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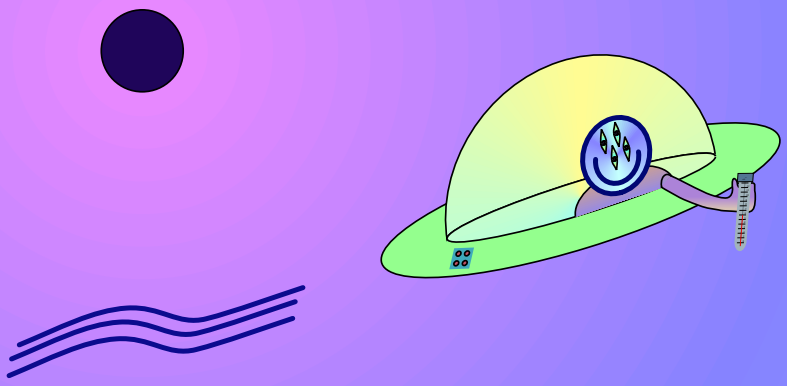
V. F. Mukhanov and S. Winitzki

Introduction to Quantum Fields in Classical Backgrounds



Lecture notes – 2004

Introduction to Quantum Fields in Classical Backgrounds

VIATCHESLAV F. MUKHANOV and SERGEI WINITZKI

DRAFT of August 4, 2005

Introduction to Quantum Fields in Classical Backgrounds

Department of Physics, Ludwig-Maximilians University, Munich, Germany.

This book is an elementary introduction to quantum field theory in curved spacetime. The text is accompanied by exercises and may be used as a base for a one-semester graduate or advanced undergraduate course.

Cover art by S. Winitzki

Contents

Preface

This book is an expanded and reorganized version of the lecture notes for a course taught (in German) at the Ludwig-Maximilians University, Munich, in the spring semester of 2003. The course is an elementary introduction to the basic concepts of quantum field theory in classical backgrounds. A certain level of familiarity with general relativity and quantum mechanics is required, although many of the necessary results are derived in the text.

The audience consisted of advanced undergraduates and beginning graduate students. There were 11 three-hour lectures. Each lecture was accompanied by exercises that are an integral part of the exposition and encapsulate longer but straightforward calculations or illustrative numerical results. Detailed solutions were given for all exercises. However, students could skip the solutions while still being able to follow the lectures. Exercises marked by an asterisk * are more difficult or cumbersome.

The book covers limited but essential material: quantization of free scalar fields; driven and time-dependent harmonic oscillators; mode expansions and Bogolyubov transformations; particle creation by classical backgrounds; quantum scalar fields in the de Sitter spacetime and growth of fluctuations; the Unruh effect; the Hawking radiation; the Casimir effect; quantization by path integrals; energy-momentum tensor for fields; effective action and backreaction; regularization of functional determinants using zeta functions and heat kernels. Topics such as quantization of higher-spin or interacting fields in curved spacetime, direct renormalization of the energy-momentum tensor, and the theory of cosmological perturbations are left out.

The emphasis of this course is rather heavily on concepts and not on computational results. Most of the required calculations have been simplified to the barest possible minimum that still contains all relevant physics. For instance, only free scalar fields are considered for quantization; background spacetimes are always chosen to be conformally flat; the Casimir effect, the Unruh effect and the Hawking radiation are computed for massless scalar fields in suitable 1+1-dimensional spacetimes. Thus a fairly modest computational effort suffices to explain important conceptual issues such as the nature of vacuum and particles in curved spacetimes, thermal effects of gravitation, and backreaction. This should prepare students for more advanced and technically demanding treatments suggested below.

The selection of the material and the initial composition of the lectures are due to Slava Mukhanov whose assistant I have been. I reworked the exposition and added many explanations and examples that the limited timespan of the spring semester did not allow us to present. The numerous remarks serve to complement and extend the presentation of the main material and may be skipped at first reading.

I am grateful to Andrei Barvinsky, Josef Gaßner, and Matthew Parry for discussions and valuable comments on the manuscript. Special thanks are due to Alex Vikman who worked through the text, corrected a number of mistakes, provided a calculation of the energy-momentum tensor in the last chapter, and prompted other important revisions.

The entire book was typeset with the excellent LyX and TEX document preparation system on computers running DEBIAN GNU/LINUX. I wish to express my gratitude to the creators and maintainers of this outstanding free software.

Sergei Winitzki, December 2004

Suggested literature

The following books offer a more extensive coverage of the subject and can be studied as a continuation of this introductory course.

N. D. BIRRELL and P. C. W. DAVIES, *Quantum fields in curved space* (Cambridge University Press, 1982).

S. A. FULLING, *Aspects of quantum field theory in curved space-time* (Cambridge University Press, 1989).

A. A. GRIB, S. G. MAMAEV, and V. M. MOSTEPANENKO, *Vacuum quantum effects in strong fields* (Friedmann Laboratory Publishing, St. Petersburg, 1994).

Part I

Canonical quantization

1 Overview. A taste of quantum fields

Summary: The vacuum state of classical and quantum oscillators. Particle interpretation of field theory. Examples of particle creation by external fields.

We start with a few elementary observations concerning the description of vacuum in quantum theory.

1.1 The harmonic oscillator and its vacuum state

The *vacuum* is the physical state corresponding to the intuitive notions of "the absence of anything" or "an empty space." Generally, the vacuum is defined as the state with the lowest possible energy. However, the classical and the quantum descriptions of the vacuum state are radically different. To get an idea of this difference, let us compare a classical oscillator with a quantized one.

A classical harmonic oscillator is described by a coordinate $q(t)$ satisfying

$$\ddot{q} + \omega^2 q = 0. \tag{1.1}$$

The solution of this equation is unique if we specify initial conditions $q\,(t_0)$ and $\dot{q}\,(t_0)$. We may identify the "vacuum state" of the oscillator as the state without motion, i.e. $q(t) \equiv 0$. This lowest-energy state is the solution of Eq. (1.1) with the initial conditions $q(0) = \dot{q}(0) = 0$.

When the oscillator is quantized, the classical coordinate q and the momentum $p = \dot{q}$ (for simplicity, we assume a unit mass of the oscillator) are replaced by operators $\hat{q}(t)$ and $\hat{p}(t)$ satisfying the Heisenberg commutation relation

$$[\hat{q}(t), \hat{p}(t)] = i\hbar.$$

Now the solution $\hat{q}(t) \equiv 0$ is impossible because the commutation relation is not satisfied. The vacuum state of the quantum oscillator is described by the normalized wave function

$$\psi(q) = \left[\frac{\omega}{\pi\hbar}\right]^{\frac{1}{4}} \exp\left(-\frac{\omega q^2}{2\hbar}\right).$$

Generally, the energy of the vacuum state is called the *zero-point energy*; for the harmonic oscillator, it is $E_0 = \frac{1}{2}\hbar\omega$. In the vacuum state, the position q fluctuates around $q = 0$ with a typical amplitude $\delta q \sim \sqrt{\hbar/\omega}$ and the measured trajectories $q(t)$ resemble a random walk around $q = 0$. Thus a quantum oscillator has a more complicated vacuum state than a classical one.

To simplify the formulae, we shall almost always use the units in which $\hbar = c = 1$.

1.2 Free quantum fields and vacuum

A classical field is described by a function of spacetime $\phi(\mathbf{x}, t)$, where $\mathbf{x}$ is a three-dimensional coordinate in space and t is the time (in some reference frame). The function $\phi(\mathbf{x}, t)$ takes values in some finite-dimensional vector space (with either real or complex coordinates).

The simplest example of a field is a real scalar field $\phi(\mathbf{x}, t)$; its values are real numbers. A free massive classical scalar field satisfies the Klein-Gordon equation

$$\frac{\partial^2 \phi}{\partial t^2} - \sum_{j=1}^{3} \frac{\partial^2 \phi}{\partial x_j^2} + m^2 \phi \equiv \ddot{\phi} - \Delta\phi + m^2\phi = 0. \tag{1.2}$$

If the initial conditions $\phi(\mathbf{x}, t_0)$ and $\dot{\phi}(\mathbf{x}, t_0)$ are specified, the solution $\phi(\mathbf{x}, t)$ for $t > t_0$ is unique. The solution with zero initial conditions is $\phi(\mathbf{x}, t) \equiv 0$ which is the classical vacuum state ("no field").

To simplify the equations of motion, it is convenient to use the spatial Fourier decomposition,

$$\phi(\mathbf{x}, t) = \int \frac{d^3\mathbf{k}}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot\mathbf{x}} \phi_{\mathbf{k}}(t), \tag{1.3}$$

where we integrate over all three-dimensional vectors $\mathbf{k}$. After the Fourier decomposition, the partial differential equation (1.2) is replaced by infinitely many ordinary differential equations, with one equation for each $\mathbf{k}$:

$$\ddot{\phi}_{\mathbf{k}} + \left(k^2 + m^2\right) \phi_{\mathbf{k}} = 0.$$

In other words, each complex function $\phi_{\mathbf{k}}(t)$ satisfies the harmonic oscillator equation with the frequency

$$\omega_k \equiv \sqrt{k^2 + m^2},$$

where $k \equiv |\mathbf{k}|$. The functions $\phi_{\mathbf{k}}(t)$ are called the *modes* of the field ϕ (abbreviated from "Fourier modes"). Note that the replacement of the field ϕ by a collection of oscillators $\phi_{\mathbf{k}}$ is a formal mathematical procedure. The oscillators "move" in the *configuration space* (i.e. in the space of values of the field ϕ), not in the real three-dimensional space.

To quantize the field, each mode $\phi_{\mathbf{k}}(t)$ is quantized as a separate harmonic oscillator. We replace the classical coordinates $\phi_{\mathbf{k}}$ and momenta $\pi_{\mathbf{k}} \equiv \dot{\phi}^*_{\mathbf{k}}$ by operators $\hat{\phi}_{\mathbf{k}}$, $\hat{\pi}_{\mathbf{k}}$ and postulate the equal-time commutation relations

$$\left[\hat{\phi}_{\mathbf{k}}(t), \hat{\pi}_{\mathbf{k}'}(t)\right] = i\delta\left(\mathbf{k} + \mathbf{k}'\right). \tag{1.4}$$

Quantization in a box

It is useful to begin by considering a field $\phi(\mathbf{x}, t)$ not in the entire infinite space but in a box of finite volume V, with some conditions imposed on the field ϕ at the box

boundary. The volume V should be large enough so that the artificially introduced box and the boundary conditions are physically irrelevant. For instance, we might choose the box as a cube with side L and volume $V = L^3$ and impose the *periodic* boundary conditions,

$$\phi(x = 0, y, z, t) = \phi(x = L, y, z, t)$$

and similarly for y and z. The Fourier decomposition can be written as

$$\begin{aligned} \phi_{\mathbf{k}}(t) &= \frac{1}{\sqrt{V}} \int d^3\mathbf{x}\, \phi(\mathbf{x}, t)\, e^{-i\mathbf{k}\cdot\mathbf{x}}, \\ \phi(\mathbf{x}, t) &= \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \phi_{\mathbf{k}}(t) e^{i\mathbf{k}\cdot\mathbf{x}}, \end{aligned} \tag{1.5}$$

where the sum goes over three-dimensional wave numbers $\mathbf{k}$ with components of the form

$$k_x = \frac{2\pi n_x}{L}, \quad n_x = 0, \pm 1, \pm 2, \ldots$$

and similarly for k_y and k_z. The normalization factor $\sqrt{V}$ in Eq. (1.5) is a mathematical convention chosen to simplify some formulae (we could rescale the modes $\phi_{\mathbf{k}}$ by any constant). Indeed, the Dirac δ function in Eq. (1.4) is replaced by the Kronecker symbol $\delta_{\mathbf{k}+\mathbf{k}',0}$ without any normalization factors, and the total energy of the field ϕ in the box is simply the sum of energies of all oscillators $\phi_{\mathbf{k}}$,

$$E = \sum_{\mathbf{k}} \left[\frac{1}{2} \left| \dot{\phi}_{\mathbf{k}} \right|^2 + \frac{1}{2} \omega_k^2 \left| \phi_{\mathbf{k}} \right|^2 \right].$$

Vacuum wave functional

Since all modes $\phi_{\mathbf{k}}$ of a free field ϕ are decoupled, the vacuum state of the field can be characterized by a *wave functional* which is the product of the ground state wave functions of all modes,

$$\Psi[\phi] \propto \prod_{\mathbf{k}} \exp\left(-\frac{\omega_k \left| \phi_{\mathbf{k}} \right|^2}{2} \right) = \exp\left[-\frac{1}{2} \sum_{\mathbf{k}} \omega_k \left| \phi_{\mathbf{k}} \right|^2 \right]. \tag{1.6}$$

Strictly speaking, Eq. (1.6) is valid only for a field quantized in a box as described above. (Incidentally, if the modes $\phi_{\mathbf{k}}$ were normalized differently than shown in Eq. (1.5), there would be a volume factor in front of ω_k.)

The wave functional (1.6) gives the quantum-mechanical amplitude for measuring a certain field configuration $\phi(\mathbf{x}, t)$ at some fixed time t. This amplitude is time-independent, so the vacuum is a stationary state. The field fluctuates in the vacuum state and the field configuration can be visualized as a random small deviation from zero (see Fig. 1.1).

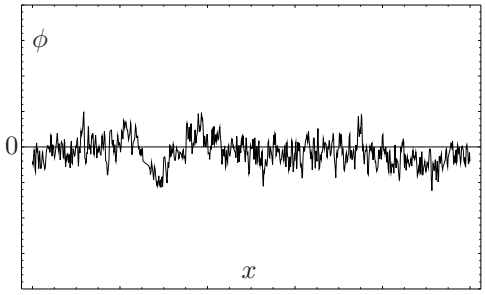


Figure 1.1: A field configuration $\phi(x)$ that could be measured in the vacuum state.

In the limit of very large volume of the box, we replace sums by integrals,

$$\sum_{\mathbf{k}} \to \frac{V}{(2\pi)^3} \int d^3\mathbf{k}, \quad \phi_{\mathbf{k}} \to \sqrt{\frac{(2\pi)^3}{V}} \phi_{\mathbf{k}}, \tag{1.7}$$

and the wave functional (1.6) becomes

$$\Psi[\phi] \propto \exp\left[-\frac{1}{2} \int d^3\mathbf{k} \, |\phi_{\mathbf{k}}|^2 \, \omega_k\right]. \tag{1.8}$$

Exercise 1.1

The vacuum wave functional (1.8) contains the integral

$$I \equiv \int d^3\mathbf{k} \, |\phi_{\mathbf{k}}|^2 \sqrt{k^2 + m^2}, \tag{1.9}$$

where $\phi_{\mathbf{k}}$ are the field modes defined by Eq. (1.3). The integral (1.9) can be expressed directly through the function $\phi(\mathbf{x})$,

$$I = \int d^3\mathbf{x} \, d^3\mathbf{y} \, \phi(\mathbf{x}) \, K(\mathbf{x}, \mathbf{y}) \, \phi(\mathbf{y}).$$

Determine the required kernel $K(\mathbf{x}, \mathbf{y})$.

1.3 The zero-point energy

We now compute the energy of the vacuum (the zero-point energy) of a free quantum field quantized in a box. Each oscillator $\phi_{\mathbf{k}}$ is in the ground state and has the energy $\frac{1}{2}\omega_k$, so the total zero-point energy of the field is

$$E_0 = \sum_{\mathbf{k}} \frac{1}{2} \omega_k.$$

Replacing the sum by an integral according to Eq. (1.7), we obtain the following expression for the zero-point energy density,

$$\frac{E_0}{V} = \int \frac{d^3\mathbf{k}}{(2\pi)^3}\frac{1}{2}\omega_k. \tag{1.10}$$

This integral diverges at the upper bound as $\sim k^4$. Taken at face value, this would indicate an infinite energy *density* of the vacuum state. If we impose a cutoff at the Planck scale (there is surely some new physics at higher energies), then the vacuum energy density will be of order 1 in Planck units, which corresponds to a mass density of about 10^{94}g/cm^3. This is much more per 1cm^3 than the mass of the entire observable Universe ($\sim 10^{55}$g)! Such a huge energy density would lead to strong gravitational effects which are not actually observed.

The standard way to avoid this problem is to *postulate* that the infinite energy density given by Eq. (1.10) does not contribute to gravitation. In effect this constant infinite energy is subtracted from the energy of the system ("renormalization" of zero-point energy).

1.4 Quantum fluctuations in the vacuum state

1.4.1 Amplitude of fluctuations

From the above consideration of harmonic oscillators we know that the typical amplitude of fluctuations $\delta\phi_{\mathbf{k}}$ in the mode $\phi_{\mathbf{k}}$ is

$$\delta\phi_{\mathbf{k}} \equiv \sqrt{\left\langle \left|\phi_{\mathbf{k}}\right|^2 \right\rangle} \sim \omega_k^{-1/2}. \tag{1.11}$$

Field values cannot be observed at a point; in a realistic experiment, only averages of field values over a region of space can be measured. The next exercise shows that if ϕ_L is the average of $\phi(x)$ over a volume L^3, the typical fluctuation of ϕ_L is

$$\delta\phi_L \sim \sqrt{\frac{k_L^3}{\omega_{k_L}}}, \quad k_L \equiv L^{-1}. \tag{1.12}$$

Exercise 1.2

The average value of a field $\phi(\mathbf{x})$ over a volume L^3 is defined by the integral over a cube-shaped region,

$$\phi_L \equiv \frac{1}{L^3}\int_{-L/2}^{L/2} dx \int_{-L/2}^{L/2} dy \int_{-L/2}^{L/2} dz\, \phi(\mathbf{x}).$$

Justify the following order-of-magnitude estimate of the typical amplitude of fluctuations $\delta\phi_L$,

$$\delta\phi_L \sim \left[(\delta\phi_k)^2 k^3\right]^{1/2}, \quad k = L^{-1},$$

where $k \equiv |\mathbf{k}|$ and $\delta\phi_k$ is the typical amplitude of vacuum fluctuations in the mode $\phi_{\mathbf{k}}$.
Hint: The "typical amplitude" δx of a quantity x fluctuating around 0 is $\delta x = \sqrt{\langle x^2 \rangle}$.

The wave number $k_L \sim L^{-1}$ characterizes the scale L. As a function of L, the amplitude of fluctuations given by Eq. (1.12) diverges as L^{-1} for small $L \ll m^{-1}$ and decays as $L^{-3/2}$ for large $L \gg m^{-1}$.

1.4.2 Observable effects of vacuum fluctuations

Quantum fluctuations are present in the vacuum state and have observable consequences that cannot be explained by any other known physics. The three well-known effects are the spontaneous emission of radiation by hydrogen atoms, the Lamb shift, and the Casimir effect. All these effects have been observed experimentally.

The spontaneous emission by a hydrogen atom is the transition between the electron states $2p \to 1s$ with the production of a photon. This effect can be explained only by an interaction of electrons with vacuum fluctuations of the electromagnetic field. Without these fluctuations, the hydrogen atom would have remained forever in the stable $2p$ state.

The Lamb shift is a small difference between the energies of the $2p$ and $2s$ states of the hydrogen atom. This shift occurs because the electron clouds in these states have different geometries and interact differently with vacuum fluctuations of the electromagnetic field. The measured energy difference corresponds to the frequency ≈ 1057MHz which is in a good agreement with the theoretical prediction.

The Casimir effect is manifested by a force of attraction between two parallel *uncharged* conducting plates. The force decays with the distance L between the plates as $F \sim L^{-4}$. This effect can be explained only by considering the shift of the zero-point energy of the electromagnetic field due to the presence of the conductors.

1.5 Particle interpretation of quantum fields

The classical concept of particles involves point-like objects moving along certain trajectories. Experiments show that this concept does not actually apply to subatomic particles. For an adequate description of photons and electrons and other elementary particles, one needs to use a relativistic quantum field theory (QFT) in which the basic objects are not particles but quantum fields. For instance, the quantum theory of photons and electrons (quantum electrodynamics) describes the interaction of the electromagnetic field with the electron field. Quantum states of the fields are interpreted in terms of corresponding particles. Experiments are then described by computing probabilities for specific field configurations.

A quantized mode $\hat{\phi}_{\mathbf{k}}$ has excited states with energies $E_{n,\mathbf{k}} = \left(\frac{1}{2} + n\right)\omega_k$, where $n = 0, 1, ...$ The energy $E_{n,\mathbf{k}}$ is greater than the zero-point energy by $\Delta E = n\omega_k = n\sqrt{k^2 + m^2}$ which is equal to the energy of n relativistic particles of mass m and momentum $\mathbf{k}$. Therefore the excited state with the energy $E_{n,\mathbf{k}}$ is interpreted as describing n particles of momentum $\mathbf{k}$. We also refer to such states as having the *occupation number* n.

A classical field corresponds to states with large occupation numbers $n \gg 1$. In that case, quantum fluctuations can be very small compared with expectation values of the field.

A free, noninteracting field in a state with certain occupation numbers will forever remain in the same state. On the other hand, occupation numbers for interacting fields can change with time. An increase in the occupation number in a mode $\phi_{\mathbf{k}}$ is interpreted as production of particles with momentum $\mathbf{k}$.

1.6 Quantum field theory in classical backgrounds

"Traditional" QFT deals with problems of finding cross-sections for transitions between different particle states, such as scattering of one particle on another. For instance, typical problems of quantum electrodynamics are:

1. Given the initial state (at time $t \to -\infty$) of an electron with momentum $\mathbf{k}_1$ and a photon with momentum $\mathbf{k}_2$, find the cross-section for the scattering into the final state (at $t \to +\infty$) where the electron has momentum $\mathbf{k}_3$ and the photon has momentum $\mathbf{k}_4$.
   This problem is formulated in terms of quantum fields in the following manner. Suppose that ψ is the field representing electrons. The initial configuration is translated into a state of the mode $\psi_{\mathbf{k}_1}$ with the occupation number 1 and all other modes of the field ψ having zero occupation numbers. The initial configuration of "oscillators" of the electromagnetic field is analogous—only the mode with momentum $\mathbf{k}_2$ is occupied. The final configuration is similarly translated into the language of field modes.

2. Initially there is an electron and a positron with momenta $\mathbf{k}_{1,2}$. Find the cross-section for their annihilation with the emission of two photons with momenta $\mathbf{k}_{3,4}$.

These problems are solved by applying perturbation theory to a system of infinitely many coupled quantum oscillators. The required calculations are usually quite tedious.

In this book we study quantum fields interacting with a strong external field called the *background*. It is assumed that the background field is adequately described by a classical theory and does not need to be quantized. In other words, our subject is *quantum fields in classical backgrounds*. A significant simplification comes from considering quantum fields that interact *only* with classical backgrounds but not with other quantum fields. Such quantum fields are also called *free* fields, even though they are coupled to the background.

Typical problems of interest to us are:

1. To compute probabilities for transitions between various states of a harmonic oscillator in a background field. A transition between oscillator states can describe, for instance, the process of particle creation by a classical field.

2. To determine the shift of the energy levels of an oscillator due to the presence of the background. The energy shift cannot be ignored since the zero-point energy of the oscillator is already subtracted. It is likely that the additional energy shift can contribute to gravity via the Einstein equation.

3. To calculate the backreaction of a quantum field on the classical background. For example, quantum effects in a gravitational field induce corrections to the energy-momentum tensor of a matter field. The corrections are of order R^2, where R is the Riemann curvature scalar, and contribute to the Einstein equation.

1.7 Examples of particle creation

1.7.1 Time-dependent oscillator

A nonstationary gravitational background influences quantum fields in such a way that the frequencies ω_k of the modes become time-dependent, $\omega_k(t)$. We shall examine this situation in detail in chapter 6. For now, let us consider a harmonic oscillator with a time-dependent frequency $\omega(t)$. Such oscillators usually exhibit transitions between energy levels. As a simple example, we study an oscillator $q(t)$ which satisfies the following equations of motion,

$$\ddot{q}(t) + \omega_0^2 q(t) = 0, \ t < 0 \text{ or } t > T;$$
$$\ddot{q}(t) - \Omega_0^2 q(t) = 0, \ 0 < t < T,$$

where ω_0 and Ω_0 are real constants.

Exercise 1.3
For the above equations of motion, take the solution $q(t) = q_1 \sin \omega_0 t$ for $t < 0$ and show that for $t > T$ the solution is of the form

$$q(t) = q_2 \sin(\omega_0 t + \alpha),$$

where α is a constant and, assuming that $\Omega_0 T \gg 1$,

$$q_2 \approx \frac{1}{2} q_1 \sqrt{1 + \frac{\omega_0^2}{\Omega_0^2}} \exp(\Omega_0 T).$$

The exercise shows that for $\Omega_0 T \gg 1$ the oscillator has a large amplitude $q_2 \gg q_1$ at late times $t > T$. The state of the oscillator is then interpreted as a state with many particles. Thus there is a prolific particle production if $\Omega_0 T \gg 1$.

Exercise 1.4
Estimate the number of particles at $t > T$ in the problem considered in Exercise 1.3, assuming that the oscillator is in the ground state at $t < 0$.

1.7.2 The Schwinger effect

A static electric field in empty space can create electron-positron (e^+e^-) pairs. This effect, called the *Schwinger effect*, is currently on the verge of being experimentally verified.

To understand the Schwinger effect qualitatively, we may imagine a virtual e^+e^- pair in a constant electric field of strength E. If the particles move apart from each other to a distance l, they will receive the energy leE from the electric field. If this energy exceeds the rest mass of the two particles, $leE \geq 2m_e$, the pair will become real and the particles will continue to move apart. The typical separation of the virtual pair is of order of the Compton wavelength $2\pi/m_e$. More precisely, the probability of separation by a distance l turns out to be $P \sim \exp(-\pi m_e l)$. Therefore the probability of creating an e^+e^- pair is

$$P \sim \exp\left(-\frac{m_e^2}{eE}\right). \tag{1.13}$$

The exact formula for the probability P can be obtained from a full (but rather lengthy) consideration using quantum electrodynamics.

Exercise 1.5

Suppose that the probability for a pair production in an electric field of intensity E is given by Eq. (1.13), where m_e and e are the mass and the charge of an electron. Consider strongest electric fields available in a laboratory today and compute the corresponding probability for producing an e^+e^- pair.

Hint: Rewrite Eq. (1.13) in the SI units.

1.7.3 Production of particles by gravity

Generally, a static gravitational field does not produce particles (black holes provide an important exception). We can visualize this by picturing a virtual particle-antiparticle pair in a static field of gravity: both virtual particles fall together and never separate sufficiently far to become real particles. However, a time-dependent gravitational field (a nonstationary spacetime) generally leads to some particle production. A nonstationary gravitational field exists, for example, in expanding universes, or during the formation of a black hole through gravitational collapse.

One would expect that a nonrotating black hole cannot produce any particles since its gravitational field is static. It came as a surprise when Hawking in 1973 discovered that static black holes nevertheless create particles with the blackbody thermal distribution at temperature

$$T = \frac{\hbar c^3}{8\pi G M},$$

where M is the mass of the black hole and G is Newton's constant.

We can outline a qualitative picture of the Hawking radiation using a consideration with virtual particle-antiparticle pairs. One particle of the pair may happen to be just outside of the black hole horizon while the other particle is inside it. The particle inside the horizon inevitably falls onto the black hole center, while the other particle

can escape and may be detected by stationary observers far from the black hole. The existence of the horizon is crucial for particle production; without horizons, a static gravitational field does not create particles.

1.7.4 The Unruh effect

This effect concerns an accelerated particle detector in empty space. Although all fields are in their vacuum states, the accelerated detector will nevertheless find a distribution of particles with a thermal spectrum (a heat bath). The temperature of this heat bath is called the *Unruh temperature* and is expressed as $T = a/(2\pi)$, where a is the acceleration of the detector (both the temperature and the acceleration are given in Planck units).

In principle, the Unruh effect can be used to heat water in an accelerated container. The energy for heating the water comes from the agent that accelerates the container.

> **Exercise 1.6**
> A glass of water is moving with a constant acceleration. Determine the smallest acceleration that makes the water boil due to the Unruh effect.

2 Reminder: Classical and quantum mechanics

Summary: Action in classical mechanics. Functional derivatives. Lagrangian and Hamiltonian mechanics. Canonical quantization in Heisenberg picture. Operators and vectors in Hilbert space. Dirac notation. Schrödinger equation.

2.1 Lagrangian formalism

Quantum theories are built by applying a quantization procedure to classical theories. The starting point of a classical theory is the action principle.

2.1.1 The action principle

The evolution of a classical physical system is described by a function $q(t)$, where q is a generalized coordinate (which may be a vector) and t is the time. The trajectory $q(t)$ is determined by the requirement that an action functional[1]

$$S\left[q(t)\right] = \int_{t_1}^{t_2} L\left(t, q(t), \dot{q}(t), \ddot{q}(t), ...\right) dt \tag{2.1}$$

is extremized. Here $t_{1,2}$ are two fixed moments of time at which one specifies boundary conditions, e.g. $q(t_1) = q_1$ and $q(t_2) = q_2$. The function $L\left(t, q, \dot{q}, ...\right)$ is called the *Lagrangian* of the system; different Lagrangians describe different systems. For example, the Lagrangian of a harmonic oscillator with unit mass and a constant frequency ω is

$$L\left(q, \dot{q}\right) = \frac{1}{2}\left(\dot{q}^2 - \omega^2 q^2\right). \tag{2.2}$$

This Lagrangian does not depend explicitly on the time t.

2.1.2 Equations of motion

The requirement that the function $q(t)$ extremizes the action usually leads to a differential equation for $q(t)$. We shall now derive this equation for the action

$$S\left[q\right] = \int_{t_1}^{t_2} L\left(t, q, \dot{q}\right) dt. \tag{2.3}$$

[1] See Appendix A.1 for more details concerning functionals.

> **Remark:** Our derivation does not apply to Lagrangians involving higher derivatives such as $\ddot{q}$. Note that in those cases one would need to impose more boundary conditions than merely $q(t_1) = q_1$ and $q(t_2) = q_2$.

If the function $q(t)$ is an extremum of the action functional (2.3), then a small perturbation $\delta q(t)$ will change the value of $S[q]$ by terms which are quadratic in $\delta q(t)$. In other words, the variation

$$\delta S[q, \delta q] \equiv S[q + \delta q] - S[q]$$

should have no first-order terms in δq. To obtain the resulting equation for $q(t)$, we compute the variation of the functional S:

$$\begin{aligned}
\delta S[q; \delta q] &= S[q(t) + \delta q(t)] - S[q(t)] \\
&= \int_{t_1}^{t_2} \left[\frac{\partial L(t, q, \dot{q})}{\partial q} \delta q(t) + \frac{\partial L(t, q, \dot{q})}{\partial \dot{q}} \delta \dot{q}(t) \right] dt + O\left(\delta q^2\right) \\
&= \delta q(t) \frac{\partial L}{\partial \dot{q}} \Big|_{t_1}^{t_2} + \int_{t_1}^{t_2} \left[\frac{\partial L}{\partial q} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} \right] \delta q(t) dt + O\left(\delta q^2\right). \qquad (2.4)
\end{aligned}$$

To satisfy the boundary conditions $q(t_{1,2}) = q_{1,2}$, we must choose the perturbation $\delta q(t)$ such that $\delta q(t_{1,2}) = 0$. Therefore the boundary terms in Eq. (2.4) vanish and we obtain the variation δS as the following functional of $q(t)$ and $\delta q(t)$,

$$\delta S = \int_{t_1}^{t_2} \left[\frac{\partial L(t, q, \dot{q})}{\partial q} - \frac{d}{dt} \frac{\partial L(t, q, \dot{q})}{\partial \dot{q}} \right] \delta q(t) dt + O\left(\delta q^2\right). \qquad (2.5)$$

The condition that the variation is second-order in δq means that the first-order terms should vanish for any $\delta q(t)$. This is possible only if the expression in the square brackets in Eq. (2.5) vanishes. Thus we obtain the *Euler-Lagrange equation*

$$\frac{\partial L(t, q, \dot{q})}{\partial q} - \frac{d}{dt} \frac{\partial L(t, q, \dot{q})}{\partial \dot{q}} = 0. \qquad (2.6)$$

This is the classical equation of motion for a mechanical system described by the Lagrangian $L(t, q, \dot{q})$.

Example: For the harmonic oscillator with the Lagrangian (2.2), the Euler-Lagrange equation reduces to

$$\ddot{q} + \omega^2 q = 0. \qquad (2.7)$$

Generally the path $q(t)$ that extremizes the action and satisfies boundary conditions is unique. However, there are cases when the extremum is not unique or even does not exist.

> **Exercise 2.1**
> Find the trajectory $q(t)$ satisfying Eq. (2.7) with the boundary conditions $q(t_1) = q_1$, $q(t_2) = q_2$. Indicate the conditions for the existence and the uniqueness of the solution.

2.1.3 Functional derivatives

The variation of a functional can always be written in the following form:

$$\delta S = \int \frac{\delta S}{\delta q(t)} \delta q(t) dt + O\left(\delta q^2\right). \tag{2.8}$$

The expression denoted by $\delta S/\delta q(t)$ in Eq. (2.8) is called the *functional derivative* (or the *variational derivative*) of $S[q]$ with respect to $q(t)$.

If the functional $S[q]$ is given by Eq. (2.3), then we compute the functional derivative $\delta S/\delta q(t_0)$ at an intermediate time t_0 from Eq. (2.5), disregarding the boundary terms:

$$\frac{\delta S}{\delta q\left(t_0\right)} = \left[\frac{\partial L\left(t, q, \dot{q}\right)}{\partial q} - \frac{d}{dt}\frac{\partial L\left(t, q, \dot{q}\right)}{\partial \dot{q}}\right]_{t=t_0}.$$

Here the functions $q(t)$ and $\dot{q}(t)$ must be evaluated at $t = t_0$ after taking all derivatives. For brevity, one usually writes the above expression as

$$\frac{\delta S}{\delta q\left(t\right)} = \frac{\partial L\left(t, q, \dot{q}\right)}{\partial q} - \frac{d}{dt}\frac{\partial L\left(t, q, \dot{q}\right)}{\partial \dot{q}}. \tag{2.9}$$

Example: For a harmonic oscillator with the Lagrangian (2.2) we get

$$\frac{\delta S}{\delta q\left(t\right)} = -\omega^2 q\left(t\right) - \ddot{q}\left(t\right). \tag{2.10}$$

It is important to keep track of the argument t in the functional derivative $\delta S/\delta q(t)$. A functional $S[q]$ generally depends on all the values $q(t)$ at all $t = t_1, t_2, ...$, and thus may be visualized as a function of infinitely many variables,

$$S[q(t)] = \text{“}S\left(q_1, q_2, q_3, ...\right)\text{”},$$

where $q_i \equiv q(t_i)$. The partial derivative of this “function” with respect to one of its arguments, say $q_1 \equiv q(t_1)$, is analogous to the functional derivative $\delta S/\delta q(t_1)$. Clearly the derivative $\delta S/\delta q(t_1)$ is not the same as $\delta S/\delta q(t_2)$, so we cannot define a derivative “with respect to the function q” without specifying a particular value of t.

For a functional of $S[\phi]$ of a field $\phi(\mathbf{x}, t)$, the functional derivative with respect to $\phi(\mathbf{x}, t)$ retains the arguments $\mathbf{x}$ and t and is written as $\delta S/\delta\phi(\mathbf{x}, t)$.

> **Remark: boundary terms in functional derivatives.** While deriving Eq. (2.9), we omitted the boundary terms
>
> $$\delta q(t) \frac{\partial L}{\partial \dot{q}}\bigg|_{t_1}^{t_2}.$$
>
> However, the definition (2.8) of the functional derivative (if applied pedantically) requires one to rewrite these boundary terms as integrals of $\delta q(t)$, e.g.
>
> $$\delta q \frac{\partial L}{\partial \dot{q}}\bigg|_{t=t_1} = \int \delta\left(t - t_1\right) \delta q(t) \frac{\partial L\left(t, q, \dot{q}\right)}{\partial \dot{q}} dt,$$

and to compute the functional derivative as

$$\frac{\delta S}{\delta q(t)} = \frac{\partial L\left(t,q,\dot{q}\right)}{\partial q} - \frac{d}{dt}\frac{\partial L\left(t,q,\dot{q}\right)}{\partial \dot{q}} + \left[\delta\left(t-t_2\right) - \delta\left(t-t_1\right)\right]\frac{\partial L\left(t,q,\dot{q}\right)}{\partial \dot{q}}.$$

The omission of the boundary terms is adequate for the derivation of the Euler-Lagrange equation because the perturbation $\delta q(t)$ vanishes at $t = t_{1,2}$ and the functional derivatives with respect to $q(t_1)$ or $q(t_2)$ are never required. For this reason we shall usually omit the boundary terms in functional derivatives.

To evaluate functional derivatives, it is convenient to convert functionals to the integral form. Sometimes the Dirac δ function must be used for this purpose. (See Appendix A.1 to recall the definition and the properties of the δ function.)

Example 1: For the functional

$$A\left[q\right] \equiv \int q^3 dt$$

the functional derivative is

$$\frac{\delta A\left[q\right]}{\delta q\left(t_1\right)} = 3q^2\left(t_1\right).$$

Example 2: The functional

$$\begin{aligned} B\left[q\right] &\equiv 3\sqrt{q(1)} + \sin\left[q(2)\right] \\ &= \int \left[3\delta(t-1)\sqrt{q(t)} + \delta(t-2)\sin q(t)\right] dt \end{aligned}$$

has the functional derivative

$$\frac{\delta B\left[q\right]}{\delta q(t)} = \frac{3\delta(t-1)}{2\sqrt{q(1)}} + \delta(t-2)\cos\left[q(2)\right].$$

Example 3: Field in three dimensions. For the following functional $S\left[\phi\right]$ depending on a field $\phi\left(\mathbf{x},t\right)$,

$$S\left[\phi\right] = \frac{1}{2}\int d^3\mathbf{x}\, dt (\nabla\phi)^2,$$

the functional derivative with respect to $\phi\left(\mathbf{x},t\right)$ is found after an integration by parts:

$$\frac{\delta S\left[\phi\right]}{\delta\phi\left(\mathbf{x},t\right)} = -\Delta\phi\left(\mathbf{x},t\right).$$

The boundary terms have been omitted because the integration in $S\left[\phi\right]$ is performed over the entire spacetime and the field ϕ is assumed to decay sufficiently rapidly at infinity.

Remark: alternative definition. The functional derivative of a functional may be equivalently defined using the δ function,

$$\frac{\delta A[q]}{\delta q(t_1)} = \left.\frac{d}{ds}\right|_{s=0} A[q(t) + s\delta(t - t_1)].$$

As this formula shows, the functional derivative describes the infinitesimal change in the functional $A[q]$ under a perturbation which consists of changing the function $q(t)$ at one point $t = t_1$. One can prove that the definition (2.8) of the functional derivative is equivalent to the above formula.

The δ function is not really a function but a distribution, so if we wish to be more rigorous, we have to reformulate the above definition:

$$\frac{\delta A[q]}{\delta q(t_1)} = \lim_{n\to\infty} \left.\frac{d}{ds}\right|_{s=0} A[q_n(t)],$$

where $q_n(t)$, $n = 1, 2, ...$ is a sequence of functions that converges to $q(t) + s\delta(t - t_1)$ in the distributional sense. Most calculations, however, can be performed without regard for these subtleties by formally manipulating the δ function under the functional $A[q]$.

Second functional derivative

A derivative of a function with many arguments is still a function of many arguments. Therefore the functional derivative is itself again a functional of $q(t)$ and we may define the second functional derivative,

$$\frac{\delta^2 S}{\delta q(t_1)\,\delta q(t_2)} \equiv \frac{\delta}{\delta q(t_2)}\left\{\frac{\delta S}{\delta q(t_1)}\right\}.$$

Exercise 2.2

The action $S[q(t)]$ of a harmonic oscillator is the functional

$$S[q] = \frac{1}{2}\int \left(\dot{q}^2 - \omega^2 q^2\right) dt.$$

Compute the second functional derivative

$$\frac{\delta^2 S[q]}{\delta q(t_1)\,\delta q(t_2)}.$$

2.2 Hamiltonian formalism

The starting point of a canonical quantum theory is a classical theory in the Hamiltonian formulation. The Hamiltonian formalism is based on the Legendre transform of the Lagrangian $L(t, q, \dot{q})$ with respect to the velocity $\dot{q}$.

Legendre transform

Given a function $f(x)$, one can introduce a new variable p instead of x,

$$p \equiv \frac{df}{dx}, \tag{2.11}$$

and replace the function $f(x)$ by a new function $g(p)$ defined by

$$g(p) \equiv px(p) - f.$$

Here we imply that x has been expressed through p using Eq. (2.11); the function $f(x)$ must be such that p, which is the slope of $f(x)$, is uniquely related to x. The new function $g(p)$ is called the *Legendre transform* of $f(x)$. A nice property of the Legendre transform is that the old variable x and the old function $f(x)$ are recovered by taking the Legendre transform of $g(p)$. In other words, the Legendre transform is its own inverse. This happens because $x = dg(p)/dp$.

The Hamiltonian

To define the Hamiltonian, one performs the Legendre transform of the Lagrangian $L(t, q, \dot{q})$ to replace $\dot{q}$ by a new variable p (the *canonical momentum*). The variables t and q do not participate in the Legendre transform and remain as parameters. The relation between the velocity $\dot{q}$ and the momentum p is

$$p = \frac{\partial L(t, q, \dot{q})}{\partial \dot{q}}. \tag{2.12}$$

The ubiquitously used notation $\partial/\partial\dot{q}$ means simply the partial derivative of $L(t, q, \dot{q})$ with respect to its third argument.

> **Remark:** If the coordinate q is a multi-dimensional vector, $q \equiv q_j$, the Legendre transform is performed with respect to each velocity $\dot{q}_j$ and the momentum vector p_j is introduced. In field theory there is a continuous set of "coordinates," so we need to use a functional derivative when defining the momenta.

Assuming that Eq. (2.12) can be solved for the velocity $\dot{q}$ as a function of t, q and p,

$$\dot{q} = v(p; q, t), \tag{2.13}$$

one defines the *Hamiltonian* $H(p, q, t)$ by

$$H(p, q, t) \equiv \left[p\dot{q} - L(t, q, \dot{q})\right]_{\dot{q}=v(p;q,t)}. \tag{2.14}$$

In the above expression, $\dot{q}$ is replaced by the function $v(p; q, t)$.

> **Remark: the existence of the Legendre transform.** The possibility of performing the Legendre transform hinges on the invertibility of Eq. (2.12) which requires that the Lagrangian $L(t, q, \dot{q})$ should be a suitably nondegenerate function of the velocity $\dot{q}$. Many physically important theories, such as the Dirac theory of the electron or Einstein's general relativity, are described by Lagrangians that do not admit a Legendre transform in the velocities. In those cases (not considered in this book) a more complicated formalism is needed to obtain an adequate Hamiltonian description of the theory.

2.2.1 The Hamilton equations of motion

The Euler-Lagrange equations of motion are second-order differential equations for $q(t)$. We shall now derive the Hamilton equations which are first-order equations for the variables $q(t)$ and $p(t)$.

Rewriting Eq. (2.6) with the help of Eq. (2.12), we get

$$\frac{dp}{dt} = \left.\frac{\partial L\left(t,q,\dot{q}\right)}{\partial q}\right|_{\dot{q}=v(p;q,t)}, \tag{2.15}$$

where the substitution $\dot{q} = v$ must be carried out after the differentiation $\partial L/\partial q$. The other equation is (2.13),

$$\frac{dq}{dt} = v\left(p;q,t\right). \tag{2.16}$$

The equations (2.15)-(2.16) can be rewritten in terms of the Hamiltonian $H(p,q,t)$ defined by Eq. (2.14). After some straightforward algebra, one obtains

$$\frac{\partial H}{\partial q} = \frac{\partial}{\partial q}(pv - L) = p\frac{\partial v}{\partial q} - \frac{\partial L}{\partial q} - \frac{\partial L}{\partial \dot{q}}\frac{\partial v}{\partial q} = -\frac{\partial L}{\partial q}, \tag{2.17}$$

$$\frac{\partial H}{\partial p} = \frac{\partial}{\partial p}(pv - L) = v + p\frac{\partial v}{\partial p} - \frac{\partial L}{\partial \dot{q}}\frac{\partial v}{\partial p} = v. \tag{2.18}$$

Therefore Eqs. (2.15)-(2.16) become

$$\dot{q} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial q}. \tag{2.19}$$

These are the Hamilton equations of motion.

Example: For a harmonic oscillator described by the Lagrangian (2.2), we obtain the canonical momentum $p = \dot{q}$ and the Hamiltonian

$$H(p,q) = p\dot{q} - L = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 q^2. \tag{2.20}$$

The Hamilton equations are

$$\dot{q} = p, \quad \dot{p} = -\omega^2 q.$$

Derivation using differential forms. The calculation leading from Eq. (2.14) to Eq. (2.17) is more elegant in the language of 1-forms in the two-dimensional phase space (q,p). The time dependence of L and H is not essential for this derivation and we omit it here. The Lagrangian is expressed through p using Eq. (2.13), and its differential is the 1-form

$$dL = \frac{\partial L}{\partial q}dq + \frac{\partial L}{\partial v}dv = \frac{\partial L}{\partial q}dq + pdv.$$

Here dv is the 1-form obtained by differentiating the function $v\left(p;q,t\right)$; here we do not need to expand $v\left(p;q,t\right)$ in dq and dp, although such expansion would pose no technical difficulty. The differential of the Hamiltonian is

$$dH = d(pv - L) = vdp - \frac{\partial L}{\partial q}dq, \tag{2.21}$$

which is equivalent to Eqs. (2.17)-(2.18).

