.3)$$

To solve the functional equation (5.5.2) under these constraints we use Lagrange multipliers $\beta \vec{v}$ and β for these four constraints, respectively. Then we can vary (5.5.2) independently with respect to \vec{p}_1 , \vec{p}_2 , $\vec{p}_{1'}$, and $\vec{p}_{2'}$. This leads to

$$\partial_{\vec{p}} \phi + \beta \vec{p}/m + \beta \vec{v} = 0 \quad (5.5.4)$$

with the general solution

$$\phi(t, \vec{x}, \vec{p}) = -\beta(t, \vec{x}) \left[\frac{\vec{p}^2}{2m} - \vec{v}(t, \vec{x}) \cdot \vec{p} \right] - \Omega(t, \vec{x}). \quad (5.5.5)$$

It is important to note that the Lagrange multipliers \vec{v} and β must be **momentum independent**. Using this in our ansatz leads to

$$f(t, \vec{x}, \vec{p}) = A(t, \vec{x}) \exp \left[-\beta(t, \vec{x}) \frac{\vec{p}^2}{2m} - \vec{v}(t, \vec{x}) \vec{p} \right] \quad (5.5.6)$$

with

$$A(t, \vec{x}) = \exp[-\Omega(t, \vec{x})]. \quad (5.5.7)$$

Obviously $A(t, \vec{x})$ is related to the spatial particle distribution

$$n(t, \vec{x}) = \int_{\mathbb{R}^3} d^3 \vec{p} f(t, \vec{x}, \vec{p}) = A(t, \vec{x}) \exp \left[\frac{\beta(t, \vec{x}) m}{2} \vec{v}^2(t, \vec{x}) \right] \left(\frac{2\pi m}{\beta(t, \vec{x})} \right)^{3/2}. \quad (5.5.8)$$

This implies that we can write

$$f(t, \vec{x}, \vec{p}) = \left(\frac{\beta(t, \vec{x})}{2\pi m} \right)^{3/2} n(t, \vec{x}) \exp \left[-\frac{\beta(t, \vec{x})}{2m} (\vec{p} - m\vec{v}(t, \vec{x}))^2 \right]. \quad (5.5.9)$$

This is the **Maxwell-Boltzmann distribution of local thermal equilibrium**.

Global thermal equilibrium is the stationary solution of the Boltzmann equation $f_{\text{eq}}(t, \vec{x}, \vec{p}) = f_{\text{eq}}(\vec{x}, \vec{p})$. Of course then also $\dot{S} = 0$ and thus the distribution is given by the Maxwell-Boltzmann distribution with $n = n(\vec{x})$, $\beta = \beta(\vec{x})$, and $\vec{v} = \vec{v}(t, \vec{x})$.

We can read off immediately from (5.5.9) that the mean momentum for a particle in the gas located around \vec{x} is given by

$$\langle \vec{p} \rangle_{t, \vec{x}} = \frac{1}{n(t, \vec{x})} \int d^3 \vec{p} f(t, \vec{x}, \vec{p}) = m \vec{v}(t, \vec{x}). \quad (5.5.10)$$

This means that the collective motion of the fluid is described by the **velocity field** $\vec{v}(t, \vec{x})$.

Next we derive the equations of motion for the functions n , \vec{v} and β , assuming the initial values of these fields as given, from the Boltzmann equation. They follow from the **conservation laws** for particle number, energy, and momentum.

To that end we multiply the Boltzmann equation (5.3.18) with the corresponding single-particle quantities 1, $E = \vec{p}^2/(2m)$, and \vec{p} and integrate over \vec{p} . Using the form (5.4.13) for the collision functional gives always 0 for the contribution from the collision integral, because energy and momentum are conserved in the elastic two-particle collisions considered here.

So integrating the Boltzmann equation (5.3.18) simply over \vec{p} gives the continuity equation,

$$\partial_t n(t, \vec{x}) + \partial_{\vec{x}} \left\langle \frac{\vec{p}}{m} \right\rangle_{\vec{p}} = \partial_t n(t, \vec{x}) + \partial_{\vec{x}} [n(t, \vec{x}) \vec{v}(t, \vec{x})] = 0. \quad (5.5.11)$$

In the second step we have used (5.5.9) for the phase-space distribution in local thermal equilibrium. Defining the mass density by

$$\rho(t, \vec{x}) = mn(t, \vec{x}), \quad (5.5.12)$$

this can be written as

$$\partial_t \rho(t, \vec{x}) + \partial_{\vec{x}} [\rho(t, \vec{x}) \vec{v}(t, \vec{x})] = 0, \quad (5.5.13)$$

which is the local form of the **conservation of mass**, which holds in non-relativistic mechanics.

Multiplying the Boltzmann equation by \vec{p} , integrating over \vec{p} and using again (5.5.9) gives

$$\partial_t (v_k \rho) + \frac{\partial}{\partial x_l} \Pi_{lk} = 0 \quad (5.5.14)$$

with the **stress tensor**

$$\Pi_{lk}(t, \vec{x}) = \frac{1}{m} \int_{\mathbb{R}^3} \frac{d^3 \vec{p}}{p} p_k f(t, \vec{x}, \vec{p}) = \rho(t, \vec{x}) \left(v_l(t, \vec{x}) v_k(t, \vec{x}) + \frac{1}{\beta(t, \vec{x}) m} \delta_{lk} \right). \quad (5.5.15)$$