It would be incorrect to say that H is a function of p and q and not of the velocity v because the differential dv does not appear in Eq. (2.21). In fact, any function of v, e.g. the Lagrangian $L(t, q, v)$, would become a function of (p, q, t) once v is expressed through p and q. The Hamilton equations can be obtained using the Lagrangian L, as Eq. (2.17) shows, but the Hamiltonian $H(p, q, t)$ is more convenient.

2.2.2 The action principle

The Hamilton equations can be derived from the action principle

$$S_H\left[q(t), p(t)\right] = \int \left[p\dot{q} - H(p, q, t)\right] dt. \tag{2.22}$$

In this formulation, the *Hamiltonian action* S_H is a functional of two functions $q(t)$ and $p(t)$ which are varied independently to extremize S_H.

Exercise 2.3

a) Derive Eqs. (2.19) by extremizing the action (2.22). Find the appropriate boundary conditions for $p(t)$ and $q(t)$.

b) Show that the Hamilton equations imply $dH/dt = 0$ when $H(p, q)$ does not depend explicitly on the time t.

c) Show that the expression $p\dot{q} - H$ evaluated on the classical trajectories $p(t)$, $q(t)$ satisfying Eqs. (2.19) is equal to the Lagrangian $L\left(q, \dot{q}, t\right)$.

2.3 Quantization of Hamiltonian systems

To quantize a classical system, one replaces the canonical variables $q(t)$, $p(t)$ by non-commuting operators $\hat{q}(t)$, $\hat{p}(t)$ for which one postulates the commutation relation

$$[\hat{q}(t), \hat{p}(t)] = i\hbar\,\hat{1}. \tag{2.23}$$

(We shall frequently omit the identity operator $\hat{1}$ in such formulae.) The operators $\hat{q}$, $\hat{p}$ may be represented by linear transformations ("matrices") acting in a suitable vector space (the space of *quantum states*). Since Eq. (2.23) cannot be satisfied by any finite-dimensional matrices,[2] the space of quantum states needs to be infinite-dimensional.

It is a standard result in quantum mechanics that the relation (2.23) expresses the physical impossibility to measure the coordinate and the momentum simultaneously (*Heisenberg's uncertainty principle*). Note that commutation relations for unequal times, for instance $[\hat{q}\left(t_1\right), \hat{p}\left(t_2\right)]$, are not postulated but *derived* for each particular physical system from its equations of motion.

[2] This is easy to prove by considering the trace of a commutator. If $\hat{A}$ and $\hat{B}$ are arbitrary finite-dimensional matrices, then $\mathrm{Tr}\,[\hat{A}, \hat{B}] = \mathrm{Tr}\hat{A}\hat{B} - \mathrm{Tr}\hat{B}\hat{A} = 0$ which contradicts Eq. (2.23). In an infinite-dimensional space, this argument does not hold because the trace is not defined for all operators and thus we cannot assume that $\mathrm{Tr}\hat{A}\hat{B} = \mathrm{Tr}\hat{B}\hat{A}$.

It is not always necessary to specify a representation of $\hat{q}$ and $\hat{p}$ as particular operators in a certain vector space. For many calculations these symbols can be manipulated purely algebraically, using only the commutation relation.

Exercise 2.4
Simplify the expression $\hat{q}\hat{p}^2\hat{q} - \hat{p}^2\hat{q}^2$ using Eq. (2.23).

Heisenberg equations of motion

Having replaced the classical quantities $q(t)$ and $p(t)$ by operators, we may look for equations of motion analogous to Eqs. (2.19),

$$\frac{d\hat{q}}{dt} = ..., \quad \frac{d\hat{p}}{dt} = ...$$

The classical equations must be recovered in the limit of $\hbar \to 0$. Therefore the quantum equations of motion should have the same form, perhaps with some additional terms of order $\hbar$ or higher,

$$\frac{d\hat{q}}{dt} = \frac{\partial H}{\partial p}(\hat{p}, \hat{q}, t) + O(\hbar), \quad \frac{d\hat{p}}{dt} = -\frac{\partial H}{\partial q}(\hat{p}, \hat{q}, t) + O(\hbar). \tag{2.24}$$

In these equations, the operators $\hat{p}$, $\hat{q}$ are substituted into $\partial H/\partial q$, $\partial H/\partial p$ *after* taking the derivatives.

To make the theory simpler, one usually does not add any extra terms of order $\hbar$ to Eqs. (2.24) and writes them as

$$\frac{d\hat{q}}{dt} = \frac{\partial H}{\partial p}(\hat{p}, \hat{q}, t), \quad \frac{d\hat{p}}{dt} = -\frac{\partial H}{\partial q}(\hat{p}, \hat{q}, t). \tag{2.25}$$

Of course, ultimately the correct form of the quantum equations of motion is decided by their agreement with experimental data. Presently, the theory based on Eqs. (2.25) is in excellent agreement with experiments.

By using the identity

$$[\hat{q}, f(\hat{p}, \hat{q})] = i\hbar \frac{\partial f}{\partial p}(\hat{p}, \hat{q})$$

and the analogous identity for $\hat{p}$ (see Exercise 2.5), we can rewrite Eqs. (2.24) in the following purely algebraic form,

$$\frac{d\hat{q}}{dt} = -\frac{i}{\hbar}\left[\hat{q}, \hat{H}\right], \quad \frac{d\hat{p}}{dt} = -\frac{i}{\hbar}\left[\hat{p}, \hat{H}\right]. \tag{2.26}$$

These are the Heisenberg equations of motion for the operators $\hat{q}(t)$ and $\hat{p}(t)$.

Exercise 2.5
a) Using the canonical commutation relation, prove that

$$[\hat{q}, \hat{q}^m\hat{p}^n] = i\hbar n\hat{q}^m\hat{p}^{n-1}.$$

Symbolically this relation can be written as

$$[\hat{q}, \hat{q}^m \hat{p}^n] = i\hbar \frac{\partial}{\partial \hat{p}} (\hat{q}^m \hat{p}^n) .$$

Derive the similar relation for $\hat{p}$,

$$[\hat{p}, \hat{p}^m \hat{q}^n] = -i\hbar \frac{\partial}{\partial \hat{q}} (\hat{p}^m \hat{q}^n) .$$

b) Suppose that $f(p, q)$ is an analytic function with a series expansion in p, q that converges for all p and q. The operator $f(\hat{p}, \hat{q})$ is defined by substituting the operators $\hat{p}$, $\hat{q}$ into that expansion (here the ordering of $\hat{q}$ and $\hat{p}$ is arbitrary but fixed). Show that

$$[\hat{q}, f(\hat{p}, \hat{q})] = i\hbar \frac{\partial}{\partial \hat{p}} f(\hat{p}, \hat{q}) . \tag{2.27}$$

Here it is implied that the derivative $\partial/\partial\hat{p}$ acts on each $\hat{p}$ with no change to the operator ordering, e.g.

$$\frac{\partial}{\partial \hat{p}} (\hat{p}^3 \hat{q} \hat{p}^2 \hat{q}) = 3\hat{p}^2 \hat{q} \hat{p}^2 \hat{q} + 2\hat{p}^3 \hat{q} \hat{p} \hat{q}.$$

Exercise 2.6

Show that an observable $\hat{A} \equiv f(\hat{p}, \hat{q})$, where $f(p, q)$ is an analytic function, satisfies the equation

$$\frac{d}{dt} \hat{A} = -\frac{i}{\hbar} \left[\hat{A}, \hat{H}\right] . \tag{2.28}$$

The operator ordering problem

The classical Hamiltonian may happen to be a function of p and q of the form (e.g.) $H(p, q) = 2p^2 q$. Since $\hat{p}\hat{q} \neq \hat{q}\hat{p}$, it is not *a priori* clear whether the corresponding quantum Hamiltonian should be $\hat{p}^2\hat{q} + \hat{q}\hat{p}^2$, or $2\hat{p}\hat{q}\hat{p}$, or perhaps some other combination of the noncommuting operators $\hat{p}$ and $\hat{q}$. The difference between the possible quantum Hamiltonians is of order $\hbar$ or higher, so the classical limit $\hbar \to 0$ is the same for any choice of the operator ordering. The ambiguity of the choice of the quantum Hamiltonian is called the *operator ordering problem*.

The choice of the operator ordering needs to be physically motivated in each case when it is not unique. In principle, only a precise measurement of quantum effects could unambiguously determine the correct operator ordering in such cases.

All examples considered in this book admit a unique and natural choice of operator ordering. For example, frequently used Hamiltonians of the form

$$H(\hat{p}, \hat{q}) = \frac{1}{2m} \hat{p}^2 + U(\hat{q}),$$

which describe a nonrelativistic particle in a potential U, obviously do not exhibit the operator ordering problem.

2.4 Dirac notation and Hilbert spaces

Quantum operators such as $\hat{p}$ and $\hat{q}$ can be represented by linear transformations in suitable infinite-dimensional Hilbert spaces. In this section we summarize the properties of Hilbert spaces and also introduce the Dirac notation. We shall always consider vector spaces over the field $\mathbb{C}$ of complex numbers.

Infinite-dimensional vector spaces

A vector in a *finite*-dimensional space can be visualized as a collection of components, e.g. $\vec{a} \equiv (a_1, a_2, a_3, a_4)$, where each a_k is a (complex) number. To describe vectors in infinite-dimensional spaces, one must use infinitely many components. An important example of an infinite-dimensional complex vector space is the space L^2 of square-integrable functions, i.e. the set of all complex-valued functions $\psi(q)$ such that the integral

$$\int_{-\infty}^{+\infty} |\psi(q)|^2 \, dq$$

converges. One can check that a linear combination of two such functions, $\lambda_1\psi_1(q) + \lambda_2\psi_2(q)$, with constant coefficients $\lambda_{1,2} \in \mathbb{C}$, is again an element of the same vector space. A function $\psi \in L^2$ can be thought of as a set of infinitely many "components" $\psi_q \equiv \psi(q)$ with a continuous "index" q.

It turns out that the space of quantum states of a point mass is exactly the space L^2 of square-integrable functions $\psi(q)$, where q is the spatial coordinate of the particle. In that case the function $\psi(q)$ is called the *wave function*. Quantum states of a two-particle system belong to the space of functions $\psi(q_1, q_2)$, where $q_{1,2}$ are the coordinates of each particle. In quantum field theory, the "coordinates" are field configurations $\phi(x)$ and the wave function is a functional, $\psi[\phi(x)]$.

The Dirac notation

Linear algebra is used in many areas of physics, and the Dirac notation is a convenient shorthand for calculations with vectors and linear operators. This notation is used for both finite- and infinite-dimensional vector spaces.

To denote a vector, Dirac proposed to write a symbol such as $|a\rangle$, $|x\rangle$, $|\lambda\rangle$, that is, a label inside the special brackets $|\rangle$. Linear combinations of vectors are written as $2|v\rangle - 3i|w\rangle$.

A linear operator $\hat{A} : V \to V$ acting in the space V transforms a vector $|v\rangle$ into the vector $\hat{A}|v\rangle$. (An operator $\hat{A}$ is *linear* if

$$\hat{A}(|v\rangle + \lambda|w\rangle) = \hat{A}|v\rangle + \lambda\hat{A}|w\rangle$$

for any $|v\rangle, |w\rangle \in V$ and $\lambda \in \mathbb{C}$.) For example, the identity operator $\hat{1}$ that does not change any vectors, $\hat{1}|v\rangle = |v\rangle$, is obviously a linear operator.

Linear forms acting on vectors, $f : V \to \mathbb{C}$, are *covectors* (vectors from the dual space) and are denoted by $\langle f|$. A linear form $\langle f|$ acts on a vector $|v\rangle$ and yields the number written as $\langle f|v\rangle$.

Usually a scalar product is defined in the space V. The scalar product of vectors $|v\rangle$ and $|w\rangle$ can be written as $(|v\rangle, |w\rangle)$ and is a complex number. The scalar product establishes a correspondence between vectors and covectors: each vector $|v\rangle$ defines a covector $\langle v|$ which is the linear map $|w\rangle \to (|v\rangle, |w\rangle)$. So the Dirac notation allows us to write scalar products somewhat more concisely as $(|v\rangle, |w\rangle) = \langle v|w\rangle$.

If $\hat{A}$ is a linear operator, the notation $\langle v| \hat{A} |w\rangle$ means the scalar product of the vectors $|v\rangle$ and $\hat{A}|w\rangle$. The quantity $\langle v| \hat{A} |w\rangle$ is also called the *matrix element* of the operator $\hat{A}$ with respect to the states $|v\rangle$ and $|w\rangle$.

The Dirac notation is convenient because the labels inside the brackets $|...\rangle$ are typographically separated from other symbols in a formula. So for instance one might denote specific vectors by $|0\rangle$, $|1\rangle$ (eigenvectors with integer eigenvalues), or by $|\psi\rangle$, $|a_i b_j\rangle$, or even by $\left|_{(out)} n_1, n_2, ...\right\rangle$, without risk of confusion. Note that the symbol $|0\rangle$ is the commonly used designation for the vacuum state, rather than the zero vector; the latter is denoted simply by 0.

If $|v\rangle$ is an eigenvector of an operator $\hat{A}$ with eigenvalue v, one writes

$$\hat{A}|v\rangle = v|v\rangle .$$

There is no confusion between the eigenvalue v (which is a number) and the vector $|v\rangle$ labeled by its eigenvalue.

Hermiticity

The scalar product in a complex vector space is *Hermitian* if $(\langle v|w\rangle)^* = \langle w|v\rangle$ for all vectors $|v\rangle$ and $|w\rangle$ (the asterisk * denotes the complex conjugation). In that case the *norm* $\langle v|v\rangle$ of a vector $|v\rangle$ is a real number.

A Hermitian scalar product allows one to define the *Hermitian conjugate* $\hat{A}^\dagger$ of an operator $\hat{A}$ via the identity

$$\langle v| \hat{A}^\dagger |w\rangle = \left(\langle w| \hat{A} |v\rangle\right)^* ,$$

which should hold for all vectors $|v\rangle$ and $|w\rangle$. Note that an operator $\hat{A}^\dagger$ is uniquely specified if its matrix elements $\langle v| \hat{A}^\dagger |w\rangle$ with respect to all vectors $|v\rangle$, $|w\rangle$ are known. For example, it is easy to prove that $\hat{1}^\dagger = \hat{1}$.

The operation of Hermitian conjugation has the properties

$$(\hat{A} + \hat{B})^\dagger = \hat{A}^\dagger + \hat{B}^\dagger; \quad (\lambda \hat{A})^\dagger = \lambda^* \hat{A}^\dagger; \quad (\hat{A}\hat{B})^\dagger = \hat{B}^\dagger \hat{A}^\dagger .$$

An operator $\hat{A}$ is called *Hermitian* if $\hat{A}^\dagger = \hat{A}$, *anti-Hermitian* if $\hat{A}^\dagger = -\hat{A}$, and *unitary* if $\hat{A}^\dagger \hat{A} = \hat{A}\hat{A}^\dagger = \hat{1}$.

According to a postulate of quantum mechanics, the result of a measurement of some quantity is always an eigenvalue of the operator $\hat{A}$ corresponding to that quantity. Eigenvalues of a Hermitian operator are always real. This motivates an important assumption made in quantum mechanics: the operators corresponding to all observables are Hermitian.

> **Example:** The operators of position $\hat{q}$ and momentum $\hat{p}$ are Hermitian, $\hat{q}^\dagger = \hat{q}$ and $\hat{p}^\dagger = \hat{p}$. The commutator of two Hermitian operators $\hat{A}$, $\hat{B}$ is anti-Hermitian: $[\hat{A}, \hat{B}]^\dagger = -[\hat{A}, \hat{B}]$. Accordingly, the commutation relation for $\hat{q}$ and $\hat{p}$ contains the imaginary unit i. The operator $\hat{p}\hat{q}$ is neither Hermitian nor anti-Hermitian: $(\hat{p}\hat{q})^\dagger = \hat{q}\hat{p} = \hat{p}\hat{q} + i\hbar\hat{1} \neq \pm\hat{p}\hat{q}$.

Eigenvectors of a Hermitian operator corresponding to different eigenvalues are always orthogonal. This is easy to prove: if $|v_1\rangle$ and $|v_2\rangle$ are eigenvectors of a Hermitian operator $\hat{A}$ with eigenvalues v_1 and v_2, then $v_{1,2}$ are real, so $\langle v_1| \hat{A} = v_1 \langle v_1|$, and $\langle v_1| \hat{A} |v_2\rangle = v_2 \langle v_1|v_2\rangle = v_1 \langle v_1|v_2\rangle$. Therefore $\langle v_1|v_2\rangle = 0$ if $v_1 \neq v_2$.

Hilbert spaces

In an N-dimensional vector space one can find a finite set of basis vectors $|e_1\rangle$, ..., $|e_N\rangle$ such that any vector $|v\rangle$ is uniquely expressed as a linear combination

$$|v\rangle = \sum_{n=1}^{N} v_n |e_n\rangle .$$

The coefficients v_n are called *components* of the vector $|v\rangle$ in the basis $\{|e_n\rangle\}$. In an orthonormal basis satisfying $\langle e_m|e_n\rangle = \delta_{mn}$, the scalar product of two vectors $|v\rangle$, $|w\rangle$ is expressed through their components v_n, w_n as

$$\langle v|w\rangle = \sum_{n=1}^{N} v_n^* w_n .$$

By definition, a vector space is infinite-dimensional if no finite set of vectors can serve as a basis. In that case, one might expect to have an infinite basis $|e_1\rangle$, $|e_2\rangle$, ..., such that any vector $|v\rangle$ is uniquely expressible as an infinite linear combination

$$|v\rangle = \sum_{n=1}^{\infty} v_n |e_n\rangle . \tag{2.29}$$

However, the convergence of this infinite series is a nontrivial issue. For instance, if the basis vectors $|e_n\rangle$ are orthonormal, then the norm of the vector $|v\rangle$ is

$$\langle v|v\rangle = \left(\sum_{m=1}^{\infty} v_m^* \langle e_n| \right) \left(\sum_{n=1}^{\infty} v_n |e_n\rangle \right) = \sum_{n=1}^{\infty} |v_n|^2 . \tag{2.30}$$

This series must converge if the vector $|v\rangle$ has a finite norm, so the numbers v_n cannot be arbitrary. We cannot expect that e.g. the sum $\sum_{n=1}^{\infty} n^2 |e_n\rangle$ represents a well-defined vector. Now, if the coefficients v_n do fall off sufficiently rapidly so that the

series (2.30) is finite, it may seem plausible that the infinite linear combination (2.29) converges and uniquely specifies the vector $|v\rangle$. However, this statement does not hold in all infinite-dimensional spaces. The required properties of the vector space are known in functional analysis as completeness and separability.[3]

A *Hilbert space* is a complete vector space with a Hermitian scalar product. When defining a quantum theory, one always chooses a separable Hilbert space as the space of quantum states. In that case, there exists a countable basis $\{|e_n\rangle\}$ and all vectors can be expanded as in Eq. (2.29). Once an orthonormal basis is chosen, all vectors $|v\rangle$ are unambiguously represented by collections $(v_1, v_2, ...)$ of their components. Therefore a separable Hilbert space can be visualized as the space of infinite rows of complex numbers, $|v\rangle \equiv (v_1, v_2, ...)$, such that the sum $\sum_{n=1}^{\infty} |v_n|^2$ converges. The convergence requirement guarantees that all scalar products $\langle v|w\rangle = \sum_{n=1}^{\infty} v_n^* w_n$ are finite.

Example: The space $L^2[a, b]$ of square-integrable wave functions $\psi(q)$ defined on an interval $a < q < b$ is a separable Hilbert space, although it may appear to be "much larger" than the space of infinite rows of numbers. The scalar product of two wave functions $\psi_{1,2}(q)$ is defined by

$$\langle \psi_1 | \psi_2 \rangle = \int_a^b \psi_1^*(q) \psi_2(q) dq.$$

The canonical operators $\hat{p}$, $\hat{q}$ can be represented as linear operators in the space L^2 that act on functions $\psi(q)$ as

$$\hat{p} : \psi(q) \to -i\hbar \frac{\partial \psi}{\partial q}, \quad \hat{q} : \psi(q) \to q\psi(q). \tag{2.31}$$

It is straightforward to verify the commutation relation (2.23).

> **Remark:** When one wishes to quantize a field $\phi(x)$ defined in infinite space, there are certain mathematical problems with the definition of a separable Hilbert space of quantum states. To obtain a mathematically consistent definition, one needs to enclose the field in a finite box and impose boundary conditions.

Decomposition of unity

If $\{|e_n\rangle\}$ is an orthonormal basis in a separable Hilbert space, the identity operator has the decomposition

$$\hat{1} = \sum_{n=1}^{\infty} |e_n\rangle \langle e_n| .$$

[3] A normed vector space is *complete* if all Cauchy sequences in it converge to a limit; then all norm-convergent infinite sums always have an unique vector as their limit. The space is *separable* if there exists a countable set of vectors $\{|e_n\rangle\}$ which is everywhere dense in the space. Separability ensures that that all vectors can be approximated arbitrarily well by *finite* combinations of the basis vectors.

This formula is called the *decomposition of unity* and is derived for Hilbert spaces in essentially the same way as in standard linear algebra. The combination $|e_n\rangle \langle e_n|$ denotes the operator which acts on vectors $|v\rangle$ as

$$|v\rangle \to (|e_n\rangle \langle e_n|) |v\rangle \equiv \langle e_n|v\rangle |e_n\rangle .$$

This operator describes a projection onto the one-dimensional subspace spanned by $|e_n\rangle$. The decomposition of unity shows that the identity operator $\hat{1}$ is a sum of projectors onto all basis vectors.

Generalized eigenvectors

We can build an *eigenbasis* in a Hilbert space if we take all eigenvectors of a suitable Hermitian operator. The operator must have a purely discrete spectrum so that its eigenbasis is countable.

In calculations it is often convenient to use the eigenbasis of an operator with a continuous spectrum, for example the position operator $\hat{q}$. The eigenvalues of this operator are all possible positions q of a particle. However, it turns out that the operator $\hat{q}$ cannot have any eigenvectors in a separable Hilbert space. Nevertheless, it is possible to consider the basis of "generalized vectors" $|q\rangle$ that are the eigenvectors of $\hat{q}$ in a larger vector space. A vector $|\psi\rangle$ is expressed through the basis $\{|q\rangle\}$ as

$$|\psi\rangle = \int dq\, \psi(q) |q\rangle .$$

Note that $|\psi\rangle$ belongs to the Hilbert space while the generalized vectors $|q\rangle$ do not. This situation is quite similar to distributions (generalized functions) such as $\delta(x-y)$ that give well-defined values only after an integration with some function $f(x)$.

We define the basis state $|q_1\rangle$ as an eigenvector of the operator $\hat{q}$ with the eigenvalue q_1 (here q_1 goes over all possible positions of the particle). In other words, the basis states satisfy

$$\hat{q} |q_1\rangle = q_1 |q_1\rangle .$$

The conjugate basis consists of the covectors $\langle q_1|$ such that $\langle q_1| \hat{q} = q_1 \langle q_1|$.

Now we consider the normalization of the basis $\{|q\rangle\}$. Since the operator $\hat{q}$ is Hermitian, its eigenvectors are orthogonal:

$$\langle q_1|q_2\rangle = 0 \text{ for } q_1 \neq q_2.$$

If the basis $|q\rangle$ plays the role of an orthonormal basis, the decomposition of unity should look like this,

$$\hat{1} = \int dq\ |q\rangle \langle q| .$$

Hence for an arbitrary state $|\psi\rangle$ we find

$$\int dq\, \psi(q) |q\rangle = |\psi\rangle = \hat{1} |\psi\rangle = \left[\int dq\, |q\rangle \langle q|\right] |\psi\rangle = \int dq\, \langle q|\psi\rangle |q\rangle ,$$

therefore $\psi(q) = \langle q|\psi\rangle$. Further, we compute

$$\langle q|\psi\rangle = \langle q| \int dq' \, |q'\rangle \, \psi(q') = \int dq' \psi(q') \, \langle q|q'\rangle \, .$$

The identity $\psi(q) = \int dq' \psi(q') \, \langle q|q'\rangle$ can be satisfied for all functions $\psi(q)$ only if

$$\langle q|q'\rangle = \delta(q - q').$$

Thus we have derived the *delta-function normalization* of the basis $|q\rangle$. It is clear that the vectors $|q\rangle$ cannot be normalized in the usual way because $\langle q|q\rangle = \delta(0)$ is undefined. Generally, we should expect that matrix elements such as $\langle q| \, \hat{A} \, |q'\rangle$ are distributions and not simply functions of q and q'.

The basis $|p\rangle$ of generalized eigenvectors of the momentum operator $\hat{p}$ has similar properties. Let us now perform some calculations with generalized eigenbases $\{|p\rangle\}$ and $\{|q\rangle\}$.

The matrix element $\langle q_1| \, \hat{p} \, |q_2\rangle$

The first example is a computation of $\langle q_1| \, \hat{p} \, |q_2\rangle$. At this point we only need to know that $|q\rangle$ are eigenvectors of the operator $\hat{q}$ which is related to $\hat{p}$ through the commutation relation (2.23). We consider the following matrix element,

$$\langle q_1| \, [\hat{q}, \hat{p}] \, |q_2\rangle = i\hbar\delta \, (q_1 - q_2) = (q_1 - q_2) \, \langle q_1| \, \hat{p} \, |q_2\rangle \, .$$

It follows that $\langle q_1| \, \hat{p} \, |q_2\rangle = F \, (q_1, q_2)$ where F is a distribution that satisfies the equation

$$i\hbar\delta \, (q_1 - q_2) = (q_1 - q_2) \, F \, (q_1, q_2) \, . \tag{2.32}$$

To solve Eq. (2.32), we cannot simply divide by $q_1 - q_2$ because both sides are distributions and $x^{-1}\delta(x)$ is undefined. So we use the Fourier representation of the δ function,

$$\delta(q) = \frac{1}{2\pi} \int e^{ipq} dp,$$

denote $q \equiv q_1 - q_2$, and apply the Fourier transform to Eq. (2.32),

$$i\hbar = \int qF \, (q_1, q_1 - q) \, e^{-ipq} dq = i\frac{\partial}{\partial p} \int F \, (q_1, q_1 - q) \, e^{-ipq} dq.$$

Integrating over p, we find

$$\hbar p + C \, (q_1) = \int F \, (q_1, q_1 - q) \, e^{-ipq} dq,$$

where $C(q_1)$ is an undetermined function. The inverse Fourier transform yields

$$F \, (q_1, q_2) = \frac{1}{2\pi} \int (\hbar p + C) e^{ipq} dp = \left[-i\hbar \frac{\partial}{\partial q_1} + C \, (q_1) \right] \delta \, (q_1 - q_2) \, ,$$

so the result is

$$\langle q_1|\,\hat{p}\,|q_2\rangle = -i\hbar\delta'\left(q_1-q_2\right)+C\left(q_1\right)\delta\left(q_1-q_2\right). \tag{2.33}$$

The function $C(q_1)$ cannot be found from the commutation relations alone. The reason is that we may replace the operator $\hat{p}$ by $\hat{p}+c(\hat{q})$, where c is an arbitrary function, without changing the commutation relations. This transformation would change the matrix element $\langle q_1|\,\hat{p}\,|q_2\rangle$ by the term $c(q_1)\delta(q_1-q_2)$. So we could redefine the operator $\hat{p}$ to remove the term proportional to $\delta(q_1-q_2)$ in the matrix element $\langle q_1|\,\hat{p}\,|q_2\rangle$, so as to obtain

$$\langle q_1|\,\hat{p}\,|q_2\rangle = -i\hbar\delta'\left(q_1-q_2\right). \tag{2.34}$$

> **Remark:** If the operators $\hat{p}$, $\hat{q}$ are specified as particular linear operators in some Hilbert space, such that Eq. (2.33) holds with $C(q)\neq 0$, we can remove the term $C(q_1)\delta(q_1-q_2)$ and obtain the standard result (2.34) by redefining the basis vectors $|q\rangle$ themselves. Multiplying each vector $|q\rangle$ by a q-dependent phase,
>
> $$|\tilde{q}\rangle \equiv e^{-ic(q)}\,|q\rangle\,,$$
>
> we obtain
>
> $$\langle\tilde{q_1}|\hat{p}|\tilde{q_2}\rangle = \hbar c'(q)\delta\left(q_1-q_2\right)-i\hbar\delta'\left(q_1-q_2\right)+C\left(q_1\right)\delta\left(q_1-q_2\right).$$
>
> Now the function $c(q)$ can be chosen to cancel the term $C(q_1)\delta(q_1-q_2)$.

The matrix element $\langle p|q\rangle$

To compute $\langle p|q\rangle$, we consider the matrix element $\langle p|\,\hat{p}\,|q\rangle$ and use the decomposition of unity,

$$\langle p|\,\hat{p}\,|q\rangle = p\,\langle p|q\rangle = \langle p|\left[\int dq_1\,|q_1\rangle\,\langle q_1|\right]\hat{p}\,|q\rangle = \int dq_1\,\langle p|q_1\rangle\,\langle q_1|\,\hat{p}\,|q\rangle\,.$$

It follows from Eq. (2.34) that

$$p\,\langle p|q\rangle = i\hbar\frac{\partial}{\partial q}\,\langle p|q\rangle\,.$$

Similarly, by considering $\langle p|\,\hat{q}\,|q\rangle$ we find

$$q\,\langle p|q\rangle = i\hbar\frac{\partial}{\partial p}\,\langle p|q\rangle\,.$$

Integrating these identities over q and p respectively, we obtain

$$\langle p|q\rangle = C_1(p)\exp\left[\frac{ipq}{\hbar}\right],\quad \langle p|q\rangle = C_2(q)\exp\left[\frac{ipq}{\hbar}\right],$$

where $C_1(p)$ and $C_2(q)$ are arbitrary functions. The last two equations are compatible only if $C_1(p) = C_2(q) = \text{const}$, therefore

$$\langle p|q\rangle = C \exp\left[\frac{ipq}{\hbar}\right]. \tag{2.35}$$

The constant C is determined (up to an irrelevant phase factor) by the normalization condition to be $C = (2\pi\hbar)^{-1/2}$. (See Exercise 2.7.) Thus

$$(\langle q|p\rangle)^* = \langle p|q\rangle = \frac{1}{\sqrt{2\pi\hbar}} \exp\left(\frac{ipq}{\hbar}\right). \tag{2.36}$$

Exercise 2.7

Let $|q\rangle$, $|p\rangle$ be the δ-normalized eigenvectors of the position and the momentum operators in a one-dimensional space, i.e.

$$\hat{p}\,|p_1\rangle = p_1\,|p_1\rangle\,, \quad \langle p_1|p_2\rangle = \delta\,(p_1 - p_2)\,,$$

and the same for $\hat{q}$. Show that the coefficient C in Eq. (2.35) satisfies $|C| = (2\pi\hbar)^{-1/2}$.

2.5 Evolution in quantum theory

So far we considered time-dependent operators $\hat{q}(t)$, $\hat{p}(t)$ that act on fixed state vectors $|\psi\rangle$; this description of quantized systems is called the *Heisenberg picture*. For an observable $\hat{A} = f\,(\hat{p}, \hat{q})$, we can write the general solution of Eq. (2.28) as

$$\hat{A}(t) = \exp\left[\frac{i}{\hbar}\,(t - t_0)\,\hat{H}\right] \hat{A}\,(t_0) \exp\left[-\frac{i}{\hbar}\,(t - t_0)\,\hat{H}\right]. \tag{2.37}$$

If we set $t_0 = 0$ in Eq. (2.37), the expectation value of $\hat{A}(t)$ in a state $|\psi_0\rangle$ is

$$\langle A(t)\rangle \equiv \langle\psi_0|\,\hat{A}(t)\,|\psi_0\rangle = \langle\psi_0|\,e^{\frac{i}{\hbar}\hat{H}t}\hat{A}_0 e^{-\frac{i}{\hbar}\hat{H}t}\,|\psi_0\rangle\,.$$

This relation can be rewritten using a time-dependent state

$$|\psi(t)\rangle \equiv e^{-\frac{i}{\hbar}\hat{H}t}\,|\psi_0\rangle \tag{2.38}$$

and the time-independent operator $\hat{A}_0$ as

$$\langle A(t)\rangle = \langle\psi(t)|\,\hat{A}_0\,|\psi(t)\rangle\,.$$

This approach to quantum theory (where the operators are time-independent but quantum states are time-dependent) is called the *Schrödinger picture*. It is clear that the state vector (2.38) satisfies the *Schrödinger equation*,

$$i\hbar\frac{\partial}{\partial t}\,|\psi(t)\rangle = \hat{H}\,|\psi(t)\rangle\,. \tag{2.39}$$

Example: the harmonic oscillator. The space of quantum states of a harmonic oscillator is the Hilbert space L^2 in which the operators $\hat{p}$, $\hat{q}$ are defined by Eqs. (2.31). Since the Hamiltonian of the harmonic oscillator is given by Eq. (2.20), the Schrödinger equation becomes

$$i\hbar\frac{\partial}{\partial t}\psi(q) = -\frac{\hbar^2}{2}\frac{\partial^2}{\partial q^2}\psi(q) + \frac{1}{2}\omega^2 q^2\psi(q).$$

The procedure of quantization is formally similar in nonrelativistic mechanics (a small number of particles), in solid state physics (a very large but finite number of nonrelativistic particles), and in relativistic field theory (infinitely many degrees of freedom).

Remark: Schrödinger equations. The use of a Schrödinger equation does *not* imply nonrelativistic physics. There is a widespread confusion about the role of the Schrödinger equation vs. that of the basic relativistic field equations (the Klein-Gordon equation, the Dirac equation, or the Maxwell equations). It would be a mistake to think that the Dirac equation and the Klein-Gordon equation are "relativistic forms" of the Schrödinger equation (although some textbooks say that). This was how the Dirac and the Klein-Gordon equations were discovered, but their actual place in quantum theory is quite different. The three named field equations describe *classical* relativistic fields of spin 0, $1/2$ and 1 respectively. These equations need to be quantized to obtain a quantum field theory. Their role is quite analogous to that of the harmonic oscillator equation: they provide a classical Hamiltonian for quantization. The Schrödinger equations corresponding to the Klein-Gordon, the Dirac and the Maxwell equations describe quantum theories of these classical fields. (In practice, Schrödinger equations are very rarely used in quantum field theory because in most cases it is much easier to work in the Heisenberg picture.)

Remark: second quantization. The term "second quantization" is frequently used to refer to quantum field theory, whereas "first quantization" means ordinary quantum mechanics. However, this is an obsolete terminology originating from the historical development of QFT as a relativistic extension of quantum mechanics. In fact, a quantization procedure can only be applied to a *classical* theory and yields the corresponding quantum theory. One does not quantize a *quantum* theory for a second time. It is more logical to say "quantization of fields" instead of "second quantization."

Historically it was not immediately realized that relativistic particles can be described only by quantized fields and not by quantum mechanics of points. At first, fields were regarded as wave functions of point particles. Old QFT textbooks present the picture of (1) quantizing a point particle to obtain a wave function that satisfies the Schrödinger equation, (2) "generalizing" the Schrödinger equation to the Klein-Gordon or the Dirac equation, and (3) "second-quantizing" the "relativistic wave function" to obtain a quantum field theory. The confusion between Schrödinger equations and relativistic wave equations has been cleared, but the old illogical terminology of "first" and "second" quantization persists. It is unnecessary to talk about a "second-quantized Dirac equation" if the Dirac equation is actually quantized only once.

The modern view is that one must describe relativistic particles by fields. Therefore one starts right away with a classical relativistic field equation, such as the Dirac equation (for the electron field) and the Maxwell equations (for the photon field), and applies the quantization procedure (only once) to obtain the relativistic quantum theory of photons and electrons.

3 Quantizing a driven harmonic oscillator

Summary: Driven harmonic oscillator. Quantization in the Heisenberg picture. "In" and "out" states. Calculations of matrix elements. Green's functions.

The quantum-mechanical description of a harmonic oscillator driven by an external force is a computationally simple problem that allows us to introduce important concepts such as Green's functions, "in" and "out" states, and particle production.

3.1 Classical oscillator under force

We consider a unit-mass harmonic oscillator driven by a force $J(t)$ which is assumed to be a known function of time. The classical equation of motion

$$\ddot{q} = -\omega^2 q + J(t)$$

can be derived from the Lagrangian

$$L\left(t, q, \dot{q}\right) = \frac{1}{2}\dot{q}^2 - \frac{1}{2}\omega^2 q^2 + J(t)q.$$

The corresponding Hamiltonian is

$$H(p, q) = \frac{p^2}{2} + \frac{\omega^2 q^2}{2} - J(t)q, \tag{3.1}$$

and the Hamilton equations are

$$\dot{q} = p, \quad \dot{p} = -\omega^2 q + J(t).$$

Note that the Hamiltonian depends explicitly on the time t.

Before quantizing the oscillator, it is convenient to introduce two new (complex-valued) dynamical variables $a^{\pm}(t)$ instead of $p(t)$, $q(t)$:

$$a^-(t) \equiv \sqrt{\frac{\omega}{2}}\left[q(t) + \frac{i}{\omega}p(t)\right], \quad a^+(t) \equiv \left[a^-(t)\right]^* = \sqrt{\frac{\omega}{2}}\left[q(t) - \frac{i}{\omega}p(t)\right].$$

The inverse relations then are

$$p = \frac{\sqrt{\omega}}{i\sqrt{2}}\left(a^- - a^+\right), \quad q = \frac{1}{\sqrt{2\omega}}\left(a^- + a^+\right). \tag{3.2}$$

The equation of motion for the variable $a^-(t)$ is straightforward to derive,

$$\frac{d}{dt}a^- = -i\omega a^- + \frac{i}{\sqrt{2\omega}}J(t). \tag{3.3}$$

(The conjugate variable $a^+(t)$ satisfies the complex conjugate equation.) The solution of Eq. (3.3) with the initial condition $a^-|_{t=0} = a^-_{in}$ can be readily found,

$$a^-(t) = a^-_{in}e^{-i\omega t} + \frac{i}{\sqrt{2\omega}}\int_0^t J(t')e^{i\omega(t'-t)}dt'. \tag{3.4}$$

Exercise 3.1
Derive Eq. (3.4).

3.2 Quantization

We quantize the oscillator in the Heisenberg picture by introducing operators $\hat{p}$, $\hat{q}$ with the commutation relation $[\hat{q}, \hat{p}] = i$. (From now on, we use the units where $\hbar = 1$.) The variables $a^\pm$ are also replaced by operators $\hat{a}^-$ and $\hat{a}^+$ called the *annihilation* and *creation* operators respectively. These operators satisfy the commutation relation $[\hat{a}^-, \hat{a}^+] = 1$ (see Exercise 3.2) and are not Hermitian since $(\hat{a}^-)^\dagger = \hat{a}^+$ and $(\hat{a}^+)^\dagger = \hat{a}^-$.

Exercise 3.2
The creation and annihilation operators $\hat{a}^+(t)$, $\hat{a}^-(t)$ are defined by

$$\hat{a}^\pm(t) = \sqrt{\frac{\omega}{2}}\left[\hat{q}(t) \mp \frac{i}{\omega}\hat{p}(t)\right].$$

Using the commutation relation $[\hat{q}, \hat{p}] = i$, show that $\left[\hat{a}^-(t), \hat{a}^+(t)\right] = 1$ for all t.

The classical Hamiltonian (3.1) is replaced by the operator $\hat{H} = H(\hat{p}, \hat{q}, t)$. Using the relations (3.2), the operator $\hat{H}$ can be expressed through the creation and annihilation operators $\hat{a}^\pm$ as

$$\hat{H} = \frac{\omega}{2}\left(\hat{a}^+\hat{a}^- + \hat{a}^-\hat{a}^+\right) - \frac{\hat{a}^+ + \hat{a}^-}{\sqrt{2\omega}}J(t) = \frac{\omega}{2}\left(2\hat{a}^+\hat{a}^- + 1\right) - \frac{\hat{a}^+ + \hat{a}^-}{\sqrt{2\omega}}J(t).$$

3.2.1 The "in" and "out" regions

To simplify the calculations, we consider a special case when the force $J(t)$ is nonzero only for a certain time interval $0 < t < T$. Thus the oscillator is unperturbed in the remaining two intervals which are called the "in" region, $t \le 0$, and the "out" region, $t \ge T$ (see Fig. 3.1). It is interesting to find the relation between the states of the oscillator in the "in" and the "out" regions (the evolution of the oscillator in the intermediate region $0 < t < T$ is less important for our present purposes).

The solution for the "in" region with the initial condition $\hat{a}^-(0) = \hat{a}^-_{in}$ is

$$\hat{a}^-(t) = \hat{a}^-_{in}e^{-i\omega t}.$$

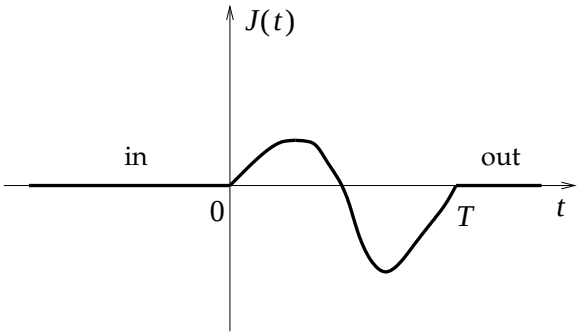


Figure 3.1: The external force $J(t)$ and the "in"/"out" regions.

For consistency, the operator $\hat{a}^-_{in}$ must satisfy the commutation relation $\left[\hat{a}^-_{in}, \hat{a}^+_{in}\right] = 1$. The solution for the "out" region is found from Eq. (3.4) and can be written as

$$\hat{a}^-(t) = \hat{a}^-_{out} e^{-i\omega t},$$

where $\hat{a}^-_{out}$ is the time-independent operator defined by

$$\hat{a}^-_{out} \equiv \hat{a}^-_{in} + \frac{i}{\sqrt{2\omega}} \int_0^T e^{i\omega t'} J(t') dt' \equiv \hat{a}^-_{in} + J_0. \tag{3.5}$$

Substituting the operators $\hat{a}^{\pm}(t)$ into the Hamiltonian, we obtain

$$\hat{H} = \begin{cases} \omega \left(\hat{a}^+_{in}\hat{a}^-_{in} + \frac{1}{2}\right), & t \le 0, \\ \omega \left(\hat{a}^+_{out}\hat{a}^-_{out} + \frac{1}{2}\right), & t \ge T. \end{cases} \tag{3.6}$$

It is clear that the Hamiltonian is time-independent in the "in" and "out" regions.

3.2.2 Excited states

Quantum states of the oscillator correspond to vectors in an appropriate Hilbert space. The construction of this Hilbert space for a free (unforced) oscillator is well-known: the vacuum state $|0\rangle$ is postulated as the eigenstate of the annihilation operator $\hat{a}^-$ with eigenvalue 0, and the excited states $|n\rangle$, where $n = 1, 2, ...$, are defined by

$$|n\rangle = \frac{1}{\sqrt{n!}} (\hat{a}^+)^n |0\rangle . \tag{3.7}$$

(The factors $\sqrt{n!}$ are needed for normalization, namely $\langle m|n\rangle = \delta_{mn}$.) The Hilbert space is spanned by the orthonormal basis $\{|n\rangle\}$, where $n = 0, 1, ...$; in other words, all states of the oscillator are of the form

$$|\psi\rangle = \sum_{n=0}^{\infty} \psi_n |n\rangle , \quad \sum_{n=0}^{\infty} |\psi_n|^2 < \infty. \tag{3.8}$$

> **Remark: why is $\{|n\rangle\}$ a complete basis?** A description of a quantum system must include not only the algebra of quantum operators but also a specification of a Hilbert space in which these operators act. For instance, the Hilbert space (3.8) cannot be derived from the commutation relation $[\hat{q}, \hat{p}] = i\hbar$ without additional assumptions. In fact, if one *assumes* the existence of a unique normalized eigenvector $|0\rangle$ such that $\hat{a}^- |0\rangle = 0$, as well as the diagonalizability of the Hamiltonian, then one can prove that the vectors $\{|n\rangle\}$ form a complete basis in the Hilbert space. This is a standard result and we omit the proof. Details can be found e.g. in the book by P. A. M. DIRAC, *Principles of quantum mechanics* (Oxford, 1948). Ultimately, it is the agreement of the resulting theory with experiments that determines whether a particular Hilbert space is suitable for describing a particular physical system; for a harmonic oscillator, the space (3.8) is adequate.

In the present case, there are two free regions (the "in" and the "out" regions) where the driving force is absent, and thus there are two annihilation operators, $\hat{a}^-_{in}$ and $\hat{a}^-_{out}$. Therefore we can define two vacuum states, the "in" vacuum $|0_{in}\rangle$ and the "out" vacuum $|0_{out}\rangle$, by the eigenvalue equations

$$\hat{a}^-_{in} |0_{in}\rangle = 0, \quad \hat{a}^-_{out} |0_{out}\rangle = 0.$$

It follows from Eq. (3.6) that the vectors $|0_{in}\rangle$ and $|0_{out}\rangle$ are the lowest-energy states for $t \leq 0$ and for $t \geq T$ respectively. We can easily check that the states $|0_{in}\rangle$ and $|0_{out}\rangle$ are different:

$$\hat{a}^-_{out} |0_{in}\rangle = \left(\hat{a}^-_{in} + J_0\right) |0_{in}\rangle = J_0 |0_{in}\rangle .$$

The state $|0_{in}\rangle$ is an eigenstate of the operator $\hat{a}^-_{out}$ with eigenvalue J_0. Conversely, $\hat{a}^-_{in} |0_{out}\rangle = -J_0 |0_{out}\rangle$.