Defining the **pressure** of the gas as

$$P(t, \vec{x}) = \frac{\rho(t, \vec{x})}{\beta(t, \vec{x}) m} = \frac{n(t, \vec{x})}{\beta(t, \vec{x})} \quad (5.5.16)$$

leads to the **ideal-gas equation of state**

$$P(t, \vec{x}) = n(t, \vec{x}) T(t, \vec{x}) \quad (5.5.17)$$

when we identify

$$T(t, \vec{x}) = \frac{1}{\beta(t, \vec{x})} \quad (5.5.18)$$

with the **temperature of the gas**, measured in units of energy, i.e., setting the Boltzmann constant $k_B = 1$. The stress tensor (5.5.15) thus reads

$$\Pi_{lk}(t, \vec{x}) = \rho(t, \vec{x}) v_l(t, \vec{x}) v_k(t, \vec{x}) + P(t, \vec{x}) \delta_{lk}. \quad (5.5.19)$$

5.5 · Local equilibrium

The equation (5.5.14) thus reads

$$\rho \partial_t \vec{v} + \vec{v} [\partial_t \rho + \partial_{\vec{x}} \cdot (\rho \vec{v})] + \rho (\vec{v} \cdot \partial_{\vec{x}}) \vec{v} = -\partial_{\vec{x}} P. \quad (5.5.20)$$

Using (5.5.13) leads to the **Euler equation for the ideal fluid**,

$$\rho \partial_t \vec{v} + \rho (\vec{v} \cdot \partial_{\vec{x}}) \vec{v} = -\partial_{\vec{x}} P. \quad (5.5.21)$$

This is just the local form of Newton's equation of motion, where the potential for the force per unit volume is given by momentum. On the left-hand side the **material time derivative**

$$D_t \vec{v} = \partial_t \vec{v} + (\vec{v} \cdot \partial_{\vec{x}}) \vec{v} \quad (5.5.22)$$

occurs. This gives the time derivative of the velocity of a fluid element moving against the inertial reference frame.

The equation describing energy conservation follows from the Boltzmann equation (5.3.18) by multiplying with $E = \vec{p}^2/(2m)$ and integrating over \vec{p} . Again with (5.5.9) this gives

$$\partial_t \epsilon(t, \vec{x}) + \partial_{\vec{x}} \cdot \vec{S}(t, \vec{x}) \quad (5.5.23)$$

with the **energy density**

$$\epsilon = \int_{\mathbb{R}^3} d^3 \vec{p} \frac{\vec{p}^2}{2m} f(t, \vec{x}, \vec{p}) = \frac{1}{2} \sum_{j=1}^3 \Pi_{jj} \stackrel{(5.5.19)}{=} \frac{\rho}{2} \vec{v}^2 + \frac{3}{2} P \quad (5.5.24)$$

and the **energy flow**

$$\vec{S} = \int_{\mathbb{R}^3} d^3 \vec{p} \frac{\vec{p}}{m} \frac{\vec{p}^2}{2m} f(t, \vec{x}, \vec{p}) = \vec{v} \left(\frac{\rho}{2} \vec{v}^2 + \frac{5}{2} nT \right) = \vec{v}(\epsilon + P). \quad (5.5.25)$$

Both expressions consist of a contribution due to the collective motion and the local thermal fluctuations (heat): In (5.5.24) $\rho \vec{v}^2/2$ is the kinetic energy of the fluid element per unit volume and according to (5.5.17) $3/2P = 3/2nT$ is the energy due to the fluctuating thermal motion of the particles in the fluid element. In (5.5.25) one has the flow of the collective part of the energy out of the volume element and the **enthalpy density** $h = \epsilon + P = 3/2nT + nT = 5/2nT$. The second form of writing the energy flow shows the reason why the enthalpy rather the inner thermal energy has to occur in the energy flux: Part of the energy flux is that additionally to the energy the particles carry as kinetic energy from their collective motion and heat energy with them, which gives the term $\vec{v}\epsilon$, there acts also a force on the particles given as the (negative) gradient of the pressure P , and that has to be added in the energy balance as a flow of the corresponding kind of potential energy out of this fluid element, and that's taken account of by the contribution $\vec{v}P$.

Appendix A

Noether's Theorem

In this chapter we consider the very important connection between **symmetries and conservation laws**. As we shall see, any continuous Symmetry of the action functional defines a quantity that is conserved with time under the dynamical evolution of the system. This allows an elegant definition of observables like energy, momentum, and angular momentum, which arise as the conservation laws from the **Poincaré symmetries** of Minkowski space under temporal and spatial translations, and rotations, respectively. As we also shall prove, the symmetry under boosts is equivalent to the conservation of the center-of-energy velocity.

A.1 Symmetries of the action

Let's consider an arbitrary set of fields ϕ_j and an infinitesimal symmetry transformation of the space-time coordinates and fields of the

$$x'^{\mu} = x^{\mu} + \delta\eta^a t_a^{\mu}(x), \quad \phi'_j(x') = \phi_j(x) + \delta\eta^a T_{aj}(\phi). \quad (\text{A.1.1})$$

Therein the $\delta\eta^a$ are some infinitesimal independent parameters of the transformation (e.g., angles for a rotation). To evaluate the variation of the action, we first have to calculate the variation of the field derivatives, which do *not* commute the the derivatives as in Hamilton's principle, because here the spactime coordinates are varied. We find

$$\delta(\partial_{\nu}\phi_j) = \partial'_{\nu}\phi'_j(x') - \partial_{\nu}\phi_j(x) = \frac{\partial x^{\rho}}{\partial x'^{\nu}} \partial_{\rho}\phi_j(x') - \partial_{\nu}\phi_j(x). \quad (\text{A.1.2})$$

Up to $\mathcal{O}(\delta\eta^2)$

$$\frac{\partial x^{\rho}}{\partial x'^{\nu}} = \delta^{\rho}_{\nu} - \delta\eta^a \partial_{\nu} t_a^{\rho}, \quad (\text{A.1.3})$$

which follows from

$$\frac{\partial x^{\rho}}{\partial x'^{\nu}} \frac{\partial x'^{\nu}}{\partial x^{\sigma}} = \delta^{\rho}_{\sigma}. \quad (\text{A.1.4})$$