> **Remark: coherent states.** Eigenstates of the annihilation operator with nonzero eigenvalues are called *coherent states*. One can show that coherent states minimize the uncertainty in both the coordinate and the momentum.

Using the creation operators $\hat{a}^+_{in}$ and $\hat{a}^+_{out}$, we build two sets of excited states,

$$|n_{in}\rangle = \frac{1}{\sqrt{n!}} \left(\hat{a}^+_{in}\right)^n |0_{in}\rangle , \quad |n_{out}\rangle = \frac{1}{\sqrt{n!}} \left(\hat{a}^+_{out}\right)^n |0_{out}\rangle , \quad n = 0, 1, 2, ...$$

The factors $\sqrt{n!}$ are needed for normalization, namely $\langle n_{in}| n_{in}\rangle = 1$ and $\langle n_{out}| n_{out}\rangle = 1$ for all n. It can be easily verified that the vectors $|n_{in}\rangle$ are eigenstates of the Hamiltonian (3.6) for $t \leq 0$ (but not for $t \geq T$), and similarly for $|n_{out}\rangle$:

$$\hat{H}(t) |n_{in}\rangle = \omega \left(n + \frac{1}{2}\right) |n_{in}\rangle , \quad t \leq 0;$$
$$\hat{H}(t) |n_{out}\rangle = \omega \left(n + \frac{1}{2}\right) |n_{out}\rangle , \quad t \geq T.$$

Therefore the vectors $|n_{in}\rangle$ are interpreted as n-particle states of the oscillator for $t \leq 0$, while for $t \geq T$ the n-particle states are $|n_{out}\rangle$.

> **Remark: interpretation of the "in" and "out" states.** We are presently working in the Heisenberg picture where quantum states are time-independent and operators depend on

time. One may prepare the oscillator in a state $|\psi\rangle$, and the state of the oscillator remains the same throughout all time t. However, the physical interpretation of this state changes with time because the state $|\psi\rangle$ is interpreted with help of the time-dependent operators $\hat{H}(t)$, $\hat{a}^-(t)$, etc. For instance, we found that at late times ($t \geq T$) the vector $|0_{in}\rangle$ is not the lowest-energy state any more, and the vectors $|n_{in}\rangle$ are not eigenstates of energy which they were at early times ($t \leq 0$). This happens because the energy of the system changes with time due to the external force $J(t)$. Without this force, we would have $\hat{a}^-_{in} = \hat{a}^-_{out}$ and the state $|0_{in}\rangle$ would describe the vacuum at all times.

3.2.3 Relation between "in" and "out" states

The states $|n_{out}\rangle$, where $n = 0, 1, 2, ...$, form a complete basis in the Hilbert space of the harmonic oscillator. However, the set of states $|n_{in}\rangle$ is another complete basis. Therefore the vector $|0_{in}\rangle$ must be expressible as a linear combination of the "out" states,

$$|0_{in}\rangle = \sum_{n=0}^{\infty} \Lambda_n |n_{out}\rangle , \tag{3.9}$$

where Λ_n are suitable coefficients. One can show that these coefficients Λ_n satisfy the recurrence relation

$$\Lambda_{n+1} = \frac{J_0}{\sqrt{n+1}} \Lambda_n . \tag{3.10}$$

Exercise 3.3
Derive Eq. (3.10) for all $n \geq 0$ using Eq. (3.5).

The solution of the recurrence relation (3.10) is easily found,

$$\Lambda_n = \frac{J_0^n}{\sqrt{n!}} \Lambda_0 .$$

The constant Λ_0 is fixed by the requirement $\langle 0_{in}| 0_{in}\rangle = 1$. Using Eq. (3.9), we get

$$\langle 0_{in}| 0_{in}\rangle = \sum_{n=0}^{\infty} |\Lambda_n|^2 = 1 \;\Rightarrow\; |\Lambda_0| = \exp\left[-\frac{1}{2}|J_0|^2\right] .$$

The only remaining freedom is the choice of the phase of Λ_0.

We found that the vacuum state $|0_{in}\rangle$ is expressed as the linear combination

$$|0_{in}\rangle = \exp\left[-\frac{1}{2}|J_0|^2\right] \sum_{n=0}^{\infty} \frac{J_0^n}{\sqrt{n!}} |n_{out}\rangle , \tag{3.11}$$

or equivalently

$$|0_{in}\rangle = \exp\left[-\frac{1}{2}|J_0|^2 + J_0 \hat{a}^+_{out}\right] |0_{out}\rangle .$$

This formula is similar to the definition of a coherent state of the harmonic oscillator. Indeed, one can verify that $|0_{in}\rangle$ is an eigenstate of $\hat{a}^-_{out}$ with eigenvalue J_0.

The relation (3.11) shows that the state describing the early-time vacuum is a superposition of excited states at late times, having the probability $|\Lambda_n|^2$ for the occupation number n. We thus conclude that the presence of the external force $J(t)$ leads to particle production.

3.3 Calculations of matrix elements

An expectation value of an operator, such as $\langle 0_{in}| \hat{A}(t) |0_{in}\rangle$, is an experimentally measurable quantity. As before, we are interested only in describing measurements performed either for times $t \leq 0$ (the "in" region) or for $t \geq T$ (the "out" region).

Unlike expectation values, an "in-out" matrix element $\langle 0_{out}| \hat{A}(t) |0_{in}\rangle$ is not a directly measurable quantity (and is generally a complex number). As we shall see in Chapter 12, such matrix elements are nevertheless useful as intermediate results in some calculations. Therefore we shall now compute various expectation values and matrix elements using explicit formulae for the operators $\hat{a}^{\pm}_{in,out}$.

Example 1: Consider the expectation value of the Hamiltonian $\hat{H}(t)$ in the "in" vacuum state $|0_{in}\rangle$. For $t \leq 0$, the state $|0_{in}\rangle$ is an eigenstate of $\hat{H}(t)$ with the eigenvalue $\frac{1}{2}\omega$, hence

$$\langle 0_{in}| \hat{H}(t) |0_{in}\rangle = \frac{\omega}{2}, \quad t \leq 0.$$

For $t \geq T$, we use Eqs. (3.5) and (3.6) to find

$$\langle 0_{in}| \hat{H}(t) |0_{in}\rangle = \langle 0_{in}| \omega \left(\frac{1}{2} + \hat{a}^{+}_{out} \hat{a}^{-}_{out} \right) |0_{in}\rangle = \left(\frac{1}{2} + |J_0|^2 \right) \omega, \quad t \geq T.$$

It is apparent from this expression that the energy of the oscillator after applying the force $J(t)$ becomes larger than the zero-point energy $\frac{1}{2}\omega$. The constant $|J_0|^2$ is expressed through $J(t)$ as

$$|J_0|^2 = \frac{1}{2\omega} \int_0^T dt_1 \int_0^T dt_2 e^{i\omega(t_1 - t_2)} J(t_1) J(t_2).$$

Example 2. The occupation number operator

$$\hat{N}(t) \equiv \hat{a}^{+}(t) \hat{a}^{-}(t)$$

has the expectation value

$$\langle 0_{in}| \hat{N}(t) |0_{in}\rangle = \begin{cases} 0, & t \leq 0; \\ |J_0|^2, & t \geq T. \end{cases} \tag{3.12}$$

Example 3. The in-out matrix element of $\hat{N}(t)$ is

$$\langle 0_{out}| \hat{N}(t) |0_{in}\rangle = 0, \quad t \leq 0 \text{ or } t \geq T.$$

Example 4. Let us calculate the expectation value of the position operator,

$$\hat{q}(t) = \frac{1}{\sqrt{2\omega}} \left(\hat{a}^-(t) + \hat{a}^+(t) \right), \tag{3.13}$$

in the "in" vacuum state. For $t \leq 0$ this expectation value is zero,

$$\langle 0_{in}| \, \hat{q}(t \leq 0) \, |0_{in}\rangle = 0.$$

For $t \geq T$, we use Eq. (3.5) together with

$$\hat{a}^-(t \geq T) = \hat{a}^-_{out} e^{-i\omega t}$$

and obtain

$$\langle 0_{in}| \, \hat{q}(t) \, |0_{in}\rangle = \frac{1}{\sqrt{2\omega}} \left(J_0 e^{-i\omega t} + J_0^* e^{i\omega t} \right) = \int_0^T \frac{\sin \omega(t-t')}{\omega} J(t') dt'. \tag{3.14}$$

Green's functions

It follows from Eq. (3.14) that the expectation value of $\hat{q}(t)$ is the solution of the driven oscillator equation

$$\ddot{q} + \omega^2 q = J(t)$$

with initial conditions $q(0) = \dot{q}(0) = 0$. Introducing the *retarded Green's function* of the harmonic oscillator,

$$G_{ret}(t,t') \equiv \frac{\sin \omega(t-t')}{\omega} \theta(t-t'), \tag{3.15}$$

the solution (3.14) can be rewritten as

$$q(t) = \int_{-\infty}^{+\infty} J(t') G_{ret}(t,t') dt'. \tag{3.16}$$

Example 5: The in-out matrix element of the position operator $\hat{q}$ is

$$\frac{\langle 0_{out}| \, \hat{q}(t \leq 0) \, |0_{in}\rangle}{\langle 0_{out}|0_{in}\rangle} = \frac{e^{-i\omega t}}{\sqrt{2\omega}} \frac{\langle 0_{out}| \, \hat{a}^+_{in} \, |0_{in}\rangle}{\langle 0_{out}|0_{in}\rangle} = -J_0 \frac{e^{-i\omega t}}{\sqrt{2\omega}},$$
$$\frac{\langle 0_{out}| \, \hat{q}(t \geq T) \, |0_{in}\rangle}{\langle 0_{out}|0_{in}\rangle} = \frac{e^{-i\omega t}}{\sqrt{2\omega}} \frac{\langle 0_{out}| \, \hat{a}^-_{out} \, |0_{in}\rangle}{\langle 0_{out}|0_{in}\rangle} = J_0 \frac{e^{-i\omega t}}{\sqrt{2\omega}}.$$

In general, these matrix elements are complex numbers since

$$\frac{1}{\sqrt{2\omega}} J_0 e^{-i\omega t} = \frac{i}{2\omega} \int_0^T e^{-i\omega(t-t')} J(t') dt'.$$

This expression can be rewritten in the form (3.16) if we use the *Feynman Green's function*

$$G_F(t,t') \equiv \frac{ie^{-i\omega|t-t'|}}{2\omega} \tag{3.17}$$

instead of the retarded Green's function G_{ret}.

Other matrix elements such as $\langle 0_{in}|\,\hat{q}\,(t_1)\,\hat{q}\,(t_2)\,|0_{in}\rangle$ can be computed in a similar way. In Chapter 12 we shall study Green's functions of the harmonic oscillator in more detail.

Exercise 3.4

Consider a harmonic oscillator driven by an external force $J(t)$. The Green's functions $G_{ret}(t,t')$ and $G_F(t,t')$ are defined by Eqs. (3.15) and (3.17). For $t_{1,2} \geq T$, show that:

(a) The expectation value of $\hat{q}\,(t_1)\,\hat{q}\,(t_2)$ in the "in" state is

$$\begin{aligned}&\langle 0_{in}|\,\hat{q}\,(t_1)\,\hat{q}\,(t_2)\,|0_{in}\rangle \\ &= \frac{1}{2\omega}e^{i\omega(t_2-t_1)} + \int_0^T dt_1' \int_0^T dt_2' J\left(t_1'\right) J\left(t_2'\right) G_{ret}\left(t_1,t_1'\right) G_{ret}\left(t_2,t_2'\right).\end{aligned}$$

(b) The in-out matrix element of $\hat{q}\,(t_1)\,\hat{q}\,(t_2)$ is

$$\begin{aligned}&\frac{\langle 0_{out}|\,\hat{q}\,(t_1)\,\hat{q}\,(t_2)\,|0_{in}\rangle}{\langle 0_{out}|\,0_{in}\rangle} \\ &= \frac{1}{2\omega}e^{i\omega(t_2-t_1)} + \int_0^T dt_1' \int_0^T dt_2' J\left(t_1'\right) J\left(t_2'\right) G_F\left(t_1,t_1'\right) G_F\left(t_2,t_2'\right).\end{aligned}$$

4 From harmonic oscillators to fields

Summary: Collections of quantum oscillators. Field quantization. Mode expansion of a quantum field. Zero-point energy. Schrödinger equation for quantum fields.

4.1 Quantization of free fields

A free field can be treated as a collection of infinitely many harmonic oscillators. To quantize a scalar field, we shall generalize the method used in quantum mechanics for describing a finite set of oscillators.

The classical action describing N harmonic oscillators with coordinates q_1, ..., q_N is

$$S\left[q_i\right] = \frac{1}{2}\int \left[\sum_{i=1}^{N} \dot{q}_i^2 - \sum_{i,j=1}^{N} M_{ij} q_i q_j\right] dt, \tag{4.1}$$

where the symmetric and positive-definite matrix M_{ij} describes the coupling between the oscillators.

By choosing an appropriate set of normal coordinates $\tilde{q}_\alpha$ that are linear combinations of q_i, the oscillators can be decoupled (see Exercise 4.1). The matrix M is diagonal in the new coordinates, $M_{\alpha\beta} = \delta_{\alpha\beta}\omega_\alpha^2$ (here no summation over α is implied).

Exercise 4.1

Find a linear transformation

$$\tilde{q}_\alpha = \sum_{i=1}^{N} C_{\alpha i} q_i$$

leading to the new decoupled coordinates $\tilde{q}_\alpha$ and reducing the action (4.1) to the form

$$S\left[\tilde{q}_\alpha\right] = \frac{1}{2}\int \sum_{\alpha=1}^{N} \left(\dot{\tilde{q}}_\alpha^2 - \omega_\alpha^2 \tilde{q}_\alpha^2\right) dt,$$

where ω_α are the eigenfrequencies.

The variables $\tilde{q}_\alpha$ are called the *normal modes*. For brevity, we shall omit the tilde and write q_α instead of $\tilde{q}_\alpha$.

The modes q_α are quantized (in the Heisenberg picture) by introducing the operators $\hat{q}_\alpha(t)$, $\hat{p}_\alpha(t)$ and imposing the standard commutation relations

$$[\hat{q}_\alpha, \hat{p}_\beta] = i\delta_{\alpha\beta}, \quad [\hat{q}_\alpha, \hat{q}_\beta] = [\hat{p}_\alpha, \hat{p}_\beta] = 0.$$

The creation and annihilation operators $\hat{a}^{\pm}_{\alpha}(t)$ are defined by

$$\hat{a}^{\pm}_{\alpha}(t) = \sqrt{\frac{\omega_\alpha}{2}} \left(\hat{q}_\alpha(t) \mp \frac{i}{\omega_\alpha} \hat{p}_\alpha(t) \right)$$

and obey the equations of motion similar to Eq. (3.3),

$$\frac{d}{dt} \hat{a}^{\pm}_{\alpha}(t) = \pm i\omega_\alpha \hat{a}^{\pm}_{\alpha}(t).$$

Their general solutions are

$$\hat{a}^{\pm}_{\alpha}(t) = {}^{(0)}\hat{a}^{\pm}_{\alpha} e^{\pm i\omega_\alpha t},$$

where ${}^{(0)}\hat{a}^{\pm}_{\alpha}$ are operator-valued integration constants satisfying the commutation relation

$$\left[{}^{(0)}\hat{a}^{-}_{\alpha}, {}^{(0)}\hat{a}^{+}_{\beta} \right] = \delta_{\alpha\beta}.$$

Below we shall never need the time-dependent operators $\hat{a}^{\pm}_{\alpha}(t)$. Therefore we drop the cumbersome superscript ${}^{(0)}$ and denote the time-*independent* creation and annihilation operators simply by $\hat{a}^{\pm}_{\alpha}$.

Using these operators $\hat{a}^{\pm}_{\alpha}$, we can define the Hilbert space of states for the oscillator system by the usual procedure. The vacuum state $|0, ..., 0\rangle$ is the unique common eigenvector of all annihilation operators $\hat{a}^{-}_{\alpha}$ with eigenvalue 0,

$$\hat{a}^{-}_{\alpha} |0, ..., 0\rangle = 0 \text{ for } \alpha = 1, ..., N.$$

The state $|n_1, n_2, ..., n_N\rangle$ having the occupation number n_α in the oscillator q_α is defined by

$$|n_1, ..., n_N\rangle = \left[\prod_{\alpha=1}^{N} \frac{(\hat{a}^{+}_{\alpha})^{n_\alpha}}{\sqrt{n_\alpha!}} \right] |0, 0, ..., 0\rangle . \tag{4.2}$$

The Hilbert space is spanned by the states $|n_1, ..., n_N\rangle$ with all possible choices of occupation numbers n_α.

4.1.1 From oscillators to fields

A *classical field* is described by a function of spacetime, $\phi(\mathbf{x}, t)$, characterizing the local strength or intensity of the field. To visualize a field as a physical system analogous to a collection of oscillators q_i, we might imagine that a separate harmonic oscillator $\phi_{\mathbf{x}}(t)$ is attached to each point $\mathbf{x}$ in space. (Note that the oscillators $\phi_{\mathbf{x}}(t)$ "move" in the configuration space, i.e. in the space of values of the field ϕ.) The spatial coordinate $\mathbf{x}$ is an index labeling the oscillators $\phi_{\mathbf{x}}(t)$, similarly to the discrete index i for the oscillators q_i. In this way one may interpret the field $\phi(\mathbf{x}, t) \equiv \phi_{\mathbf{x}}(t)$ as the coordinate of the oscillator corresponding to the point $\mathbf{x}$.

Using this analogy, we treat the field $\phi(\mathbf{x}, t)$ as an infinite collection of oscillators. In the action (4.1), sums over i must be replaced by integrals over $\mathbf{x}$, so that the action

for ϕ is of the form

$$S[\phi] = \frac{1}{2}\int dt \left[\int d^3\mathbf{x}\,\dot{\phi}^2(\mathbf{x},t) - \int d^3\mathbf{x}\,d^3\mathbf{y}\,\phi(\mathbf{x},t)\,\phi(\mathbf{y},t)\,M(\mathbf{x},\mathbf{y})\right]. \tag{4.3}$$

Here the function M is yet to be determined.

A relativistic theory must be invariant under transformations of the Poincaré group describing the time and space shifts (translations), spatial rotations, and Lorentz transformations (boosts). The simplest Poincaré-invariant action for a real scalar field $\phi(\mathbf{x},t)$ is

$$\begin{aligned} S[\phi] &= \frac{1}{2}\int d^4x \left[\eta^{\mu\nu}(\partial_\mu\phi)(\partial_\nu\phi) - m^2\phi^2\right] \\ &= \frac{1}{2}\int d^3\mathbf{x}\,dt \left[\dot{\phi}^2 - (\nabla\phi)^2 - m^2\phi^2\right], \end{aligned} \tag{4.4}$$

where $\eta^{\mu\nu} = \mathrm{diag}(1,-1,-1,-1)$ is the Minkowski metric (in this chapter we consider only the flat spacetime) and the Greek indices label four-dimensional coordinates: $x^0 \equiv t$ and $(x^1,x^2,x^3) \equiv \mathbf{x}$. The action (4.4) has the form (4.3) if we set

$$M(\mathbf{x},\mathbf{y}) = \left[-\Delta_{\mathbf{x}} + m^2\right]\delta(\mathbf{x}-\mathbf{y}). \tag{4.5}$$

The invariance of the action (4.4) under translations is obvious; its Lorentz invariance is the subject of the following exercise.

Exercise 4.2
Show that the scalar field action (4.4) remains unchanged under a Lorentz transformation

$$x^\mu \to \tilde{x}^\mu = \Lambda^\mu_\nu x^\nu, \quad \phi(\mathbf{x},t) \to \tilde{\phi}(\mathbf{x},t) = \phi\left(\tilde{\mathbf{x}},\tilde{t}\right), \tag{4.6}$$

where the transformation matrix Λ^μ_ν satisfies $\eta_{\mu\nu}\Lambda^\mu_\alpha\Lambda^\nu_\beta = \eta_{\alpha\beta}$.

To derive the equation of motion for ϕ, we calculate the functional derivative of the action with respect to $\phi(\mathbf{x},t)$,

$$\frac{\delta S}{\delta\phi(\mathbf{x},t)} = \ddot{\phi}(\mathbf{x},t) - \Delta\phi(\mathbf{x},t) + m^2\phi(\mathbf{x},t) = 0. \tag{4.7}$$

Exercise 4.3
Derive Eq. (4.7) from the action (4.4).

The equation of motion (4.7) shows that the "oscillators" $\phi(\mathbf{x},t) \equiv \phi_{\mathbf{x}}(t)$ are coupled. This can be intuitively understood as follows: The Laplacian $\Delta\phi$ contains second derivatives of ϕ that may be visualized as

$$\frac{d^2\phi_x}{dx^2} \approx \frac{\phi_{x+\delta x} - 2\phi_x + \phi_{x-\delta x}}{(\delta x)^2},$$

so the evolution of the oscillator ϕ_x depends on the oscillators at adjacent points $x \pm \delta x$.

To decouple the oscillators $\phi_{\mathbf{x}}$, we apply the Fourier transform,

$$\phi_{\mathbf{k}}(t) \equiv \int \frac{d^3\mathbf{x}}{(2\pi)^{3/2}} e^{-i\mathbf{k}\cdot\mathbf{x}} \phi(\mathbf{x}, t), \tag{4.8}$$

$$\phi(\mathbf{x}, t) \equiv \int \frac{d^3\mathbf{k}}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot\mathbf{x}} \phi_{\mathbf{k}}(t). \tag{4.9}$$

As in Chapter 1, the complex functions $\phi_{\mathbf{k}}(t)$ are called the *modes* of the field ϕ. From Eqs. (4.7)-(4.9) it is straightforward to derive the following equations for the modes:

$$\frac{d^2}{dt^2}\phi_{\mathbf{k}}(t) + \left(k^2 + m^2\right)\phi_{\mathbf{k}}(t) = 0. \tag{4.10}$$

These equations describe an infinite set of decoupled harmonic oscillators with frequencies

$$\omega_k \equiv \sqrt{k^2 + m^2}.$$

Using Eq. (4.9), one can also express the action (4.4) through the modes $\phi_{\mathbf{k}}$,

$$S = \frac{1}{2}\int dt\, d^3\mathbf{k} \left(\dot{\phi}_{\mathbf{k}}\dot{\phi}_{-\mathbf{k}} - \omega_k^2 \phi_{\mathbf{k}}\phi_{-\mathbf{k}}\right). \tag{4.11}$$

Exercise 4.4
Show that the modes $\phi_{\mathbf{k}}(t)$ of a real field $\phi(\mathbf{x}, t)$ satisfy the relation $(\phi_{\mathbf{k}})^* = \phi_{-\mathbf{k}}$.

4.1.2 Quantizing fields in flat spacetime

To prepare for quantization, we need to introduce the canonical momenta and to obtain the classical Hamiltonian for the field ϕ. Note that the action (4.4) is an integral of the Lagrangian over *time* (but not over space), $S[\phi] = \int L[\phi]\, dt$, so the Lagrangian $L[\phi]$ is

$$L[\phi] = \int \mathcal{L} d^3\mathbf{x}; \quad \mathcal{L} \equiv \frac{1}{2}\eta^{\mu\nu}\phi_{,\mu}\phi_{,\nu} - \frac{1}{2}m^2\phi^2,$$

where $\mathcal{L}$ is the Lagrangian *density*. To define the canonical momenta and the Hamiltonian, one must use the Lagrangian $L[\phi]$, not the Lagrangian density $\mathcal{L}$. Hence the momenta $\pi(\mathbf{x}, t)$ are computed as the functional derivatives

$$\pi(\mathbf{x}, t) \equiv \frac{\delta L[\phi]}{\delta\dot{\phi}(\mathbf{x}, t)} = \dot{\phi}(\mathbf{x}, t),$$

and then the classical Hamiltonian is

$$H = \int \pi(\mathbf{x}, t)\,\dot{\phi}(\mathbf{x}, t)\, d^3\mathbf{x} - L = \frac{1}{2}\int d^3\mathbf{x}\left[\pi^2 + (\nabla\phi)^2 + m^2\phi^2\right]. \tag{4.12}$$

Remark: Lorentz invariance. To quantize a field theory, we use the Hamiltonian formalism which explicitly separates the time coordinate t from the spatial coordinate $\mathbf{x}$. However, if the classical theory is relativistic (Lorentz-invariant), the resulting quantum theory is also relativistic.

To quantize the field, we introduce the operators $\hat{\phi}(\mathbf{x},t)$ and $\hat{\pi}(\mathbf{x},t)$ with the standard commutation relations

$$[\hat{\phi}(\mathbf{x},t)\,,\,\hat{\pi}(\mathbf{y},t)] = i\delta(\mathbf{x}-\mathbf{y})\,; \quad [\hat{\phi}(\mathbf{x},t)\,,\,\hat{\phi}(\mathbf{y},t)] = [\hat{\pi}(\mathbf{x},t)\,,\,\hat{\pi}(\mathbf{y},t)] = 0. \tag{4.13}$$

The modes $\phi_{\mathbf{k}}(t)$ also become operators $\hat{\phi}_{\mathbf{k}}(t)$. The commutation relation for the modes can be derived from Eq. (4.13) by performing Fourier transforms in $\mathbf{x}$ and $\mathbf{y}$. After some algebra, we find

$$[\hat{\phi}_{\mathbf{k}_1}(t),\,\hat{\pi}_{\mathbf{k}_2}(t)] = i\delta(\mathbf{k}_1+\mathbf{k}_2)\,.$$

Note the plus sign in $\delta(\mathbf{k}_1+\mathbf{k}_2)$: it shows that the variable which is conjugate to $\phi_{\mathbf{k}}$ is not $\pi_{\mathbf{k}}$ but $\pi_{-\mathbf{k}} = \pi^*_{\mathbf{k}}$. This is also evident from the action (4.11).

Quite similarly to Sec. 4.1, we first introduce the time-dependent creation and annihilation operators:

$$\hat{a}^-_{\mathbf{k}}(t) \equiv \sqrt{\frac{\omega_k}{2}}\left(\hat{\phi}_{\mathbf{k}} + \frac{i\hat{\pi}_{\mathbf{k}}}{\omega_k}\right);\ \hat{a}^+_{\mathbf{k}}(t) \equiv \sqrt{\frac{\omega_k}{2}}\left(\hat{\phi}_{-\mathbf{k}} - \frac{i\hat{\pi}_{-\mathbf{k}}}{\omega_k}\right).$$

The equations of motion for the operators $\hat{a}^\pm_{\mathbf{k}}(t)$,

$$\frac{d}{dt}\hat{a}^\pm_{\mathbf{k}}(t) = \pm i\omega_k \hat{a}^\pm_{\mathbf{k}}(t),$$

have the general solution $\hat{a}^\pm_{\mathbf{k}}(t) = {}^{(0)}\hat{a}^\pm_{\mathbf{k}} e^{\pm i\omega_k t}$, where the time-independent operators ${}^{(0)}\hat{a}^\pm_{\mathbf{k}}$ satisfy the relations (note the signs of $\mathbf{k}$ and $\mathbf{k}'$)

$$\left[\hat{a}^-_{\mathbf{k}},\,\hat{a}^+_{\mathbf{k}'}\right] = \delta(\mathbf{k}-\mathbf{k}')\,; \quad \left[\hat{a}^-_{\mathbf{k}},\,\hat{a}^-_{\mathbf{k}'}\right] = \left[\hat{a}^+_{\mathbf{k}},\,\hat{a}^+_{\mathbf{k}'}\right] = 0. \tag{4.14}$$

In Eq. (4.14) we omitted the superscript ${}^{(0)}$ for brevity; below we shall always use the time-independent creation and annihilation operators and denote them by $\hat{a}^\pm_{\mathbf{k}}$.

Remark: complex oscillators. The modes $\phi_{\mathbf{k}}(t)$ are complex variables; each $\phi_{\mathbf{k}}$ may be thought of as a pair of real-valued oscillators, $\phi_{\mathbf{k}} = \phi^{(1)}_{\mathbf{k}} + i\phi^{(2)}_{\mathbf{k}}$. Accordingly, the operators $\hat{\phi}_{\mathbf{k}}$ are not Hermitian and $(\hat{\phi}_{\mathbf{k}})^\dagger = \hat{\phi}_{-\mathbf{k}}$. In principle, one could rewrite the theory in terms of Hermitian variables, but it is mathematically more convenient to keep the complex modes $\phi_{\mathbf{k}}$.

The Hilbert space of field states is built in the standard fashion. We postulate the vacuum state $|0\rangle$ such that $\hat{a}^-_{\mathbf{k}}|0\rangle = 0$ for all $\mathbf{k}$. The state with occupation numbers n_s in each mode with momentum $\mathbf{k}_s$ (where $s = 1, 2, ...$ is an index that enumerates the excited modes) is defined similarly to Eq. (4.2),

$$|n_1,\,n_2,\,...\rangle = \left[\prod_s \frac{(\hat{a}^+_{\mathbf{k}_s})^{n_s}}{\sqrt{n_s!}}\right]|0\rangle\,. \tag{4.15}$$

We write $|0\rangle$ instead of $|0,0,...\rangle$ for brevity. The vector (4.15) describes a state with n_s particles having momentum $\mathbf{k}_s$ (where $s = 1, 2, ...$). The Hilbert space of quantum states is spanned by the vectors $|n_1,\, n_2,\, ...\rangle$ with all possible choices of the numbers n_s.

The quantum Hamiltonian of the free scalar field can be written as

$$\hat{H} = \frac{1}{2}\int d^3\mathbf{k}\left[\hat{\pi}_{\mathbf{k}}\hat{\pi}_{-\mathbf{k}} + \omega_k^2\hat{\phi}_{\mathbf{k}}\hat{\phi}_{-\mathbf{k}}\right],$$

which yields

$$\hat{H} = \int d^3\mathbf{k}\frac{\omega_k}{2}\left(\hat{a}_{\mathbf{k}}^-\hat{a}_{\mathbf{k}}^+ + \hat{a}_{\mathbf{k}}^+\hat{a}_{\mathbf{k}}^-\right) = \int d^3\mathbf{k}\frac{\omega_k}{2}\left[2\hat{a}_{\mathbf{k}}^+\hat{a}_{\mathbf{k}}^- + \delta^{(3)}(0)\right]. \tag{4.16}$$

> **Exercise 4.5**
> Derive this relation.

Thus we have quantized the scalar field $\phi(\mathbf{x}, t)$ in the Heisenberg picture. Quantum observables such as $\hat{\phi}(\mathbf{x}, t)$ and $\hat{H}$ are represented by linear operators in the Hilbert space, and the quantum states of the field ϕ are interpreted in terms of particles.

4.1.3 A first look at mode expansions

We now give a brief introduction to mode expansions which offer a shorter and computationally more convenient way to quantize fields. A more detailed treatment is given in Chapter 6.

The mode operator $\hat{\phi}_{\mathbf{k}}(t)$ can be expressed through the creation and annihilation operators,

$$\hat{\phi}_{\mathbf{k}}(t) = \frac{1}{\sqrt{2\omega_k}}\left(\hat{a}_{\mathbf{k}}^- e^{-i\omega_k t} + \hat{a}_{-\mathbf{k}}^+ e^{i\omega_k t}\right).$$

Substituting this into Eq. (4.9), we obtain the following expansion of the field operator $\hat{\phi}(\mathbf{x}, t)$,

$$\hat{\phi}(\mathbf{x}, t) = \int \frac{d^3\mathbf{k}}{(2\pi)^{3/2}}\frac{1}{\sqrt{2\omega_k}}\left[\hat{a}_{\mathbf{k}}^- e^{-i\omega_k t + i\mathbf{k}\cdot\mathbf{x}} + \hat{a}_{-\mathbf{k}}^+ e^{i\omega_k t + i\mathbf{k}\cdot\mathbf{x}}\right],$$

which we then rewrite by changing $\mathbf{k} \to -\mathbf{k}$ in the second term to make the integrand manifestly Hermitian:

$$\hat{\phi}(\mathbf{x}, t) = \int \frac{d^3\mathbf{k}}{(2\pi)^{3/2}}\frac{1}{\sqrt{2\omega_k}}\left[\hat{a}_{\mathbf{k}}^- e^{-i\omega_k t + i\mathbf{k}\cdot\mathbf{x}} + \hat{a}_{\mathbf{k}}^+ e^{i\omega_k t - i\mathbf{k}\cdot\mathbf{x}}\right]. \tag{4.17}$$

This relation is called the *mode expansion* of the quantum field $\hat{\phi}$.

It is easy to see that the commutation relations (4.13) between $\hat{\phi}$ and $\hat{\pi}$ are equivalent to the relations (4.14), while the equations of motion (4.7) are identically satisfied by the ansatz (4.17) with time-independent operators $\hat{a}_{\mathbf{k}}^{\pm}$. Therefore we may quantize the field $\phi(\mathbf{x}, t)$ by simply postulating the commutation relations (4.14) and the mode expansion (4.17), without introducing the operators $\hat{\phi}_{\mathbf{k}}$ and $\hat{\pi}_{\mathbf{k}}$ explicitly. The Hilbert space of quantum states is constructed and interpreted as above.

Mode functions

Note the occurrence of the functions $e^{-i\omega_k t}$ in the time dependence of the modes $\hat{\phi}_{\mathbf{k}}$. These functions are complex-valued solutions of the harmonic oscillator equation with frequency ω_k. In chapter 6 we shall show that for quantum fields in gravitational backgrounds the "oscillator frequency" ω_k becomes time-dependent. In that case, we need to replace $e^{-i\omega_k t}$ by *mode functions* $v_{\mathbf{k}}(t)$ which are certain complex-valued solutions of the equation

$$\ddot{v}_{\mathbf{k}} + \omega_k^2(t) v_{\mathbf{k}} = 0.$$

The mode expansion is written more generally as

$$\hat{\phi}(\mathbf{x}, t) = \int \frac{d^3\mathbf{k}}{(2\pi)^{3/2}} \frac{1}{\sqrt{2}} \left[\hat{a}^-_{\mathbf{k}} v^*_{\mathbf{k}}(t) e^{i\mathbf{k}\cdot\mathbf{x}} + \hat{a}^+_{\mathbf{k}} v_{\mathbf{k}}(t) e^{-i\mathbf{k}\cdot\mathbf{x}} \right]. \tag{4.18}$$

(The commutation relation for the operators $\hat{a}^\pm_{\mathbf{k}}$ remains unchanged.) From Eq. (4.17) we can read off the mode functions of a free field in flat space,

$$v_k(t) = \frac{1}{\sqrt{\omega_k}} e^{i\omega_k t}, \quad \omega_k = \sqrt{k^2 + m^2}. \tag{4.19}$$

In this case the mode functions depend only on the magnitude of the wave number k, so we write v_k and not $v_{\mathbf{k}}$.

> **Remark: quantitative meaning of mode functions.** Equation (4.18) relates $\hat{\phi}$ to $\hat{a}^\pm_{\mathbf{k}}$ and $v_{\mathbf{k}}$. Since the operators $\hat{a}^\pm_{\mathbf{k}}$ are dimensionless and normalized to 1 through the commutation relation, the order of magnitude of ϕ is the same as that of v_k. We shall show in chapter 7 (Sec. 7.1.2) that $|v_k|$ characterizes the typical amplitude of vacuum fluctuations of the field ϕ. For instance, the mode functions (4.19) indicate that the typical fluctuation in the mode $\phi_{\mathbf{k}}$ is of order $1/\sqrt{\omega_k}$. This result is already familiar from Eq. (1.11) of Sec. 1.4.

4.2 Zero-point energy

It is easy to see from Eq. (4.16) that the vacuum state $|0\rangle$ is an eigenstate of the Hamiltonian with the eigenvalue

$$E_0 = \langle 0 | \hat{H} | 0 \rangle = \frac{1}{2} \delta^{(3)}(0) \int d^3\mathbf{k}\, \omega_k. \tag{4.20}$$

This expression, which we expect to describe the total energy of the field in the vacuum state, is obviously divergent: the factor $\delta^{(3)}(0)$ is infinite, and also the integral

$$\int d^3\mathbf{k}\, \omega_k = \int_0^\infty 4\pi k^2 \sqrt{m^2 + k^2}\, dk$$

diverges at the upper limit.

Explaining the presence of $\delta^{(3)}(0)$

The origin of the divergent factor $\delta^{(3)}(0)$ is relatively easy to understand: it is the infinite volume of all space. Indeed, the factor $\delta^{(3)}(0)$ arises from the commutation relation (4.14) when we evaluate $\delta^{(3)}(\mathbf{k}-\mathbf{k}')$ at $\mathbf{k}=\mathbf{k}'$; note that $\delta^{(3)}(\mathbf{k})$ has the dimension of 3-volume. For a field quantized in a finite box of volume V (see Sec. 1.2), the vacuum energy is given by Eq. (1.10),

$$E_0 = \frac{1}{2}\sum_{\mathbf{k}} \omega_k \approx \frac{1}{2}\frac{V}{(2\pi)^3}\int d^3\mathbf{k}\,\omega_k.$$

Comparing this with Eq. (4.20), we find that the formally infinite factor $\delta^{(3)}(0)$ arises when the box volume V grows to infinity. Dividing the energy E_0 by the volume V and taking the limit $V\to\infty$, we obtain the zero-point energy density

$$\lim_{V\to\infty}\frac{E_0}{V} = \frac{1}{2}\int \frac{d^3\mathbf{k}}{(2\pi)^3}\omega_k. \tag{4.21}$$

Renormalizing the zero-point energy

The energy density (4.21) is infinite because the integral $\int d^3\mathbf{k}\,\omega_k$ diverges at $|\mathbf{k}|\to\infty$. This is called an *ultraviolet divergence* because large values of k correspond to large energies. The formal reason for this divergence is the presence of infinitely many oscillators $\phi_{\mathbf{k}}(t)$, each having the zero-point energy $\frac{1}{2}\omega_k$.

This is the first of several divergences encountered in quantum field theory. In the case of a free scalar field in the flat spacetime, there is a simple recipe to circumvent this problem. The energy of an excited state $|n_1,\,n_2,\,...\rangle$ can be computed using Eqs. (4.14)-(4.16). Since

$$[\hat{a}^-_{\mathbf{k}},(\hat{a}^+_{\mathbf{k}'})^n] = n(\hat{a}^+_{\mathbf{k}})^{n-1}\delta(\mathbf{k}-\mathbf{k}'),$$

we obtain

$$E(n_1,n_2,...) = E_0 + \int d^3\mathbf{k}\left(\sum_s n_s\delta(\mathbf{k}-\mathbf{k}_s)\right)\omega_k = E_0 + \sum_s n_s\omega_{k_s}.$$

Thus the energy of a state is always a sum of the divergent quantity E_0 and a finite state-dependent contribution. The presence of the zero-point energy E_0 cannot be detected by measuring transitions between the excited states of the field. So the divergent term E_0 can be simply subtracted away.

The subtraction is conveniently performed by modifying the Hamiltonian (4.16) so that all annihilation operators $\hat{a}^-_{\mathbf{k}}$ appear to the right of all creation operators $\hat{a}^+_{\mathbf{k}}$ (this form is called *normal-ordered*). For the free field, we set

$$\hat{H} \equiv \int d^3\mathbf{k}\,\omega_k\hat{a}^+_{\mathbf{k}}\hat{a}^-_{\mathbf{k}}.$$

After this redefinition, the vacuum state becomes an eigenstate of *zero* energy:

$$\langle 0|\,\hat{H}\,|0\rangle = 0.$$

The resulting quantum theory agrees with experiments.

4.3 The Schrödinger equation for a quantum field

So far we have been working in the Heisenberg picture, but fields can be quantized also in the Schrödinger picture. Here we first consider the Schrödinger equation for a collection of harmonic oscillators and then generalize that equation to quantum fields.

The action describing a set of N harmonic oscillators is given by Eq. (4.1). In the coordinates q_i, $p_i \equiv \dot{q}_i$, where $i = 1, 2, ..., N$, the Hamiltonian is

$$H = \frac{1}{2}\sum_i p_i^2 + \frac{1}{2}\sum_{i,j} M_{ij} q_i q_j.$$

To quantize this system in the Schrödinger picture, we introduce time-*independent* operators $\hat{p}_i$, $\hat{q}_i$ which act on time-dependent states $|\psi(t)\rangle$. The Hamiltonian becomes an operator $\hat{H} = H(\hat{p}_i, \hat{q}_i)$. The Hilbert space is spanned by the basis vectors $|q_1, ..., q_N\rangle$ which are the generalized eigenvectors of the position operators q_i. A state vector $|\psi(t)\rangle$ can then be decomposed into a linear combination

$$|\psi(t)\rangle = \int dq_1 ... dq_N \psi(q_1, ..., q_N, t)\,|q_1, ..., q_N\rangle\,,$$

where the wave function $\psi(q_1, ..., q_N, t)$ is

$$\psi(q_1, ..., q_N, t) = \langle q_1, ..., q_N|\psi(t)\rangle\,.$$

The momentum operators $\hat{p}_i$ in this representation act on the wave function as derivatives $-i\partial/\partial q_i$, and the Schrödinger equation takes the form

$$i\frac{\partial\psi}{\partial t} = \hat{H}\psi = \frac{1}{2}\sum_{i,j}\left(-\delta_{ij}\frac{\partial^2}{\partial q_i \partial q_j} + M_{ij} q_i q_j\right)\psi. \tag{4.22}$$

To generalize the Schrödinger equation to quantum fields, we need to replace the oscillator coordinates q_i by field values $\phi(\mathbf{x})$ and the wave function $\psi(q_1, ..., q_N, t)$ by a wave functional $\Psi[\phi(\mathbf{x}), t]$. Note that the spatial coordinate $\mathbf{x}$ plays the role of the index i, so Ψ is a functional of $\phi(\mathbf{x})$ which is a function only of space; the time dependence is contained in the functional Ψ. The probability for measuring a field configuration $\phi(\mathbf{x})$ at time t is proportional to $|\Psi[\phi(\mathbf{x}), t]|^2$.

The partial derivative $\partial/\partial q_i$ is replaced by the functional derivative $\delta/\delta\phi(\mathbf{x})$ and the sum over i by an integral over space, $\int d^3\mathbf{x}$. Thus we obtain the following equation as a direct generalization of Eq. (4.22):

$$i\frac{\partial}{\partial t}\Psi[\phi,t] = -\frac{1}{2}\int d^3\mathbf{x}\frac{\delta^2\Psi[\phi,t]}{\delta\phi(\mathbf{x})\,\delta\phi(\mathbf{x})} + \frac{1}{2}\int d^3\mathbf{x}\,d^3\mathbf{y}\,M(\mathbf{x},\mathbf{y})\,\phi(\mathbf{x})\,\phi(\mathbf{y})\,\Psi[\phi,t]\,.$$

This is the Schrödinger equation for a scalar field ϕ; the kernel $M(\mathbf{x},\mathbf{y})$ is given by Eq. (4.5).

We wrote the Schrödinger equation for a relativistic quantum field rather as a proof of concept than as a practical device for calculations. It is rather difficult to solve this equation directly (a formal solution may be found as a path integral). Usually one needs additional insight to extract information from this equation. The Schrödinger picture is rarely used in quantum field theory.

5 Overview of classical field theory

Summary: Action principle for classical fields. Minimal and conformal coupling to gravity. Internal symmetries and gauge invariance. Action for gauge fields. The energy-momentum tensor for fields. Conservation of the EMT.

5.1 Choosing the action functional

Classical field theory is based on the action principle: the field equations are the conditions of extremizing the action functional,

$$S\left[\phi\right] = \int d^4x\, \mathcal{L}\left(\phi_i, \partial_\mu \phi_i, ...\right) \tag{5.1}$$

where the Lagrangian density $\mathcal{L}$ depends on the field and its derivatives. (For brevity, spacetime derivatives are denoted by commas, e.g. $\partial_\mu \phi \equiv \phi_{,\mu}$.) The main focus of this section is the choice of an appropriate action functional for a classical field. The field under consideration may be a scalar field with one or more components ϕ_i, a vector field, a spinor field, and so on. For instance, the gravitational field is described by the metric $g_{\alpha\beta}(x)$ which is a tensor of rank 2.

> **Remark: fermions.** A classical theory of fermionic fields can be built by considering spinor fields $\psi^\mu(x)$ with values in an anticommutative (Grassmann) algebra, so that $\psi^\mu \psi^\nu = -\psi^\nu \psi^\mu$. The assumption of anticommutativity is necessary to obtain the correct anticommutation relations in the quantum theory. Consideration of fermionic fields is beyond the scope of this book.

5.1.1 Requirements for the action functional

To choose an action for a field, we use the following guiding principles:

1. The action is real-valued and has an extremum.
   Without this condition, one cannot formulate the action principle as "the classical trajectory is an extremum of the action."

2. The action is a local functional of the fields and their derivatives.
   A *local functional* is one of the form (5.1) where the Lagrangian density $\mathcal{L}$ is a function of all fields at one and the same point. An example of a nonlocal functional is
   $$\int d^4x\, d^4x' \phi^\mu(x - x') \psi_{,\mu}(x').$$

This functional directly couples the values of the fields ϕ and ψ at distant points x and x'.
Local theories have so far been successful in describing experiments, so there was no need to consider nonlocal theories which are much more complicated.

3. The equations of motion for the fields contain derivatives of at most second order.
This requirement means that it is sufficient to specify initial values of the fields and their first derivatives, or alternatively initial and final values, to fix the solution uniquely. In the next section we shall show that this requirement is satisfied when the Lagrangian contains only the fields and their first derivatives, $\mathcal{L} = \mathcal{L}\left(\phi^i, \phi^i_{,\mu}\right)$.

4. When the background spacetime is flat (i.e. if gravity is negligible), the action is Poincaré-invariant.
The Poincaré group of transformations encompasses four shifts of the coordinates x^μ, three spatial rotations and three Lorentz transformations (boosts). This requirement constrains possible Lagrangians quite strongly. The Poincaré invariance enforces the Lorentz invariance, the rotational invariance, and additionally prohibits Lagrangian densities $\mathcal{L}$ that explicitly depend on $\mathbf{x}$ or t.

5. For an arbitrary curved background spacetime, the action has a generally covariant form (invariant under arbitrary coordinate transformations).
This requirement comes from general relativity: A field theory is compatible with general relativity if it is formulated in a coordinate-independent manner.

6. If the fields have additional physical symmetries, the action should respect them.
Fields can have *internal symmetries* such as gauge symmetries. For example, the conservation of electric charge in electrodynamics can be viewed as a consequence of an internal symmetry of the complex-valued spinor field ψ^μ which describes the electrons. Namely, the Lagrangian of electrodynamics is invariant under the gauge transformations

$$\psi^\mu(x) \to e^{i\alpha}\psi^\mu(x),$$

where α is a real constant. These transformations form the $U(1)$ *gauge group*. Another example is the theory of electroweak interactions where the action is invariant under transformations of the $SU(2) \times U\,(1)$ gauge group. (See Sec. 5.2 for more details on gauge symmetry.)
Quantization of multicomponent fields with gauge symmetries is complicated, and in this book we shall quantize only scalar fields.

5.1.2 Equations of motion for fields

The action principle states that a classical field $\phi^i(x)$ must be an extremum of the action functional. The variation of the action under a small change $\delta\phi^i(x)$ of the field

$\phi^i(x)$ is

$$\delta S = \int d^4x \frac{\delta S}{\delta \phi^i(x)} \delta\phi^i(x) + O\left(\left[\delta\phi^i\right]^2\right).$$

This yields the Euler-Lagrange equation of motion for the field,

$$\frac{\delta S}{\delta \phi^i(x)} = 0.$$

The currently established field theories (electrodynamics, gravitation, weak and strong interactions) are described by Lagrangian densities which depend only on the fields and their first derivatives, $\mathcal{L} = \mathcal{L}\left(\phi^i, \phi^i_{,\mu}\right)$. For such Lagrangians, the variation of the action is given by the formula

$$\delta S = \int d^4x \left(\frac{\partial \mathcal{L}\left(\phi^i, \phi^i_{,\mu}\right)}{\partial \phi^j} - \frac{\partial}{\partial x^\mu} \frac{\partial \mathcal{L}\left(\phi^i, \phi^i_{,\mu}\right)}{\partial \phi^j_{,\mu}} \right) \delta\phi^j(x) + O\left(\left[\delta\phi^i\right]^2\right),$$

where the summations over μ and j are implied. The boundary terms vanish if

$$\frac{\partial \mathcal{L}}{\partial \phi^j_{,\mu}} \delta\phi^j \to 0 \text{ sufficiently rapidly as } |\mathbf{x}| \to \infty,\ |t| \to \infty,$$

which is the usual assumption. Thus we obtain the following equations of motion for the fields ϕ^i,

$$\frac{\delta S\left[\phi\right]}{\delta \phi^j(x)} = \frac{\partial \mathcal{L}\left(\phi^i, \phi^i_{,\mu}\right)}{\partial \phi^j} - \frac{\partial}{\partial x^\mu} \frac{\partial \mathcal{L}\left(\phi^i, \phi^i_{,\mu}\right)}{\partial \phi^j_{,\mu}} = 0. \tag{5.2}$$

These equations conform to the third requirement section 5.1.1 because they contain ϕ^i, $\phi^i_{,\mu}$, and $\phi^i_{,\mu\nu}$, but no higher derivatives.

The formula (5.2) holds for all Lagrangians that depend on fields and their first derivatives. If a Lagrangian for a field ϕ contains second-order derivatives such as $\phi_{,\mu\nu}$, the corresponding equations of motion will generally contain derivatives of third and fourth order.

5.1.3 Real scalar field

The Lagrangian density for a real-valued scalar field $\phi(x)$ in the Minkowski spacetime is

$$\mathcal{L}\left(\phi, \partial_\mu \phi\right) = \frac{1}{2} \eta^{\mu\nu} \phi_{,\mu} \phi_{,\nu} - V(\phi), \tag{5.3}$$

where $\eta^{\mu\nu} \equiv \mathrm{diag}(1, -1, -1, -1)$ is the Minkowski metric and $V(\phi)$ is a potential that describes the self-interaction of the field. A *free* (i.e. noninteracting) field has the potential

$$V(\phi) = \frac{1}{2} m^2 \phi^2.$$

This is the simplest nontrivial potential; an additional linear term $A\phi$ can be removed by a field redefinition $\phi(x) = \tilde{\phi}(x) + \phi_0$. The parameter m is the rest mass of the

particles described by the field ϕ. The Lagrangian density (5.3) satisfies all conditions of Sec. 5.1.1 except the requirement of general covariance.

To make a Poincaré-invariant action generally covariant, we need to adjust it in several ways:

1. Replace $\eta_{\mu\nu}$ by the general spacetime metric $g_{\mu\nu}$.

2. Replace spatial derivatives by covariant derivatives, e.g. $\phi_{,\mu} \to \phi_{;\mu}$. (This makes no difference for a scalar field since covariant derivatives of a scalar function are the same as ordinary spacetime derivatives.)

3. Replace the Minkowski volume element $d^3\mathbf{x}\,dt$ by the covariant volume element $d^4x\sqrt{-g}$, where $g \equiv \det g_{\mu\nu}$ is the determinant of the covariant metric tensor.

Covariant volume element

The expression d^4x does not give the correct volume element if the coordinates x are not Cartesian or if the spacetime is curved. Here is a simple calculation to motivate the choice of $d^4x\sqrt{-g}$ as the volume element.

We consider a two-dimensional Euclidean plane with Cartesian coordinates x, y and introduce arbitrary curvilinear coordinates $\tilde{x}$, $\tilde{y}$ and a metric $g_{ij}(x)$ (here $i, j = 1, 2$). Infinitesimal increments $d\tilde{x}$, $d\tilde{y}$ of the coordinates define an area element corresponding to the infinitesimal parallelogram spanned by vectors $(d\tilde{x}, 0)$ and $(0, d\tilde{y})$. The lengths of the sides of this parallelogram are $l_1 = \sqrt{g_{11}}\,|d\tilde{x}|$ and $l_2 = \sqrt{g_{22}}\,|d\tilde{y}|$, while the angle θ between the vectors is found from the cosine theorem, $l_1 l_2 \cos\theta = g_{12} d\tilde{x} d\tilde{y}$. Thus the infinitesimal area dA of the parallelogram is equal to

$$dA = l_1 l_2 \sin\theta = \sqrt{g_{11}g_{22} - (g_{12})^2}\,|d\tilde{x}|\,|d\tilde{y}| = \sqrt{\det g_{ij}}\,|d\tilde{x}|\,|d\tilde{y}|\,.$$

It is not difficult to show that the volume element in any number of dimensions is given by the formula $dV = d^n x\sqrt{|g(x)|}$. If $\mathbf{u}_1$, ..., $\mathbf{u}_n$ are some vectors in a Euclidean space and let $G_{ij} \equiv \mathbf{u}_i \cdot \mathbf{u}_j$ be the $n \times n$ matrix of their pairwise scalar products. Then the volume of the n-dimensional parallelepiped spanned by the vectors $\mathbf{u}_i$ is $V = \sqrt{|\det G|}$. To prove this statement, we consider the matrix U of coordinates of the vectors $\mathbf{u}_i$ in an orthonormal basis $\mathbf{e}_i$, i.e. $\mathbf{u}_i = \sum_j U_i^j \mathbf{e}_j$. A standard definition of the determinant of a linear transformation is the volume of the image of a unit parallelepiped after the transformation. This gives the volume V as $\det U$. Then we observe that $G = U^T U$, therefore $\det G = (\det U)^2 = V^2$ and $V = \sqrt{|\det G|}$.

In general relativity, the spacetime has a metric with signature $(+,-,-,-)$ and the determinant $\det g_{\mu\nu}$ is always negative (except at singular points where it may be zero or infinite). Therefore we change the sign of g and write the volume element as $d^4x\sqrt{-g}$.

Minimal coupling to gravity

Above we listed the three modifications of the action which are necessary to enforce general covariance. These modifications produce a generally covariant action out of a Poincaré-invariant action. The new action explicitly depends on $g_{\mu\nu}$ and thus describes a field coupled to gravity. For instance, a generally covariant action for a scalar field is

$$S = \int d^4x\sqrt{-g}\left[\frac{1}{2}g^{\mu\nu}\phi_{,\mu}\phi_{,\nu} - V(\phi)\right]. \tag{5.4}$$

This form of coupling is called the *minimal coupling* to gravity; it describes the minimal required interaction of a field with gravitation which necessarily follows from the requirement of compatibility with general relativity. There are other forms of coupling to gravity, for example, the conformal coupling (see below). These couplings are called *nonminimal* and are usually expressed by additional terms in the action. These additional terms couple fields to the curvature tensor $R_{\mu\nu\rho\sigma}$ and violate the strong equivalence principle ("*all* local effects of gravity are equivalent to accelerated coordinate systems in a flat spacetime") because the field is directly influenced by the curvature which, if nonzero, cannot be imitated by an accelerated reference frame in the flat spacetime. One needs a justification to introduce nonminimal terms into the Lagrangian; nonminimally coupled field theories are usually more complicated.

Conformal coupling

A frequently used nonminimally coupled model is the *conformally coupled* scalar field described by the action

$$S = \int d^4x\sqrt{-g}\left[\frac{1}{2}g^{\mu\nu}\phi_{,\mu}\phi_{,\nu} - V(\phi) - \frac{\xi}{2}R\phi^2\right], \tag{5.5}$$

where R is the Ricci curvature scalar and ξ is a constant parameter chosen as $\xi = \frac{1}{6}$. In effect, the additional term describes a "mass" that depends on the curvature of the spacetime. With $\xi = \frac{1}{6}$ the theory has an additional symmetry, namely the action (5.5) is invariant under conformal transformations of the metric,

$$g_{\mu\nu} \to \tilde{g}_{\mu\nu} = \Omega^2(x)g_{\mu\nu}, \tag{5.6}$$

where the conformal factor $\Omega^2(x)$ is an arbitrary nonvanishing function of spacetime.[1] The importance of conformal transformations comes from the fact that several important spacetimes, such as spatially flat Friedmann-Robertson-Walker (FRW) spacetimes used in cosmology, are *conformally flat*. A spacetime is conformally flat if in some coordinates its metric is $g_{\mu\nu} = \Omega^2(x)\eta_{\mu\nu}$, where $\eta_{\mu\nu}$ is the flat Minkowski metric and $\Omega^2(x) \neq 0$ is some function. These spacetimes can be mapped to the flat spacetime by a conformal transformation. If a field theory is conformally invariant, this

[1] Verifying the conformal invariance of the above action takes a fair amount of algebra. We omit the details of this calculation which can be found in chapter 6 of the book *Aspects of quantum field theory in curved space-time* by S. FULLING (Cambridge, 1989).

transformation reduces the action to that of a field in the flat Minkowski spacetime. In effect, a conformal field in a conformally flat spacetime is totally decoupled from gravity.

The equation of motion for a conformally coupled field ϕ follows from the action (5.5),

$$\partial_\alpha \frac{\partial \mathcal{L}}{\partial \phi_{,\alpha}} - \frac{\partial \mathcal{L}}{\partial \phi} = \left(\sqrt{-g} g^{\alpha\beta} \phi_{,\beta}\right)_{,\alpha} + \frac{\partial V}{\partial \phi} + \xi R \phi \sqrt{-g} = 0. \tag{5.7}$$

This equation can be rewritten in a manifestly covariant form as

$$\phi^{;\alpha}_{;\alpha} + \frac{\partial V}{\partial \phi} + \xi R \phi = 0. \tag{5.8}$$

This is similar to the Klein-Gordon equation,

$$\phi^{;\alpha}_{;\alpha} + m^2 \phi = 0,$$

except for the covariant derivatives and the nonminimal coupling term $\xi R \phi$ which can be interpreted as a curvature-dependent mass.

Gauss's law with covariant derivatives

When computing the variation of a generally covariant action such as the action (5.4), one needs to integrate by parts. A useful shortcut in such calculations is an analog of Gauss's law with covariant derivatives. The covariant divergence of a vector field A^μ can be written as

$$A^\mu_{;\mu} = \frac{1}{\sqrt{-g}} \partial_\mu \left(\sqrt{-g} A^\mu\right).$$

Assuming that the contribution of the boundary terms vanishes, we obtain

$$\int d^n x \sqrt{-g} A^\mu_{;\mu} B = -\int d^n x \sqrt{-g} A^\mu B_{,\mu}. \tag{5.9}$$

This formula can be used to integrate by parts: we set $A^\mu \equiv \phi_{,\alpha} g^{\alpha\mu}$, $B \equiv \psi$ and find

$$\int d^4 x \sqrt{-g} \phi_{,\alpha} \psi_{,\beta} g^{\alpha\beta} = -\int d^4 x \sqrt{-g} \left(\phi_{,\alpha} g^{\alpha\beta}\right)_{;\beta} \psi.$$

Note that the covariant derivative of the metric is zero, $g^{;\alpha}_{\alpha\beta} = 0$, so we may lower or raise the indices under covariant derivatives at will; for example, $A^\mu_{;\mu} = A^{;\mu}_{\mu}$.

5.2 Gauge symmetry and gauge fields

Gauge fields naturally appear if the action for a field is invariant under a group of internal symmetry transformations and this symmetry is made local, i.e. when different symmetry transformations are applied at different spacetime points x. We shall now study this construction on some examples.

5.2.1 The $U(1)$ gauge symmetry

Let us consider a complex scalar field $\phi(x)$ with the action

$$S[\phi] = \int d^4x\sqrt{-g}\left[\frac{1}{2}g^{\alpha\beta}\phi_{,\alpha}\phi^*_{,\beta} - V(\phi\phi^*)\right]. \tag{5.10}$$

It is clear that the action (5.10) is generally covariant and describes a minimal coupling to gravity. This action is also invariant under the *gauge transformation*

$$\phi(x) \to \tilde{\phi}(x) = e^{i\alpha}\phi(x), \tag{5.11}$$

where α is an arbitrary real constant. These transformations form the $U(1)$ symmetry group which is the *gauge group* in the theory of a complex scalar field.

The symmetry transformation (5.11) is called *internal* because it only changes the value of the field $\phi(x)$ within its space of values but does not change the point x. Other symmetry transformations such as Lorentz rotations or mirror reflections involve also the spacetime coordinates and are not called internal.

> **Remark: conservation of charge.** According to Noether's theorem, the invariance under transformations (5.11) leads to the conservation of total charge,
>
> $$\frac{d}{dt}\int d^3\mathbf{x}\left(\phi^*\frac{\partial\phi}{\partial t} - \phi\frac{\partial\phi^*}{\partial t}\right) = 0.$$

The transformation (5.11) is called *global* because the values $\phi(x)$ are transformed in the same way at all points x. An important discovery was that this global symmetry can be made *local*, with an arbitrary function $\alpha(x)$ instead of a constant α:

$$\phi(x) \to \tilde{\phi}(x) = e^{i\alpha(x)}\phi(x). \tag{5.12}$$

The action (5.10) is not invariant under local gauge transformations because the derivative $\phi_{,\mu}$ transforms as

$$\phi_{,\mu}(x) \to \tilde{\phi}_{,\mu}(x) = e^{i\alpha(x)}\left(\phi_{,\mu} + i\alpha_{,\mu}\phi\right),$$

instead of $\tilde{\phi}_{,\mu} = e^{i\alpha(x)}\phi_{,\mu}$. To achieve the invariance under local gauge transformations, one introduces an additional vector field A^μ called the *gauge field* which compensates the extra term in the derivative $\phi_{,\mu}$. Namely, all derivatives of the field ϕ in the Lagrangian are replaced by the modified derivatives D_μ,

$$\phi_{,\mu} \to D_\mu\phi \equiv \phi_{,\mu} + iA_\mu\phi, \tag{5.13}$$

which are called *gauge-covariant derivatives*, in analogy with the covariant derivative in general relativity,

$$f^\alpha_{;\mu} = f^\alpha_{,\mu} + \Gamma^\alpha_{\beta\mu}f^\beta.$$

One then postulates that the gauge transformation of the field A^μ is given by the following special rule,

$$A_\mu \to \tilde{A}_\mu \equiv A_\mu - \alpha_{,\mu}. \tag{5.14}$$

Then it is straightforward to verify that the covariant derivative of ϕ transforms according to the local transformation law:

$$\tilde{D}_\mu \tilde{\phi} = \left(\partial_\mu + i\tilde{A}_\mu\right)\left(e^{i\alpha(x)}\phi\right) = e^{i\alpha(x)} D_\mu \phi,$$

and that the modified action

$$S\left[\phi, A\right] = \int d^4x\sqrt{-g}\left[\frac{1}{2}g^{\alpha\beta}\left(D_\alpha\phi\right)\left(D_\beta\phi\right)^* - V\left(\phi\phi^*\right)\right] \tag{5.15}$$

is invariant under local gauge transformations (5.12)-(5.14). Note that the transformation law for A_μ can be chosen at will since all we need is *some* transformation law for the fields which makes the action invariant.

> **Remark: minimal coupling.** The introduction of the gauge field A_μ, the covariant derivative D_μ, and the transformation law (5.14) may appear arbitrary at this stage. In fact, it follows from geometric considerations (based on the theory of fiber bundles) that this is the minimum necessary modification of the action (5.10) that ensures local gauge invariance. Therefore the coupling of the field ϕ to the gauge field manifested in the action (5.15) is called *minimal coupling*.
>
> Building a gauge-invariant action is quite similar to building a generally covariant action. This is so because gravity may be also viewed as a gauge field that arises in a field theory after localizing the symmetry of coordinate transformations. One can derive the minimal coupling to gravity from the equivalence principle as the minimum necessary modification of the flat-space action.

> **Remark: elementary particles.** In QFT, each field describes a certain family of particles. The present picture of fundamental interactions divides all elementary particles into "matter" and "gauge" particles. Namely, "matter particles" interact by forces mediated by "gauge particles," i.e. particles that correspond to gauge fields. For example, electrons are matter particles while photons are gauge particles that transmit the electromagnetic interaction between electrons. Similarly, quarks are matter particles that interact through gluons (gauge particles of the $SU(3)$ symmetry group). It is also remarkable that that all presently known matter particles are fermions, while all gauge particles are bosons.

5.2.2 Action for gauge fields

The action (5.15) describes a scalar field ϕ coupled to the vector field A^μ and to gravity. To obtain the total action of the system, we need to add to Eq. (5.15) some further terms describing the dynamics of the gauge field A_μ itself and the dynamics of gravitation. As before, we need to find an action that is generally covariant and invariant under local gauge transformations. For instance, one cannot add a mass term $m^2 g_{\mu\nu}A^\mu A^\nu$ because this term is not invariant under the gauge transformation (5.14).

The standard form of a gauge-invariant action for the field A_μ is built using the antisymmetric *field strength* tensor

$$F_{\mu\nu} \equiv A_{\nu;\mu} - A_{\mu;\nu} = A_{\nu,\mu} - A_{\mu,\nu}. \tag{5.16}$$

The Christoffel symbols in the covariant derivatives in Eq. (5.16) cancel because of antisymmetrization. One can check that the tensor $F_{\mu\nu}$ is invariant under gauge transformations. So any scalar quantity built from $F_{\mu\nu}$ would be an acceptable (gauge-invariant and generally covariant) term in the action.

The simplest such quantity is the *Yang-Mills* term, $F_{\mu\nu}F^{\mu\nu} \equiv g^{\alpha\beta}g^{\mu\nu}F_{\alpha\mu}F_{\beta\nu}$. The action

$$S\left[A_\mu\right] = -\frac{1}{16\pi}\int d^4x\sqrt{-g}F_{\mu\nu}F^{\mu\nu} \tag{5.17}$$

describes classical electrodynamics coupled to gravity (in vacuum); the field A_μ is proportional to the electromagnetic 4-potential. It is a standard result that Maxwell's equations follow from this action. The combined action (5.15) and (5.17) describes a field of charged relativistic particles of spin 0 (scalar mesons) interacting with the electromagnetic field (photons) and with gravity.

> **Remark: conformal invariance of electrodynamics.** The action (5.17) describes the dynamics of photons as well as the interaction between photons and gravity. We notice that a conformal transformation (5.6) leaves the action invariant since $\sqrt{-g}$ changes by the factor Ω^4 while $g^{\alpha\beta}$ is multiplied by the factor Ω^{-2}. Therefore the evolution of electromagnetic field in any conformally flat spacetime is exactly the same as in the flat Minkowski spacetime (after a conformal transformation). In particular, the gravitational field does not produce electromagnetic waves in conformally flat spacetimes.

The action for gravity is not as straightforward to derive. The simplest theory of gravity is Einstein's general relativity defined by the *Einstein-Hilbert action*,

$$S^{\text{grav}} = -\frac{1}{16\pi G}\int d^4x\sqrt{-g}(R+2\Lambda). \tag{5.18}$$

Here G is Newton's gravitational constant, R is the Ricci curvature scalar and Λ is a constant parameter (the cosmological constant). The Einstein equations are obtained by extremizing this action with respect to $g^{\alpha\beta}$.

> **Exercise 5.1**
> Derive the Einstein equations in vacuum ("pure gravity") from the action
>
> $$S^{\text{grav}} = -\frac{1}{16\pi G}\int R\sqrt{-g}d^4x$$
>
> using the *Palatini* method, namely by varying the action with respect to the metric $g_{\mu\nu}$ and the Christoffel symbol $\Gamma^\mu_{\alpha\beta}$ independently, as if they were unrelated functions.
>
> *Hint:* Write the curvature scalar through the Ricci tensor,
>
> $$R = g^{\alpha\beta}R_{\alpha\beta} = g^{\alpha\beta}\left(\partial_\mu\Gamma^\mu_{\alpha\beta} - \partial_\beta\Gamma^\mu_{\alpha\mu} + \Gamma^\mu_{\alpha\beta}\Gamma^\nu_{\mu\nu} - \Gamma^\nu_{\alpha\mu}\Gamma^\mu_{\beta\nu}\right). \tag{5.19}$$
>
> (We use the sign convention of Landau and Lifshitz.) First find the variation of $R\sqrt{-g}$ with respect to Γ and establish the standard relation between Γ and g, assuming that $\Gamma^\mu_{\alpha\beta}$ is symmetric in α,β:
>
> $$\Gamma^\mu_{\alpha\beta} = \frac{1}{2}g^{\mu\nu}\left(g_{\alpha\nu,\beta} + g_{\beta\nu,\alpha} - g_{\alpha\beta,\nu}\right). \tag{5.20}$$

Then compute the variation of $R\sqrt{-g}$ with respect to $g^{\alpha\beta}$ (note the variation of the determinant) and finally obtain the vacuum Einstein equation as

$$\frac{\delta S^{\text{grav}}}{\delta g^{\alpha\beta}} = -\frac{\sqrt{-g}}{16\pi G}\left(R_{\alpha\beta} - \frac{1}{2}g_{\alpha\beta}R\right) = 0. \tag{5.21}$$

Remark: alternative theories of gravity. At the moment, general relativity agrees with available gravitation experiments. However, we cannot probe strongly curved spacetimes and it is natural to expect that general relativity may be an approximation to a more accurate theory. For instance, the action might contain terms of the form R^2, $R_{\mu\nu}R^{\mu\nu}$, or $R_{\mu\nu\rho\sigma}R^{\mu\nu\rho\sigma}$. The effect of these terms would be to modify the Einstein equations in the high-curvature regime. Such terms greatly complicate the theory and may be introduced only with sufficient justification. All such theories must necessarily agree with Einstein's general relativity in the Newtonian limit of small curvature (weak gravity). Therefore any differences between the alternative theories of gravity can be manifested only when the gravitational field is extremely strong. Such experiments are presently impossible.

5.3 Energy-momentum tensor for fields

The main result of this section is that the energy-momentum tensor (EMT) of a field is related to the functional derivative of the action with respect to the metric $g^{\alpha\beta}$.

We consider a generally covariant action

$$S\left[\phi_i, g_{\mu\nu}\right] = S^{\text{grav}}\left[g_{\mu\nu}\right] + S^{m}\left[\phi_i, g_{\mu\nu}\right]$$

describing a set of matter fields ϕ_i coupled to gravity. Here S^{grav} is the gravitational action (5.18) and S^m is the action for the matter fields. (The coupling to gravity does not have to be minimal.) The equations of motion for the gravitational field are obtained by varying the action S with respect to $g^{\alpha\beta}$,

$$\frac{\delta S\left[\phi_i, g_{\mu\nu}\right]}{\delta g^{\alpha\beta}} = \frac{\delta}{\delta g^{\alpha\beta}} S^{\text{grav}}\left[g_{\mu\nu}\right] + \frac{\delta}{\delta g^{\alpha\beta}} S^{m}\left[\phi_i, g_{\mu\nu}\right] = 0.$$

We know that the result must be the Einstein equation:

$$R_{\alpha\beta} - \frac{1}{2}g_{\alpha\beta}R = 8\pi G T_{\alpha\beta}, \tag{5.22}$$

where $T_{\alpha\beta}$ is the combined energy-momentum tensor of the fields ϕ_i. As shown in Exercise 5.1 (p. 59), the functional derivative of S^{grav} with respect to $g^{\alpha\beta}$ gives (up to a factor) the LHS of Eq. (5.22). Therefore we expect Eq. (5.22) to coincide with

$$-\frac{\sqrt{-g}}{16\pi G}\left(R_{\alpha\beta} - \frac{1}{2}g_{\alpha\beta}R\right) = -\frac{\delta S^m}{\delta g^{\alpha\beta}}.$$

This requirement immediately leads to the relation

$$T_{\alpha\beta} = \frac{2}{\sqrt{-g}}\frac{\delta S^m}{\delta g^{\alpha\beta}}. \tag{5.23}$$

Equation (5.23) can be viewed as a convenient *definition* of the EMT of matter fields. The resulting tensor $T_{\alpha\beta}$ is symmetric and covariantly conserved (see the next section),

$$T^{;\alpha}_{\alpha\beta} = 0. \tag{5.24}$$

> **Remark:** Strictly speaking, the above derivation shows only that if the Einstein equation follows from the action of matter fields combined with the Einstein-Hilbert action for gravity, then the total EMT of all matter must be given by Eq. (5.23).

Example: The energy-momentum tensor for the field ϕ with the action (5.4) is

$$T_{\alpha\beta}(x) = \frac{2}{\sqrt{-g}}\frac{\delta S}{\delta g^{\alpha\beta}(x)} = \phi_{,\alpha}\phi_{,\beta} - g_{\alpha\beta}\left[\frac{1}{2}g^{\mu\nu}\phi_{,\mu}\phi_{,\nu} - V(\phi)\right].$$

5.3.1 Conservation of the EMT

In this section we show that the tensor $T_{\alpha\beta}$ defined by Eq. (5.23) is covariantly conserved, $T^{;\alpha}_{\alpha\beta} = 0$, as long as the matter action S^m is generally covariant and the field ϕ_i satisfies its equation of motion,

$$\frac{\delta S^m\left[\phi_i\right]}{\delta\phi_i(x)} = 0. \tag{5.25}$$

The requirement (5.25) is natural: in mechanics, the energy is conserved only when the equations of motions are satisfied.

To derive the conservation law, we consider an infinitesimal coordinate transformation

$$x^\alpha \to \tilde{x}^\alpha = x^\alpha + \xi^\alpha(x),$$

where $\xi^\alpha(x)$ is the generator of the transformation. (Note that the transformation depends on the point x.) The matter fields ϕ_i are transformed according to

$$\phi_i(x) \to \tilde{\phi}_i(x) = \phi_i(x) + \delta\phi_i(x),$$

where $\delta\phi_i(x)$ is determined for each field according to its spin. The metric (being a field of spin 2) is transformed according to

$$g^{\alpha\beta} \to \tilde{g}^{\alpha\beta} = g^{\alpha\beta} + \xi^{\alpha;\beta} + \xi^{\beta;\alpha} + O\left(|\xi|^2\right).$$

We know that the total action is invariant under this transformation, therefore the variation δS must vanish:

$$0 = \delta S = \int \frac{\delta S^m}{\delta g^{\alpha\beta}(x)}\left(\xi^{\alpha;\beta} + \xi^{\beta;\alpha}\right)d^4x + \int \frac{\delta S^m}{\delta\phi_i(x)}\delta\phi_i(x)d^4x. \tag{5.26}$$

Since the field ϕ_i satisfies Eq. (5.25), the second term vanishes. Expressing the first term through the tensor $T_{\alpha\beta}$, we get

$$\int T_{\alpha\beta}\xi^{\beta;\alpha}\sqrt{-g}d^4x = \int \left[\left(T_{\alpha\beta}\xi^{\beta}\right)^{;\alpha} - T^{;\alpha}_{\alpha\beta}\xi^{\beta}\right]\sqrt{-g}d^4x$$
$$= -\int T^{;\alpha}_{\alpha\beta}\xi^{\beta}\sqrt{-g}d^4x = 0. \tag{5.27}$$

Here we used the relation (5.9) and assumed that ξ^α vanishes at infinity sufficiently quickly. Since Eq. (5.27) must be satisfied for arbitrary $\xi^\alpha(x)$, we conclude that the conservation law $T^{;\alpha}_{\alpha\beta} = 0$ holds.

> **Remark:** The absence of the covariant volume factor $\sqrt{-g}$ in Eq. (5.26) is not a mistake; the result is nevertheless a covariant quantity. The derivative with respect to ξ^α is calculated using the chain rule, e.g.
>
> $$\delta S^m = \int \frac{\delta S^m}{\delta g^{\alpha\beta}(x)}\delta g^{\alpha\beta}(x)d^4x,$$
>
> and the rule requires a simple integration over x. The correct covariant behavior is supplied by the functionals S^{grav} and S^m.

In a flat spacetime, the laws of energy and momentum conservation follow from the invariance of the action under spacetime translations. In the presence of gravitation the spacetime is curved, so in general the spacetime translations are not a physical symmetry any more. However, the action is covariant with respect to arbitrary coordinate transformations. The corresponding conservation law is the covariant conservation of the EMT, Eq. (5.24). Because of the presence of the covariant derivative in Eq. (5.24), it does not actually express a conservation of energy or momentum of the matter field ϕ_i. That equation would be a conservation law if it had the form$\partial_\mu\left(\sqrt{-g}T^{\mu\nu}\right) = 0$, but instead it can be shown that

$$\partial_\mu\left(\sqrt{-g}T^{\mu\nu}\right) = -\sqrt{-g}\Gamma^\nu_{\mu\lambda}T^{\mu\lambda} \neq 0. \tag{5.28}$$

The energy of the matter fields alone, described by the energy-momentum tensor $T_{\alpha\beta}$, is not necessarily conserved; the gravitational field can change the energy and the momentum of matter.

6 Quantum fields in expanding universe

Summary: Scalar field in a FRW universe. Mode functions. Bogolyubov transformations. Choice of the vacuum state. Particle creation.

The principal task of this chapter is to study the influence of time-dependent gravitational backgrounds on quantum fields. To focus on the essential physics and to avoid cumbersome calculations, we shall consider a free scalar field in a homogeneous and isotropic universe.

6.1 Scalar field in FRW universe

A minimally coupled real scalar field $\phi(x)$ in a curved spacetime is described by the action (5.4),

$$S = \int \sqrt{-g} d^4x \left[\frac{1}{2} g^{\alpha\beta} \phi_{,\alpha} \phi_{,\beta} - V(\phi) \right]. \tag{6.1}$$

The equation of motion for the field ϕ is Eq. (5.7) with $\xi = 0$,

$$g^{\mu\nu} \phi_{,\mu\nu} + \frac{1}{\sqrt{-g}} \left(g^{\mu\nu} \sqrt{-g} \right)_{,\mu} \phi_{,\nu} + \frac{\partial V}{\partial \phi} = 0. \tag{6.2}$$

For a free massive field, one sets $V(\phi) = \frac{1}{2} m^2 \phi^2$.

In this chapter we consider an important class of spacetimes—homogeneous and isotropic Friedmann-Robertson-Walker (FRW) spacetimes with flat spatial sections (called for brevity *flat FRW*) characterized by metrics of the form

$$ds^2 \equiv g_{\mu\nu} dx^\mu dx^\nu = dt^2 - a^2(t) d\mathbf{x}^2, \tag{6.3}$$

where $d\mathbf{x}^2$ is the usual Euclidean metric and $a(t)$ is the scale factor. Note that it is only the three-dimensional spatial sections which are flat; the four-dimensional geometry of such spacetimes is usually curved.

A flat FRW spacetime is a conformally flat spacetime (this notion was discussed in Sec. 5.1.3). To explicitly transform the metric (6.3) into a conformally flat form, we replace the coordinate t by the *conformal time* η,

$$\eta(t) \equiv \int_{t_0}^{t} \frac{dt}{a(t)},$$

where t_0 is an arbitrary constant. The scale factor $a(t)$ expressed through the new variable η is denoted by $a(\eta)$. In the coordinates $(\mathbf{x}, \eta)$ the line element takes the form

$$ds^2 = a^2(\eta)\left[d\eta^2 - d\mathbf{x}^2\right], \tag{6.4}$$

so the metric tensor is $g_{\mu\nu} = a^2\eta_{\mu\nu}$, $g^{\mu\nu} = a^{-2}\eta^{\mu\nu}$, and we have $\sqrt{-g} = a^4$. The field equation (6.2) in the coordinates $(\mathbf{x}, \eta)$ with $V(\phi) = \frac{1}{2}m^2\phi^2$ becomes

$$\phi'' + 2\frac{a'}{a}\phi' - \Delta\phi + m^2a^2\phi = 0, \tag{6.5}$$

where the prime $'$ denotes derivatives with respect to η. It is convenient to introduce the auxiliary field $\chi \equiv a(\eta)\phi$ and to rewrite Eq. (6.5) as

$$\chi'' - \Delta\chi + \left(m^2a^2 - \frac{a''}{a}\right)\chi = 0. \tag{6.6}$$

Exercise 6.1
Derive Eq. (6.6) from Eq. (6.5).

Comparing Eqs. (6.6) and (4.7), we find that the field $\chi(x)$ obeys the usual equation of motion of a field in the Minkowski spacetime, except for the time-dependent *effective mass*

$$m_{\text{eff}}^2(\eta) \equiv m^2a^2 - \frac{a''}{a}. \tag{6.7}$$

The action (6.1) can be rewritten in terms of the field χ,

$$S = \frac{1}{2}\int d^3\mathbf{x}\, d\eta \left(\chi'^2 - (\nabla\chi)^2 - m_{\text{eff}}^2(\eta)\chi^2\right), \tag{6.8}$$

and is analogous to the action (4.4).

Exercise 6.2
Derive the action (6.8) from Eq. (6.1) with $V(\phi) = \frac{1}{2}m^2\phi^2$ and the metric (6.4).

Thus the dynamics of a scalar field ϕ in a flat FRW spacetime is mathematically equivalent to the dynamics of the auxiliary field χ in the Minkowski spacetime. All information about the influence of the gravitational field on ϕ is encapsulated in the time-dependent mass $m_{\text{eff}}(\eta)$ defined by Eq. (6.7). Note that the action (6.8) for the field χ is explicitly time-dependent, so the energy of the field χ is generally not conserved. In quantum theory this leads to the possibility of particle creation; the energy for new particles is supplied by the gravitational field.

6.1.1 Mode functions

Expanding the field χ in Fourier modes,

$$\chi(\mathbf{x}, \eta) = \int \frac{d^3\mathbf{k}}{(2\pi)^{3/2}}\chi_{\mathbf{k}}(\eta)e^{i\mathbf{k}\cdot\mathbf{x}}, \tag{6.9}$$

we obtain from Eq. (6.6) the decoupled equations of motion for the modes $\chi_{\mathbf{k}}(\eta)$,

$$\chi''_{\mathbf{k}} + \left[k^2 + m^2 a^2(\eta) - \frac{a''}{a}\right] \chi_{\mathbf{k}} \equiv \chi''_{\mathbf{k}} + \omega_k^2(\eta)\chi_{\mathbf{k}} = 0. \tag{6.10}$$

> **Remark: other spacetimes.** The decoupling of the field modes hinges on the separation of the time coordinate in the Klein-Gordon equation and on the expansion of the field χ through the eigenfunctions of the spatial Laplace operator at a fixed time. In flat space, these eigenfunctions are $\exp(i\mathbf{kx})$; another solvable case is a static, spherically symmetric spacetime with a metric $g_{\alpha\beta}(r)$ that depends only on the radial coordinate r. However, the field equations in a general spacetime are not separable. In such cases, the mode decoupling cannot be performed explicitly and quantization is difficult.

We now need a few mathematical facts about time-dependent oscillator equations such as Eq. (6.10),

$$\ddot{x} + \omega^2(t)x = 0. \tag{6.11}$$

This equation has a two-dimensional space of solutions. Any two linearly independent solutions $x_1(t)$ and $x_2(t)$ are a basis in that space. The expression

$$W[x_1, x_2] \equiv \dot{x}_1 x_2 - x_1 \dot{x}_2$$

is called the *Wronskian* of the two functions $x_1(t)$ and $x_2(t)$. Standard properties of the Wronskian are summarized in the following exercise.

> **Exercise 6.3**
> Show that the Wronskian $W[x_1, x_2]$ is time-independent if $x_{1,2}(t)$ satisfy Eq. (6.11). Prove that $W[x_1, x_2] \neq 0$ if and only if $x_1(t)$ and $x_2(t)$ are two linearly independent solutions.

If $\{x_1(t), x_2(t)\}$ is a basis of solutions, it is convenient to define the complex function $v(t) \equiv x_1(t) + ix_2(t)$. Then $v(t)$ and $v^*(t)$ are linearly independent and form a basis in the space of *complex* solutions of Eq. (6.11). It is easy to check that

$$\mathrm{Im}\,(\dot{v}v^*) = \frac{\dot{v}v^* - \dot{v}^*v}{2i} = \frac{1}{2i}W[v, v^*] = -W[x_1, x_2] \neq 0,$$

and thus the quantity $\mathrm{Im}\,(\dot{v}v^*)$ is a nonzero real constant. If $v(t)$ is multiplied by a constant, $v(t) \to \lambda v(t)$, the Wronskian $W[v, v^*]$ changes by the factor $|\lambda|^2$, therefore we may normalize $v(t)$ to a prescribed value of $\mathrm{Im}\,(\dot{v}v^*)$ by choosing the constant λ.

A complex solution $v(t)$ of Eq. (6.11) is called a *mode function* if $v(t)$ is normalized by the condition $\mathrm{Im}\,(\dot{v}v^*) = 1$. It follows from Exercise 6.3 that any solution $v(t)$ normalized by $\mathrm{Im}\,(\dot{v}v^*) = 1$ is necessarily such that $v(t)$ and $v^*(t)$ are a basis of linearly independent complex solutions of Eq. (6.11).

> **Remark: How to find a mode function.** There exist infinitely many mode functions for Eq. (6.18). For instance, the solution $v(t)$ with the initial conditions $v(t_0) = 1$, $\dot{v}(t_0) = i$ at some $t = t_0$ is a mode function since it satisfies the normalization condition $\mathrm{Im}\,(\dot{v}v^*) = 1$. If exact solutions of Eq. (6.11) are not available in an analytic form, mode functions $v(t)$ must be found by approximate methods (e.g. numerically).

If some complex solution $f(t)$ of Eq. (6.11) is known, one can compute the Wronskian of f and f^* which is always a pure imaginary number. If $W[f, f^*] = 0$, the solution $f(t)$ cannot be used to produce a mode function. If, on the other hand, $W[f, f^*] \equiv 2i\lambda \neq 0$, then a mode function is obtained from $f(t)$ by an appropriate rescaling, namely $v(t) = f\lambda^{-1/2}$ if $\lambda > 0$ and $v(t) = f^* |\lambda|^{-1/2}$ if $\lambda < 0$. There still remains the freedom of multiplying $v(t)$ by a phase $e^{i\alpha}$ with a real constant α.

6.1.2 Mode expansions

All modes $\chi_{\mathbf{k}}(\eta)$ with equal $|\mathbf{k}| = k$ are complex solutions of the same equation (6.10). If a mode function $v_k(\eta)$ of that equation is chosen, the general solution $\chi_{\mathbf{k}}(\eta)$ can be expressed as a linear combination of v_k and v_k^* as

$$\chi_{\mathbf{k}}(\eta) = \frac{1}{\sqrt{2}} \left[a_{\mathbf{k}}^- v_k^*(\eta) + a_{-\mathbf{k}}^+ v_k(\eta) \right], \tag{6.12}$$

where $a_{\mathbf{k}}^{\pm}$ are complex constants of integration that depend on the vector $\mathbf{k}$ (but not on η). The index $-\mathbf{k}$ in the second term of Eq. (6.12) and the factor $\frac{1}{\sqrt{2}}$ are chosen for later convenience.

Since χ is real, $\chi_{\mathbf{k}}^* = \chi_{-\mathbf{k}}$ and it follows from Eq. (6.12) that $a_{\mathbf{k}}^+ = \left(a_{\mathbf{k}}^-\right)^*$. Combining Eqs. (6.9) and (6.12), we find

$$\begin{aligned} \chi(\mathbf{x}, \eta) &= \int \frac{d^3\mathbf{k}}{(2\pi)^{3/2}} \frac{1}{\sqrt{2}} \left[a_{\mathbf{k}}^- v_k^*(\eta) + a_{-\mathbf{k}}^+ v_k(\eta) \right] e^{i\mathbf{k}\cdot\mathbf{x}} \\ &= \int \frac{d^3\mathbf{k}}{(2\pi)^{3/2}} \frac{1}{\sqrt{2}} \left[a_{\mathbf{k}}^- v_k^*(\eta) e^{i\mathbf{k}\cdot\mathbf{x}} + a_{\mathbf{k}}^+ v_k(\eta) e^{-i\mathbf{k}\cdot\mathbf{x}} \right]. \end{aligned} \tag{6.13}$$

Note that the integration variable $\mathbf{k}$ was changed ($\mathbf{k} \to -\mathbf{k}$) in the second term of Eq. (6.13) to make the integrand a manifestly real expression.

The relation (6.13) is called the *mode expansion* of the field $\chi(\mathbf{x}, \eta)$ w.r.t. the mode functions $v_k(\eta)$. At this point the choice of the mode functions is still arbitrary.

The coefficients $a_{\mathbf{k}}^{\pm}$ are easily expressed through $\chi_{\mathbf{k}}(\eta)$ and $v_k(\eta)$:

$$a_{\mathbf{k}}^- = \sqrt{2} \frac{v_k' \chi_{\mathbf{k}} - v_k \chi_{\mathbf{k}}'}{v_k' v_k^* - v_k v_k^{*\prime}} = \sqrt{2} \frac{W[v_k, \chi_{\mathbf{k}}]}{W[v_k, v_k^*]}; \quad a_{\mathbf{k}}^+ = \left(a_{\mathbf{k}}^-\right)^*. \tag{6.14}$$

Note that the numerators and denominators in Eq. (6.14) are time-independent since they are Wronskians of solutions of the same oscillator equation.

Remark: isotropy of mode functions. In Eq. (6.12) we expressed all $\chi_{\mathbf{k}}(\eta)$ with $|\mathbf{k}| = k$ through the *same* mode function $v_k(\eta)$, written with the scalar index k. We call this the *isotropic* choice of the mode functions $v_k(\eta)$. This convenient simplification is possible because ω_k depends only on $k = |\mathbf{k}|$. (The modes $\chi_{\mathbf{k}}$ and the coefficients $a_{\mathbf{k}}^{\pm}$ must have the vector index $\mathbf{k}$.) Of course, the mode functions $v_{\mathbf{k}}(\eta)$ can also be chosen anisotropically; below we shall discuss this in more detail.

6.2 Quantization of scalar field

The field $\chi(x)$ can be quantized in the standard fashion by introducing the equal-time commutation relations,

$$[\hat{\chi}(\mathbf{x},\eta),\,\hat{\pi}(\mathbf{y},\eta)] = i\delta(\mathbf{x}-\mathbf{y}), \tag{6.15}$$

where $\hat{\pi} = d\hat{\chi}/d\eta \equiv \hat{\chi}'$ is the canonical momentum. The quantum Hamiltonian is

$$\hat{H}(\eta) = \frac{1}{2}\int d^3\mathbf{x}\left(\hat{\pi}^2 + (\nabla\hat{\chi})^2 + m_{\rm eff}^2(\eta)\hat{\chi}^2\right). \tag{6.16}$$

Then the modes $\hat{\chi}_{\mathbf{k}}(t)$ and the creation and annihilation operators $\hat{a}^{\pm}_{\mathbf{k}}$ are defined as in chapter 4.