Using (A.1.1) and (A.1.3) in (A.1.2) we finally get

$$\delta(\partial_{\nu}\phi_j) = \delta\eta^a \left\{ \partial_{\nu} T_j^{\mu}[\phi(x)] - [\partial_{\nu} t_j^{\rho}(x)] \partial_{\rho}\phi_j(x) \right\}. \quad (\text{A.1.5})$$

Then we need the variation of the four-volume element,

$$\delta d^4x = d^4x' - d^4x = \left[\det \left(\frac{\partial x'}{\partial x} \right) - 1 \right] d^4x. \quad (\text{A.1.6})$$

To find the Jacobian of the symmetry transformation up to $\mathcal{O}(\delta\eta^2)$, we use its defining expression in terms of the matrix elements and skip any contribution of higher than first order in the $\delta\eta$'s. This gives (*check!*)

$$\delta d^4x' = \delta\eta^a \partial_\mu t_a^\mu d^4x. \quad (\text{A.1.7})$$

Using (A.1.3), (A.1.5), and (A.1.7) we find after some elementary manipulations and integration by parts

$$\delta S = \int_{\mathbb{R}^4} d^4x \delta\eta^a \left\{ \left[\frac{\partial \mathcal{L}}{\partial \phi_j} - \partial_\nu \frac{\partial \mathcal{L}}{\partial (\partial_\nu \phi_j)} \right] T_{aj} + \partial_\nu \left[\frac{\partial \mathcal{L}}{\partial (\partial_\nu \phi_k)} \partial_\mu \phi_k - \mathcal{L} \delta_\mu^\nu \right] t_a^\mu \right\}. \quad (\text{A.1.8})$$

Since the $\delta\eta^a$ are independent variables by assumption, the integral must vanish separately for each a . This means that the expression in the curly bracket is a total four-divergence of a current,

$$\left[\frac{\partial \mathcal{L}}{\partial \phi_j} - \partial_\nu \frac{\partial \mathcal{L}}{\partial (\partial_\nu \phi_j)} \right] T_{aj} + \partial_\nu \left[\frac{\partial \mathcal{L}}{\partial (\partial_\nu \phi_k)} \partial_\mu \phi_k - \mathcal{L} \delta_\mu^\nu \right] t_a^\mu = \partial_\sigma j_a^\sigma. \quad (\text{A.1.9})$$

Using the functional derivative of the action,

$$\frac{\delta S}{\delta \phi_j} := \frac{\partial \mathcal{L}}{\partial \phi_j} - \partial_\nu \frac{\partial \mathcal{L}}{\partial (\partial_\nu \phi_j)} \quad (\text{A.1.10})$$

We find after working out the ∂_ν derivative that (A.1.9) takes the form

$$\frac{\delta S}{\delta \phi_j} \left[T_{aj} - (\partial_\mu \phi_j) t_a^\mu \right] = \partial_\nu j_a^\nu. \quad (\text{A.1.11})$$

A.2 Noether currents and conserved quantities

Since further the field equations of motion are given by the stationarity of the action functional under variations of the ϕ_j , i.e., the vanishing of the functional derivative (A.1.10), we conclude for any **solution of the field equations**

$$\partial_\nu j_a^\nu = 0, \quad (\text{A.2.1})$$

which is **Noether's Theorem** [Noe18]:

For each one-parameter subgroup of a Lie-group representation on the fields and spacetime coordinates, for which the action is invariant, there exists a conserved current.

It is important to note that the **Noether currents**, defined by (A.1.11), are *not* unique, but we can always define a new current,

$$j_a'^{\mu} = j_a^\mu + \partial_\nu \omega_a^{\mu\nu} \quad (\text{A.2.2})$$

where $\omega_a^{\mu\nu}$ are arbitrary antisymmetric 2nd-rank tensor fields. Obviously if j_a^μ is a conserved current, the $j_a'^{\mu}$ are also conserved and define the same conserved quantities (*why?*)

$$\int_{\mathbb{R}^3} d^3\vec{x} \partial_\nu \omega_a^{0\nu} = 0. \quad (\text{A.2.3})$$

Appendix B

Imaginary-time formalism

B.1 Bosons

B.1.1 Bosonic Matsubara sums

The imaginary-time formalism leads to Feynman rules that are even more similar to the vacuum case than the real-time Feynman rules. Up to some changes in factors i , the most profound difference between the vacuum and the imaginary-time Feynman rules at finite temperature is that instead of energy integrals but sums over the discrete Matsubara frequencies. These can be evaluated as a integral in the complex energy plane by making use of the theorem of residues. Our task is to calculate sums of the form

$$H(\beta) = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} h(i\omega_n) \quad \text{with} \quad \omega_n = \frac{2\pi n}{\beta}. \quad (\text{B.1.1})$$

Usually in the physical calculations one can find a complex function $h(z)$ which is identical to the series for $z = i\omega_n$ and is analytic in an open strip around the complete imaginary axis and has poles and branch points¹ only along the real axis. Then the usual trick is to use the function

$$S_B(p_0) = \frac{1}{2} \coth\left(\frac{\beta p_0}{2}\right), \quad (\text{B.1.2})$$

which has simple poles at $p_0 = i\omega_n$ with residuum $1/\beta$ and is analytic everywhere else in the complex p_0 plane. Thus we can write the series in the form

$$H(\beta) = \int_C \frac{dp_0}{2\pi i} S_B(p_0) h(p_0). \quad (\text{B.1.3})$$

The integration path is given in (B.1). Since both, the function h and the function (B.1.2), have no singularities in the open four sectors of the p_0 plane the integral along the red paths is 0. Now only the parts parallel and close to the real axis contribute to this integral since h has to go to zero for $z \rightarrow \infty$ faster than $1/z$. Thus, the integral along the four red lines close to the real axis gives $-[H(\beta) - h(0)]/\beta$. Due to the residuum theorem the integral along the little green path around the point $p_0 = 0$, which has to be chosen such, that its vertical parts do not intersect a possibly existing branch cut of h along the real axis, gives $-h(0)/\beta$. The vertical parts of the green box cancel the corresponding vertical parts