However, a quicker way to quantize the field is based on the mode expansion (6.13) which can be used for quantum fields in the same way as for classical fields. The mode expansion for the field operator $\hat{\chi}$ is found by replacing the constants $a^{\pm}_{\mathbf{k}}$ in Eq. (6.13) by time-independent operators $\hat{a}^{\pm}_{\mathbf{k}}$,

$$\hat{\chi}(\mathbf{x},\eta) = \int \frac{d^3\mathbf{k}}{(2\pi)^{3/2}}\frac{1}{\sqrt{2}}\left(e^{i\mathbf{k}\cdot\mathbf{x}}v_k^*(\eta)\hat{a}^-_{\mathbf{k}} + e^{-i\mathbf{k}\cdot\mathbf{x}}v_k(\eta)\hat{a}^+_{\mathbf{k}}\right), \tag{6.17}$$

where $v_k(\eta)$ are mode functions obeying the equations

$$v_k'' + \omega_k^2(\eta)v_k = 0, \quad \omega_k(\eta) \equiv \sqrt{k^2 + m_{\rm eff}^2(\eta)}. \tag{6.18}$$

The operators $\hat{a}^{\pm}_{\mathbf{k}}$ satisfy the usual commutation relations for creation and annihilation operators,

$$\left[\hat{a}^-_{\mathbf{k}},\,\hat{a}^+_{\mathbf{k}'}\right] = \delta(\mathbf{k}-\mathbf{k}'), \quad \left[\hat{a}^-_{\mathbf{k}},\,\hat{a}^-_{\mathbf{k}'}\right] = \left[\hat{a}^+_{\mathbf{k}},\,\hat{a}^+_{\mathbf{k}'}\right] = 0. \tag{6.19}$$

The next exercise shows that the commutation relations (6.15) and (6.19) are consistent if the mode functions $v_k(\eta)$ are normalized by

$$\mathrm{Im}\,(v_k'v_k^*) = \frac{v_k'v_k^* - v_kv_k'^*}{2i} \equiv \frac{W[v_k,v_k^*]}{2i} = 1. \tag{6.20}$$

Therefore, quantization of the field $\hat{\chi}$ can be accomplished by postulating the mode expansion (6.17), the commutation relations (6.19) and the normalization (6.20). (The choice of the mode functions $v_{\mathbf{k}}(\eta)$ will be made later on.) The technique of mode expansions is a shortcut to quantization which avoids introducing the canonical momentum $\hat{\pi}(\mathbf{x},\eta)$ explicitly.[1]

[1] One can also show, by using the operator analog of Eq. (6.14), that the commutation relations (6.15) follow from (6.19) and (6.20).

Exercise 6.4
Use the mode expansion of the scalar field in the form

$$\hat{\chi}(\mathbf{x},\eta) = \frac{1}{\sqrt{2}} \int \frac{d^3\mathbf{k}}{(2\pi)^{3/2}} \left[e^{i\mathbf{k}\cdot\mathbf{x}} v_{\mathbf{k}}^*(\eta) \hat{a}_{\mathbf{k}}^- + e^{-i\mathbf{k}\cdot\mathbf{x}} v_{\mathbf{k}}(\eta) \hat{a}_{\mathbf{k}}^+ \right] \tag{6.21}$$

to show that Eqs. (6.15) and (6.19) require the normalization condition

$$v_{\mathbf{k}}' v_{\mathbf{k}}^* - v_{\mathbf{k}} v_{\mathbf{k}}'^* = 2i. \tag{6.22}$$

Isotropy of modes is *not* to be assumed (the mode functions $v_{\mathbf{k}}$ have the vector index $\mathbf{k}$).

The mode expansion (6.17) can be visualized as the general solution of the field equation (6.6), where the operators $\hat{a}_{\mathbf{k}}^{\pm}$ are integration constants. The mode expansion can also be viewed as a *definition* of the operators $\hat{a}_{\mathbf{k}}^{\pm}$ through the field operator $\hat{\chi}(\mathbf{x},\eta)$. Explicit formulae relating $\hat{a}_{\mathbf{k}}^{\pm}$ to $\hat{\chi}$ and $\hat{\pi} \equiv \hat{\chi}'$ are analogous to Eq. (6.14). Clearly, the definition of $\hat{a}_{\mathbf{k}}^{\pm}$ depends on the choice of the mode functions $v_k(\eta)$.

Remark: complex scalar field. If χ were a complex field, then $(\chi_{\mathbf{k}})^* \neq \chi_{-\mathbf{k}}$ and Eq. (6.12) would give $\left(a_{\mathbf{k}}^-\right)^* \neq a_{\mathbf{k}}^+$. In that case we cannot use Eq. (6.12) but instead introduce two sets of creation and annihilation operators, e.g. $\hat{a}_{\mathbf{k}}^{\pm}$ and $\hat{b}_{\mathbf{k}}^{\pm}$, satisfying $(\hat{a}_{\mathbf{k}}^-)^\dagger = \hat{a}_{\mathbf{k}}^+$ and $(\hat{b}_{\mathbf{k}}^-)^\dagger = \hat{b}_{\mathbf{k}}^+$, and the mode expansion would be

$$\hat{\chi}(\mathbf{x},\eta) = \int \frac{d^3\mathbf{k}}{(2\pi)^{3/2}} \frac{1}{\sqrt{2}} \left(e^{i\mathbf{k}\cdot\mathbf{x}} v_k^*(\eta) \hat{a}_{\mathbf{k}}^- + e^{-i\mathbf{k}\cdot\mathbf{x}} v_k(\eta) \hat{b}_{\mathbf{k}}^+ \right).$$

This agrees with the picture of a complex field as a set of two real fields. The operators $\hat{a}_{\mathbf{k}}^+$ and $\hat{b}_{\mathbf{k}}^+$ describe the creation of respectively particles and antiparticles. (A real field describes particles that are their own antiparticles.)

6.2.1 The vacuum state and particle states

Once the operators $\hat{a}_{\mathbf{k}}^{\pm}$ are determined, the vacuum state $|0\rangle$ is defined as the eigenstate of all annihilation operators $\hat{a}_{\mathbf{k}}^-$ with eigenvalue 0, i.e. $\hat{a}_{\mathbf{k}}^- |0\rangle = 0$ for all $\mathbf{k}$. An excited state $|m_{\mathbf{k}_1}, n_{\mathbf{k}_2}, ...\rangle$ with the occupation numbers $m, n, ...$ in the modes $\chi_{\mathbf{k}_1}$, $\chi_{\mathbf{k}_2}$, ..., is constructed by

$$|m_{\mathbf{k}_1}, n_{\mathbf{k}_2}, ...\rangle \equiv \frac{1}{\sqrt{m!n!...}} \left[\left(\hat{a}_{\mathbf{k}_1}^+\right)^m \left(\hat{a}_{\mathbf{k}_2}^+\right)^n ... \right] |0\rangle . \tag{6.23}$$

We write $|0\rangle$ instead of $|0_{\mathbf{k}_1}, 0_{\mathbf{k}_2}, ...\rangle$ for brevity. An arbitrary quantum state $|\psi\rangle$ is a linear combination of these states,

$$|\psi\rangle = \sum_{m,n,...} C_{mn...} |m_{\mathbf{k}_1}, n_{\mathbf{k}_2}, ...\rangle .$$

If the field is in the state $|\psi\rangle$, the probability for measuring the occupation number m in the mode $\chi_{\mathbf{k}_1}$, the number n in the mode $\chi_{\mathbf{k}_2}$, etc., is $|C_{mn...}|^2$.

Let us now comment on the role of the mode functions. Complex solutions $v_k(\eta)$ of a second-order differential equation (6.18) with one normalization condition (6.20)

are parametrized by one complex parameter. Multiplying $v_k(\eta)$ by a constant phase $e^{i\alpha}$ introduces an extra phase $e^{\pm i\alpha}$ in the operators $\hat{a}_k^{\pm}$, which can be compensated by a constant phase factor $e^{i\alpha}$ in the state vectors $|0\rangle$ and $|m_{\mathbf{k}_1}, n_{\mathbf{k}_2}, ...\rangle$. There remains one real free parameter that distinguishes physically inequivalent mode functions. With each possible choice of the functions $v_k(\eta)$, the operators $\hat{a}_{\mathbf{k}}^{\pm}$ and consequently the vacuum state and particle states are different. As long as the mode functions satisfy Eqs. (6.18) and (6.20), the commutation relations (6.19) hold and thus the operators $\hat{a}_{\mathbf{k}}^{\pm}$ formally resemble the creation and annihilation operators for particle states. However, we do not yet know whether the operators $\hat{a}_{\mathbf{k}}^{\pm}$ obtained with some choice of $v_k(\eta)$ actually correspond to physical particles and whether the quantum state $|0\rangle$ describes the physical vacuum. The correct commutation relations alone do not guarantee the validity of the physical interpretation of the operators $\hat{a}_{\mathbf{k}}^{\pm}$ and of the state $|0\rangle$. For this interpretation to be valid, the mode functions must be *appropriately selected*; we postpone the consideration of this important issue until Sec. 6.3 below. In the rest of this section we shall formally study the consequences of choosing several sets of mode functions to quantize the field ϕ.

6.2.2 Bogolyubov transformations

Suppose two sets of isotropic mode functions $u_k(\eta)$ and $v_k(\eta)$ are chosen. Since u_k and u_k^* are a basis, the function v_k is a linear combination of u_k and u_k^*,

$$v_k^*(\eta) = \alpha_k u_k^*(\eta) + \beta_k u_k(\eta), \tag{6.24}$$

with η-independent complex coefficients α_k and β_k. If both sets $v_k(\eta)$ and $u_k(\eta)$ are normalized by Eq. (6.20), it follows that the coefficients α_k and β_k satisfy

$$|\alpha_k|^2 - |\beta_k|^2 = 1. \tag{6.25}$$

In particular, $|\alpha_k| \geq 1$.

Exercise 6.5
Derive Eq. (6.25).

Using the mode functions $u_k(\eta)$ instead of $v_k(\eta)$, one obtains an alternative mode expansion which defines another set $\hat{b}_{\mathbf{k}}^{\pm}$ of creation and annihilation operators,

$$\hat{\chi}(\mathbf{x}, \eta) = \int \frac{d^3\mathbf{k}}{(2\pi)^{3/2}} \frac{1}{\sqrt{2}} \left(e^{i\mathbf{k}\cdot\mathbf{x}} u_k^*(\eta) \hat{b}_{\mathbf{k}}^- + e^{-i\mathbf{k}\cdot\mathbf{x}} u_k(\eta) \hat{b}_{\mathbf{k}}^+ \right). \tag{6.26}$$

The expansions (6.17) and (6.26) express the same field $\hat{\chi}(\mathbf{x}, \eta)$ through two different sets of functions, so the $\mathbf{k}$-th Fourier components of these expansions must agree,

$$e^{i\mathbf{k}\cdot\mathbf{x}} \left[u_k^*(\eta) \hat{b}_{\mathbf{k}}^- + u_k(\eta) \hat{b}_{-\mathbf{k}}^+ \right] = e^{i\mathbf{k}\cdot\mathbf{x}} \left[v_k^*(\eta) \hat{a}_{\mathbf{k}}^- + v_k(\eta) \hat{a}_{-\mathbf{k}}^+ \right].$$

A substitution of v_k through u_k using Eq. (6.24) gives the following relation between the operators $\hat{b}_{\mathbf{k}}^{\pm}$ and $\hat{a}_{\mathbf{k}}^{\pm}$:

$$\hat{b}_{\mathbf{k}}^- = \alpha_k \hat{a}_{\mathbf{k}}^- + \beta_k^* \hat{a}_{-\mathbf{k}}^+, \quad \hat{b}_{\mathbf{k}}^+ = \alpha_k^* \hat{a}_{\mathbf{k}}^+ + \beta_k \hat{a}_{-\mathbf{k}}^-. \tag{6.27}$$

The relation (6.27) and the complex coefficients α_k, β_k are called respectively the *Bogolyubov transformation* and the *Bogolyubov coefficients*.[2]

The old operators $\hat{a}^{\pm}_{\mathbf{k}}$ are expressed through the new operators $\hat{b}^{\pm}_{\mathbf{k}}$ in a similar way.

Exercise 6.6

Suppose that the two sets $\hat{a}^{\pm}_{\mathbf{k}}$, $\hat{b}^{\pm}_{\mathbf{k}}$ of creation and annihilation operators for a real scalar field are related by the Bogolyubov transformation

$$\hat{b}^{-}_{\mathbf{k}} = \alpha_{\mathbf{k}}\hat{a}^{-}_{\mathbf{k}} + \beta^{*}_{-\mathbf{k}}\hat{a}^{+}_{-\mathbf{k}}, \quad \hat{b}^{+}_{\mathbf{k}} = \alpha^{*}_{\mathbf{k}}\hat{a}^{+}_{\mathbf{k}} + \beta_{-\mathbf{k}}\hat{a}^{-}_{-\mathbf{k}}. \tag{6.28}$$

Isotropy of Bogolyubov coefficients is not assumed, so $\alpha_{\mathbf{k}}$ and $\beta_{\mathbf{k}}$ depend on the vector $\mathbf{k}$. Express the operators $\hat{a}^{\pm}_{\mathbf{k}}$ through $\hat{b}^{\pm}_{\mathbf{k}}$.

Hint: First show that for a real scalar field, $\alpha_{\mathbf{k}} = \alpha_{-\mathbf{k}}$ and $\beta_{\mathbf{k}} = \beta_{-\mathbf{k}}$.

Remark: Quantum states defined by an exponential of a quadratic combination of creation operators acting on the vacuum, as in Eq. (6.29), are called *squeezed vacuum* states. The b-vacuum is therefore a squeezed vacuum state with respect to the a-vacuum. Similarly, the a-vacuum is a squeezed b-vacuum state.

The two sets of annihilation operators $\hat{a}^{-}_{\mathbf{k}}$ and $\hat{b}^{-}_{\mathbf{k}}$ define the corresponding vacua $\left|{}_{(a)}0\right\rangle$ and $\left|{}_{(b)}0\right\rangle$ which we call the "a-vacuum" and the "b-vacuum." Two parallel sets of excited states are built from the two vacua using Eq. (6.23). We refer to these states as a-particle and b-particle states. So far the physical interpretation of the a- and b-particles remains unspecified. In chapters 7-9 we shall apply this formalism to study specific physical effects and the interpretation of excited states corresponding to various mode functions will be fully explained.

The b-vacuum can be expressed as a superposition of a-particle states (Exercise 6.7):

$$\left|{}_{(b)}0\right\rangle = \left[\prod_{\mathbf{k}} \frac{1}{|\alpha_{\mathbf{k}}|^{1/2}} \exp\left(-\frac{\beta^{*}_{\mathbf{k}}}{2\alpha_{\mathbf{k}}}\hat{a}^{+}_{\mathbf{k}}\hat{a}^{+}_{-\mathbf{k}}\right)\right] \left|{}_{(a)}0\right\rangle . \tag{6.29}$$

A similar relation expresses the a-vacuum as a linear combination of b-particle states. From Eq. (6.29) it is clear that the b-vacuum state contains a-particles in pairs of opposite momentum $\mathbf{k}$ and $-\mathbf{k}$.

Exercise 6.7

The b-vacuum state $\left|{}_{(b)}0_{\mathbf{k},-\mathbf{k}}\right\rangle$ of the mode $\chi_{\mathbf{k}}$ is defined by

$$\hat{b}^{-}_{\mathbf{k}}\left|{}_{(b)}0_{\mathbf{k},-\mathbf{k}}\right\rangle = 0, \quad \hat{b}^{-}_{-\mathbf{k}}\left|{}_{(b)}0_{\mathbf{k},-\mathbf{k}}\right\rangle = 0.$$

Show that the b-vacuum is expanded through a-particle states $\left|{}_{(a)}m_{\mathbf{k}}, n_{-\mathbf{k}}\right\rangle$ as

$$\left|{}_{(b)}0_{\mathbf{k},-\mathbf{k}}\right\rangle = \frac{1}{|\alpha_{\mathbf{k}}|}\sum_{n=0}^{\infty}\left(-\frac{\beta^{*}_{\mathbf{k}}}{\alpha_{\mathbf{k}}}\right)^{n}\left|{}_{(a)}n_{\mathbf{k}}, n_{-\mathbf{k}}\right\rangle$$

and derive Eq. (6.29). The Bogolyubov coefficients $\alpha_{\mathbf{k}}$ and $\beta_{\mathbf{k}}$ in Eq. (6.28) are known.

Note that the b-vacuum state (6.29) is normalized by the infinite product $\prod_{\mathbf{k}}|\alpha_{\mathbf{k}}|$. This product converges only if $|\alpha_{\mathbf{k}}|$ rapidly tends to 1 at large $|\mathbf{k}|$, or more precisely if $|\beta_{\mathbf{k}}|^2 \to 0$ faster than k^{-3} at $k \to \infty$. If this is not the case, the vacuum state $\left|{}_{(b)}0\right\rangle$ is not normalizable and the Bogolyubov transformation is not well-defined.

[2] The prononciation is close to the American "bogo-lube-of" with the third syllable stressed.

Computing the Bogolyubov coefficients

To determine the Bogolyubov coefficients α_k and β_k, it is necessary to know the mode functions $v_k(\eta)$ and $u_k(\eta)$ and their derivatives at *only one* value of η, say $\eta = \eta_0$. From Eq. (6.24) and its derivative at $\eta = \eta_0$, we find

$$\begin{aligned} v_k^*(\eta_0) &= \alpha_k u_k^*(\eta_0) + \beta_k u_k(\eta_0)\,, \\ v_k^{*\prime}(\eta_0) &= \alpha_k u_k^{*\prime}(\eta_0) + \beta_k u_k'(\eta_0)\,. \end{aligned}$$

This system of equations can be solved for α_k and β_k using Eq. (6.20):

$$\alpha_k = \left.\frac{u_k' v_k^* - u_k v_k^{*\prime}}{2i}\right|_{\eta_0}, \quad \beta_k^* = \left.\frac{u_k' v_k - u_k v_k'}{2i}\right|_{\eta_0}. \tag{6.30}$$

These relations hold at any time η_0 (note that the numerators are Wronskians and thus are time-independent). For instance, knowing only the asymptotics of $v_k(\eta)$ and $u_k(\eta)$ at $\eta \to -\infty$ would suffice to compute α_k and β_k.

> **Remark: Anisotropic mode expansions.** In this book we always use isotropic mode functions $v_k(\eta)$ because in all cases under consideration the modes $\chi_{\mathbf{k}}$ with constant $|\mathbf{k}|$ satisfy the same equation. An anisotropic choice of mode functions would be an unnecessary complication. However, anisotropic mode functions are needed in some cases, so it is useful to know which relations depend on the assumption of isotropy. Here we list the relevant changes to the formalism for anisotropic mode functions. Note that the results of Exercises 6.4 to 6.8 below are valid without the assumption of isotropy.
>
> For a real scalar field χ with anisotropic mode functions $v_{\mathbf{k}}(\eta)$, the relation (6.12) is replaced by
>
> $$\chi_{\mathbf{k}}(\eta) = \frac{1}{\sqrt{2}}\left[a_{\mathbf{k}}^- v_{\mathbf{k}}^*(\eta) + a_{-\mathbf{k}}^+ v_{\mathbf{k}}(\eta)\right]. \tag{6.31}$$
>
> The identity $v_{\mathbf{k}}(\eta) = v_{-\mathbf{k}}(\eta)$ must still hold, as follows from the relations $(\chi_{\mathbf{k}})^* = \chi_{-\mathbf{k}}$, $(a_{\mathbf{k}}^-)^* = a_{\mathbf{k}}^+$ and Eq. (6.31). [For a complex field, $(\chi_{\mathbf{k}})^* \neq \chi_{-\mathbf{k}}$ and mode functions may be chosen with $v_{\mathbf{k}}(\eta) \neq v_{-\mathbf{k}}(\eta)$.] The mode expansion is Eq. (6.21). The coefficients $\alpha_{\mathbf{k}}$, $\beta_{\mathbf{k}}$ that relate $v_{\mathbf{k}}(\eta)$ to $u_{\mathbf{k}}(\eta)$ also depend on the vector $\mathbf{k}$, namely $v_{\mathbf{k}}^* = \alpha_{\mathbf{k}} u_{\mathbf{k}}^* + \beta_{\mathbf{k}}$. The Bogolyubov transformation is given by Eq. (6.28). The normalization condition is unchanged, $|\alpha_{\mathbf{k}}|^2 - |\beta_{\mathbf{k}}|^2 = 1$. The formulae expressing the Bogolyubov coefficients through the mode functions at a fixed time $\eta = \eta_0$ are the same as Eq. (6.30) but with the vector index $\mathbf{k}$.

6.2.3 Mean particle number

Here we calculate the mean number of b-particles of the mode $\chi_{\mathbf{k}}$ in the a-vacuum state. The expectation value of the b-particle number operator $\hat{N}_{\mathbf{k}}^{(b)} = \hat{b}_{\mathbf{k}}^+ \hat{b}_{\mathbf{k}}^-$ in the state $\left|{}_{(a)}0\right\rangle$ is found using Eq. (6.27):

$$\begin{aligned} \left\langle {}_{(a)}0\right| \hat{N}^{(b)} \left|{}_{(a)}0\right\rangle &= \left\langle {}_{(a)}0\right| \hat{b}_{\mathbf{k}}^+ \hat{b}_{\mathbf{k}}^- \left|{}_{(a)}0\right\rangle \\ &= \left\langle {}_{(a)}0\right| \left(\alpha_k^* \hat{a}_{\mathbf{k}}^+ + \beta_k \hat{a}_{-\mathbf{k}}^-\right)\left(\alpha_k \hat{a}_{\mathbf{k}}^- + \beta_k^* \hat{a}_{-\mathbf{k}}^+\right) \left|{}_{(a)}0\right\rangle \\ &= \left\langle {}_{(a)}0\right| \left(\beta_k \hat{a}_{-\mathbf{k}}^-\right)\left(\beta_k^* \hat{a}_{-\mathbf{k}}^+\right) \left|{}_{(a)}0\right\rangle = |\beta_k|^2\, \delta^{(3)}(0). \end{aligned} \tag{6.32}$$

The divergent factor $\delta^{(3)}(0)$ is a consequence of considering an infinite spatial volume. As discussed in Sec. 4.2 (p. 48), this divergent factor would be replaced by the box volume V if we quantized the field in a finite box. Therefore we can remove this factor and obtain the mean *density* of b-particles in the mode $\chi_{\mathbf{k}}$,

$$n_k = |\beta_k|^2 . \tag{6.33}$$

The Bogolyubov coefficient β_k is dimensionless and the density n_k is the mean number of particles per spatial volume $d^3\mathbf{x}$ and per wave number $d^3\mathbf{k}$, so that $\int n_k d^3\mathbf{k}\, d^3\mathbf{x}$ is the (dimensionless) total mean number of b-particles in the a-vacuum state.

The combined mean density of particles in all modes is $\int d^3\mathbf{k}\, |\beta_k|^2$. This integral is finite if $|\beta_k|^2 \to 0$ faster than k^{-3} at large k. Note that the same condition guarantees the normalizability of the b-vacuum in Eq. (6.29). In other words, the Bogolyubov transformation is well-defined only if the the total particle density is finite.

6.3 Choice of vacuum

In the theory developed so far, the particle interpretation depends on the choice of the mode functions. For instance, the a-vacuum $\left|{}_{(a)}0\right\rangle$ defined above is a state without a-particles but with b-particle density n_k in each mode $\chi_{\mathbf{k}}$. A natural question to ask is whether the a-particles or the b-particles are the correct representation of the observable particles. The problem at hand is to determine the mode functions that describe the "actual" physical vacuum and particles.

6.3.1 The instantaneous lowest-energy state

In chapter 4 the vacuum state was defined as the eigenstate with the lowest energy. However, in the present case the Hamiltonian (6.16) explicitly depends on time and thus does not have time-independent eigenstates that could serve as the vacuum.

One possible prescription for the vacuum state is to select a particular moment of time, $\eta = \eta_0$, and to define the vacuum $\left|{}_{\eta_0}0\right\rangle$ as the lowest-energy eigenstate of the *instantaneous* Hamiltonian $\hat{H}(\eta_0)$. To obtain the mode functions that correspond to the vacuum $\left|{}_{\eta_0}0\right\rangle$, we first compute the expectation value $\left\langle {}_{(v)}0\right| \hat{H}(\eta_0) \left|{}_{(v)}0\right\rangle$ in the vacuum state $\left|{}_{(v)}0\right\rangle$ determined by arbitrarily chosen mode functions $v_k(\eta)$. Then we shall minimize that expectation value with respect to all possible choices of $v_k(\eta)$. (A standard result in linear algebra is that the minimization of $\langle x| \hat{A} |x\rangle$ with respect to all normalized vectors $|x\rangle$ is equivalent to finding the eigenvector $|x\rangle$ of the operator $\hat{A}$ with the smallest eigenvalue.)

We start with Eq. (6.21) with so far unspecified mode functions $v_{\mathbf{k}}(\eta)$ that depend on the vector $\mathbf{k}$. (Isotropy of mode functions is not assumed in this calculation.) The mode functions $v_{\mathbf{k}}(\eta)$ define the operators $\hat{a}^{\pm}_{\mathbf{k}}$ through which the Hamiltonian (6.16) is expressed as follows (see Exercise 6.8):

$$\hat{H}(\eta) = \frac{1}{4}\int d^3\mathbf{k} \left[\hat{a}^-_{\mathbf{k}}\hat{a}^-_{-\mathbf{k}}F^*_{\mathbf{k}} + \hat{a}^+_{\mathbf{k}}\hat{a}^+_{-\mathbf{k}}F_{\mathbf{k}} + \left(2\hat{a}^+_{\mathbf{k}}\hat{a}^-_{\mathbf{k}} + \delta^{(3)}(0)\right) E_{\mathbf{k}}\right], \tag{6.34}$$

where the coefficients $F_{\mathbf{k}}$ and $E_{\mathbf{k}}$ are defined by

$$E_{\mathbf{k}} \equiv \left|v'_{\mathbf{k}}\right|^2 + \omega_k^2(\eta)\left|v_{\mathbf{k}}\right|^2, \tag{6.35}$$

$$F_{\mathbf{k}} \equiv v'^2_{\mathbf{k}} + \omega_k^2(\eta) v^2_{\mathbf{k}}. \tag{6.36}$$

Exercise 6.8
Use the mode expansion (6.21) to obtain Eqs. (6.34)-(6.36) from Eq. (6.16).

Since $\hat{a}^-_{\mathbf{k}} \left|{}_{(v)}0\right\rangle = 0$, the expectation value of the instantaneous Hamiltonian in the state $\left|{}_{(v)}0\right\rangle$ is

$$\left\langle {}_{(v)}0\right| \hat{H}\left(\eta_0\right) \left|{}_{(v)}0\right\rangle = \frac{1}{4}\delta^{(3)}(0) \int d^3\mathbf{k}\; E_{\mathbf{k}}|_{\eta=\eta_0}\,.$$

As discussed above, the divergent factor $\delta^{(3)}(0)$ is a harmless manifestation of the infinite total volume of space. We obtain the energy density

$$\varepsilon = \frac{1}{4}\int d^3\mathbf{k}\; E_{\mathbf{k}}|_{\eta=\eta_0} = \frac{1}{4}\int d^3\mathbf{k}\left(\left|v'_{\mathbf{k}}\right|^2 + \omega_k^2(\eta_0)\left|v_{\mathbf{k}}\right|^2\right), \tag{6.37}$$

and the task is to determine the mode functions $v_{\mathbf{k}}(\eta)$ that minimize ε. It is clear that the contribution $\frac{1}{4}E_{\mathbf{k}}$ of each mode $\chi_{\mathbf{k}}$ must be minimized separately.

At fixed $\mathbf{k}$, the choice of the mode function $v_{\mathbf{k}}(\eta)$ may be specified by a set of initial conditions at $\eta = \eta_0$,

$$v_{\mathbf{k}}(\eta_0) = q, \quad v'_{\mathbf{k}}(\eta_0) = p,$$

where the parameters p and q are complex numbers satisfying the normalization constraint which follows from Eq. (6.22),

$$q^* p - p^* q = 2i. \tag{6.38}$$

Now we need to find such p and q that minimize the expression $|p|^2 + \omega_k^2 |q|^2$. If some p and q minimize $|p|^2 + \omega_k^2 |q|^2$, then so do $e^{i\lambda}p$ and $e^{i\lambda}q$ for arbitrary real λ; this is the freedom of choosing the overall phase of the mode function. We may choose this phase to make q real and write $p = p_1 + ip_2$ with real $p_{1,2}$. Then Eq. (6.38) yields

$$q = \frac{2i}{p - p^*} = \frac{1}{p_2} \;\Rightarrow\; E_{\mathbf{k}} = p_1^2 + p_2^2 + \frac{\omega_k^2(\eta_0)}{p_2^2}. \tag{6.39}$$

If $\omega_k^2(\eta_0) > 0$, the function $E_{\mathbf{k}}\left(p_1, p_2\right)$ has a minimum with respect to $p_{1,2}$ at $p_1 = 0$ and $p_2 = \sqrt{\omega_k(\eta_0)}$. Therefore the desired initial conditions for the mode function are

$$v_{\mathbf{k}}\left(\eta_0\right) = \frac{1}{\sqrt{\omega_k(\eta_0)}}, \quad v'_{\mathbf{k}}(\eta_0) = i\sqrt{\omega_k(\eta_0)} = i\omega_k v_{\mathbf{k}}(\eta_0). \tag{6.40}$$

On the other hand, for $\omega_k^2(\eta_0) < 0$ the function $E_{\mathbf{k}}$ in Eq. (6.39) has no minimum because the expression $p_2^2 + \omega_k^2(\eta_0) p_2^{-2}$ varies from $-\infty$ to $+\infty$. In that case the instantaneous lowest-energy vacuum does not exist.

Discussion and remarks

The main result of the above calculation is Eq. (6.40). A mode function satisfying the conditions (6.40) defines a certain set of operators $\hat{a}^{\pm}_{\mathbf{k}}$ and the corresponding vacuum $|_{\eta_0}0\rangle$. For this mode function one finds $E_{\mathbf{k}}|_{\eta=\eta_0} = 2\omega_k$ and $F_{\mathbf{k}}|_{\eta=\eta_0} = 0$, so the Hamiltonian at time η_0 is related to the operators $\hat{a}^{\pm}_{\mathbf{k}}$ by

$$\hat{H}\,(\eta_0) = \int d^3\mathbf{k}\,\omega_k(\eta_0)\left[\hat{a}^{+}_{\mathbf{k}}\hat{a}^{-}_{\mathbf{k}} + \frac{1}{2}\delta^{(3)}(0)\right]. \tag{6.41}$$

Therefore the instantaneous Hamiltonian is diagonal in the eigenbasis of the occupation number operators $\hat{N}_{\mathbf{k}} = \hat{a}^{+}_{\mathbf{k}}\hat{a}^{-}_{\mathbf{k}}$ (this eigenbasis consists of the vacuum state $|_{\eta_0}0\rangle$ and the excited states derived from it). Accordingly, the state $|_{\eta_0}0\rangle$ is sometimes called the *vacuum of instantaneous diagonalization*.

Since the initial conditions (6.40) are the same for all $\mathbf{k}$ such that $|\mathbf{k}| = k$, the resulting mode functions $v_{\mathbf{k}}(\eta)$ are isotropic, $v_{\mathbf{k}} \equiv v_k$. This isotropy has a physical origin which can be understood as follows. The vacuum mode functions were chosen by minimization of the instantaneous energy. Since the Hamiltonian of the scalar field in a FRW spacetime is isotropic (invariant under spatial rotations), the lowest-energy state of the field in that spacetime is isotropic as well.

It also follows that the instantaneous vacuum states at different times are related by isotropic Bogolyubov coefficients α_k and β_k. Therefore, if particles are produced, the occupation numbers are equal in all modes with fixed $|\mathbf{k}| = k$. In situations with a preferred direction, for example in the presence of anisotropic external fields, one may find that $\omega_{\mathbf{k}}(\eta)$ depends on the vector $\mathbf{k}$ and the lowest energy is achieved by a vacuum state with anisotropic mode functions $v_{\mathbf{k}}(\eta)$. The Bogolyubov coefficients $\alpha_{\mathbf{k}}$, $\beta_{\mathbf{k}}$ and thus the rate of particle production can be anisotropic in those cases.

> **Remark: zero-point energy.** As before, the zero-point energy density of the quantum field in the vacuum state $|_{\eta_0}0\rangle$ is divergent,
>
> $$\frac{1}{4}\int d^3\mathbf{k}\,E_{\mathbf{k}}(\eta_0) = \frac{1}{2}\int d^3\mathbf{k}\,\omega_k(\eta_0).$$
>
> This quantity is time-dependent and cannot be simply subtracted away because the zero-point energy at one time generally differs from that at another time by a formally infinite amount. A more sophisticated renormalization procedure (beyond the scope of this book) is needed to obtain correct values of energy density.

For a scalar field in the Minkowski spacetime, ω_k is time-independent and the prescription (6.40) yields the standard mode functions (4.19) which remain the vacuum mode functions at all times. But this is not the case for a time-dependent gravitational background, because then $\omega_k(\eta) \neq$ const and the mode function selected by the initial conditions (6.40) imposed at a time η_0 will generally differ from the mode function selected at another time $\eta_1 \neq \eta_0$. In other words, the state $|_{\eta_0}0\rangle$ is not an energy eigenstate at time η_1. In fact, there are no states which remain instantaneous eigenstates of the Hamiltonian at all times. This statement can be derived formally from Eq. (6.34). A vacuum state annihilated by $\hat{a}^{-}_{\mathbf{k}}$ could remain an eigenstate of the

Hamiltonian only if $F_{\mathbf{k}} = 0$ for all η, i.e.

$$F_{\mathbf{k}} = (v_k')^2 + \omega_k^2(\eta) v_k^2 = 0.$$

This differential equation has exact solutions of the form

$$v_k(\eta) = C \exp\left[\pm i \int \omega_k(\eta) d\eta\right].$$

However, for $\omega_k(\eta) \neq$ const these solutions are incompatible with Eq. (6.18), therefore an all-time eigenstate is impossible.

We can compare the instantaneous vacuum states $|_{\eta_1} 0\rangle$ and $|_{\eta_2} 0\rangle$ defined at two different times $\eta_1 \neq \eta_2$. There exists a Bogolyubov transformation with some coefficients α_k and β_k that relates the corresponding creation and annihilation operators. Then Eqs. (6.32), (6.41) yield the expectation value of energy at time $\eta = \eta_2$ in the vacuum state $|_{\eta_1} 0\rangle$:

$$\langle_{\eta_1} 0| \hat{H}(\eta_2) |_{\eta_1} 0\rangle = \delta^3(0) \int d^3\mathbf{k}\, \omega_k(\eta_2) \left[\frac{1}{2} + |\beta_k|^2\right].$$

This energy is larger than the minimum value unless $\beta_k = 0$ for all k (this would be the case in the Minkowski spacetime). This shows once again that for a general FRW spacetime the vacuum state $|_{\eta_1} 0\rangle$ is normally an excited state at another time $\eta = \eta_2$.

> **Remark: minimized fluctuations.** One might try to define the vacuum state by minimizing the amplitude of quantum fluctuations of the field at a time η_0, instead of minimizing the instantaneous energy. But such a prescription does not yield a definite vacuum state. The expectation value of the mean squared fluctuation is
>
> $$\langle_{(v)} 0| \int \chi^2(x) d^3\mathbf{x} \,|_{(v)} 0\rangle = \frac{1}{2}\delta^{(3)}(0) \int d^3\mathbf{k}\, |v_k(\eta_0)|^2 .$$
>
> Now the quantity $|v_k(\eta_0)|^2$ must be minimized separately for each $\mathbf{k}$. However, the value of the mode function $v_k(\eta_0)$ at one time $\eta = \eta_0$ can be made arbitrarily small without violating the normalization condition (6.20). The Heisenberg uncertainty principle disallows small uncertainties in both $\hat{\chi}$ and $\hat{\pi}$ *at the same time*, so there exist quantum states with arbitrarily small (but nonzero) fluctuations in the field $\hat{\chi}$ and a correspondingly large uncertainty in the canonical momentum $\hat{\pi} = \hat{\chi}'$. There is no state with the smallest amplitude of fluctuations.

6.3.2 The meaning of vacuum

Minimization of the instantaneous energy is certainly not the only possible way to define the vacuum state. For example, we could instead minimize the average energy for a certain period of time or the number of particles with respect to some other vacua. There is no unique "best" prescription available for a general curved spacetime.

The physical reason for this ambiguity is explained by the following qualitative argument. The usual definitions of the vacuum and of "particles with momentum $\mathbf{k}$" in

the Minkowski spacetime are based on the decomposition of fields into plane waves $\exp(i\mathbf{kx} - i\omega_k t)$. In quantum theory, a particle with momentum p is described by a wavepacket which has a certain spread Δp of the momentum. The spread should be sufficiently small, $\Delta p \ll p$, for the momentum of the particle to be well-defined. The spatial size λ of the wavepacket is related to the spread Δp by $\lambda \Delta p \sim 1$, therefore $\lambda \gg 1/p$. However, the geometry of a curved spacetime may significantly vary across a region of size λ. In that case, the plane waves are a poor approximation to solutions of the wave equation and so particles with momentum p cannot be defined in the usual way. The notion of a particle with momentum p is meaningful only if the spacetime is very close to Minkowski on distance and time scales of order p^{-1}.

Spatial flatness alone is not sufficient for the applicability of the particle interpretation; the relevant quantity is the four-dimensional curvature. Even in a spatially flat FRW spacetime it is quite possible that the vacuum and particle states cannot be reasonably defined for some modes. An example is a nonstationary metric with the scale factor $a(\eta)$ such that at some time η the square of the effective frequency

$$\omega_k^2(\eta) = k^2 + m^2 a^2 - \frac{a''}{a}$$

is negative, $\omega_k^2 < 0$ (i.e. the frequency ω_k is imaginary). In this case the modes $\chi_{\mathbf{k}}(\eta)$ do not oscillate but behave as growing and decaying exponents, so the analogy with a harmonic oscillator breaks down. Formally, with $\omega_k^2 < 0$ one can still define a mode expansion with respect to a set of normalized mode functions $v_k(\eta)$ and obtain the creation and annihilation operators $a_{\mathbf{k}}^{\pm}$, the vacuum state, and the corresponding excited states. But the interpretation of such states in terms of physical particles is not justified. For instance, some "excited" states defined in this way will have a lower mean energy than the "vacuum" state. This happens because the expectation value (6.37) of the energy density is not necessarily positive when $\omega_k^2 < 0$. As we have seen, the state with the lowest instantaneous energy does not exist in that case; there are states with arbitrarily low energy. In fact, for $\omega_k^2 < 0$ the condition $F_{\mathbf{k}}(\eta_0) = 0$ leads to $v_k' = c v_k$ with real c, which contradicts Eq. (6.20). Thus there are no instantaneous eigenstates $|0\rangle$ of the Hamiltonian satisfying $a_{\mathbf{k}}^- |0\rangle = 0$. The prescription of instantaneous lowest-energy vacuum completely fails when $\omega_k^2(\eta) < 0$.

Even in cases when a well-defined vacuum is available, one cannot simply postulate some prescription of the vacuum state as the "correct" one. The reason is that in general relativity a non-inertial coordinate system is equivalent to the presence of gravitation, while the field ϕ is coupled to gravity. Therefore the result of any prescription of the vacuum state, defined in terms of some physical experiment with the field ϕ, depends on the coordinate system of the observer. As we shall see in Chapter 8, an accelerated observer in the Minkowski space detects particles in an inertial observer's vacuum state. In a general spacetime, no preferred coordinate system can be selected and therefore no naturally defined "true" vacuum state can be found.

The absence of a generally valid definition of the vacuum state does not mean that we are unable to make predictions for specific experiments. For instance, we may consider a hypothetical device that prepares the field $\hat{\phi}(x)$ in the lowest-energy state

within a box of finite volume. We may assume that the device works by extracting energy from the field in the box instantaneously (as quickly as possible). In the Minkowski spacetime this device prepares the field in the standard vacuum state. The same device may be used in an FRW spacetime to prepare the field in an instantaneous lowest-energy vacuum state (assuming that $\omega_k^2 > 0$ for all relevant modes $\chi_{\mathbf{k}}$). The resulting quantum state depends on the time and place where we run the device, as well as on the reference frame in which the device is at rest; this reflects the ambiguity of the vacuum state in a curved spacetime. However, if the vacuum preparation device is known to move along a certain trajectory, one can compute the quantum state of the prepared field and make predictions about any experiments involving this field.

We conclude that "vacuum" and "particles" are approximate concepts that are inherently ambiguous in the presence of gravitation. One observer's particle may be another observer's vacuum. In contrast, quantities defined directly through the field $\hat{\phi}$, e.g. expectation values $\langle\psi|\,\hat{\phi}(x)\,|\psi\rangle$ in some state $|\psi\rangle$, are unambiguous. In this sense, field observables are more fundamental than particle occupation numbers.

6.3.3 Vacuum at short distances

We have seen that the instantaneous vacuum state at time η cannot be defined when $\omega_k^2(\eta) < 0$. But since $\omega_k^2(\eta) = k^2 + m_{\text{eff}}^2(\eta)$, there always exist large enough wavenumbers k for which $\omega_k^2 > 0$ even if $m_{\text{eff}}^2 < 0$, namely

$$k^2 > k_{\min}^2(\eta) \equiv -m_{\text{eff}}^2(\eta) = \frac{a''}{a} - m^2 a^2. \tag{6.42}$$

Therefore the instantaneous vacuum is well-defined for modes $\chi_{\mathbf{k}}$ with wavelengths shorter than the scale $L_{\max} \sim k_{\min}^{-1}$ (large values of k correspond to short distances). In cosmological applications, the relevant scales $L_{\max}$ are usually larger than the size of the observable universe ($\sim 10^{29}$cm), and the absence of an adequate vacuum state for larger-scale modes is unimportant.

A natural length scale in a curved spacetime is the radius of curvature; on much shorter scales, the spacetime looks approximately flat. The field modes with wavelengths much shorter than the curvature radius are almost unaffected by gravitation. These are the modes $\chi_{\mathbf{k}}$ with large k such that $|m_{\text{eff}}(\eta)| \ll k$ and thus $\omega_k \approx k$. Then the mode functions are approximately those of Eq. (4.19),

$$v_k(\eta) \approx \frac{1}{\sqrt{k}} e^{ik\eta}. \tag{6.43}$$

This gives a natural definition of the vacuum for modes with sufficiently short wavelengths, $L \ll L_{\max} \sim |m_{\text{eff}}|^{-1}$.

6.3.4 Adiabatic vacuum

There are situations where the lowest-energy vacuum prescription fails in such a way that we must doubt the physical interpretation of the instantaneous vacuum states.

If a lowest-energy state $|_{\eta_1}0\rangle$ is defined at some time η_1, this state will generally be a state with particles with respect to the vacuum $|_{\eta_2}0\rangle$ defined at another time η_2. At first sight this may not look problematic because *some* particle production is expected in a gravitational background. However, it turns out that in some anisotropic spacetimes the total density of such "η_2-particles" is *infinite* when all modes are counted, even when the geometry changes slowly with time and the interval (η_1, η_2) is small. This outcome is generic and occurs in a broad class of spacetimes.[3] Thus, particle states defined through the vacuum $|_\eta 0\rangle$ are not always an adequate description of the actual physical particles at time η. This motivates us to consider another prescription for vacuum that does not exhibit infinite particle production.

Often the frequency $\omega_k(\eta)$ is a slowly-changing function for some range of η. This range is called the *adiabatic regime*[4] of $\omega_k(\eta)$. It is assumed that $\omega_k^2(\eta) > 0$ within the adiabatic regime. Then the WKB approximation for Eq. (6.18) yields approximate solutions of the form

$$v_k^{(\text{approx})}(\eta) = \frac{1}{\sqrt{\omega_k(\eta)}} \exp\left[i \int_{\eta_0}^{\eta} \omega_k(\eta) d\eta\right]. \tag{6.44}$$

A quantitative condition for $\omega_k(\eta)$ to be a *slowly-changing function* of η is that the relative change of $\omega_k(\eta)$ during one oscillation period $\Delta\eta = 2\pi/\omega_k$ is negligibly small,

$$\left|\frac{\omega_k(\eta+\Delta\eta) - \omega_k(\eta)}{\omega_k(\eta)}\right| \approx \left|\frac{\omega_k'}{\omega_k}\Delta\eta\right| = 2\pi\left|\frac{\omega_k'}{\omega_k^2}\right| \ll 1. \tag{6.45}$$

This inequality is called the adiabaticity condition. The adiabatic regime is precisely the range of η where this condition holds. Note that according to this definition, a slowly-changing function does not need to be approximately constant; e.g., the function $\omega_k(\eta) = c\eta^2$ has an adiabatic regime for $|\eta| \gg |c|^{-1/3}$ where $\omega_k(\eta)$ is growing.

The mode functions $v_k(\eta)$ of the *adiabatic vacuum* $|_{\eta_0}0_{ad}\rangle$ *at time* η_0 are defined by the requirement that the function $v_k(\eta)$ and its derivative $v_k'(\eta)$ should be equal to the value and the derivative of the WKB function (6.44) at $\eta = \eta_0$, i.e.

$$v_k(\eta_0) = \frac{1}{\sqrt{\omega_k(\eta_0)}}, \quad \left.\frac{dv_k}{d\eta}\right|_{\eta=\eta_0} = \left(i\omega_k - \frac{1}{2}\frac{\omega_k'}{\omega_k}\right)\left.\frac{1}{\sqrt{\omega_k}}\right|_{\eta=\eta_0}.$$

It is easy to check that the normalization (6.20) holds.

In general, the adiabatic vacuum $|_{\eta_0}0_{ad}\rangle$ is not an eigenstate of the Hamiltonian and does not minimize the energy $E_{\mathbf{k}}$ in the modes $\chi_{\mathbf{k}}$ at $\eta = \eta_0$. However, the expectation value of energy in the mode $\chi_{\mathbf{k}}$ at time $\eta = \eta_0$ in the state $|_{\eta_0}0_{ad}\rangle$ is only slightly higher than the minimum value $\frac{1}{4}\left.E_{\mathbf{k}}\right|_{\min} = \frac{1}{2}\omega_k(\eta_0)$:

$$\frac{1}{4}E_{\mathbf{k}} = \frac{1}{4}\left(|v_{\mathbf{k}}'|^2 + \omega_k^2|v_{\mathbf{k}}|^2\right) = \frac{1}{2}\omega_k + \frac{1}{16}\frac{\omega_k'^2}{\omega_k^3} \approx \frac{1}{2}\omega_k.$$

[3] More details are given in S. A. FULLING, *Aspects of quantum field theory in curved space-time* (Cambridge University Press, 1989), chapter 7, section "Particle observables at finite times."

[4] In the physics literature, the word *regime* stands for "an interval of values for a variable." It should be clear from the context which interval for which variable is implied.

We would like to stress that the mode functions $v_k(\eta)$ must be computed as *exact* solutions of Eq. (6.18) that match the WKB functions at one point $\eta = \eta_0$. The WKB formula (6.44) is merely an approximation to the exact mode functions and the precision of that approximation is insufficient for some calculations. For instance, the WKB approximation does not yield the correct Bogolyubov coefficients between vacua defined at different times $\eta = \eta_1$ and $\eta = \eta_2$, even if the adiabaticity condition (6.45) holds. (A method of computing the Bogolyubov coefficients in the adiabatic regime is presented in Appendix B.)

All vacuum prescriptions agree if $\omega_k(\eta)$ is exactly constant, $\omega_k(\eta) \equiv \omega_k^{(0)}$, in some range $\eta_1 < \eta < \eta_2$. In that case, it is easy to verify that the natural definition of the vacuum with the mode functions (4.19) is also the result of the lowest-energy prescription. The same mode functions are found in the RHS of Eq. (6.44) because the WKB approximation is exact in the range $\eta_1 < \eta < \eta_2$.

Besides a time-independent ω_k, another interesting case is when the frequency $\omega_k(\eta)$ has a *strongly adiabatic* regime at early times, i.e. the LHS of Eq. (6.45) tends to zero at $\eta \to -\infty$ for all k. In that case we can define the mode functions of the adiabatic vacuum by imposing the condition (6.40) at $\eta_0 \to -\infty$. The resulting vacuum state is the naturally unique state that minimizes the energy in the infinite past.

> **Remark: the "in-out" transition.** We may consider the case when $\omega_k(\eta)$ tends to a constant both in the distant past and in the far future. This happens if a non-negligible gravitational field is present only for a certain period of time, e.g. $\eta_1 < \eta < \eta_2$. In that case, there are natural "in" (at $\eta < \eta_1$) and "out" (at $\eta > \eta_2$) vacuum states. The relation between the corresponding mode functions is described by a certain set of Bogolyubov coefficients $\alpha_{\mathbf{k}}$ and $\beta_{\mathbf{k}}$. Since the choice of the "in" and "out" vacuum states is unique, we obtain an unambiguous prediction for the total number density of particles, $n_{\mathbf{k}} = |\beta_{\mathbf{k}}|^2$. This is the density of particles produced by gravity in the spacetime where the field was initially (at $\eta < \eta_1$) in the natural vacuum state. The created particles are observed at late times $\eta > \eta_2$, when gravity is inactive and the definition of particles is again unambiguous. However, the choice of vacuum states at intermediate times η between η_1 and η_2 is ambiguous and particle numbers at these times are not well-defined.

6.4 A quantum-mechanical analogy

The oscillator equation for the mode functions, Eq. (6.18), is formally similar to the stationary Schrödinger equation for the wave function $\psi(x)$ of a quantum-mechanical particle in a one-dimensional potential $V(x)$,

$$\frac{d^2\psi}{dx^2} + (E - V(x))\,\psi = 0.$$

The two equations are related by the replacements $\eta \to x$ and $\omega_k^2(\eta) \to E - V(x)$.

To illustrate the analogy, we may consider the case when the potential $V(x)$ is almost constant for $x < x_1$ and for $x > x_2$ but varies in the intermediate region (see Fig. 6.1). An incident wave $\psi(x) = \exp(-ipx)$ comes from large positive x and is scattered off the potential. A reflected wave $\psi_R(x) = R\exp(ipx)$ is produced in the region

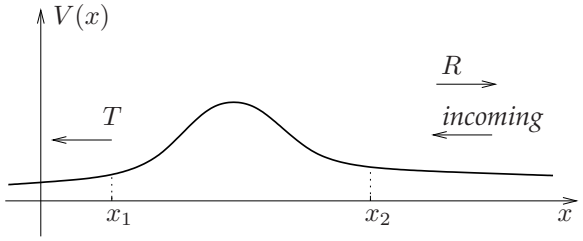


Figure 6.1: Quantum-mechanical analogy: motion in a potential $V(x)$.

$x > x_2$ and a transmitted wave $\psi_T(x) = T\exp(-ipx)$ in the region $x < x_1$. For most potentials, the reflection amplitude R is nonzero. The conservation of probability gives the constraint $|R|^2 + |T|^2 = 1$.

The solution $\psi(x)$ behaves similarly to the mode function $v_k(\eta)$ in the case when $\omega_k(\eta)$ is approximately constant at $\eta < \eta_1$ and at $\eta > \eta_2$. If we define the mode function $v_k(\eta)$ by the instantaneous vacuum condition $v_k' = i\omega_k v_k$ at some $\eta_0 < \eta_1$, then at $\eta > \eta_2$ the function $v_k(\eta)$ will be a superposition of positive and negative exponents $\exp(\pm i\omega_k\eta)$. The relation between R and T is similar to the normalization condition (6.25) for the Bogolyubov coefficients. We have seen that a nontrivial Bogolyubov transformation (with $\beta_k \neq 0$) signifies the presence of particles. Therefore we come to the qualitative conclusion that particle production is manifested by a mixing of positive and negative exponentials in the mode functions.

We emphasize that the analogy with quantum mechanics is purely mathematical. When we consider a quantum field, the modes $\chi_{\mathbf{k}}(\eta)$ are not particles moving in real space and η is not a spatial coordinate. The mode functions $v_k(\eta)$ do not represent reflected or transmitted waves. The quantum-mechanical analogy can be used only to visualize the qualitative behavior of the mode functions $v_k(\eta)$.

> **Remark: "positive" and "negative" frequency.** The function $v_k(\eta) \propto \exp(i\omega_k\eta)$ is sometimes called the positive-frequency solution and the conjugate function $v_k^*(\eta) \propto \exp(-i\omega_k\eta)$ the negative-frequency solution. Alternatively, these solutions are called positive-energy and negative-energy. This terminology historically comes from the old interpretation of QFT as the theory of quantized wave functions (the "second quantization"). The classical field $\phi(\mathbf{x}, t)$ was thought to be a "wave function" and the Schrödinger equation
>
> $$i\frac{\partial\phi}{\partial t} = E\phi$$
>
> was used to interpret the functions $\phi(t) \propto \exp(\pm i\omega t)$ as having positive or negative energy. Particle creation was described as a "mixing of positive- and negative-energy modes." However, Eq. (6.6) does not have the meaning of a Schrödinger equation and the mode functions $v_k(\eta)$ are not wave functions.

7 Quantum fields in de Sitter spacetime

Summary: Correlation functions. Amplitude of quantum fluctuations. Particle production and fluctuations: a worked-out example. Field quantization in de Sitter spacetime. Bunch-Davies vacuum. Evolution of quantum fluctuations.

7.1 Amplitude of quantum fluctuations

In the previous chapter the focus was on particle production. The main observable to compute was the average particle number $\langle \hat{N} \rangle$ in a certain quantum state. Now we consider another important quantity—the amplitude of field fluctuations. This quantity is well-defined even for those quantum states that cannot be meaningfully interpreted in terms of particles.

7.1.1 Correlation functions

To characterize the amplitude of quantum fluctuations of a field $\hat{\chi}(\mathbf{x}, \eta)$ in some quantum state $|\psi\rangle$, one may use the equal-time correlation function

$$\langle \psi | \hat{\chi}(\mathbf{x}, \eta) \hat{\chi}(\mathbf{y}, \eta) | \psi \rangle .$$

For simplicity, we consider correlation functions in a vacuum state $|\psi\rangle = |0\rangle$. (The choice of the vacuum state will be discussed below.)

If the vacuum state $|0\rangle$ is determined by a set of mode functions $v_k(\eta)$, the correlation function is given by the formula

$$\langle 0 | \hat{\chi}(\mathbf{x}, \eta) \hat{\chi}(\mathbf{y}, \eta) | 0 \rangle = \int_0^\infty \frac{k^2 dk}{4\pi^2} |v_k(\eta)|^2 \frac{\sin kL}{kL}, \tag{7.1}$$

where $L \equiv |\mathbf{x} - \mathbf{y}|$.

Exercise 7.1
Derive Eq. (7.1) from the mode expansion (6.17).

We can perform a qualitative estimate of the RHS of Eq. (7.1). The main contribution to the integral comes from wave numbers $k \sim L^{-1}$, therefore the magnitude of the correlation function is estimated as

$$\langle 0 | \hat{\chi}(\mathbf{x}, \eta) \hat{\chi}(\mathbf{y}, \eta) | 0 \rangle \sim k^3 |v_k|^2 , \quad k \sim \frac{1}{L}. \tag{7.2}$$

Note that the quantity L in Eqs. (7.1)-(7.2) is defined as the difference between the coordinate values, $L = |\mathbf{x} - \mathbf{y}|$, which is not the same as the physically observed distance L_p between these points, $L_p = a(\eta)L$. The scale L is called the *comoving distance* to distinguish it from the physical distance L_p.

7.1.2 Fluctuations of averaged fields

Another way to characterize fluctuations on scales L is to average the field $\hat{\chi}(\mathbf{x}, \eta)$ over a region of size L (e.g. a cube with sides $L \times L \times L$). The averaged operator $\hat{\chi}_L$ such as

$$\hat{\chi}_L(\eta) \equiv \frac{1}{L^3} \int_{L\times L\times L} \hat{\chi}(\mathbf{x}, \eta)\, d^3\mathbf{x}$$

can be used to describe measurements of the field $\hat{\chi}$ with a device that cannot resolve distances smaller than L. The amplitude $\delta\chi_L(\eta)$ of fluctuations in $\hat{\chi}_L(\eta)$ in a quantum state $|\psi\rangle$ is found from

$$\delta\chi_L^2(\eta) \equiv \langle\psi| \left[\hat{\chi}_L(\eta)\right]^2 |\psi\rangle .$$

A convenient way to describe spatial averaging over arbitrary domains is by using window functions. A *window function* for scale L is any function $W(\mathbf{x})$ which is of order 1 for $|\mathbf{x}| \lesssim L$, rapidly decays for $|\mathbf{x}| \gg L$, and satisfies the normalization condition

$$\int W(\mathbf{x})\, d^3\mathbf{x} = 1. \tag{7.3}$$

The prototypical example of a window function is the *Gaussian window*

$$W_G(\mathbf{x}) = \frac{1}{(2\pi)^{3/2}} \exp\left(-\frac{1}{2}|\mathbf{x}|^2\right)$$

which selects $|\mathbf{x}| \lesssim 1$. A given window function can be easily modified to select another scale, for instance if $W_L(\mathbf{x})$ is a window for the scale L, then

$$W_{L'}(\mathbf{x}) \equiv \frac{L^3}{L'^3} W_L\left(\frac{L}{L'}\mathbf{x}\right)$$

yields a window that selects the scale L'.

The basic use of window functions is to integrate $W(\mathbf{x})$ with an $\mathbf{x}$-dependent quantity $f(\mathbf{x})$. The result is the *window-averaged quantity*

$$f_L \equiv \int f(\mathbf{x})\, W(\mathbf{x})\, d^3\mathbf{x}.$$

By construction, the main contribution to the averaged quantity f_L comes from the values $f(\mathbf{x})$ at $|\mathbf{x}| \lesssim L$. The normalization (7.3) guarantees that a spatially constant quantity does not change after the averaging.

Vacuum fluctuations of a spatially averaged field

We define the averaged field operator $\hat{\chi}_L(\eta)$ by integrating the product of $\hat{\chi}(\mathbf{x},\eta)$ with a window function that selects the scale L,

$$\hat{\chi}_L(\eta) \equiv \int d^3\mathbf{x}\, \hat{\chi}(\mathbf{x},\eta)\, W_L(\mathbf{x}).$$

The amplitude of vacuum fluctuations in $\hat{\chi}_L(\eta)$ can be computed as a function of L. The calculation is similar to that of Exercise 7.1. It is natural to suppose that the window function $W_L(\mathbf{x})$ is of the form

$$W_L(\mathbf{x}) = \frac{1}{L^3} W\left(\frac{\mathbf{x}}{L}\right),$$

where $W(\mathbf{x})$ is a fixed (L-independent) window profile. Then it is convenient to introduce the Fourier image $w(\mathbf{k})$ of this window profile,

$$w(\mathbf{k}) \equiv \int d^3\mathbf{x}\, W(\mathbf{x})\, e^{-i\mathbf{k}\cdot\mathbf{x}}.$$

The function $w(\mathbf{k})$ satisfies $w|_{\mathbf{k}=0} = 1$ and decays rapidly for $|\mathbf{k}| \gtrsim 1$. (Self-test exercise: prove these statements!) It follows that the Fourier image of $W_L(\mathbf{x})$ is

$$\int d^3\mathbf{x}\, W_L(\mathbf{x}) e^{-i\mathbf{k}\cdot\mathbf{x}} = w(\mathbf{k}L).$$

We now use the mode expansion (6.17) for the field operator $\hat{\chi}(\mathbf{x},\eta)$, assuming that the mode functions $v_k(\eta)$ are given. After some straightforward algebra we find

$$\langle 0| \left[\int d^3\mathbf{x}\, W_L(\mathbf{x}) \hat{\chi}(\mathbf{x},\eta)\right]^2 |0\rangle = \frac{1}{2}\int \frac{d^3\mathbf{k}}{(2\pi)^3} |v_k|^2 |w(\mathbf{k}L)|^2.$$

Since the function $w(\mathbf{k}L)$ is of order 1 for $|\mathbf{k}| \lesssim L^{-1}$ and almost zero for $|\mathbf{k}| \gtrsim L^{-1}$, we can estimate the above integral as follows,

$$\frac{1}{2}\int \frac{d^3\mathbf{k}}{(2\pi)^3} |v_k|^2 |w(\mathbf{k}L)|^2 \sim \int_0^{L^{-1}} k^2 |v_k|^2\, dk \sim \frac{1}{L^3} |v_k|^2.$$

Thus the amplitude of fluctuations $\delta\chi_L$ is (up to a factor of order 1)

$$\delta\chi_L^2 \sim k^3 |v_k|^2, \text{ where } k \sim L^{-1}. \tag{7.4}$$

The results (7.2) and (7.4) coincide, therefore the correlation function at a distance L and the mean square fluctuation $\delta\chi_L^2$ (for any choice of the window function W_L) are both order-of-magnitude estimates of the same characteristic of the field $\hat{\chi}$. We call this characteristic *the amplitude of fluctuations on scales* L and denote it by $\delta\chi_L(\eta)$. This quantity is defined only up to a factor of order 1 and is a function of time η and of the comoving scale L. Expressed through the wavenumber $k \equiv 2\pi L^{-1}$, the fluctuation amplitude is usually called the *spectrum of fluctuations*.

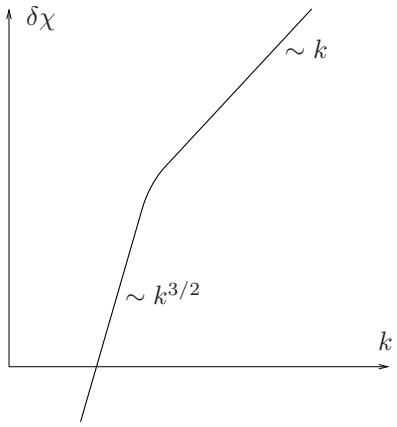


Figure 7.1: A sketch of the spectrum of fluctuations $\delta\chi_L$ in the Minkowski space; $L \equiv 2\pi k^{-1}$. (The logarithmic scaling is used for both axes.)

> **Remark: dependence on window functions.** It is clear that the result of averaging over a domain depends on the exact shape of that domain, and thus the fluctuation amplitude $\delta\chi_L$ depends on the particular window profile $W(\mathbf{x})$. However, the qualitative behavior of $\delta\chi_L$ as a function of the scale L is the same regardless of the shape of the window. To remove the dependence on the window profile, we first perform the calculations with an arbitrary window $W(\mathbf{x})$. The resulting expression contains a window-dependent factor of order 1 which is discarded, as we have done in the derivation of Eq. (7.4). The rest is the window-independent result we are looking for.

7.1.3 Fluctuations in vacuum and nonvacuum states

Intuitively one may expect that quantum fluctuations in an excited state are larger than those in the vacuum state. To verify this, let us now compute the spectrum of fluctuations for a scalar field in the Minkowski space.

The vacuum mode functions are $v_k(\eta) = \omega_k^{-1/2} \exp(i\omega_k\eta)$, where $\omega_k = \sqrt{k^2+m^2}$. So the spectrum of fluctuations in vacuum is

$$\delta\chi_L(\eta) = k^{3/2}|v_k(\eta)| = \frac{k^{3/2}}{(k^2+m^2)^{1/4}}. \tag{7.5}$$

This time-independent spectrum is sketched in Fig. 7.1. When measured with a high-resolution device (small L or large k), the field shows large fluctuations. On the other hand, if the field is averaged over a large volume ($L \to \infty$), the amplitude of fluctuations tends to zero.

Now we consider the (nonvacuum) state $|b\rangle$ annihilated by operators $\hat{b}_{\mathbf{k}}^-$ which are related to the initial annihilation operators $\hat{a}_{\mathbf{k}}^-$ by Bogolyubov transformations of

the form (6.27). Instead of performing a new calculation, we use the mode expansion (6.26) with the new mode functions u_k. The result is the same as Eq. (7.4) with the mode functions $u_k(\eta)$ instead of $v_k(\eta)$:

$$\delta\chi_L^{(b)} = k^{3/2}\,|u_k(\eta)| = k^{3/2}\,|\alpha_k v_k(\eta) - \beta_k^* v_k^*(\eta)|\,.$$

Substitution of the expression (4.19) for $v_k(\eta)$ gives

$$\delta\chi_L^{(b)} = \frac{k^{3/2}}{\sqrt{\omega_k}}\left[|\alpha_k|^2 + |\beta_k|^2 - 2\mathrm{Re}\left(\alpha_k\beta_k e^{2i\omega_k\eta}\right)\right]^{1/2}. \tag{7.6}$$

Comparing this result with the spectrum (7.5) in the vacuum state, we obtain

$$\frac{\left(\delta\chi_L^{(b)}\right)^2}{\left(\delta\chi_L\right)^2} = 1 + 2\,|\beta_k|^2 - 2\mathrm{Re}\left(\alpha_k\beta_k e^{2i\omega_k\eta}\right). \tag{7.7}$$

The oscillating term $\mathrm{Re}\left(\alpha_k\beta_k e^{2i\omega_k\eta}\right)$ in Eq. (7.7) cannot be ignored in general. However, if the quantity (7.7) is averaged over a sufficiently long time $\Delta\eta \gg \omega_k^{-1}$, the oscillations cancel and the result is simply $1 + 2\,|\beta_k|^2$.

This calculation shows that fluctuations in a nonvacuum state are typically larger than those in the vacuum state. Nevertheless, at a particular time η the oscillating term may be negative and the fluctuation amplitude $\delta\chi_L^{(b)}(\eta)$ may be smaller than the time-averaged value $\delta\chi_L(\eta)$.

7.2 A worked-out example

To illustrate the relation of quantum fluctuations and particle production, we now explicitly perform the required calculations for a scalar field in a specially chosen FRW spacetime. To make the computations easier, we choose the effective mass $m_{\mathrm{eff}}(\eta)$ as follows,

$$m_{\mathrm{eff}}^2(\eta) = \begin{cases} m_0^2, & \eta < 0 \text{ and } \eta > \eta_1; \\ -m_0^2, & 0 < \eta < \eta_1. \end{cases} \tag{7.8}$$

In the two regimes $\eta < 0$ and $\eta > \eta_1$ the vacuum states are defined naturally; these states are called the "in" vacuum $|0_{in}\rangle$ and the "out" vacuum $|0_{out}\rangle$. We assume that the field is initially ($\eta < 0$) in the "in" vacuum state. Our present goals are:

1. To compute the mean particle number at $\eta > \eta_1$.
2. To compute the mean energy in produced particles.
3. To estimate the amplitude of quantum fluctuations.

We work in the Heisenberg picture where the field $\hat{\chi}$ is at all times the "in" vacuum state. Note that the correct physical vacuum at late times $\eta > \eta_1$ is the "out" vacuum.

Mode functions

The mode functions $v_k(\eta)$ are solutions of the time-dependent oscillator equation

$$\frac{d^2}{d\eta^2}v_k + \omega_k^2(\eta)v_k = 0.$$

The "in" vacuum is described by the standard Minkowski mode functions,

$$v_k^{(in)}(\eta) = \frac{1}{\sqrt{\omega_k}}e^{i\omega_k\eta}, \quad \eta < 0. \tag{7.9}$$

At $\eta > 0$ the functions $v_k^{(in)}(\eta)$ are given by more complicated expressions (as we will see below). The mode functions of the "out" vacuum can be chosen as

$$v_k^{(out)}(\eta) = \frac{1}{\sqrt{\omega_k}}e^{i(\eta-\eta_1)\omega_k}, \quad \eta > \eta_1.$$

The task at hand is to represent the "in" mode functions at $\eta > \eta_1$ as linear combinations of the "out" mode functions.

Since the frequency $\omega_k(\eta)$ is discontinuous at $\eta = 0$ and $\eta = \eta_1$, the mode functions $v_k^{(in)}(\eta)$ and their derivatives must be matched at these points. The resulting expression is (see Exercise 7.2)

$$v_k^{(in)}(\eta) = \frac{1}{\sqrt{\omega_k}}\left[\alpha_k^* e^{i\omega_k(\eta-\eta_1)} + \beta_k^* e^{-i\omega_k(\eta-\eta_1)}\right], \quad \eta > \eta_1,$$

where the Bogolyubov coefficients α_k, β_k are given by the formulae

$$\alpha_k = \frac{e^{-i\Omega_k\eta_1}}{4}\left(\sqrt{\frac{\omega_k}{\Omega_k}} + \sqrt{\frac{\Omega_k}{\omega_k}}\right)^2 - \frac{e^{i\Omega_k\eta_1}}{4}\left(\sqrt{\frac{\omega_k}{\Omega_k}} - \sqrt{\frac{\Omega_k}{\omega_k}}\right)^2,$$

$$\beta_k = \frac{1}{4}\left(\frac{\Omega_k}{\omega_k} - \frac{\omega_k}{\Omega_k}\right)\left(e^{i\Omega_k\eta_1} - e^{-i\Omega_k\eta_1}\right) = \frac{1}{2}\left(\frac{\Omega_k}{\omega_k} - \frac{\omega_k}{\Omega_k}\right)\sin(\Omega_k\eta_1).$$

Here we have denoted $\omega_k \equiv \sqrt{k^2 + m_0^2}$ and $\Omega_k \equiv \sqrt{k^2 - m_0^2}$.

> **Exercise 7.2**
> Consider a real scalar field with the effective mass (7.8). Verify that the mode functions (7.9) are expressed through the "out" mode functions $v_k^{(out)}(\eta)$ at $\eta > \eta_1$ with the Bogolyubov coefficients given above.

Particle number density

At late times $\eta > \eta_1$ the physical vacuum is $|0_{out}\rangle$ while the field is in the state $|0_{in}\rangle$. Therefore the mean particle number density n_k in a mode $\chi_{\mathbf{k}}$ at $\eta > \eta_1$ is

$$n_k = |\beta_k|^2 = \frac{m_0^4}{|k^4 - m_0^4|}\left|\sin\left(\eta_1\sqrt{k^2 - m_0^2}\right)\right|^2. \tag{7.10}$$

Note that this expression remains finite at $k \to m_0$.

We now distinguish two limiting cases: $k \gg m_0$ (ultrarelativistic particles) and $k \ll m_0$ (wavelengths much larger than the curvature scale).

When $k \gg m_0$, one may approximate $\omega_k \approx \Omega_k$. Assuming that $m_0\eta_1$ is not large, we expand Eq. (7.10) in the small parameter (m_0/k) and obtain, after some algebra,

$$n_k = \frac{m_0^4}{k^4}\sin^2(k\eta_1) + O\left(\frac{m_0^5}{k^5}\right).$$

It follows that $n_k \ll 1$; in other words, very few particles are created.

The situation is different for $k \ll m_0$ because $\Omega_k = i\sqrt{m_0^2 - k^2}$ is imaginary and therefore $|\sin(\eta_1\Omega_k)|$ in Eq. (7.10) may become large. Since $\Omega_k \approx i\omega_k$, we get

$$\beta_k \approx \sin(im_0\eta_1) = i\sinh(m_0\eta_1).$$

The leading asymptotic of n_k can be found (assuming $m_0\eta_1 \lesssim 1$) as

$$n_k = \sinh^2(m_0\eta_1)\left[1 + O\left(\frac{k^2}{m_0^2}\right)\right]. \tag{7.11}$$

If $m_0\eta_1 \gg 1$, the density of produced particles is exponentially large. In that case, Eq. (7.11) is valid only when $k \ll \sqrt{m_0/\eta_1}$, since it is based on the approximation $\exp(\eta_1|\Omega_k|) \approx \exp(m_0\eta_1)$.

> **Remark: normalization of Bogolyubov coefficients.** In highly excited quantum states, both $|\alpha_k|$ and $|\beta_k|$ may be large but they still remain normalized by $|\alpha_k|^2 - |\beta_k|^2 = 1$.

Particle energy density

The energy density in produced particles (after subtracting the zero-point energy) is

$$\varepsilon_0 = \int d^3\mathbf{k}\, n_k\omega_k = \int_0^\infty dk\, 4\pi k^2 n_k\sqrt{k^2 + m_0^2}. \tag{7.12}$$

Since $n_k \sim k^{-4}$ at large k, the above integral logarithmically diverges at the upper (ultraviolet) limit. This divergence is a consequence of the discontinuity in the frequency $\omega_k(\eta)$ and would disappear if we chose a smooth function for $\omega_k(\eta)$. For the purposes of qualitative estimation, we may ignore this divergence and assume that the integral is cut off at some $k = k_{\max}$. For large $m_0\eta_1 \gg 1$, the main contribution to the integral comes from small $k \lesssim m_0$ for which $\omega_k \sim m_0$. The value of n_k at these k is given by Eq. (7.11) and therefore we obtain the following rough estimate,

$$\varepsilon_0 \sim m_0\int_0^{m_0} dk\, k^2\exp(2m_0\eta_1) \sim m_0^4\exp(2m_0\eta_1).$$

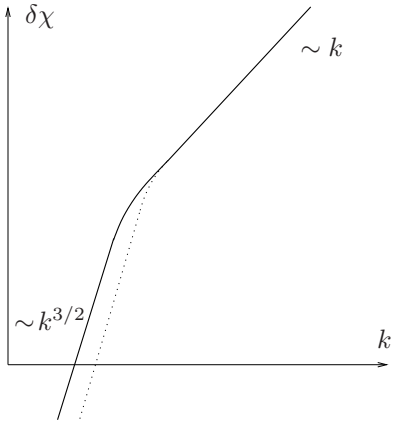


Figure 7.2: A sketch of the spectrum $\delta\chi_L$ after particle creation; $L \equiv 2\pi k^{-1}$. (The logarithmic scaling is used for both axes.) The dotted line is the spectrum in the Minkowski space.

Exercise 7.3*

Derive a more precise asymptotic estimate for ε_0. Assuming that the integral in Eq. (7.12) is performed over $0 < k < k_{\max}$, show that for $m_0\eta_1 \gg 1$ the dominant contribution to the integral comes from $k \approx \sqrt{m_0/\eta}$ and then obtain the leading asymptotic

$$\varepsilon_0 \propto \frac{m_0^4}{(m_0\eta_1)^{3/2}} \exp(2m_0\eta_1) .$$

Amplitude of fluctuations

The amplitude of fluctuations at late times $\eta > \eta_1$ is found from Eq. (7.6),

$$\delta\chi_L(\eta) = \frac{k^{3/2}}{\sqrt{\omega_k}} \left[1 + 2|\beta_k|^2 - 2\mathrm{Re}\left(\alpha_k\beta_k e^{2i\omega_k\eta}\right)\right]^{1/2} .$$

This function rapidly oscillates with time η. After an averaging over time, the value of $\delta\chi_L$ is of order

$$\delta\chi_L \sim \frac{k^{3/2}}{\sqrt{\omega_k}} \left(1 + 2|\beta_k|^2\right)^{1/2} \sim \begin{cases} k, & k \gg m_0; \\ k^{3/2} m_0^{-1/2} \exp(m_0\eta_1), & k \ll m_0. \end{cases}$$

Comparing with the spectrum (7.5) of fluctuations in the Minkowski space, we find an enhancement by the factor $\exp(m_0\eta_1)$ on large scales (see Fig. 7.2).

7.3 Field quantization in de Sitter spacetime

The *de Sitter spacetime* is the solution of the vacuum Einstein equations with a positive cosmological constant Λ. This is a cosmologically relevant spacetime in which (as we shall see) the particle interpretation of field states is usually absent, while the amplitude of fluctuations is an important quantity to compute.

To describe the geometry of this spacetime, we use the spatially flat metric

$$ds^2 = dt^2 - a^2(t)d\mathbf{x}^2 \tag{7.13}$$

with the scale factor $a(t)$ defined by

$$a(t) = a_0 e^{Ht}. \tag{7.14}$$

The Hubble parameter $H = \dot{a}/a > 0$ is a fixed constant. For convenience, we redefine the origin of time t to set $a_0 = 1$, so that $a(t) = \exp(Ht)$. The de Sitter spacetime has a constant four-dimensional curvature characterized by the Ricci scalar $R = -12H^2$.

> **Remark: derivation of $a(t) \propto \exp(Ht)$.** The de Sitter metric (7.13)-(7.14) can be derived from the Einstein equation for a universe filled with homogeneous matter with the equation of state $p = -\varepsilon$. The presence of matter with this equation of state is equivalent to a cosmological constant because the conservation of energy,
>
> $$\frac{d\varepsilon}{dt} = -3(\varepsilon + p)\frac{\dot{a}}{a} = 0,$$
>
> forces $\varepsilon = \text{const}$, and then the energy-momentum tensor of matter is
>
> $$T^{\mu\nu} = (\varepsilon + p)u^\mu u^\nu - pg^{\mu\nu} = \varepsilon g^{\mu\nu}.$$
>
> The 0-0th component of the Einstein equation for a flat FRW spacetime yields the equation
>
> $$\left(\frac{\dot{a}}{a}\right)^2 = \frac{8\pi G}{3}\varepsilon,$$
>
> which has the solution
>
> $$a(t) = a_0 \exp\left(t\sqrt{\frac{8\pi G\varepsilon}{3}}\right) \equiv a_0 \exp(Ht),$$
>
> where
>
> $$H \equiv \sqrt{\frac{8\pi G\varepsilon}{3}}$$
>
> is the (time-independent) Hubble parameter.

Incompleteness of the coordinates $(t, \mathbf{x})$

The coordinates t and $\mathbf{x}$ used in the metric (7.13) vary from $-\infty$ to $+\infty$ and yet do not cover the entire de Sitter spacetime. To show this, one may consider a timelike trajectory $\mathbf{x}(t)$ of a freely falling observer and compute the observer's proper time

along that trajectory. One finds that the infinite interval $(-\infty, 0)$ of the coordinate t corresponds to a *finite* proper time interval of the moving observer. In a spacetime without boundaries, an observer should be able to move for arbitrarily long proper time intervals. Therefore the coordinates $(t, \mathbf{x})$ cover only a portion of the observer's worldline.

Here is an explicit derivation of this result. A freely falling observer moves along a timelike worldline $\mathbf{x}(t)$ that extremizes the proper time functional $\tau\,[\mathbf{x}]$,

$$\tau\,[\mathbf{x}(t)] \equiv \int dt \sqrt{1 - a^2(t)\dot{\mathbf{x}}^2}.$$

The variation of the functional $\tau\,[\mathbf{x}]$ with respect to $\mathbf{x}(t)$ must vanish, therefore

$$\frac{\delta\tau\,[\mathbf{x}(t)]}{\delta\mathbf{x}(t)} = 0 \;\Rightarrow\; \frac{d}{dt}\frac{a^2(t)\dot{\mathbf{x}}}{\sqrt{1 - a^2(t)\dot{\mathbf{x}}^2}} \equiv \frac{d}{dt}\mathbf{p} = 0 \;\Rightarrow\; \mathbf{p} = \text{const}.$$

The integral of motion $\mathbf{p}$ is equal to the momentum of a unit-mass observer. The trajectory $\mathbf{x}(t)$ can now be found explicitly. However, we need only the relation

$$a^2\dot{\mathbf{x}}^2 = \frac{p^2}{p^2 + a^2}, \quad p \equiv |\mathbf{p}|\,.$$

If the observer's initial velocity is nonzero, $\dot{\mathbf{x}}(0) \neq 0$, then $p \neq 0$ and it follows that the proper time τ_0 elapsed for the observer during the interval $-\infty < t < 0$ is finite:

$$\tau_0 = \int_{-\infty}^{0} dt \sqrt{1 - a^2(t)\dot{\mathbf{x}}^2} = \int_{-\infty}^{0} \frac{a(t)dt}{\sqrt{p^2 + a^2(t)}} = H^{-1}\sinh^{-1}\frac{1}{p} < \infty.$$

An event at the proper time $\tau = -\tau_0$ in the observer's frame corresponds to the values $t = -\infty$ and $|\mathbf{x}| = \infty$; events encountered by the observer at earlier proper times $\tau < -\tau_0$ are not covered by the coordinates $(t, \mathbf{x})$. These coordinates cover only a part of the whole spacetime as shown in Fig. 7.3. However, the incompleteness of this coordinate system is a benign problem. In cosmological applications, only a relatively small portion of the de Sitter space (shaded in Fig. 7.3) is used as an approximation to a certain epoch in the history of the universe. The coordinate system $(t, \mathbf{x})$ is completely adequate for that task, and the inability to describe events in very distant past is unimportant. At the same time, a different choice of the coordinate system would significantly complicate the calculations.

Horizons

Another feature of the de Sitter spacetime—the presence of horizons—is revealed by the following consideration of trajectories of lightrays. A null worldline $\mathbf{x}(t)$ satisfies $a^2(t)\dot{\mathbf{x}}^2(t) = 1$, which yields the solution

$$|\mathbf{x}(t)| = \frac{1}{H}\left(e^{-Ht_0} - e^{-Ht}\right)$$

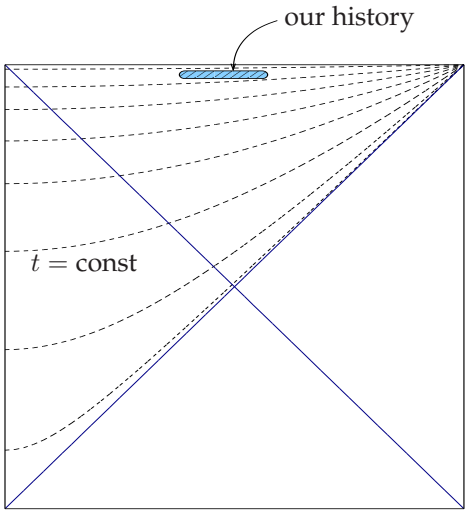


Figure 7.3: A conformal diagram of the de Sitter spacetime. The flat coordinate system $(t, \mathbf{x})$ covers only the left upper half of the diagram. Dashed lines are surfaces of constant t.

for trajectories starting at the origin, $\mathbf{x}(t_0) = 0$. Therefore all lightrays emitted at the origin at $t = t_0$ asymptotically approach the sphere $|\mathbf{x}| = r_{\max}(t_0) \equiv H^{-1} \exp(-Ht_0)$. This sphere is the *horizon* for the observer at the origin; the spacetime expands too quickly for lightrays to reach any points beyond the horizon. Similarly, observers at the origin will never receive any lightrays emitted at $t = t_0$ at points $|\mathbf{x}| > r_{\max}$.

It is easy to verify that at any time t_0 the horizon is always at the same *proper* distance $a(t_0) r_{\max}(t_0) = H^{-1}$ from the observer. This distance is called the *horizon scale*.

7.3.1 Quantization of scalar fields

To describe a real scalar field $\phi(\mathbf{x}, t)$ in the de Sitter spacetime, we first transform the coordinate t to make the metric explicitly conformally flat:

$$ds^2 = dt^2 - a^2(t) d\mathbf{x}^2 = a^2(\eta) \left(d\eta^2 - d\mathbf{x}^2 \right),$$

where the conformal time η and the scale factor $a(\eta)$ are

$$\eta = -\frac{1}{H} e^{-Ht}, \quad a(\eta) = -\frac{1}{H\eta}.$$

The conformal time η changes from $-\infty$ to 0 when the proper time t goes from $-\infty$ to $+\infty$. (Since the value of η is always negative, we shall sometimes have to write $|\eta|$ in the equations. However, it is essential that the variable η grows when t grows, so

we cannot choose $-\eta$ as the time variable. For convenience, we chose the origin of η so that the infinite future corresponds to $\eta = 0$.)

The field $\phi(\mathbf{x}, \eta)$ can now be quantized by the method of Sec. 6.2. The action for the scalar field is given by Eq. (5.4) with $V(\phi) = \frac{1}{2}m^2\phi^2$. We introduce the auxiliary field $\chi \equiv a\phi$ and use the mode expansion (6.17)-(6.18) with

$$\omega_k^2(\eta) = k^2 + m^2a^2 - \frac{a''}{a} = k^2 + \left(\frac{m^2}{H^2} - 2\right)\frac{1}{\eta^2}. \tag{7.15}$$

From this expression it is clear that the effective frequency may become imaginary, i.e. $\omega_k^2(\eta) < 0$, if $m^2 < 2H^2$. In most cosmological scenarios where the early universe is approximated by a region of the de Sitter spacetime, the relevant value of H is much larger than the masses of elementary particles. Therefore below we shall assume that $m \ll H$.

7.3.2 Mode functions

When the definition (7.15) of the effective frequency, Eq. (6.18) becomes

$$v_k'' + \left[k^2 - \left(2 - \frac{m^2}{H^2}\right)\frac{1}{\eta^2}\right]v_k = 0, \tag{7.16}$$

which can be reduced to the Bessel equation (see Exercise 7.4). The general solution is expressed through the Bessel functions $J_n(x)$ and $Y_n(x)$,

$$v_k(\eta) = \sqrt{k|\eta|}\left[AJ_n(k|\eta|) + BY_n(k|\eta|)\right], \quad n \equiv \sqrt{\frac{9}{4} - \frac{m^2}{H^2}}.$$

The normalization of the mode function, $\mathrm{Im}\,(v_k^* v_k') = 1$, constrains the constants A and B by

$$AB^* - A^*B = \frac{i\pi}{k}.$$

> **Exercise 7.4**
> Assume that $m \ll H$ and transform Eq. (7.16) by a change of variables into the Bessel equation
>
> $$s^2\frac{d^2f}{ds^2} + s\frac{df}{ds} + \left(s^2 - n^2\right)f = 0$$
>
> which has the general solution
>
> $$f(s) = AJ_n(s) + BY_n(s),$$
>
> where A and B are constants. Use the asymptotics of the Bessel functions $J_n(s)$, $Y_n(s)$ at large and small s to determine the asymptotics of the mode functions $v_k(\eta)$ for $k|\eta| \gg 1$ and $k|\eta| \ll 1$.

In the preceding exercise, the asymptotics of the mode functions $v_k(\eta)$ at very early and very late times were obtained from the Bessel functions. This can also be done using the following elementary considerations.

At very early times (large negative η), we may neglect η^{-2} and approximately set $\omega_k \approx k$. This is the same as the short-distance limit considered in Sec. 6.3.3. The approximation is valid when

$$k^2 \gg \left| \frac{a''}{a} - m^2 a^2 \right| \sim \frac{1}{\eta^2}.$$

In this limit the field modes $\hat{\chi}_{\mathbf{k}}$ are not significantly affected by gravity. The vacuum is defined as in the Minkowski space, with the mode functions

$$v_k(\eta) \approx \frac{1}{\sqrt{k}} e^{ik\eta}, \quad k\,|\eta| \gg 1. \tag{7.17}$$

At very late times ($\eta \to 0$) the term k^2 becomes negligible and we obtain

$$\omega_k^2(\eta) \approx -\left(2 - \frac{m^2}{H^2}\right) \frac{1}{\eta^2}.$$

It follows that for small masses, $m \ll H$, the frequency ω_k is imaginary. The equation for the mode functions is

$$v_k'' - \left(2 - \frac{m^2}{H^2}\right) \frac{1}{\eta^2} v_k = 0.$$

This equation is homogeneous in η, so the general solution can be written as

$$v_k(\eta) = A\,|\eta|^{n_1} + B\,|\eta|^{n_2}, \quad k\,|\eta| \ll 1, \tag{7.18}$$

where

$$n_{1,2} \equiv \frac{1}{2} \pm \sqrt{\frac{9}{4} - \frac{m^2}{H^2}} = \frac{1}{2} \pm n.$$

The dominant asymptotic at late times ($\eta \to 0$) is the term with the larger negative exponent,

$$v_k(\eta) \sim B\,|\eta|^{n_2}.$$

We found that the asymptotic forms of the mode functions depend on the value of $k\,|\eta|$. A wave with the wave number $\mathbf{k}$ has the comoving wavelength $L \sim k^{-1}$ and the physical wavelength $L_p = a(\eta)L$, therefore

$$k\,|\eta| \sim \frac{1}{L} \frac{1}{aH} = \frac{H^{-1}}{L_p}.$$

This suggests the following physical interpretation of the parameter $k\,|\eta|$. Large values of $k\,|\eta|$ correspond to wavelengths which are much shorter than the horizon distance H^{-1} at time η (the *subhorizon* modes). These modes are essentially unaffected by the curvature of the spacetime. On the other hand, small values of $k\,|\eta|$ correspond to physical wavelengths $L_p \gg H^{-1}$ stretching far beyond the horizon.

These *superhorizon* modes are significantly affected by gravity. A mode with comoving wavenumber k is subhorizon at early times and becomes superhorizon at a k-dependent time $\eta = \eta_k$ at which the physical wavelength L_p is equal to the horizon scale, i.e. $k\,|\eta_k| = 1$. The time $\eta = \eta_k$ is conventionally referred to as the moment of *horizon crossing* for the mode $\chi_{\mathbf{k}}$. Note that the existence of horizon crossing is due to an accelerated expansion of the de Sitter spacetime ($\ddot{a} > 0$); there would be no horizon crossing if the expansion were decelerating ($\ddot{a} < 0$).

7.3.3 The Bunch-Davies vacuum

Quantum fields in the de Sitter spacetime have a preferred vacuum state which is known as the *Bunch-Davies* (BD) *vacuum*, defined essentially as the Minkowski vacuum in the early-time limit ($\eta \to -\infty$) of each mode.

Before introducing the BD vacuum, let us consider the prescription of the instantaneous vacuum defined at a time $\eta = \eta_0$. If we had $\omega_k^2(\eta_0) > 0$ for all k, this prescription would yield a well-defined vacuum state. However, since $m \ll H$, there always exists a small enough k such that $k\,|\eta_0| \ll 1$ and thus $\omega_k^2(\eta_0) < 0$. It was shown in Sec. 6.3.2 that the energy in a mode $\chi_{\mathbf{k}}$ cannot be minimized when $\omega_k^2 < 0$. Therefore the instantaneous energy prescription cannot define a vacuum state of the entire quantum field (for all modes) but only for the modes $\chi_{\mathbf{k}}$ with $k\,|\eta_0| \gtrsim 1$, i.e. for the subhorizon modes at $\eta = \eta_0$. This "partial" definition of the vacuum is adequate if the time η_0 is chosen to be sufficiently early such that all observationally relevant modes $\chi_{\mathbf{k}}$ are subhorizon at $\eta = \eta_0$.