¹the branch cuts start usually away from $z = 0$

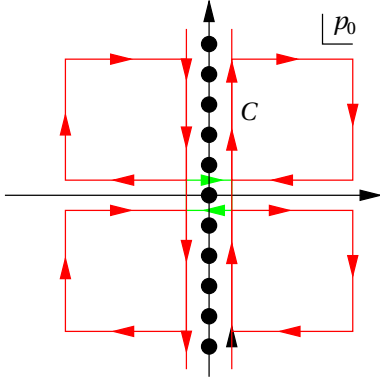


Figure B.1: The contour to calculate the Matsubara sums. The original contour C in (B.1.3) is given by the red vertical lines parallel to the imaginary axis surrounding counterclockwise the simple poles at $p_0 = i\omega_n$ of the Bose-Einstein function (B.1.2).

of the original contour C . Finally we deformed the original path C to the paths along the real axis, one a little below and one a little above the real axis. So the real-time integral is given by

$$H(\beta) = \int_{\mathbb{R}} \frac{dp_0}{2\pi i} S_B(p_0) [h(p_0 + i0^+) - h(p_0 - i0^+)]. \quad (\text{B.1.4})$$

Now

$$S_B(p_0) = \frac{1}{2} \frac{\exp(\beta p_0/2) + \exp(-\beta p_0/2)}{\exp(\beta p_0/2) - \exp(-\beta p_0/2)} = \frac{1}{2} [1 + 2f_B(p_0)]. \quad (\text{B.1.5})$$

So finally we get

$$H(\beta) = \frac{1}{2} \int_{\mathbb{R}} \frac{dp_0}{2\pi i} [1 + 2f_B(p_0)] [h(p_0 + i0^+) - h(p_0 - i0^+)]. \quad (\text{B.1.6})$$

This form of the Matsubara sum is convenient, if we have to evaluate closed diagrams without external lines, which have the meaning of correction factors to the partition sum. Such diagrams can with help of real-time quantities making use of the analytic properties of two-point functions (see the end of Sect. 2.2.5).

For imaginary-time quantities it is often more convenient to simplify (B.1.3) in a different way. We start with (B.1.6)

$$H(\beta) := \frac{1}{\beta} \sum_{\omega_n} h(i\omega_n) = \frac{1}{2} \int_{\mathcal{C}} \frac{dp_0}{2\pi i} [1 + 2f_B(p_0)] h(p_0) \quad \text{with} \quad \omega_n = \frac{2\pi i n}{\beta}, \quad n \in \mathbb{Z}. \quad (\text{B.1.7})$$

Instead of deforming the contour to one along the real axis we do a simple substitution $p_0 = -p'_0$ for the contour part left to the imaginary axis:

$$\int_{-i\infty-0^+}^{i\infty-0^+} dp_0 S_B(p_0) h(p_0) = - \int_{-i\infty+0^+}^{i\infty+0^+} \frac{dp_0}{2\pi i} S_B(p_0) h(-p_0). \quad (\text{B.1.8})$$

The part of \mathcal{C} going down parallel to the imaginary axis with, shifted slightly to the left is thus written in terms of an integral along the other branch of \mathcal{C} . This gives

$$\frac{1}{\beta} \sum_{\omega_n} h(i\omega_n) = \frac{1}{2} \int_{-i\infty+0^+}^{i\infty+0^+} \frac{dp_0}{2\pi i} [1 + 2f_B(p_0)] [h(p_0) + h(-p_0)]. \quad (\text{B.1.9})$$

Often the integral can be evaluated by closing the contour with a large semi-circle to the right half-plane. Possibly special care has to be taken to the “zero-mode contribution” which is not multiplied by a Bose distribution factor.

B.1.2 Imaginary time Green's function

With help of (B.1.9) it is easy to give a simplified expression for (3.1.57) with t along the vertical part of the modified Schwinger-Keldysh contour (see Fig. 2.2). From (3.1.56) we read off

$$A(p) = -2\text{Im } G_R(p). \quad (\text{B.1.10})$$

Now we use the spectral representation to define the *analytic Green's function*

$$G_a(p) = \int \frac{dp'_0 A(p'_0, \vec{p})}{2\pi p_0 - p'_0}, \quad p_0 \in \mathbb{C} \setminus \mathbb{R}. \quad (\text{B.1.11})$$

It is clear, that the retarded and advanced Green's functions are given as limits of p_0 to the real axis

$$G_R(p) = G_a(p_0 + i0^+, \vec{p}), \quad G_A(p) = G_a(p_0 - i0^+, \vec{p}); \quad p_0 \in \mathbb{R}. \quad (\text{B.1.12})$$

The Matsubara Green's function is defined by Eq. (3.1.33) for times $t = -i\tau$ with $\tau \in [0, \beta)$:

$$G_M(\tau_1, \vec{x}_1; \tau_2, \vec{x}_2) = -\langle T_\tau \phi(-i\tau_1, \vec{x}_1) \phi^\dagger(-i\tau_2, \vec{x}_2) \rangle. \quad (\text{B.1.13})$$

From translation invariance in space and time G_M is a function of the difference $x_1 - x_2$ only and due to the time evolution along the imaginary time axis periodic in time with period β .

For $0 < \tau < \beta$ we have

$$G_M(\tau, \vec{x}) = -\langle \phi(-i\tau, \vec{x}) \phi^\dagger(0, 0) \rangle. \quad (\text{B.1.14})$$

Now we expand G_M in a Fourier *series* in time and a Fourier integral in space:

$$G_M(\tau, \vec{x}) = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} \int \frac{d^3 \vec{p}}{(2\pi)^3} \tilde{G}_M(i\omega_n, \vec{p}) \exp(-i\omega_n \tau + i\vec{p}\vec{x}) \quad (\text{B.1.15})$$

Due to the KMS-condition $G_M(\tau + \beta, x) = G_M(\tau, x)$ the *Matsubara frequencies* are given by $\omega_n = 2\pi n/\beta$.

The next step is to show, that

$$\tilde{G}_M(i\omega_n, \vec{p}) = -G_a(i\omega_n, \vec{p}) = \int \frac{dp'_0 A(p'_0, \vec{p})}{2\pi p'_0 - i\omega_n}. \quad (\text{B.1.16})$$

For that, it is sufficient to use (B.1.14) and the fact, that the Wightman function

$$W(t, \vec{x}) = -\langle \phi(t, \vec{x}) \phi^\dagger(0, 0) \rangle \quad (\text{B.1.17})$$

is analytic in the open strip $-\beta < \text{Im } t < 0$, which we call S . Along the real axis W is identical with $-iG^{+-}(t, \vec{x})$. Thus, we obtain W from the real time function G^{+-} by analytic continuation from real t to complex t with values restricted to the open strip S . Thus, we can use (3.1.54) to obtain

$$\tilde{G}_M(i\omega_n, \vec{p}) = -\int_0^\beta d\tau \int \frac{dp_0}{2\pi} A(p_0, \vec{p}) [1 + f_B(p_0)] \exp(-p_0 \tau + i\omega_n \tau) = \int \frac{dp_0}{2\pi} \frac{A(p)}{p_0 - i\omega_n}, \quad (\text{B.1.18})$$

where we have evaluated the τ -integral and used $\exp(i\omega_n \beta) = 1$ and $1 + f_B(p_0) = -f_B(-p_0)$. This proves (B.1.16).

B.1.3 Mills representation in imaginary time

We can also give a general formula for the *Mills representation* of the Matsubara propagator, i.e., as function of imaginary time τ and momentum:

$$G'_M(\tau, \vec{p}) = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} \exp(-i\omega_n \tau) \tilde{G}_M(i\omega_n, \vec{p}). \quad (\text{B.1.19})$$

With help of (B.1.16) this can be written as

$$G'_M(\tau, \vec{p}) = \int \frac{dp_0}{2\pi} K(\tau, p_0) A(p_0, \vec{p}) = \int_0^\infty \frac{dp_0}{2\pi} \tilde{K}(\tau, p_0) A(p_0, \vec{p}). \quad (\text{B.1.20})$$

Here we have defined the kernels

$$K(\tau, p_0) = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} \frac{\exp(-i\omega_n \tau)}{p_0 - i\omega_n}, \quad \tilde{K}(\tau, p_0) = K(\tau, p_0) - K(\tau, -p_0). \quad (\text{B.1.21})$$

To obtain the second form in (B.1.20) the property $A(-p'_0, \vec{p}) = -A(p'_0, \vec{p})$ has been used.

Now we apply (B.1.9) to calculate the kernel K from (B.1.21). In this case we have to set

$$h(z) = \frac{\exp(-z\tau)}{p_0 - z}. \quad (\text{B.1.22})$$

Since $p_0 \in \mathbb{R}$, it fulfils the properties needed to apply (B.1.9). To evaluate the integral we split it in two parts, the one with a Bose-Einstein distribution factor, and the other. The first part reads

$$K_1(\tau, p_0) = \int_{-i\infty+0^+}^{i\infty+0^+} \frac{dz}{2\pi i} \frac{1}{\exp(\beta z) - 1} \left[\frac{\exp(z\tau)}{z + p_0} - \frac{\exp(-z\tau)}{z - p_0} \right]. \quad (\text{B.1.23})$$

For $0 < \tau < \beta$ we can close the contour with a big semicircle in the right plane, since its contribution to the integral vanishes, when we take the radius to infinity. This path contains only the residua from the denominators $1/(z \pm p_0)$. So we find

$$K_1(\tau, p_0) = -[\Theta(p_0) + f_B(-\beta p_0)] \exp(-p_0 \tau), \quad 0 < \tau < \infty. \quad (\text{B.1.24})$$

The second part is

$$K_2(\tau, p_0) = \int_{-i\infty+0^+}^{i\infty+0^+} \frac{dz}{2\pi i} \frac{\exp(z\tau)}{p_0 + z} \quad (\text{B.1.25})$$

For $\tau > 0$ this integral can be evaluated by closing the contour in the left plane with a big semicircle, whose contribution vanishes when taking its radius to infinity:

$$K_2(\tau, p_0) = \Theta(p_0) \exp(-p_0 \tau), \quad \tau > 0. \quad (\text{B.1.26})$$

Together with (B.1.24) this finally yields

$$K(\tau, p_0) = \frac{\exp(-p_0 \tau)}{1 - \exp(-p_0 \beta)}, \quad 0 < \tau < \beta. \quad (\text{B.1.27})$$

From this we get, cf. (B.1.21)

$$\tilde{K}(\tau, p_0) = \frac{\cosh\left(p_0 \tau - \frac{p_0 \beta}{2}\right)}{\sinh\left(\frac{p_0 \beta}{2}\right)}. \quad (\text{B.1.28})$$