The motivation for introducing the BD vacuum state is the following. The effective frequency $\omega_k(\eta)$ becomes constant in the early-time limit $\eta \to -\infty$, and thus each mode $\chi_{\mathbf{k}}$ has a strongly adiabatic regime in that limit (see Sec. 6.3.4 for a discussion of adiabatic regimes). Physically, the influence of gravity on each mode $\chi_{\mathbf{k}}$ is negligible at sufficiently early (k-dependent) times. So it is natural to define the mode functions $v_k(\eta)$ by applying the Minkowski vacuum prescription in the limit $\eta \to -\infty$, separately for each mode $\chi_{\mathbf{k}}$. This prescription can be expressed by the asymptotic relations

$$v_k(\eta) \to \frac{1}{\sqrt{\omega_k}} e^{i\omega_k \eta}, \quad \frac{v_k'(\eta)}{v_k(\eta)} \to i\omega_k, \quad \text{as } \eta \to -\infty. \tag{7.19}$$

The vacuum state determined by the mode functions $v_k(\eta)$ satisfying Eq. (7.19) is called the *Bunch-Davies vacuum*. From the result of Exercise 7.4 we can read the mode functions of the BD vacuum,

$$v_k(\eta) = \sqrt{\frac{\pi\,|\eta|}{2}} \left[J_n\left(k\,|\eta|\right) - iY_n\left(k\,|\eta|\right)\right], \quad n \equiv \sqrt{\frac{9}{4} - \frac{m^2}{H^2}}. \tag{7.20}$$

The Bunch-Davies vacuum prescription has important applications in cosmology. The de Sitter spacetime approximates the inflationary stage of the evolution of the universe. However, this approximation is valid only for a certain time interval, for instance $\eta_i < \eta < \eta_f$, while at earlier times, $\eta < \eta_i$, the spacetime is not de Sitter. Therefore the procedure of imposing the adiabatic conditions at earlier times $\eta < \eta_i$

cannot be justified, and the BD vacuum state can be used only for modes $\chi_{\mathbf{k}}$ such that $k|\eta_i| \gg 1$. The modes $\chi_{\mathbf{k}}$ with $k|\eta_i| \lesssim 1$ were superhorizon at $\eta = \eta_i$ and their quantum states are determined by the evolution of the spacetime at $\eta < \eta_i$. Unless this evolution is known, one should refrain from making predictions about the quantum state of those modes.

> **Remark: interpretation of superhorizon modes.** For $m \ll H$, all modes $\chi_{\mathbf{k}}$ with $k|\eta| < 2$ have imaginary effective frequencies $\omega_k(\eta)$ at time η. Hence, quantum states of these superhorizon modes do not have a particle interpretation. However, field modes with superhorizon wavelengths are real and their influence can be quantitatively investigated, for instance, by computing the spectrum of fluctuations. This is another illustration of the fact that field observables such as $\langle 0|\,\hat{\phi}(x)\hat{\phi}(y)\,|0\rangle$ are more fundamental than a description of quantum states in terms of particles.

7.4 Evolution of fluctuations

We now study the fluctuation amplitude $\delta\phi_L(\eta)$ in the BD vacuum state as a function of time η and scale L.

According to the formula (7.4), the amplitude of fluctuations is determined by absolute values of the mode functions. Up to now we have been mostly working with the auxiliary field $\hat{\chi}(x) = a\hat{\phi}(x)$. The mode expansion for $\hat{\phi}(x)$ is simply $a^{-1}(\eta)$ times the mode expansion for $\hat{\chi}$. Therefore, the mode functions of the field $\hat{\phi}$ are $a^{-1}(\eta)v_k(\eta)$, where $v_k(\eta)$ are the mode functions of the field $\hat{\chi}$, and the amplitude of fluctuations of $\hat{\phi}$ on a comoving scale L is

$$\delta\phi_L(\eta) = a^{-1}(\eta)k^{3/2}\,|v_k(\eta)|\,, \quad k \equiv L^{-1}. \tag{7.21}$$

To compute the time dependence of the fluctuations, we could use the exact expression (7.20). However, the correct order or magnitude of the mode function $v_k(\eta)$ can be found without cumbersome calculations.

Evolution of mode functions

The mode functions (7.20) describing the BD vacuum possess the asymptotic forms (7.17) and (7.18). We assume that the earliest available time is η_i and do not consider modes with $k|\eta_i| < 2$; their quantum state is considered to be unknown.

For a mode $\chi_{\mathbf{k}}$ with a wavelength which at $\eta = \eta_i$ was much smaller than the horizon so that $k|\eta_i| \gg 1$, the adiabatic regime lasts from η_i until the horizon crossing time η_k such that $k|\eta_k| \sim 1$. Therefore within the time interval $\eta_i < \eta < \eta_k$ the BD mode function is approximately equal to the Minkowski mode function,

$$v_k(\eta) \approx \frac{1}{\sqrt{k}}e^{ik\eta}, \quad \eta_i < \eta < \eta_k, \quad \eta_k \equiv -\frac{1}{k}. \tag{7.22}$$

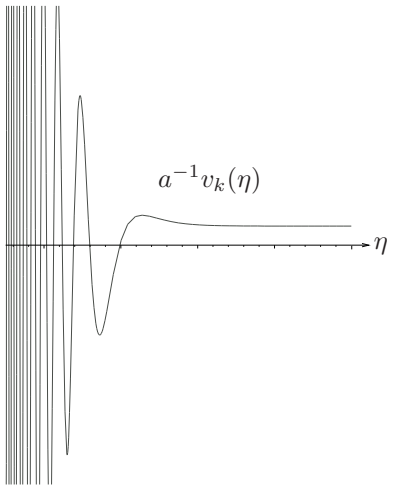


Figure 7.4: The imaginary part of the mode function $a^{-1}v_k(\eta)$ for the Bunch-Davies vacuum (massless field). The time η is plotted in logarithmic scale. The magnitude of fluctuations is constant at late times.

At $\eta = \eta_k$, we match the asymptotic solution (7.18) to this function and find

$$v_k(\eta) \sim A_k \frac{1}{\sqrt{k}} \left|\frac{\eta}{\eta_k}\right|^{n_1} + B_k \frac{1}{\sqrt{k}} \left|\frac{\eta}{\eta_k}\right|^{n_2}, \quad \eta > \eta_k,$$

where the coefficients A_k and B_k must be both of order 1 to match the value and the derivative of $v_k(\eta)$. (Exact expressions for A_k and B_k are not needed for the present estimate.) Finally, for $k\,|\eta| \ll 1$ the term multiplied by A_k is negligible, therefore

$$v_k(\eta) \sim \frac{1}{\sqrt{k}} \left|\frac{\eta}{\eta_k}\right|^{\frac{1}{2}-n}, \quad n = \sqrt{\frac{9}{4} - \frac{m^2}{H^2}}, \quad |\eta| \ll k^{-1}. \tag{7.23}$$

The mode functions of the field $\hat{\phi}$ are $a^{-1}v_k$, and at late times ($k\,|\eta| \ll 1$) we have

$$a^{-1}v_k(\eta) \propto |\eta|\, v_k(\eta) \propto |\eta|^{3/2-n}.$$

For $m \ll H$, Eq. (7.23) gives $n \approx \frac{3}{2}$ and it follows that the mode function $a^{-1}v_k(\eta)$ tends to a constant at late times. The exact mode function for $m = 0$ is plotted in Fig. 7.4 where one can see the transition from the oscillatory regime at early times to the late-time behavior.

Spectrum of fluctuations

Now we can compute the amplitude of fluctuations according to Eq. (7.21). The asymptotic forms (7.22)-(7.23) of the Bunch-Davies mode functions yield the corre-

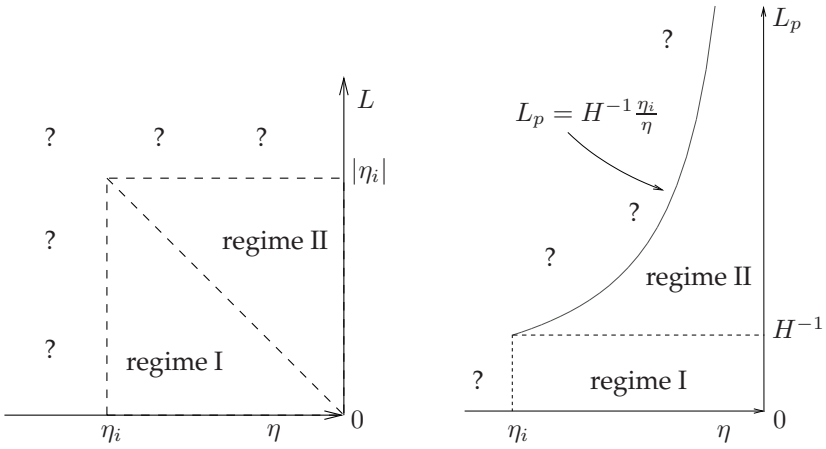


Figure 7.5: The asymptotic regimes of $\delta\phi_L$ (left) from Eq. (7.24) and $\delta\phi_{L_p}$ (right) from Eq. (7.25). Question marks indicate undetermined spectra.

sponding asymptotic estimates of $\delta\phi_L(\eta)$ in various regimes of L and η:

$$\delta\phi_L(\eta) = \begin{cases} \text{unknown}, \quad \eta < \eta_i \text{ or } L \gtrsim |\eta_i|\,; \\ H\left|L^{-1}\eta\right|, \quad L < |\eta| < |\eta_i| \quad \text{(regime I)}; \\ H\left|L^{-1}\eta\right|^{3/2-n}, \; L \gg |\eta| \quad \text{(regime II)}. \end{cases} \tag{7.24}$$

By assumption $m \ll H$, therefore $3/2 - n$ is a small positive number,

$$\frac{3}{2} - n = \frac{3}{2} - \sqrt{\frac{9}{4} - \frac{m^2}{H^2}} = \frac{1}{3}\frac{m^2}{H^2} + O\left(\frac{m^4}{H^4}\right).$$

The relevant domains of the (η, L) plane are shown in Fig. 7.5, left.

It is useful to express the function $\delta\phi_L(\eta)$ through the physical distance $L_p \equiv a(\eta)L$ measured at time η, instead of the comoving scale L. We find a simpler set of results,

$$\delta\phi_{L_p}(\eta) = \begin{cases} \text{unknown}, \quad \eta < \eta_i \text{ or } L_p \gtrsim H^{-1}\dfrac{\eta_i}{\eta}; \\ L_p^{-1}, \quad L_p < H^{-1} \quad \text{(regime I)}; \\ H\left|L_p H\right|^{n-3/2}, \; L_p > H^{-1} \quad \text{(regime II)}. \end{cases} \tag{7.25}$$

As a function of the physical length L_p, the fluctuation spectrum is independent of the time η and only the domain of applicability of the "regime II" moves with η toward larger scales (see Fig. 7.5, right).

The fluctuation spectrum $\delta\phi_{L_p}(\eta)$ at a fixed time η can be visualized using Eq. (7.25). The spectrum for $L_p < H^{-1}$ is the same as in the Minkowski spacetime, while for superhorizon scales $L_p > H^{-1}$ the spectrum becomes almost flat (*scale-invariant*) and shows much larger fluctuations than the Minkowski spacetime spectrum, $\delta\phi \sim L_p^{-1}$

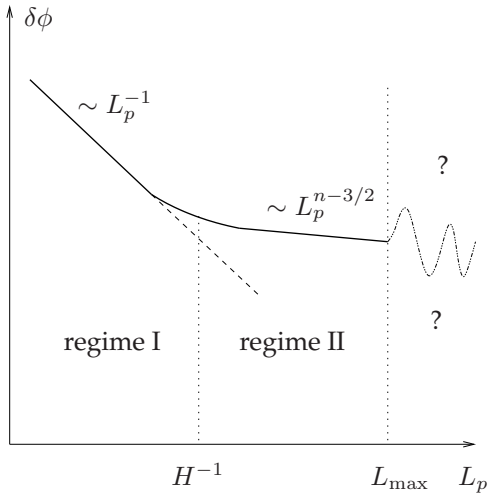


Figure 7.6: The fluctuation amplitude $\delta\phi_{L_p}(\eta)$ as function of L_p at fixed time η. The dashed line shows the amplitude of fluctuations in the Minkowski spacetime. (The logarithmic scaling is used for both axes.)

(see Fig. 7.6). The growth of fluctuations is due to the influence of gravity on the superhorizon modes of the field $\hat{\phi}$. Beyond the scale $L_{\max} = H^{-1}\frac{\eta_i}{\eta}$ the quantum state of the field is unknown.

The scale $L_{\max}$ grows with time as $L_{\max} \sim \exp(Ht)$, so the region $L_p > L_{\max}$ where the spectrum is unknown quickly moves toward extremely large scales. We can therefore picture the evolution of the spectrum as a gradual "ironing" of unknown fluctuations into the almost flat regime $H^{-1} < L_p < L_{\max}$. At sufficiently late times, fluctuations on all cosmologically interesting scales are independent of the initial conditions at $\eta = \eta_i$ and coincide with the fluctuations in the Bunch-Davies vacuum state. We find that the effect of the de Sitter expansion is to bring an arbitrary initial quantum state into the Bunch-Davies vacuum state at late times.

The growth of quantum fluctuations is used in cosmology to explain the formation of large-scale structures (galaxies and clusters of galaxies) in the early universe. The theory of *cosmological inflation* assumes the existence of a de Sitter-like epoch during which quantum fluctuations of the fields were amplified and at the same time all information about previous quantum states was moved to unobservably large scales. The resulting large quantum fluctuations act as seeds for the inhomogeneities of energy density, which then grow by gravitational collapse and eventually cause the formation of galaxies. This theory is a practical application of QFT in curved spacetime to astrophysics.

8 The Unruh effect

Summary: Uniformly accelerated motion. The Rindler spacetime in 1+1 dimensions. Quantization of massless scalar field. The Rindler and the Minkowski vacua. Density of particles. The Unruh temperature.

The Unruh effect predicts the detection of particles in vacuum by an accelerated observer. In this chapter we consider the simplest case when the observer moves with a constant acceleration through the Minkowski spacetime. Even though the field is in the vacuum state, the observer finds a distribution of particles characteristic of a thermal bath of blackbody radiation.

8.1 Kinematics of uniformly accelerated motion

First we consider the trajectory of an object moving with a constant acceleration in the Minkowski spacetime. A model of this situation is a spaceship with an infinite energy supply and a propulsion engine that exerts a constant force (but moves with the ship). The resulting motion of the spaceship is such that the acceleration of the ship in its own frame of reference (the *proper acceleration*) is constant. This is the natural definition of a uniformly accelerated motion in a relativistic theory. (An object cannot move with $d\mathbf{v}/dt = \text{const}$ for all time because velocities must be smaller than the speed of light, $|\mathbf{v}| < 1$.)

We now introduce the reference frames that will play a major role in our considerations: the laboratory frame, the proper frame, and the comoving frame. The laboratory frame is the usual inertial reference frame with the coordinates (t, x, y, z). The proper frame is the accelerated system of reference that moves together with the observer; we shall also call it the accelerated frame. The comoving frame defined at a time t_0 is the *inertial* frame in which the accelerated observer is instantaneously at rest at $t = t_0$. (Thus the term *comoving frame* actually refers to a different frame for each t_0.)

By definition, the observer's proper acceleration at time $t = t_0$ is the 3-acceleration measured in the comoving frame at time t_0. We consider a uniformly accelerated observer whose proper acceleration is time-independent and equal to a given 3-vector $\mathbf{a}$. The trajectory of such an observer may be described by a worldline $x^\mu(\tau)$, where τ is the proper time measured by the observer. The proper time parametrization implies the condition

$$u^\mu u_\mu = 1, \quad u^\mu \equiv \frac{dx^\mu}{d\tau}. \tag{8.1}$$

It is a standard result that the 4-acceleration in the laboratory frame,

$$a^\mu \equiv \frac{du^\mu}{d\tau} = \frac{d^2x^\mu}{d\tau^2},$$

is related to the three-dimensional proper acceleration $\mathbf{a}$ by

$$a^\mu a_\mu = -\left|\mathbf{a}\right|^2. \tag{8.2}$$

Derivation of Eq. (8.2). Let $u^\mu(\tau)$ be the observer's 4-velocity and let t_c be the time variable in the comoving frame defined at $\tau = \tau_0$; this is the time measured by an *inertial* observer moving with the constant velocity $u^\mu(\tau_0)$. We shall show that the 4-acceleration $a^\mu(\tau)$ in the comoving frame has components $(0, a^1, a^2, a^3)$, where a^i are the components of the acceleration 3-vector $\mathbf{a} \equiv d^2\mathbf{x}/dt_c^2$ measured in the comoving frame. It will then follow that Eq. (8.2) holds in the comoving frame, and hence it holds also in the laboratory frame since the Lorentz-invariant quantity $a^\mu a_\mu$ is the same in all frames.

Since the comoving frame moves with the velocity $u^\mu(\tau_0)$, the 4-vector $u^\mu(\tau_0)$ has the components $(1,0,0,0)$ in that frame. The derivative of the identity $u^\mu(\tau)u_\mu(\tau) = 1$ with respect to τ yields $a^\mu(\tau)u_\mu(\tau) = 0$, therefore $a^0(\tau_0) = 0$ in the comoving frame. Since $dt_c = u^0(\tau)d\tau$ and $u^0(\tau_0) = 1$, we have

$$\frac{d^2x^\mu}{dt_c^2} = \frac{1}{u^0}\frac{d}{d\tau}\left[\frac{1}{u^0}\frac{dx^\mu}{d\tau}\right] = \frac{d^2x^\mu}{d\tau^2} + \frac{dx^\mu}{d\tau}\frac{d}{d\tau}\frac{1}{u^0}.$$

It remains to compute

$$\frac{d}{d\tau}\frac{1}{u^0(\tau_0)} = -\left[u^0(\tau_0)\right]^{-2}\left.\frac{du^0}{d\tau}\right|_{\tau=\tau_0} = -a^0(\tau_0) = 0,$$

and it follows that $d^2x^\mu/d\tau^2 = d^2x^\mu/dt_c^2 = \left(0, a^1, a^2, a^3\right)$ as required. (Self-test question: why is $a^\mu = du^\mu/d\tau \neq 0$ even though $u^\mu = (1,0,0,0)$ in the comoving frame?)

We now derive the trajectory $x^\mu(\tau)$ of the accelerated observer. Without loss of generality, we may assume that the acceleration is parallel to the x axis, $\mathbf{a} \equiv (a,0,0)$, where $a > 0$, and that the observer moves only in the x direction. Then the coordinates y and z of the observer remain constant and only the functions $x(\tau)$, $t(\tau)$ need to be computed. From Eqs. (8.1)-(8.2) it is straightforward to derive the general solution

$$x(\tau) = x_0 - \frac{1}{a} + \frac{1}{a}\cosh a\tau, \quad t(\tau) = t_0 + \frac{1}{a}\sinh a\tau. \tag{8.3}$$

This trajectory has zero velocity at $\tau = 0$ (which implies $x = x_0$, $t = t_0$).

Derivation of Eq. (8.3). Since $a^\mu = du^\mu/d\tau$ and $u^2 = u^3 = 0$, the components u^0, u^1 of the velocity satisfy

$$\left(\frac{du^0}{d\tau}\right)^2 - \left(\frac{du^1}{d\tau}\right)^2 = -a^2,$$
$$\left(u^0\right)^2 - \left(u^1\right)^2 = 1.$$

We may assume that $u_0 > 0$ (the time τ grows together with t) and that $du^1/d\tau > 0$, since the acceleration is in the positive x direction. Then

$$u^0 = \sqrt{1 + (u^1)^2}; \quad \frac{du^1}{d\tau} = a\sqrt{1 + (u^1)^2}.$$

The solution with the initial condition $u^1(0) = 0$ is

$$u^1(\tau) \equiv \frac{dx}{d\tau} = \sinh a\tau, \quad u^0(\tau) \equiv \frac{dt}{d\tau} = \cosh a\tau.$$

After an integration we obtain Eq. (8.3).

The trajectory (8.3) has a simpler form if we choose the initial conditions $x(0) = a^{-1}$ and $t(0) = 0$. Then the worldline is a branch of the hyperbola $x^2 - t^2 = a^{-2}$ (see Fig. 8.1). At large $|t|$ the worldline approaches the lightcone. The observer comes in from $x = +\infty$, decelerates and stops at $x = a^{-1}$, and then accelerates back towards infinity. In the comoving frame of the observer, this motion takes infinite proper time, from $\tau = -\infty$ to $\tau = +\infty$.

From now on, we drop the coordinates y and z and work in the 1+1-dimensional spacetime (t, x).

8.1.1 Coordinates in the proper frame

To describe quantum fields as seen by an accelerated observer, we need to use the *proper coordinates* (τ, ξ), where τ is the proper time and ξ is the distance measured by the observer. The proper coordinate system (τ, ξ) is related to the laboratory frame (t, x) by some transformation functions $\tau(t, x)$ and $\xi(t, x)$ which we shall now determine.

The observer's trajectory $t(\tau)$, $x(\tau)$ should correspond to the line $\xi = 0$ in the proper coordinates. Let the observer hold a rigid measuring stick of proper length ξ_0, so that the entire stick accelerates together with the observer. Then the stick is instantaneously at rest in the comoving frame and the far endpoint of the stick has the proper coordinates (τ, ξ_0) at time τ. We shall derive the relation between the coordinates (t, x) and (τ, ξ) by computing the laboratory coordinates (t, x) of the far end of the stick as functions of τ and ξ_0.

In the comoving frame at time τ, the stick is represented by the 4-vector $s^\mu_{(\text{com})} \equiv (0, \xi_0)$ connecting the endpoints $(\tau, 0)$ and (τ, ξ_0). This comoving frame is an inertial system of reference moving with the 4-velocity $u^\mu(\tau) = dx^\mu/d\tau$. Therefore the coordinates $s^\mu_{(\text{lab})}$ of the stick in the laboratory frame can be found by applying the inverse Lorentz transformation to the coordinates $s^\mu_{(\text{com})}$:

$$\begin{bmatrix} s^0_{(\text{lab})} \\ s^1_{(\text{lab})} \end{bmatrix} = \frac{1}{\sqrt{1-v^2}} \begin{pmatrix} 1 & v \\ v & 1 \end{pmatrix} \begin{bmatrix} s^0_{(\text{com})} \\ s^1_{(\text{com})} \end{bmatrix} = \begin{pmatrix} u^0 & u^1 \\ u^1 & u^0 \end{pmatrix} \begin{bmatrix} s^0_{(\text{com})} \\ s^1_{(\text{com})} \end{bmatrix} = \begin{bmatrix} u^1\xi \\ u^0\xi \end{bmatrix},$$

where $v \equiv u^1/u^0$ is the velocity of the stick in the laboratory system. The stick is attached to the observer moving along $x^\mu(\tau)$, so the proper coordinates (τ, ξ) of the

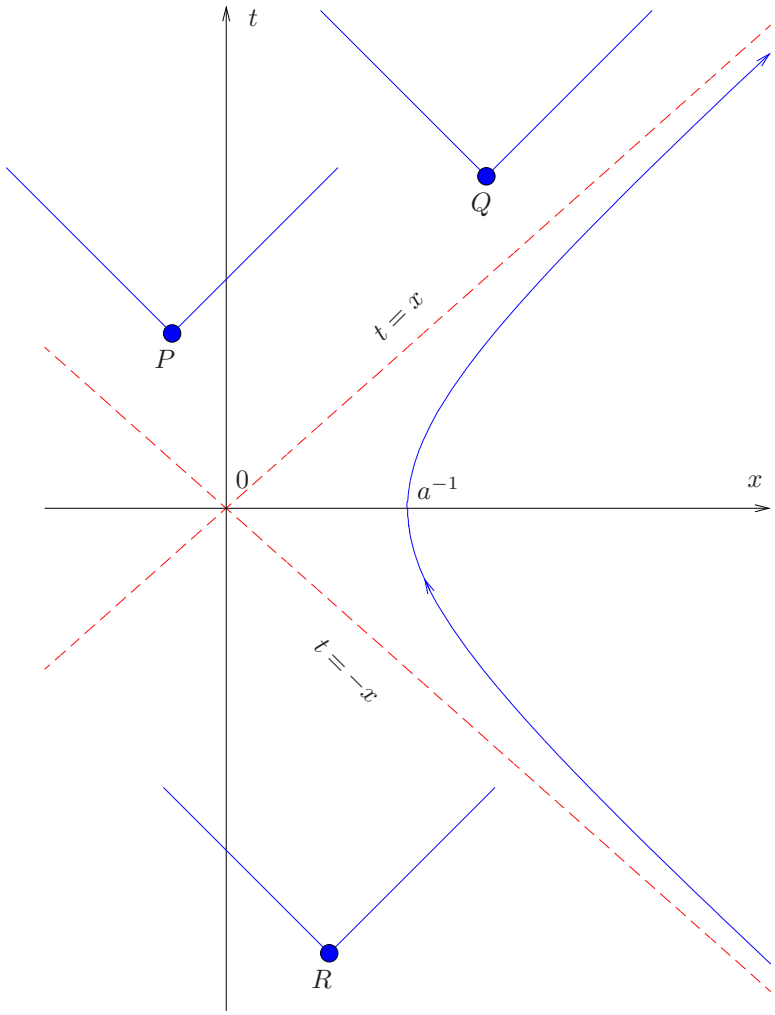


Figure 8.1: The worldline of a uniformly accelerated observer (proper acceleration $a \equiv |\mathbf{a}|$) in the Minkowski spacetime. The dashed lines show the light-cone. The observer cannot receive any signals from the events P, Q and cannot send signals to R.

far end of the stick correspond to the laboratory coordinates

$$t(\tau,\xi) = x^0(\tau) + s^0_{(\text{lab})} = x^0(\tau) + \frac{dx^1(\tau)}{d\tau}\xi, \tag{8.4}$$

$$x(\tau,\xi) = x^1(\tau) + s^1_{(\text{lab})} = x^1(\tau) + \frac{dx^0(\tau)}{d\tau}\xi. \tag{8.5}$$

Note that the relations (8.4)-(8.5) specify the proper frame for *any* trajectory $x^{0,1}(\tau)$ in the 1+1-dimensional Minkowski spacetime.

Now we can substitute Eq. (8.3) into the above relations to compute the proper coordinates for a uniformly accelerated observer. We choose the initial conditions $x^0(0) = 0$, $x^1(0) = a^{-1}$ for the observer's trajectory and obtain

$$t(\tau,\xi) = \frac{1+a\xi}{a}\sinh a\tau, \tag{8.6}$$

$$x(\tau,\xi) = \frac{1+a\xi}{a}\cosh a\tau. \tag{8.7}$$

The converse relations are

$$\tau(t,x) = \frac{1}{2a}\ln\frac{x+t}{x-t},$$
$$\xi(t,x) = -a^{-1} + \sqrt{x^2-t^2}.$$

The horizon

From Eqs. (8.6)-(8.7) it can be seen that the coordinates (τ,ξ) vary in the intervals $-\infty < \tau < +\infty$ and $-a^{-1} < \xi < +\infty$. In particular, for $\xi < -a^{-1}$ we would find $\partial t/\partial\tau < 0$, i.e. the direction of time t would be opposite to that of τ. One can verify that an accelerated observer cannot measure distances longer than a^{-1} in the direction opposite to the acceleration, for instance, the distances to the events P and Q in Fig. 8.1. A measurement of the distance to a point requires to place a clock at that point and to synchronize that clock with the observer's clock. However, the observer cannot synchronize clocks with the events P and Q because no signals can be ever received from these events. One says that the accelerated observer perceives a *horizon* at proper distance a^{-1}.

The coordinate system (8.6)-(8.7) is incomplete and covers only a "quarter" of the Minkowski spacetime, more precisely, the subdomain $x > |t|$ (see Fig. 8.2). This is the subdomain of the Minkowski spacetime accessible to a uniformly accelerated observer. For instance, the events P, Q, R cannot be described by (real) values of τ and ξ. The past lightcone $x = -t$ corresponds to the proper coordinates $\tau = -\infty$ and $\xi = -a^{-1}$. The observer can see signals from the event R, however these signals appear to have originated not from R but from the horizon $\xi = -a^{-1}$ in the infinite past $\tau = -\infty$.

Another way to see that the line $\xi = -a^{-1}$ is a horizon is to consider a line of constant proper length $\xi = \xi_0 > -a^{-1}$. It follows from Eqs. (8.6)-(8.7) that the line

$\xi = \xi_0$ is a trajectory of the form $x^2 - t^2 =$ const with the proper acceleration

$$a_0 \equiv \frac{1}{\sqrt{x^2 - t^2}} = \left(\xi_0 + a^{-1}\right)^{-1}.$$

The observer cannot hold a rigid measuring stick longer than a^{-1} because the point $\xi = -a^{-1}$ of the stick would have to move with an infinite proper acceleration, which would require an infinitely large force and is thus impossible.

8.1.2 The Rindler spacetime

The Minkowski metric in the proper coordinates (τ, ξ) is

$$ds^2 = dt^2 - dx^2 = (1 + a\xi)^2 d\tau^2 - d\xi^2. \tag{8.8}$$

The spacetime with this metric is called the Rindler spacetime. The curvature of the Rindler spacetime is everywhere zero since it differs from the Minkowski spacetime merely by a change of coordinates.

> **Exercise 8.1**
> Derive the metric (8.8) from Eqs. (8.6)-(8.7).

To develop the quantum field theory in the Rindler spacetime, we first rewrite the metric (8.8) in a conformally flat form. This can be achieved by choosing the new spatial coordinate $\tilde{\xi}$ such that $d\xi = (1 + a\xi)d\tilde{\xi}$, because in that case both $d\tau^2$ and $d\tilde{\xi}^2$ will have a common factor $(1 + a\xi)^2$. The necessary replacement is therefore

$$\tilde{\xi} \equiv \frac{1}{a} \ln(1 + a\xi).$$

Since the proper distance ξ is constrained by $\xi > -a^{-1}$, the conformal distance $\tilde{\xi}$ varies in the interval $-\infty < \tilde{\xi} < +\infty$. The metric becomes

$$ds^2 = e^{2a\tilde{\xi}}(d\tau^2 - d\tilde{\xi}^2). \tag{8.9}$$

The relation between the laboratory coordinates and the conformal coordinates is

$$t(\tau, \tilde{\xi}) = a^{-1} e^{a\tilde{\xi}} \sinh a\tau, \quad x(\tau, \tilde{\xi}) = a^{-1} e^{a\tilde{\xi}} \cosh a\tau. \tag{8.10}$$

8.2 Quantum fields in the Rindler spacetime

The goal of this section is to quantize a scalar field in the proper reference frame of a uniformly accelerated observer. To simplify the problem, we consider a massless scalar field in the 1+1-dimensional spacetime. All physical conclusions will be the same as those drawn from a four-dimensional calculation.

The action for a massless scalar field $\phi(t, x)$ is

$$S[\phi] = \frac{1}{2} \int g^{\alpha\beta} \phi_{,\alpha} \phi_{,\beta} \sqrt{-g} d^2x.$$

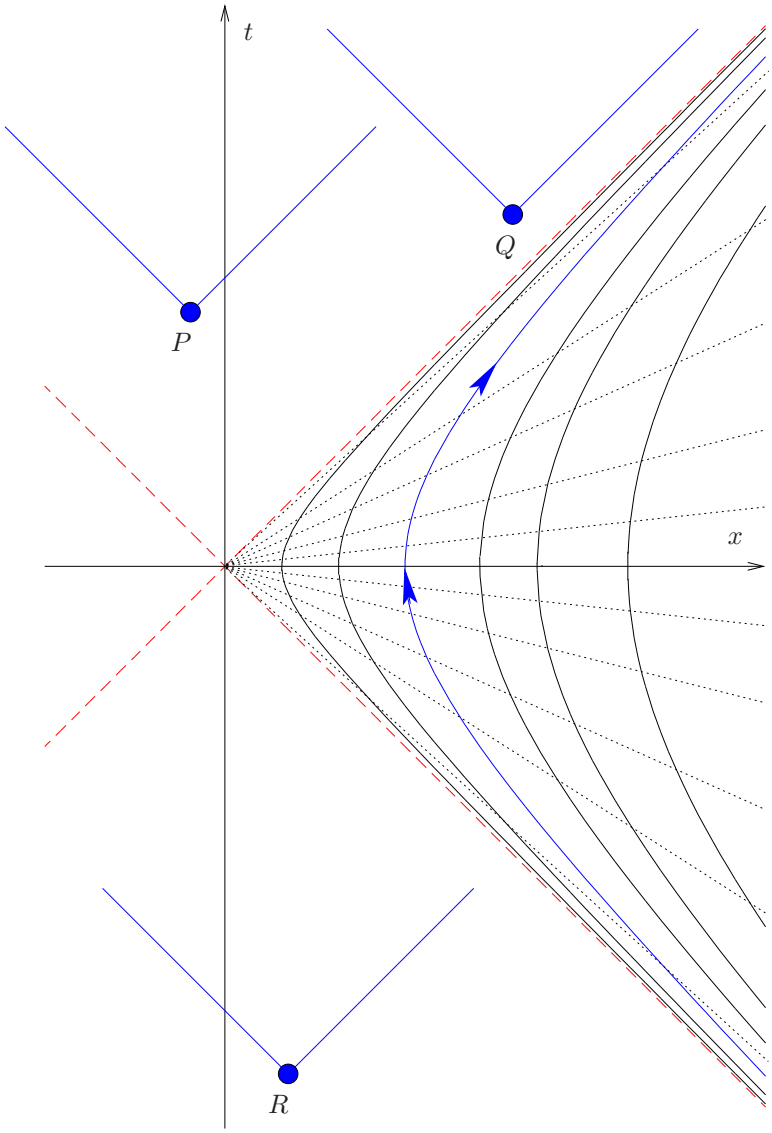


Figure 8.2: The proper coordinate system of a uniformly accelerated observer in the Minkowski spacetime. The solid hyperbolae are the lines of constant proper distance ξ; the hyperbola with arrows is $\xi = 0$, or $x^2 - t^2 = a^{-2}$. The lines of constant τ are dotted. The dashed lines show the lightcone which corresponds to $\xi = -a^{-1}$. The events P, Q, R are not covered by the proper coordinate system.

Here $x^\mu \equiv (t, x)$ is the two-dimensional coordinate. It is easy to see that this action is conformally invariant: indeed, if we replace

$$g_{\alpha\beta} \to \tilde{g}_{\alpha\beta} = \Omega^2(t, x) g_{\alpha\beta},$$

then the determinant $\sqrt{-g}$ and the contravariant metric are replaced by

$$\sqrt{-g} \to \Omega^2 \sqrt{-g}, \quad g^{\alpha\beta} \to \Omega^{-2} g^{\alpha\beta}, \tag{8.11}$$

so the factors Ω^2 cancel in the action. Therefore the minimally coupled massless scalar field in the 1+1-dimensional Minkowski spacetime is in fact *conformally* coupled. The conformal invariance causes a significant simplification of the theory in 1+1 dimensions. (Note that a minimally coupled massless scalar field in 3+1 dimensions is *not* conformally coupled!)

In the laboratory coordinates (t, x), the action is

$$S[\phi] = \frac{1}{2} \int \left[(\partial_t \phi)^2 - (\partial_x \phi)^2 \right] dt\, dx.$$

In the conformal coordinates, the metric (8.9) is equal to the flat Minkowski metric multiplied by a conformal factor $\Omega^2(\tau, \tilde{\xi}) \equiv \exp(2a\tilde{\xi})$. Therefore, due to the conformal invariance, the action has the same form in the coordinates $(\tau, \tilde{\xi})$:

$$S[\phi] = \frac{1}{2} \int \left[(\partial_\tau \phi)^2 - (\partial_{\tilde{\xi}} \phi)^2 \right] d\tau\, d\tilde{\xi}.$$

The classical equations of motion in the laboratory frame and in the accelerated frame are

$$\frac{\partial^2 \phi}{\partial t^2} - \frac{\partial^2 \phi}{\partial x^2} = 0; \quad \frac{\partial^2 \phi}{\partial \tau^2} - \frac{\partial^2 \phi}{\partial \tilde{\xi}^2} = 0,$$

with the general solutions

$$\phi(t, x) = A(t - x) + B(t + x), \quad \phi(\tau, \tilde{\xi}) = P(\tau - \tilde{\xi}) + Q(\tau + \tilde{\xi}).$$

Here A, B, P, and Q are arbitrary smooth functions. Note that a solution $\phi(t, x)$ representing a certain state of the field will be a very different function of τ and $\tilde{\xi}$.

8.2.1 Quantization

We shall now quantize the field ϕ and compare the vacuum states in the laboratory frame and in the accelerated frame.

The procedure of quantization is formally the same in both coordinate systems (t, x) and $(\tau, \tilde{\xi})$. The mode expansion in the laboratory frame is found from Eq. (4.17) with the substitution $\omega_k = |k|$:

$$\hat{\phi}(t, x) = \int_{-\infty}^{+\infty} \frac{dk}{(2\pi)^{1/2}} \frac{1}{\sqrt{2\,|k|}} \left[e^{-i|k|t + ikx} \hat{a}_k^- + e^{i|k|t - ikx} \hat{a}_k^+ \right]. \tag{8.12}$$

The normalization factor $(2\pi)^{1/2}$ is used in 1+1 dimensions instead of the factor $(2\pi)^{3/2}$ used in 3+1 dimensions. The creation and annihilation operators $\hat{a}_k^+$ defined by Eq. (8.12) satisfy the usual commutation relations and describe particles moving with momentum k either in the positive x direction ($k > 0$) or in the negative x direction ($k < 0$).

> **Remark: the zero mode.** The mode expansion (8.12) ignores the $k = 0$ solution, $\phi(t, x) = c_0 + c_1 t$, called the *zero mode*. Quantization of the zero mode in the 1+1-dimensional spacetime is a somewhat complicated technical issue. However, the zero mode does not contribute to the four-dimensional theory and we ignore it here.

The vacuum state in the laboratory frame (the *Minkowski vacuum*), denoted by $|0_M\rangle$, is the zero eigenvector of all annihilation operators $\hat{a}_k^-$,

$$\hat{a}_k^- \, |0_M\rangle = 0 \quad \text{for all } k.$$

The mode expansion in the accelerated frame is quite similar to Eq. (8.12),

$$\hat{\phi}(\tau, \tilde{\xi}) = \int_{-\infty}^{+\infty} \frac{dk}{(2\pi)^{1/2}} \frac{1}{\sqrt{2\,|k|}} \left[e^{-i|k|\tau + ik\tilde{\xi}} \hat{b}_k^- + e^{i|k|\tau - ik\tilde{\xi}} \hat{b}_k^+ \right]. \tag{8.13}$$

Note that the mode expansions (8.12) and (8.13) are decompositions of the operator $\hat{\phi}(x, t)$ into linear combinations of two different sets of basis functions with operator-valued coefficients $\hat{a}_k^\pm$ and $\hat{b}_k^\pm$. So it is to be expected that the operators $\hat{a}_k^\pm$ and $\hat{b}_k^\pm$ are different, although they satisfy similar commutation relations.

The vacuum state in the accelerated frame $|0_R\rangle$ (the *Rindler vacuum*) is defined by

$$\hat{b}_k^- \, |0_R\rangle = 0 \quad \text{for all } k.$$

Since the operators $\hat{b}_k$ differ from $\hat{a}_k$, the Rindler vacuum $|0_R\rangle$ and the Minkowski vacuum $|0_M\rangle$ are two *different* quantum states of the field $\hat{\phi}$.

At this point, a natural question to ask is whether the state $|0_M\rangle$ or $|0_R\rangle$ is the "correct" vacuum. To answer this question, we need to consider the physical interpretation of the states $|0_M\rangle$ and $|0_R\rangle$ in a particular (perhaps imaginary) physical experiment. In Sec. 6.3.2 we discussed a hypothetical device for preparing the quantum field in the lowest-energy state. If mounted onto an accelerated spaceship, the device will prepare the field in the quantum state $|0_R\rangle$. All observers moving with the ship would agree that the field in the state $|0_R\rangle$ has the lowest possible energy, while the Minkowski state $|0_M\rangle$ has a higher energy. Thus a particle detector which remains at rest in the accelerated frame will register particles when the field is in the state $|0_M\rangle$. However, in the laboratory frame the state with the lowest energy is $|0_M\rangle$ and the state $|0_R\rangle$ has a higher energy. Therefore, if the field is in the Rindler state $|0_R\rangle$ (the vacuum prepared inside the spaceship), it will appear to be in an excited state when examined by observers in the laboratory frame.

Neither of the two vacuum states is "more correct" if considered by itself, without regard for realistic physical conditions in the universe. Ultimately the choice of vacuum is determined by experiment: the correct vacuum state must be such that the

theoretical predictions agree with available experimental data. In an inertial reference frame in the Minkowski spacetime, we observe empty space that does not create any particles by itself. By virtue of this observation, we are justified to assume that fields in the empty Minkowski spacetime are in the vacuum state $|0_M\rangle$ and that any excitations in the field modes are always due to external sources. In particular, an accelerated observer moving through empty space will encounter fields in the state $|0_M\rangle$ and therefore will detect particles. This detection is the manifestation of the Unruh effect.

The rest of this chapter is devoted to a calculation relating the Minkowski frame operators $\hat{a}_k^{\pm}$ to the Rindler frame operators $\hat{b}_k^{\pm}$ through the appropriate Bogolyubov coefficients. This calculation will enable us to express the Minkowski vacuum as a superposition of excited states built on top of the Rindler vacuum and thus to compute the probability distribution for particle occupation numbers observed in the accelerated frame.

8.2.2 Lightcone mode expansions

It is convenient to introduce the lightcone coordinates[1]

$$\bar{u} \equiv t - x,\ \bar{v} \equiv t + x; \quad u \equiv \tau - \tilde{\xi},\ v \equiv \tau + \tilde{\xi}.$$

The relation between the laboratory frame and the accelerated frame has a simpler form in lightcone coordinates: from Eq. (8.10) we find

$$\bar{u} = -a^{-1}e^{-au}, \quad \bar{v} = a^{-1}e^{av}, \tag{8.14}$$

so the metric is

$$ds^2 = d\bar{u}\, d\bar{v} = e^{a(v-u)} du\, dv.$$

The field equations and their general solutions are also expressed more concisely in the lightcone coordinates:

$$\begin{aligned} &\frac{\partial^2}{\partial\bar{u}\partial\bar{v}}\phi\left(\bar{u},\bar{v}\right) = 0, \quad \phi\left(\bar{u},\bar{v}\right) = A\left(\bar{u}\right) + B\left(\bar{v}\right); \\ &\frac{\partial^2}{\partial u\partial v}\phi(u,v) = 0, \quad \phi(u,v) = P(u) + Q(v). \end{aligned} \tag{8.15}$$

The mode expansion (8.12) can be rewritten in the coordinates $\bar{u}, \bar{v}$ by first splitting the integration into the ranges of positive and negative k,

$$\begin{aligned} \hat{\phi}(t,x) = &\int_{-\infty}^{0} \frac{dk}{(2\pi)^{1/2}} \frac{1}{\sqrt{2\,|k|}} \left[e^{ikt+ikx}\hat{a}_k^- + e^{-ikt-ikx}\hat{a}_k^+\right] \\ &+ \int_{0}^{+\infty} \frac{dk}{(2\pi)^{1/2}} \frac{1}{\sqrt{2k}} \left[e^{-ikt+ikx}\hat{a}_k^- + e^{ikt-ikx}\hat{a}_k^+\right]. \end{aligned}$$

[1] The chosen notation (u, v) for the lightcone coordinates in a uniformly accelerated frame and $(\bar{u}, \bar{v})$ for the freely falling (unaccelerated) frame will be used in Chapter 9 as well.

Then we introduce $\omega = |k|$ as the integration variable with the range $0 < \omega < +\infty$ and obtain the *lightcone mode expansion*

$$\hat{\phi}(\bar{u},\bar{v}) = \int_0^{+\infty} \frac{d\omega}{(2\pi)^{1/2}} \frac{1}{\sqrt{2\omega}} \left[e^{-i\omega\bar{u}} \hat{a}_\omega^- + e^{i\omega\bar{u}} \hat{a}_\omega^+ + e^{-i\omega\bar{v}} \hat{a}_{-\omega}^- + e^{i\omega\bar{v}} \hat{a}_{-\omega}^+ \right]. \quad (8.16)$$

Lightcone mode expansions explicitly decompose the field $\hat{\phi}(\bar{u},\bar{v})$ into a sum of functions of $\bar{u}$ and functions of $\bar{v}$. This agrees with Eq. (8.15) from which we find that $A(\bar{u})$ is a linear combination of the operators $\hat{a}_\omega^\pm$ with positive momenta ω, while $B(\bar{v})$ is a linear combination of $\hat{a}_{-\omega}^\pm$ with negative momenta $-\omega$:

$$\begin{aligned}
\hat{\phi}(\bar{u},\bar{v}) &= \hat{A}(\bar{u}) + \hat{B}(\bar{v}); \\
\hat{A}(\bar{u}) &= \int_0^{+\infty} \frac{d\omega}{(2\pi)^{1/2}} \frac{1}{\sqrt{2\omega}} \left[e^{-i\omega\bar{u}} \hat{a}_\omega^- + e^{i\omega\bar{u}} \hat{a}_\omega^+ \right], \\
\hat{B}(\bar{v}) &= \int_0^{+\infty} \frac{d\omega}{(2\pi)^{1/2}} \frac{1}{\sqrt{2\omega}} \left[e^{-i\omega\bar{v}} \hat{a}_{-\omega}^- + e^{i\omega\bar{v}} \hat{a}_{-\omega}^+ \right].
\end{aligned}$$

The lightcone mode expansion in the Rindler frame has exactly the same form except for involving the coordinates (u,v) instead of $(\bar{u},\bar{v})$. We use the integration variable Ω to distinguish the Rindler frame expansion from that of the Minkowski frame,

$$\begin{aligned}
\hat{\phi}(u,v) &= \hat{P}(u) + \hat{Q}(v) \\
&= \int_0^{+\infty} \frac{d\Omega}{(2\pi)^{1/2}} \frac{1}{\sqrt{2\Omega}} \left[e^{-i\Omega u} \hat{b}_\Omega^- + e^{i\Omega u} \hat{b}_\Omega^+ + e^{-i\Omega v} \hat{b}_{-\Omega}^- + e^{i\Omega v} \hat{b}_{-\Omega}^+ \right]. \quad (8.17)
\end{aligned}$$

As before, $\hat{P}(u)$ is expanded into operators $\hat{b}_\Omega^\pm$ with positive momenta Ω and $\hat{Q}(v)$ into the operators $\hat{b}_{-\Omega}^\pm$ with negative momenta $-\Omega$. (Note that in all lightcone mode expansions, the variables ω and Ω take only *positive* values.)