B.1.4 Finite chemical potential

In the same way as we have derived (B.1.16) from (B.1.14), we can use (B.1.14) together with the boundary conditions (3.1.26) to derive the same for finite chemical potential:

$$G_M(\tau, \vec{x}) = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} \exp[-(i\omega_n + \mu)\tau] \int \frac{d^3\vec{p}}{(2\pi)^3} \exp(i\vec{p}\vec{x}) \tilde{G}_M(i\omega_n + \mu, \vec{p}), \quad (\text{B.1.29})$$

where

$$\tilde{G}_M(i\omega_n + \mu, \vec{p}) = \int \frac{dp_0}{2\pi} \frac{A(p_0, \vec{p})}{p_0 - (i\omega_n + \mu)}. \quad (\text{B.1.30})$$

We have used again the Wightman function (B.1.17), its connection to $-iG^{+-}$ and (3.1.54)². The analytic Green's function is thus given by

$$G_a(p) = \int \frac{dp'_0}{2\pi} \frac{A(p'_0, \vec{p})}{p_0 + \mu - p'_0} \quad (\text{B.1.32})$$

and the retarded Green's function is

$$G_R(p) = G_a(p_0 + i0^+, \vec{p}), \quad A(p) = -2 \text{Im} G_R(p_0 - \mu, \vec{p}). \quad (\text{B.1.33})$$

B.1.5 Imaginary-time Feynman rules

For the derivation of the imaginary-time Feynman rules one has to integrate along the vertical part of the modified Schwinger-Keldysh contour only. The Feynman rules in imaginary time are nearly the same as in the vacuum. First of all, since there is only one imaginary time line, no doubling as along the real axis, we have only one type of vertices coming from the interaction part of the action:

$$S_I[\phi] = \int d^4x \mathcal{L}(x) = -i \int_0^\beta d\tau d^3\vec{x} \mathcal{L}_I(-i\tau, \vec{x}). \quad (\text{B.1.34})$$

The $-i$ in front of the integral, coming from the substitution $t = -i\tau$, cancels the $+i$ in the exponent of the path integral. Thus, the vertex, corresponding to a certain monomial in \mathcal{L}_I , is given by the vacuum expression without the i . In the case of derivative couplings one has to set $p_0 = i\omega_n + \mu$. E.g., for the simple ϕ^4 -theory we have only the four-point vertex $\Gamma_4 = -\lambda/(4!)$ (of course in this case we have neutral particles and thus necessarily $\mu = 0$).

The free propagator can be derived much simpler directly from the Lagrangian than by doing the dispersion integral (B.1.30). One only needs to invert the quadratic form, defined by S_0 along the imaginary time axis.

$$\Delta_M(i\omega_n + \mu, \vec{p}) = -\frac{1}{(i\omega_n + \mu)^2 - \vec{p}^2 - m^2}. \quad (\text{B.1.35})$$

A line in a Feynman diagram then stands for $\Delta_M(i\omega_n + \mu, \vec{p})$, as can be derived from (3.1.68), with the time coordinates specialised to imaginary times $-i\tau_1$ and $-i\tau_2$.

²Note, that the inverse of the Fourier transform (B.1.29) in this case reads

$$\tilde{G}_M(i\omega_n + \mu, \vec{p}) = \int_0^\beta d\tau \int d^3\vec{x} \exp[(i\omega_n + \mu)\tau - i\vec{p}\vec{x}] G_M(\tau, \vec{x}). \quad (\text{B.1.31})$$

At each vertex both, energy and momentum conservation, i.e., $\sum p_0 = \sum(i\omega_n + \mu) = 0$ and $\sum \vec{p} = 0$, where the sum is taken over all momenta running into the vertex have to hold. Over all “energies” and momenta corresponding to inner lines, which are not fixed by these conditions, has to be summed or integrated, respectively. That means, to each loop four-momentum l the operator

$$\frac{1}{\beta} \sum_{n_l=-\infty}^{\infty} \int \frac{d^3 \vec{l}}{(2\pi)^3} \quad (\text{B.1.36})$$

has to be applied.

For the sums one can use (B.1.9). With this formula it is also easy to separate the “vacuum parts” from the parts depending on β and μ , which is important for renormalisation issues: One can show, that all UV-divergences can be renormalised by subtracting counterterms, which are independent of β and μ .

B.2 Fermions

B.2.1 Fermionic Matsubara sums

The Matsubara sums over fermions are evaluated with an analogous technique as explained for bosons in Sect. B.1.1. In order to pick up the Matsubara frequencies $\tilde{\omega}_n = (2n + 1)T$ we use the function

$$S_F(p_0) = \frac{1}{2} \tanh\left(\frac{p_0}{2T}\right) = \frac{1}{2}[1 - 2f_F(p_0)], \quad (\text{B.2.1})$$

which has simple poles with residuum T at $p_0 = i\tilde{\omega}_n$, and the **Fermi-Dirac distribution** is given by

$$f_F(p_0) = \frac{1}{1 + \exp(\beta p_0)}. \quad (\text{B.2.2})$$

Thus the fermionic Matsubara sums can be written as the contour integral

$$H = T \sum_{\tilde{\omega}_n} b(i\tilde{\omega}_n) = \int_C \frac{dp_0}{2\pi i} S_F(p_0) b(p_0). \quad (\text{B.2.3})$$

The contour is the same as shown in (B.1), and we have assumed that b is analytic in an entire open strip around the imaginary p_0 axis. By the same argument as for the bosons (somewhat simplified by the fact that there is no zero Matsubara frequency for fermions) leads to the analogue of (B.1.4):

$$H = \frac{1}{2} \int_{\mathbb{R}} \frac{dp_0}{2\pi i} [1 - 2f_F(p_0)] [b(p_0 + i0^+) - b(p_0 - i0^+)] \quad (\text{B.2.4})$$

For later use we note the usefull identity

$$f_F(p_0) + f_F(-p_0) = +1, \quad (\text{B.2.5})$$

which is derived by some simple algebra.

Appendix C

Wigner representation of two-point functions

In this chapter we give some purely mathematical properties of Wigner transformations of two-point functions.

C.1 Definition and analytical properties

In general two-point functions along the Schwinger-Keldysh contour are defined as the expectation values of contour-ordered field-operator products,

$$iF(x, y) = \langle \mathcal{T}_c \mathbf{A}(x) \mathbf{B}(y) \rangle. \quad (\text{C.1.1})$$

In the following it is convenient to express the contour function in the matrix representation as functions of the usual time

$$i\hat{F}(x, y) = i \begin{pmatrix} F^{11}(x, y) & F^{12}(x, y) \\ F^{21}(x, y) & F^{22}(x, y) \end{pmatrix} = \begin{pmatrix} \langle \mathcal{T}_c \mathbf{A}(x) \mathbf{B}(x) \rangle & \langle \mathbf{B}(y) \mathbf{A}(x) \rangle \\ \langle \mathbf{A}(x) \mathbf{B}(y) \rangle & \langle \mathcal{T}_a \mathbf{A}(x) \mathbf{B}(y) \rangle \end{pmatrix}. \quad (\text{C.1.2})$$

For simplicity we have assumed that the field operators are of bosonic nature. In the case of fermionic field operators, one has to include the signs when changing the order due to the contour or time ordering prescription. The upper indices refer to the location of the time arguments on the branch of the contour (1: time-ordered, 2: anti-time-ordered branches, respectively).

Obviously the various two-point functions in the matrix (C.1.2) are not independent from each other but fulfill

$$F^{11} + F^{22} = F^{12} + F^{21} = \langle \{ \mathbf{A}(x), \mathbf{B}(y) \} \rangle. \quad (\text{C.1.3})$$

One can also work with other, sometimes more convenient, linear combinations of the two-point functions. Most important are the retarded and advanced combinations

$$\begin{aligned} F_{\text{ret}}(x, y) &= F^{11}(x, y) - F^{12}(x, y) = F^{21}(x, y) - F^{22}(x, y) \\ &= \Theta(x_0 - y_0) [F^{21}(x, y) - F^{12}(x, y)], \\ F_{\text{adv}}(x, y) &= F^{11}(x, y) - F^{21}(x, y) = F^{12}(x, y) - F^{22}(x, y) \\ &= -\Theta(y_0 - x_0) [F^{21}(x, y) - F^{12}(x, y)]. \end{aligned} \quad (\text{C.1.4})$$

The **Wigner transform** of the two-point functions is defined as the Fourier transform with respect to the relative coordinates $\xi = x - y$. If the situation is not translation invariant in space and time as in

thermal equilibrium, as is the case in general non-equilibrium function, this Fourier transform will also depend on the center-momentum coordinates $X = (x + y)/2$. Thus the Wigner transform reads

$$\tilde{F}^{ij}(X, p) = \int_{\mathbb{R}^4} d^4\xi F^{ij}\left(X + \frac{\xi}{2}, X - \frac{\xi}{2}\right) \exp(ip \cdot \xi). \quad (\text{C.1.5})$$

Using the Fourier representation of the Heaviside-unitstep function,

$$\Theta(x_0 - y_0) = \int_{\mathbb{R}} \frac{dp_0}{2\pi} \frac{i}{p_0 + i0^+} \exp(-ip_0 t), \quad (\text{C.1.6})$$

using the convolution theorem, one can write the Wigner transform of the retarded Green's function (C.1.4) as

$$\tilde{F}_{\text{ret}}(X, p) = \int_{\mathbb{R}} \frac{dp'_0}{2\pi} \frac{\tilde{F}_S(X, p')}{p_0 - p'_0 + i0^+} \Big|_{\vec{p}' = \vec{p}}, \quad (\text{C.1.7})$$

where the **spectral function**, related with the two-point function under consideration, is defined as

$$\tilde{F}_S(X, p) = i[\tilde{F}^{21}(X, p) - \tilde{F}^{12}(X, p)]. \quad (\text{C.1.8})$$

This shows that the complete two-point function is determined, if the spectral function and one of the Wightman functions \tilde{F}^{21} and \tilde{F}^{12} is known. In the case of thermal equilibrium it is already sufficient to know the spectral function, because then also the Wightman functions are known, because then in addition the Martin-Kubo-Schwinger relation is valid (for details see Sect. 3.1.2).

In the special case that $\mathbf{B} = \mathbf{A}^\dagger$, which is the case for the important example of the propagator of a scalar field one has the additional relations

$$\begin{aligned} [iF^{12}(x, y)]^* &= iF^{12}(y, x), & [iF^{21}(x, y)]^* &= iF^{21}(y, x), \\ [iF^{11}(x, y)]^* &= iF^{11}(y, x), & [iF^{22}(x, y)]^* &= iF^{22}(y, x), \\ [F_{\text{ret}}(x, y)]^* &= F_{\text{adv}}(y, x). \end{aligned} \quad (\text{C.1.9})$$

These relations are found by using the hermitean conjugate under the defining expectation values of the various Green's functions (C.1.2). For the Wigner transforms it follows

$$\begin{aligned} i\tilde{F}^{12}(X, p), \quad i\tilde{F}^{21}(X, p) &\in \mathbb{R}, & [i\tilde{F}^{11}(X, p)]^* &= i\tilde{F}^{22}(X, p), & [i\tilde{F}^{22}(X, p)]^* &= i\tilde{F}^{11}(X, p), \\ [\tilde{F}_{\text{ret}}(x, p)]^* &= \tilde{F}_A(x, p). \end{aligned} \quad (\text{C.1.10})$$

This implies that in this case the spectral function (C.1.8) is real, and

$$\tilde{F}_S = i[\tilde{F}_{\text{ret}} - \tilde{F}_{\text{adv}}] = -2\text{Im} \tilde{F}_{\text{ret}}, \quad (\text{C.1.11})$$

and from (C.1.7) one finds the **Kramers-Kroenig relation**,

$$\text{Re} \tilde{F}_{\text{ret}}(X, p) = -\mathcal{P} \int_{\mathbb{R}} \frac{dp'_0}{\pi} \frac{\text{Im} \tilde{F}_{\text{ret}}(X, p')}{p'_0 - p_0} \Big|_{\vec{p}' = \vec{p}}, \quad (\text{C.1.12})$$

for the retarded Green's function.

C.2 Convolution theorem for Wigner transforms

The **convolution** of two two-point functions (with ordinary time arguments) is defined by

$$(A \odot B)(x_1, x_3) = \int_{\mathbb{R}^4} d^4 x_2 A(x_1, x_2) B(x_2, x_3). \quad (\text{C.2.1})$$

Now we want to express this expression in terms of the Wigner transforms of A and B . Using the inverse Fourier transformations, we find

$$(A \odot B)(x_1, x_3) = \int_{\mathbb{R}^4} d^4 x_2 \int_{\mathbb{R}^4} \frac{d^4 p}{(2\pi)^4} \int_{\mathbb{R}^4} \frac{d^4 q}{(2\pi)^4} \tilde{A}(X_{12}, p) \tilde{B}(X_{23}, q) \exp(-ip \cdot \xi_{12} - iq \cdot \xi_{23}), \quad (\text{C.2.2})$$

where we define

$$X_{jk} = \frac{x_j + x_k}{2}, \quad \xi_{jk} = x_j - x_k. \quad (\text{C.2.3})$$

Now we expand the Wigner transforms both Wigner transforms under the integral (C.2.2) around X_{13} :

$$\begin{aligned} \tilde{A}(X_{12}, p) &= \tilde{A}\left(X_{13} + \frac{\xi_{23}}{2}, p\right) = \exp\left(\frac{1}{2}\xi_{23} \cdot \partial_{X_{13}}\right) \tilde{A}(X_{13}, p), \\ \tilde{B}(X_{23}, q) &= \tilde{B}\left(X_{13} - \frac{\xi_{12}}{2}, q\right) = \exp\left(-\frac{1}{2}\xi_{12} \partial_{X_{13}}\right) \tilde{B}(X_{13}, q). \end{aligned} \quad (\text{C.2.4})$$

Plugging this in (C.2.2) we find

$$\begin{aligned} \widetilde{(A \odot B)}(X_{13}, p_{13}) &= \int_{\mathbb{R}^4} d^4 x_2 \int_{\mathbb{R}^4} \frac{d^4 p}{(2\pi)^4} \int_{\mathbb{R}^4} \frac{d^4 q}{(2\pi)^4} \exp(ip_{13} \cdot \xi_{13} - ip \cdot \xi_{12} - iq \cdot \xi_{23}) \\ &\quad \times \exp\left(\frac{i}{2}\partial_p^{(A)} \partial_{X_{13}}^{(B)} - \frac{i}{2}\partial_{X_{13}}^{(A)} \partial_q^{(B)}\right) A(X_{13}, p) B(X_{23}, q), \end{aligned} \quad (\text{C.2.5})$$

where the bracketed superscripts on the differentiation operators indicate which of the two functions in the product to the right has to be differentiated. We have performed a partial integration with respect to p and q to apply the derivatives to the Wigner transforms of the two-point functions rather than the exponential. Now the argument of the exponential is

$$ip_{13} \cdot \xi_{13} - ip \cdot \xi_{12} - iq \cdot \xi_{23} = p_{13} \cdot \xi_{13} + x_2 \cdot (p - q) + q \cdot x_3 - p \cdot x_1. \quad (\text{C.2.6})$$

This enables us to perform the integral over x_2 leading to a factor $(2\pi)^4 \delta^{(4)}(p - q)$ and then the integral over q which gives

$$\widetilde{(A \odot B)}(X_{13}, p_{13}) = \int_{\mathbb{R}^4} \frac{d^4 p}{(2\pi)^4} \int_{\mathbb{R}^4} d^4 \xi_{13} \exp[i(p_{13} - p) \cdot \xi_{13}] \exp(i \diamond) A(X_{13}, p) B(X_{13}, p). \quad (\text{C.2.7})$$

Finally we can also perform the remaining integrals to get

$$\widetilde{(A \odot B)}(X_{13}, p_{13}) = \exp(i \diamond) A(X_{13}, p_{13}) B(X_{13}, p_{13}). \quad (\text{C.2.8})$$

Above we have introduced the **generalized Poisson-bracket operator**

$$\diamond A(X, p) B(X, p) = \frac{1}{2} [\partial_p A(X, p) \cdot \partial_x B(X, p) - \partial_x A(X, p) \cdot \partial_p B(X, p)] = \frac{1}{2} \{A, B\}_{\text{pb}}. \quad (\text{C.2.9})$$

Appendix C · Wigner representation of two-point functions

For the special case of two-point functions in homogeneous systems, where both A and B are independent of X , (C.2.8) leads to the usual convolution theorem of Fourier transformations: The convolution in the space-time domain maps simply to the product in the energy-momentum domain. In the non-equilibrium case the expansion of the exponential operator in this equation leads to the **gradient expansion** of the Kadanoff-Baym equations and in turn to semi-classical transport equations.

C.2 · *Convolution theorem for Wigner transforms*

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