8.2.3 The Bogolyubov transformations

The relation between the operators $\hat{a}_{\pm\omega}^\pm$ and $\hat{b}_{\pm\Omega}^\pm$, which we shall presently derive, is a Bogolyubov transformation of a more general form than that considered in Sec. 6.2.2.

Since the coordinate transformation (8.14) does not mix u and v, the identity

$$\hat{\phi}(u,v) = \hat{A}(\bar{u}(u)) + \hat{B}(\bar{v}(v)) = \hat{P}(u) + \hat{Q}(v)$$

entails two separate relations for u and for v,

$$\hat{A}(\bar{u}(u)) = \hat{P}(u), \quad \hat{B}(\bar{v}(v)) = \hat{Q}(v).$$

Comparing the expansions (8.16) and (8.17), we find that the operators $\hat{a}_\omega^\pm$ with positive momenta ω are expressed through $\hat{b}_\Omega^\pm$ with positive momenta Ω, while the operators $\hat{a}_{-\omega}^\pm$ are expressed through negative-momentum operators $\hat{b}_{-\Omega}^\pm$. In other words,

there is no mixing between operators of positive and negative momentum. The relation $\hat{A}(\bar{u}) = \hat{P}(u)$ is then rewritten as

$$\begin{aligned}\hat{A}(\bar{u}) &= \int_0^{+\infty} \frac{d\omega}{(2\pi)^{1/2}} \frac{1}{\sqrt{2\omega}} \left[e^{-i\omega\bar{u}}\hat{a}_\omega^- + e^{i\omega\bar{u}}\hat{a}_\omega^+\right] \\ =\hat{P}(u) &= \int_0^{+\infty} \frac{d\Omega}{(2\pi)^{1/2}} \frac{1}{\sqrt{2\Omega}} \left[e^{-i\Omega u}\hat{b}_\Omega^- + e^{i\Omega u}\hat{b}_\Omega^+\right]. \end{aligned} \tag{8.18}$$

Here $\bar{u}$ is understood to be the function of u given by Eq. (8.14); both sides of Eq. (8.18) are equal as functions of u.

We can now express the positive-momentum operators $\hat{a}_\omega^\pm$ as explicit linear combinations of $\hat{b}_\Omega^\pm$. To this end, we perform the Fourier transform of both sides of Eq. (8.18) in u. The RHS yields

$$\int_{-\infty}^{+\infty} \frac{du}{\sqrt{2\pi}} e^{i\Omega u}\hat{P}(u) = \frac{1}{\sqrt{2\,|\Omega|}} \begin{cases} \hat{b}_\Omega^-, & \Omega > 0; \\ \hat{b}_{|\Omega|}^+, & \Omega < 0. \end{cases} \tag{8.19}$$

(The Fourier transform variable is denoted also by Ω for convenience.) The Fourier transform of the LHS of Eq. (8.18) yields an expression involving all $\hat{a}_\omega^\pm$,

$$\begin{aligned}\int_{-\infty}^{+\infty} \frac{du}{\sqrt{2\pi}} e^{i\Omega u}\hat{A}(\bar{u}) &= \int_0^{\infty} \frac{d\omega}{\sqrt{2\omega}} \int_{-\infty}^{+\infty} \frac{du}{2\pi} \left[e^{i\Omega u - i\omega\bar{u}}\hat{a}_\omega^- + e^{i\Omega u + i\omega\bar{u}}\hat{a}_\omega^+\right] \\ &\equiv \int_0^{\infty} \frac{d\omega}{\sqrt{2\omega}} \left[F(\omega,\Omega)\hat{a}_\omega^- + F(-\omega,\Omega)\hat{a}_\omega^+\right], \end{aligned} \tag{8.20}$$

where we introduced the auxiliary function[2]

$$F(\omega,\Omega) \equiv \int_{-\infty}^{+\infty} \frac{du}{2\pi} e^{i\Omega u - i\omega\bar{u}} = \int_{-\infty}^{+\infty} \frac{du}{2\pi} \exp\left[i\Omega u + i\frac{\omega}{a}e^{-au}\right]. \tag{8.21}$$

Comparing Eqs. (8.19) and (8.20) restricted to positive Ω, we find that the relation between $\hat{a}_\omega^\pm$ and $\hat{b}_\Omega^-$ is of the form

$$\hat{b}_\Omega^- = \int_0^{\infty} d\omega \left[\alpha_{\omega\Omega}\hat{a}_\omega^- + \beta_{\omega\Omega}\hat{a}_\omega^+\right], \tag{8.22}$$

where the coefficients $\alpha_{\omega\Omega}$ and $\beta_{\omega\Omega}$ are

$$\alpha_{\omega\Omega} = \sqrt{\frac{\Omega}{\omega}}F(\omega,\Omega), \quad \beta_{\omega\Omega} = \sqrt{\frac{\Omega}{\omega}}F(-\omega,\Omega); \quad \omega > 0, \Omega > 0. \tag{8.23}$$

[2] Because of the carelessly interchanged order of integration while deriving Eq. (8.20), the integral (8.21) diverges at $u \to +\infty$ and the definition of $F(\omega,\Omega)$ must be understood in the distributional sense. In Appendix A.3 it is shown how to express $F(\omega,\Omega)$ through Euler's gamma function, but we shall not need that representation.

The operators $\hat{b}^+_\Omega$ can be similarly expressed through $\hat{a}^\pm_\omega$ using the Hermitian conjugation of Eq. (8.22) and the identity

$$F^*(\omega,\Omega) = F(-\omega,-\Omega).$$

The relation (8.22) is a Bogolyubov transformation that mixes creation and annihilation operators with different momenta $\omega \neq \Omega$. In contrast, the Bogolyubov transformations considered in Sec. 6.2.2 are "diagonal," with $\alpha_{\omega\Omega}$ and $\beta_{\omega\Omega}$ proportional to $\delta(\omega-\Omega)$.

The relation between the operators $\hat{a}^\pm_{-\omega}$ and $\hat{b}^\pm_{-\Omega}$ is obtained from the equation $\hat{B}(\bar{v}) = \hat{Q}(v)$. We omit the corresponding straightforward calculations and concentrate on the positive-momentum modes; the results for negative momenta are completely analogous.

General Bogolyubov transformations

We need to briefly consider the properties of general Bogolyubov transformations,

$$\hat{b}^-_\Omega = \int_{-\infty}^{+\infty} d\omega \left[\alpha_{\omega\Omega}\hat{a}^-_\omega + \beta_{\omega\Omega}\hat{a}^+_\omega\right]. \tag{8.24}$$

The relation (8.22) is of this form except for the integration over $0<\omega<+\infty$ which is justified because the only nonzero Bogolyubov coefficients are those relating the momenta ω,Ω of equal sign, i.e. $\alpha_{-\omega,\Omega}=0$ and $\beta_{-\omega,\Omega}=0$. But for now we shall not limit ourselves to this case.

The relation for the operator $\hat{b}^+_\Omega$ is the Hermitian conjugate of Eq. (8.24).

> **Remark:** To avoid confusion in the notation, we always write the indices ω,Ω in the Bogolyubov coefficients in this order, i.e. $\alpha_{\omega\Omega}$, but never $\alpha_{\Omega\omega}$. In the calculations throughout this chapter, the integration is always over the first index ω corresponding to the momentum of a-particles.

Since the operators $\hat{a}^\pm_\omega$, $\hat{b}^\pm_\Omega$ satisfy the commutation relations

$$\left[\hat{a}^-_\omega,\hat{a}^+_{\omega'}\right] = \delta(\omega-\omega'), \quad \left[\hat{b}^-_\Omega,\hat{b}^+_{\Omega'}\right] = \delta(\Omega-\Omega'), \tag{8.25}$$

the Bogolyubov coefficients are constrained by

$$\int_{-\infty}^{+\infty} d\omega\,(\alpha_{\omega\Omega}\alpha^*_{\omega\Omega'} - \beta_{\omega\Omega}\beta^*_{\omega\Omega'}) = \delta(\Omega-\Omega'). \tag{8.26}$$

This is analogous to the normalization condition $|\alpha_{\mathbf{k}}|^2 - |\beta_{\mathbf{k}}|^2 = 1$ we had earlier.

> **Exercise 8.2**
> Derive Eq. (8.26).

Note that the origin of the δ function in Eq. (8.25) is the infinite volume of the entire space. If the field were quantized in a finite box of volume V, the momenta ω and Ω would be discrete and the δ function would be replaced by the ordinary Kronecker

symbol times the volume factor, i.e. $V\delta_{\Omega\Omega'}$. The δ function in Eq. (8.26) has the same origin. Below we shall use Eq. (8.26) with $\Omega = \Omega'$ and the divergent factor $\delta(0)$ will be interpreted as the infinite spatial volume.

Remark: inverse Bogolyubov transformations. The commutation relation $[\hat{b}^-_\Omega, \hat{b}^-_{\Omega'}] = 0$ yields another restriction on the Bogolyubov coefficients,

$$\int_{-\infty}^{+\infty} d\omega \left(\alpha_{\omega\Omega}\beta_{\omega\Omega'} - \alpha_{\omega\Omega'}\beta_{\omega\Omega}\right) = 0. \tag{8.27}$$

It follows from Eqs. (8.26), (8.27) that the inverse Bogolyubov transformation is

$$\hat{a}^-_\omega = \int_{-\infty}^{+\infty} d\Omega \left(\alpha^*_{\omega\Omega}\hat{b}^-_\Omega - \beta_{\omega\Omega}\hat{b}^+_\Omega\right).$$

This relation can be easily verified by substituting it into Eq. (8.24). One can also derive orthogonality relations similar to Eqs. (8.26), (8.27) but with the integration over Ω. We shall not need the inverse Bogolyubov transformations in this chapter.

8.2.4 Density of particles

Since the vacua $|0_M\rangle$ and $|0_R\rangle$ corresponding to the operators $\hat{a}^-_\omega$ and $\hat{b}^-_\Omega$ are different, the a-vacuum is a state with b-particles and vice versa. We now compute the density of b-particles in the a-vacuum state.

The b-particle number operator is $\hat{N}_\Omega \equiv \hat{b}^+_\Omega \hat{b}^-_\Omega$, so the average b-particle number in the a-vacuum $|0_M\rangle$ is equal to the expectation value of $\hat{N}_\Omega$,

$$\begin{aligned}\langle \hat{N}_\Omega \rangle &\equiv \langle 0_M | \hat{b}^+_\Omega \hat{b}^-_\Omega | 0_M \rangle \\ &= \langle 0_M | \int d\omega \left[\alpha^*_{\omega\Omega}\hat{a}^+_\omega + \beta^*_{\omega\Omega}\hat{a}^-_\omega\right] \int d\omega' \left[\alpha_{\omega'\Omega}\hat{a}^-_{\omega'} + \beta_{\omega'\Omega}\hat{a}^+_{\omega'}\right] | 0_M \rangle \\ &= \int d\omega \, |\beta_{\omega\Omega}|^2 .\end{aligned} \tag{8.28}$$

This is the mean number of particles observed in the accelerated frame.

In principle one can explicitly compute the Bogolyubov coefficients $\beta_{\omega\Omega}$ defined by Eq. (8.23) in terms of the Γ function (see Appendix A.3). However, we only need to evaluate the RHS of Eq. (8.28) which involves an integral over ω, and we shall use a mathematical trick that allows us to compute just that integral and avoid cumbersome calculations.

We first note that the function $F(\omega, \Omega)$ satisfies the identity

$$F(\omega, \Omega) = F(-\omega, \Omega) \exp\left(\frac{\pi\Omega}{a}\right), \quad \text{for } \omega > 0,\ a > 0. \tag{8.29}$$

Exercise 8.3*
Derive the relation (8.29) from Eq. (8.21). *Hint:* deform the contour of integration in the complex plane.

We then substitute Eq. (8.23) into the normalization condition (8.26), use Eq. (8.29) and find

$$\begin{aligned}\delta(\Omega-\Omega') &= \int_0^{+\infty} d\omega \frac{\sqrt{\Omega\Omega'}}{\omega}\left[F(\omega,\Omega)F^*(\omega,\Omega') - F(-\omega,\Omega)F^*(-\omega,\Omega')\right] \\ &= \left[\exp\left(\frac{\pi\Omega+\pi\Omega'}{a}\right)-1\right]\int_0^{+\infty} d\omega \frac{\Omega}{\omega}F^*(-\omega,\Omega)F(-\omega,\Omega).\end{aligned}$$

The last line above yields the relation

$$\int_0^{+\infty} d\omega \frac{\Omega}{\omega}F(-\omega,\Omega)F^*(-\omega,\Omega') = \left[\exp\left(\frac{2\pi\Omega}{a}\right)-1\right]^{-1}\delta(\Omega-\Omega'). \tag{8.30}$$

Setting $\Omega'=\Omega$ in Eq. (8.30), we directly compute the integral in the RHS of Eq. (8.28),

$$\langle\hat{N}_\Omega\rangle = \int_0^{+\infty} d\omega\,|\beta_{\omega\Omega}|^2 = \int_0^{+\infty} d\omega\frac{\Omega}{\omega}\,|F(-\omega,\Omega)|^2 = \left[\exp\left(\frac{2\pi\Omega}{a}\right)-1\right]^{-1}\delta(0).$$

As usual, we expect $\langle\hat{N}_\Omega\rangle$ to be divergent since it is the total number of particles in the entire space. As discussed in Sec. 4.2, the divergent volume factor $\delta(0)$ represents the volume of space, and the remaining factor is the density n_Ω of b-particles with momentum Ω:

$$\int_0^{+\infty} d\omega\,|\beta_{\omega\Omega}|^2 \equiv n_\Omega\delta(0).$$

Therefore, the mean density of particles in the mode with momentum Ω is

$$n_\Omega = \left[\exp\left(\frac{2\pi\Omega}{a}\right)-1\right]^{-1}. \tag{8.31}$$

This is the main result of this chapter.

So far we have computed n_Ω only for positive-momentum modes (with $\Omega>0$). The result for negative-momentum modes is obtained by replacing Ω by $|\Omega|$ in Eq. (8.31).

8.2.5 The Unruh temperature

A massless particle with momentum Ω has energy $E=|\Omega|$, so the formula (8.31) is equivalent to the Bose distribution

$$n(E) = \left[\exp\left(\frac{E}{T}\right)-1\right]^{-1}$$

where T is the *Unruh temperature*

$$T \equiv \frac{a}{2\pi}.$$

We found that an accelerated observer detects particles when the field ϕ is in the Minkowski vacuum state $|0_M\rangle$. The detected particles may have any momentum Ω, although the probability for registering a high-energy particle is very small. The particle distribution (8.31) is characteristic of the thermal blackbody radiation with the temperature $T = a/2\pi$, where a is the magnitude of the proper acceleration (in Planck units). An accelerated detector behaves as though it were placed in a thermal bath with temperature T. This is the Unruh effect.

> **Remark: conformal invariance.** Earlier we said that a conformally coupled field cannot exhibit particle production by gravity. This is not in contradiction with the detection of particles in accelerated frames. Conformal invariance means that identical initial conditions produce identical evolution in all conformally related frames. If the lowest-energy state is prepared in the accelerated frame (this is the Rindler vacuum $|0_R\rangle$) and later the number of particles is measured by a detector that remains accelerated in the same frame, then no particles will be registered after arbitrarily long times. This is exactly the same prediction as that obtained in the laboratory frame. Nevertheless, the vacuum state prepared in one frame of reference may be a state with particles in another frame.

A physical interpretation of the Unruh effect as seen in the laboratory frame is the following. The accelerated detector is coupled to the quantum fields and perturbs their quantum state around its trajectory. This perturbation is very small but as a result the detector registers particles, although the fields were previously in the vacuum state. The detected particles are real and the energy for these particles comes from the agent that accelerates the detector.

Finally, we note that the Unruh effect is impossible to use in practice because the acceleration required to produce a measurable temperature is enormous (see Exercise 1.6 on p. 12 for a numerical example). The energy spent by the accelerating agent is exponentially large compared with the energy in detected particles. The Unruh effect is an extremely inefficient way to produce particles.

> **Remark: more general motion.** Observers moving with a nonconstant acceleration will generally also detect particles but with a nonthermal spectrum. For a general trajectory $x^\mu(\tau)$ it is difficult to construct a proper reference frame; instead one considers a quantum-mechanical model of a detector coupled to the field $\phi(x)$ and computes the probability for observing an excited state of the detector. A calculation of this sort was first performed by W. G. Unruh; see the book by Birrell and Davies, §3.2.

9 The Hawking effect. Thermodynamics of black holes

Summary: Quantization of fields in a black hole spacetime. Choice of vacuum. Hawking radiation. Black hole evaporation. Thermodynamics of black holes.

In this chapter we consider a counter-intuitive effect: emission of particles by black holes.

9.1 The Hawking radiation

Classical general relativity describes black holes as massive objects with such a strong gravitational field that even light cannot escape their surface (the *black hole horizon*). However, quantum theory predicts that black holes emit particles moving away from the horizon. The particles are produced out of vacuum fluctuations of quantum fields present around the black hole. In effect, a black hole (BH) is not completely black but radiates a dim light as if it were an object with a low but nonzero temperature.

The theoretical prediction of radiation by black holes came as a complete surprise. It was thought that particles may be produced only by time-dependent gravitational fields. The first rigorous calculation of the rate of particle creation by a rotating BH was performed in 1974 by S. Hawking. He expected that in the limit of no rotation the particle production should disappear, but instead he found that nonrotating (static) black holes also create particles at a steady rate. This was so perplexing that Hawking thought he had made a mistake in calculations. It took some years before this theoretically derived effect (the *Hawking radiation*) was accepted by the scientific community.

An intuitive picture of the Hawking radiation involves a virtual particle-antiparticle pair at the BH horizon. It may happen that the first particle of the pair is inside the BH horizon while the second particle is outside. The first virtual particle always falls onto the BH center, but the second particle has a nonzero probability for moving away from the horizon and becoming a real radiated particle. The mass of the black hole is decreased in the process of radiation because the energy of the infalling virtual particle with respect to faraway observers is formally negative.

Another qualitative consideration is that a black hole of size R cannot capture radiation with wavelength much larger than R. It follows that particles (real or virtual) with sufficiently small energies $E \ll \hbar c/R$ might avoid falling into the BH horizon.

This argument indicates the correct order of magnitude for the energy of radiated particles, although it remains unclear whether and how the radiation is actually emitted.

The main focus of this section is to compute the density of particles emitted by a static black hole, as registered by observers far away from the BH horizon.

9.1.1 Scalar field in a BH spacetime

In quantum theory, particles are excitations of quantum fields, so we consider a scalar field in the presence of a single nonrotating black hole of mass M. The BH spacetime is described by the Schwarzschild metric,[1]

$$ds^2 = \left(1 - \frac{2M}{r}\right) dt^2 - \frac{dr^2}{1 - \frac{2M}{r}} - r^2 \left(d\theta^2 + d\varphi^2 \sin^2\theta\right).$$

This metric is singular at $r = 2M$ which corresponds to the BH horizon, while for $r < 2M$ the coordinate t is spacelike and r is timelike. Therefore the coordinates (t, r) may be used with the normal interpretation of time and space only in the exterior region, $r > 2M$.

To simplify the calculations, we assume that the field ϕ is independent of the angular variables θ, φ and restrict our attention to a 1+1-dimensional section of the spacetime with the coordinates (t, r). The line element in 1+1 dimensions,

$$ds^2 = g_{ab} dx^a dx^b, \quad x^0 \equiv t, \; x^1 \equiv r,$$

involves the reduced metric

$$g_{ab} = \begin{bmatrix} 1 - \frac{2M}{r} & 0 \\ 0 & -\left(1 - \frac{2M}{r}\right)^{-1} \end{bmatrix}.$$

The theory we are developing is a toy model (i.e. a drastically simplified version) of the full 3+1-dimensional QFT in the Schwarzschild spacetime. We expect that the main features of the full theory are preserved in the 1+1-dimensional model.

The action for a minimally coupled massless scalar field is

$$S[\phi] = \frac{1}{2} \int g^{ab} \phi_{,a} \phi_{,b} \sqrt{-g} d^2x.$$

As shown in Sec. 8.2, the field ϕ with this action is in fact conformally coupled. Because of the conformal invariance, a significant simplification occurs if the metric is brought to a conformally flat form. This is achieved by changing the coordinate $r \to r^*$, where the function $r^*(r)$ is chosen so that

$$dr = \left(1 - \frac{2M}{r}\right) dr^*.$$

[1] In our notation here and below, the asimuthal angle is φ while the scalar field is ϕ.

From this relation we find $r^*(r)$ up to an integration constant which we choose as $2M$ for convenience,

$$r^*(r) = r - 2M + 2M \ln\left(\frac{r}{2M} - 1\right). \tag{9.1}$$

The metric in the coordinates (t, r^*) is conformally flat,

$$ds^2 = \left(1 - \frac{2M}{r}\right)\left[dt^2 - dr^{*2}\right], \tag{9.2}$$

where r must be expressed through r^* using Eq. (9.1). We shall not need an explicit formula for the function $r(r^*)$.

The coordinate $r^*(r)$ is defined only for $r > 2M$ and varies in the range $-\infty < r^* < +\infty$. It is called the "tortoise coordinate" because an object approaching the horizon $r = 2M$ needs to cross an infinite coordinate distance in r^*. From Eq. (9.2) it is clear that the tortoise coordinates (t, r^*) are asymptotically the same as the Minkowski coordinates (t, r) when $r \to +\infty$, i.e. in regions far from the black hole where the spacetime is almost flat.

The action for the scalar field in the tortoise coordinates is

$$S[\phi] = \frac{1}{2}\int \left[(\partial_t \phi)^2 - (\partial_{r^*}\phi)^2\right] dt\, dr^*,$$

and the general solution of the equation of motion is of the form

$$\phi(t, r^*) = P(t - r^*) + Q(t + r^*),$$

where P and Q are arbitrary (but sufficiently smooth) functions.

In the lightcone coordinates (u, v) defined by

$$u \equiv t - r^*, \quad v \equiv t + r^*, \tag{9.3}$$

the metric is expressed as

$$ds^2 = \left(1 - \frac{2M}{r}\right) du\, dv. \tag{9.4}$$

Note that $r = 2M$ is a singularity where the metric becomes degenerate.

9.1.2 The Kruskal coordinates

The coordinate system (t, r^*) has the advantage that for $r^* \to +\infty$ it asymptotically coincides with the Minkowski coordinate system (t, r) naturally defined far away from the BH horizon. However, the coordinates (t, r^*) do not cover the black hole interior, $r < 2M$. To describe the entire spacetime, we need another coordinate system.

It is a standard result that the singularity in the Schwarzschild metric (9.4) which occurs at $r \to 2M$ is merely a *coordinate singularity* since a suitable change of coordinates yields a metric regular at the BH horizon. For instance, an observer freely falling into the black hole would see a normal, finitely curved space while crossing

the horizon line $r = 2M$. Therefore one is motivated to consider the coordinate system $(\bar{t}, \bar{r})$ describing the proper time $\bar{t}$ and the proper distance $\bar{r}$ measured by a freely falling observer at the moment of horizon crossing. This coordinate system is called the Kruskal frame.

We omit the construction of the Kruskal frame[2] and write only the final formulae. The Kruskal lightcone coordinates

$$\bar{u} \equiv \bar{t} - \bar{r}, \quad \bar{v} \equiv \bar{t} + \bar{r}$$

are related to the tortoise lightcone coordinates (9.3) by

$$\bar{u} = -4M \exp\left(-\frac{u}{4M}\right), \quad \bar{v} = 4M \exp\left(\frac{v}{4M}\right). \tag{9.5}$$

The parameters $\bar{u}$, $\bar{v}$ vary in the intervals

$$-\infty < \bar{u} < 0, \quad 0 < \bar{v} < +\infty. \tag{9.6}$$

The inverse relation between $(\bar{u}, \bar{v})$ and the tortoise coordinates (t, r^*) is then found from Eqs. (9.1) and (9.5):

$$\begin{aligned} t &= 2M \ln\left(-\frac{\bar{v}}{\bar{u}}\right), \\ \exp\left(-\frac{r^*}{2M}\right) &= -\frac{\exp\left(1 - \frac{r}{2M}\right)}{1 - \frac{r}{2M}} = -\frac{16M^2}{\bar{u}\bar{v}}. \end{aligned} \tag{9.7}$$

The BH horizon $r = 2M$ corresponds to the lines $\bar{u} = 0$ and $\bar{v} = 0$. To examine the spacetime near the horizon, we need to rewrite the metric in the Kruskal coordinates. With the substitution

$$u = -4M \ln\left(-\frac{\bar{u}}{4M}\right), \quad v = 4M \ln\frac{\bar{v}}{4M},$$

the metric (9.4) becomes

$$ds^2 = -\frac{16M^2}{\bar{u}\bar{v}}\left(1 - \frac{2M}{r}\right) d\bar{u}\, d\bar{v}.$$

Using Eqs. (9.1) and (9.7), after some algebra we obtain

$$ds^2 = \frac{2M}{r} \exp\left(1 - \frac{r}{2M}\right) d\bar{u}\, d\bar{v}, \tag{9.8}$$

where it is implied that the Schwarzschild coordinate r is expressed through $\bar{u}$ and $\bar{v}$ using the relation (9.7).

It follows from Eq. (9.8) that at $r = 2M$ the metric is $ds^2 = d\bar{u}\, d\bar{v}$, the same as in the Minkowski spacetime. Although the coordinates $\bar{u}, \bar{v}$ were defined in the ranges (9.6),

[2] A detailed derivation can be found, for instance, in §31 of the book *Gravitation* by C.W. MISNER, K. THORNE, and J. WHEELER (W. H. Freeman, San Francisco, 1973).

there is no singularity at $\bar{u} = 0$ or at $\bar{v} = 0$ and therefore the coordinate system may be extended to $\bar{u} > 0$ and $\bar{v} < 0$. Thus the Kruskal coordinates cover a larger patch of the spacetime than the tortoise coordinates (t, r^*). For instance, Eq. (9.7) relates r to $\bar{u}, \bar{v}$ also for $0 < r < 2M$, even though r^* is undefined for these r.

The *Kruskal spacetime* is the extension of the Schwarzschild spacetime described by the Kruskal coordinates $\bar{t}, \bar{r}$.

> **Remark: the physical singularity.** The Kruskal metric (9.8) is undefined at $r = 0$. A calculation shows that the spacetime curvature grows without limit as $r \to 0$. Therefore $r = 0$ (the center of the black hole) is a real singularity where general relativity breaks down. From Eq. (9.7) one finds that $r = 0$ corresponds to the line $\bar{u}\bar{v} = \bar{t}^2 - \bar{r}^2 = 16e^{-1}M^2$. This line is a singular boundary of the Kruskal spacetime; the coordinates $\bar{t}$, $\bar{r}$ vary in the domain $|\bar{t}| < \sqrt{\bar{r}^2 + 16e^{-1}M^2}$.

Since the Kruskal metric (9.8) is conformally flat, the action and the classical field equations for a conformally coupled field in the Kruskal frame have the same form as in the tortoise coordinates. For instance, the general solution for the field ϕ is $\phi(\bar{u}, \bar{v}) = A(\bar{u}) + B(\bar{v})$.

We note that Eq. (9.5) is similar to the definition (8.14) of the proper frame for a uniformly accelerated observer. The formal analogy is exact if we set $a \equiv (4M)^{-1}$. Note that a freely falling observer (with the worldline $\bar{r} = \text{const}$) has zero proper acceleration. On the other hand, a spaceship remaining at a fixed position relative to the BH must keep its engine running at a constant thrust and thus has a constant proper acceleration. To make the analogy with the Unruh effect more apparent, we chose the notation in which the coordinates $(\bar{u}, \bar{v})$ always refer to freely falling observers while the coordinates (u, v) describe accelerated frames.

9.1.3 Field quantization

In the previous section we introduced two coordinate systems corresponding to a locally inertial observer (the Kruskal frame) and a locally accelerated observer (the tortoise frame). Now we quantize the field $\phi(x)$ in these two frames and compare the respective vacuum states. The considerations are formally quite similar to those in Chapter 8.

To quantize the field $\phi(x)$, it is convenient to employ the lightcone mode expansions (defined in Sec. 8.2.2) in the coordinates (u, v) and $(\bar{u}, \bar{v})$. Because of the intentionally chosen notation, the relations (8.16) and (8.17) can be directly used to describe the quantized field $\hat{\phi}$ in the BH spacetime.

The lightcone mode expansion in the tortoise coordinates is

$$\hat{\phi}(u, v) = \int_0^{+\infty} \frac{d\Omega}{\sqrt{2\pi}} \frac{1}{\sqrt{2\Omega}} \left[e^{-i\Omega u} \hat{b}^-_\Omega + H.c. + e^{-i\Omega v} \hat{b}^-_{-\Omega} + H.c. \right],$$

where the "$H.c.$" denotes the Hermitian conjugate terms. The operators $\hat{b}^{\pm}_{\pm\Omega}$ correspond to particles detected by a stationary observer at a constant distance from the BH. The role of this observer is completely analogous to that of the uniformly accelerated observer considered in Sec. 8.1.

The lightcone mode expansion in the Kruskal coordinates is

$$\hat{\phi}\left(\bar{u},\bar{v}\right)=\int_0^{+\infty}\frac{d\omega}{\sqrt{2\pi}}\frac{1}{\sqrt{2\omega}}\left[e^{-i\omega\bar{u}}\hat{a}_{\omega}^{-}+H.c.+e^{-i\omega\bar{v}}\hat{a}_{-\omega}^{-}+H.c.\right].$$

The operators $\hat{a}_{\pm\omega}^{\pm}$ are related to particles registered by an observer freely falling into the black hole.

It is clear that the two sets of creation and annihilation operators $\hat{a}_{\pm\omega}^{\pm}$, $\hat{b}_{\pm\Omega}^{\pm}$ specify two different vacuum states, $|0_K\rangle$ ("Kruskal") and $|0_T\rangle$ ("tortoise"),

$$\hat{a}_{\pm\omega}^{-}\left|0_K\right\rangle=0;\quad\hat{b}_{\pm\Omega}^{-}\left|0_T\right\rangle=0.$$

The state $|0_T\rangle$ is also called the *Boulware vacuum*.

Exactly as in the previous chapter, the operators $\hat{b}_{\pm\Omega}^{\pm}$ can be expressed through $\hat{a}_{\pm\omega}^{\pm}$ using the Bogolyubov transformation (8.22). The Bogolyubov coefficients are found from Eq. (8.23) if the acceleration a is replaced by $(4M)^{-1}$.

The correspondence between the Rindler and the Schwarzschild spacetimes is summarized in the following table. (We stress that this analogy is precise only for a conformally coupled field in 1+1 dimensions.)

Rindler	**Schwarzschild**
Inertial observers: vacuum $\|0_M\rangle$	Observers in free fall: vacuum $\|0_K\rangle$
Accelerated observers: $\|0_R\rangle$	Observers at $r=$ const: $\|0_T\rangle$
Proper acceleration a	Proper acceleration $(4M)^{-1}$
$\bar{u}=-a^{-1}\exp(-au)$	$\bar{u}=-4M\exp\left[-u/(4M)\right]$
$\bar{v}=a^{-1}\exp(av)$	$\bar{v}=4M\exp\left[v/(4M)\right]$

9.1.4 Choice of vacuum

To find the expected number of particles measured by observers far outside of the black hole, we first need to make the correct choice of the quantum state of the field $\hat{\phi}$. In the present case, there are two candidate vacua, $|0_K\rangle$ and $|0_T\rangle$. We shall draw on the analogy with Sec. 8.2.1 to justify the choice of the Kruskal vacuum $|0_K\rangle$, which is the lowest-energy state for freely falling observers, as the quantum state of the field.

When considering a uniformly accelerated observer in the Minkowski spacetime, the correct choice of the vacuum state is $|0_M\rangle$ which is the lowest-energy state as measured by inertial observers. An accelerated observer registers this state as thermally excited. The other vacuum state, $|0_R\rangle$, can be physically realized by an accelerated vacuum preparation device occupying a very large volume of space. Consequently, the energy needed to prepare the field in the state $|0_R\rangle$ in the whole space is infinitely large. If one computes the mean energy density of the field $\hat{\phi}$ in the state $|0_R\rangle$, one finds (after subtracting the zero-point energy) that in the Minkowski frame the energy density diverges at the horizon.[3] On the other hand, the Minkowski vacuum

[3] This result can be qualitatively understood if we recall that the Rindler coordinate $\tilde{\xi}$ covers an infinite range when approaching the horizon ($\tilde{\xi}\to-\infty$ as $\xi\to-a^{-1}$). The zero-point energy density in the state $|0_R\rangle$ is constant in the Rindler frame and thus appears as an infinite concentration of energy density near the horizon in the Minkowski frame. We omit the detailed calculation.

state $|0_M\rangle$ has zero energy density everywhere.

It turns out that a very similar situation occurs in the BH spacetime. At first it may appear that the field $\hat{\phi}$ should be in the Boulware state $|0_T\rangle$ which is the vacuum measured by observers remaining at a constant distance from the black hole. However, the field $\hat{\phi}$ in the state $|0_T\rangle$ has an infinite energy density (after subtracting the zero-point energy) near the BH horizon.[4] Any energy density influences the metric via the Einstein equation. A divergent energy density indicates that the backreaction of the quantum fluctuations in the state $|0_T\rangle$ is so large near the BH horizon that the Schwarzschild metric is not a good approximation for the resulting spacetime. Thus the picture of a quantum field in the state $|0_T\rangle$ near an almost unperturbed black hole is inconsistent. On the other hand, the field $\hat{\phi}$ in the Kruskal state $|0_K\rangle$ has an everywhere finite and small energy density (when computed in the Schwarzschild frame after a subtraction of the zero-point energy). In this case, the backreaction of the quantum fluctuations on the metric is negligible. Therefore one has to employ the vacuum state $|0_K\rangle$ rather than the state $|0_T\rangle$ to describe quantum fields in the presence of a classical black hole.

Another argument for selecting the Kruskal vacuum $|0_K\rangle$ is the consideration of a star that turns into a black hole through the gravitational collapse. Before the collapse, the spacetime is almost flat and the initial state of quantum fields is the naturally defined Minkowski vacuum. It can be shown that the final quantum state of the field $\hat{\phi}$ after the collapse is the Kruskal vacuum.

9.1.5 The Hawking temperature

Observers remaining at $r = \text{const}$ far away from the black hole ($r \gg 2M$) are in an almost flat space where the natural vacuum is the Minkowski one. The Minkowski vacuum at $r \gg 2M$ is approximately the same as the Boulware vacuum $|0_T\rangle$. Since the field $\hat{\phi}$ is in the Kruskal vacuum state $|0_K\rangle$, these observers would register the presence of particles.

The calculations of Sec. 8.2.4 show that the temperature measured by an accelerated observer is $T = a/(2\pi)$, and we have seen that the correspondence between the Rindler and the Schwarzschild cases requires to set $a = (4M)^{-1}$. It follows that observers at a fixed distance $r \gg 2M$ from the black hole detect a thermal spectrum of particles with the temperature

$$T_H = \frac{1}{8\pi M}. \tag{9.9}$$

This temperature is known as the Hawking temperature. (Observers staying closer to the BH will see a higher temperature due to the inverse gravitational redshift.)

Similarly, we find that the density of observed particles with energy $E = k$ is

$$n_E = \left[\exp\left(\frac{E}{T_H}\right) - 1\right]^{-1}.$$

[4] This is analogous to the divergent energy density near the horizon in the Rindler vacuum state. We again omit the required calculations.

This formula remains valid for massive particles with mass m and momentum k, after the natural replacement $E = \sqrt{m^2 + k^2}$. One can see that the particle production is significant only for particles with very small masses $m \lesssim T_H$.

The Hawking effect is in principle measurable, although the Hawking temperature for plausible astrophysical black holes is extremely small.

Exercise 9.1

Rewrite Eq. (9.9) in the SI units and compute the Hawking temperature for black holes of masses $M_1 = M_\odot = 2 \cdot 10^{30}$kg (one solar mass), $M_2 = 10^{15}$g, and $M_3 = 10^{-5}$g (of order of the Planck mass).

Exercise 9.2

(a) Estimate the typical wavelength of photons radiated by a black hole of mass M and compare it with the size of the black hole (the Schwarzschild radius $R = 2M$).

(b) The temperature of a sufficiently small black hole can be high enough to efficiently produce baryons (e.g. protons) as components of the Hawking radiation. Estimate the required mass M of such black holes and compare their Schwarzschild radius with the size of the proton (its Compton length).

9.1.6 The Hawking effect in 3+1 dimensions

We have considered the 1+1-dimensional field $\hat{\phi}(t, r)$ that corresponds to spherically symmetric 3+1-dimensional field configurations. However, there is a difference between fields in 1+1 dimensions and spherically symmetric modes in 3+1 dimensions.

The field ϕ in 3+1 dimensions can be decomposed into spherical harmonics,

$$\phi(t, r, \theta, \varphi) = \sum_{l,m} \phi_{lm}(t, r) Y_{lm}(\theta, \varphi).$$

The mode $\phi_{00}(t, r)$ is spherically symmetric and independent of the angles θ, φ. However, the restriction of the 3+1-dimensional wave equation to the mode ϕ_{00} is not equivalent to the 1+1-dimensional problem. The four-dimensional wave equation ${}^{(4)}\Box\phi = 0$ for the spherically symmetric mode is

$$\left[{}^{(2)}\Box + \left(1 - \frac{2M}{r}\right) \frac{2M}{r^3} \right] \phi_{00}(t, r) = 0.$$

This equation represents a wave propagating in the potential

$$V(r) = \left(1 - \frac{2M}{r}\right) \frac{2M}{r^3}$$

instead of a free wave $\phi(t, r)$ considered above. The potential $V(r)$ has a barrier-like shape shown in Fig. 9.1, and a wave escaping the black hole needs to tunnel from $r \approx 2M$ to the potential-free region $r \gg 2M$. This decreases the intensity of the wave and changes the resulting distribution of produced particles by a *greybody factor* $\Gamma_{gb}(E) < 1$,

$$n_E = \Gamma_{gb}(E) \left[\exp\left(\frac{E}{T_H}\right) - 1 \right]^{-1}.$$

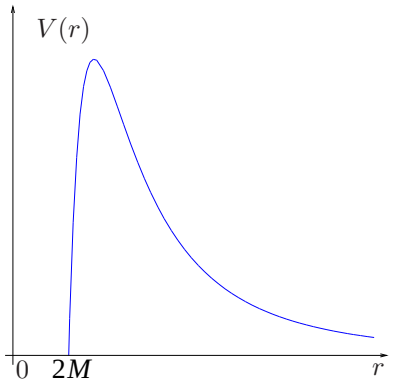


Figure 9.1: The potential $V(r)$ for the propagation of the spherically symmetric mode in 3+1 dimensions.

The computation of the greybody factor $\Gamma_{gb}(E)$ is beyond the scope of this book. This factor depends on the geometry of the radiated field mode and is different for fields of higher spin. (Of course, fermionic fields obey the Fermi instead of the Bose distribution.)

9.1.7 Remarks on other derivations

We derived the Hawking effect in one of the simplest possible cases, namely that of a conformally coupled field in a static BH spacetime restricted to 1+1 dimensions. This derivation cannot be straightforwardly generalized to the full 3+1-dimensional spacetime. For instance, a free massless scalar field is not conformally coupled in 3+1 dimensions, and spherically symmetric modes are not the only available ones. Realistic calculations must consider the production of photons or massive fermions instead of massless scalar particles. However, all such calculations yield the same temperature T_H of the black hole.

It is also important to consider a black hole formed by a gravitational collapse of matter (see Fig. 9.2). Hawking's original calculation involved wave packets of field modes that entered the collapsing region before the BH was formed (the dotted line in the figure). The BH horizon is a light-like surface, therefore massless and ultra-relativistic particles may remain near the horizon for a very long time before they escape to infinity. Since the spacetime is almost flat before the gravitational collapse, the "in" vacuum state of such modes is well-defined in the remote past. After the mode moves far away from the black hole, the "out" vacuum state is again the standard Minkowski ("tortoise") vacuum. A computation of the Bogolyubov coefficients between the "in" and the "out" vacuum states for this wave packet yields a thermal spectrum of particles with the temperature T_H.

This calculation implies that the radiation coming out of the black hole consists of particles that already existed at the time of BH formation but spent a long time near

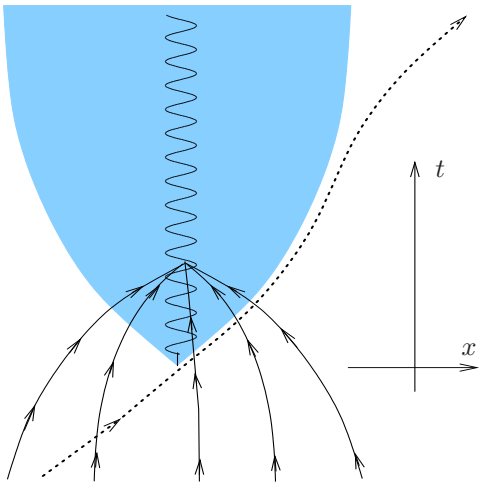


Figure 9.2: Black hole (shaded region) formed by gravitational collapse of matter (lines with arrows). The wavy line marks the singularity at the BH center. A light-like trajectory (dotted line) may linger near the horizon (the boundary of the shaded region) for a long time before escaping to infinity.

the horizon and only managed to escape at the present time. This explanation, however, contradicts the intuitive expectation that particles are created right at the present time by the gravitational field of the BH. The rate of particle creation should depend only on the present state of the black hole and not on the details of its formation in the distant past. One expects that an eternal black hole should radiate in the same way as a BH formed by gravitational collapse.

Another way to derive the Hawking radiation is to evaluate the energy-momentum tensor $T_{\mu\nu}$ of a quantum field in a BH spacetime and to verify that it corresponds to thermal excitations. However, a direct computation of the EMT is complicated and has been explicitly performed only for a 1+1-dimensional spacetime. The reason for the difficulty is that the EMT contains information about the quantum field at all points, not only the asymptotic properties at spatial infinity. This additional information is necessary to determine the backreaction of fields on the black hole during its evaporation. The detailed picture of the BH evaporation remains unknown.

There seems to be no unique physical explanation of the BH radiation. However, the resulting thermal spectrum of the created particles has been derived in many different ways and agrees with general thermodynamical arguments. There is little doubt that the Hawking radiation is a valid and in principle observable prediction of general relativity and quantum field theory.

9.2 Thermodynamics of black holes

9.2.1 Evaporation of black holes

In many situations, a static black hole of mass M behaves as a spherical body with radius $r = 2M$ and surface temperature T_H. According to the Stefan-Boltzmann law, a black body radiates the flux of energy

$$L = \gamma \sigma T_H^4 A,$$

where γ parametrizes the number of degrees of freedom available to the radiation, $\sigma = \pi^2/60$ is the Stefan-Boltzmann constant in Planck units, and

$$A = 4\pi R^2 = 16\pi M^2$$

is the surface area of the BH. The emitted flux determines the loss of energy due to radiation. The mass of the black hole decreases with time according to

$$\frac{dM}{dt} = -L = -\frac{\gamma}{15360\pi M^2}. \tag{9.10}$$

The solution with the initial condition $M|_{t=0} = M_0$ is

$$M(t) = M_0 \left(1 - \frac{t}{t_L}\right)^{1/3}, \quad t_L \equiv 5120\pi \frac{M_0^3}{\gamma}.$$

This calculation suggests that black holes are fundamentally unstable objects with the lifetime t_L during which the BH completely evaporates. Taking into account the greybody factor (see Sec. 9.1.6) would change only the numerical coefficient in the power law $t_L \sim M_0^3$.

> **Exercise 9.3**
> Estimate the lifetime of black holes with masses $M_1 = M_\odot = 2 \cdot 10^{30}$kg, $M_2 = 10^{15}$g, $M_3 = 10^{-5}$g.

It is almost certain that the final stage of the BH evaporation cannot be described by classical general relativity. The radius of the BH eventually reaches the Planck scale 10^{-33}cm and one expects unknown effects of quantum gravity to dominate in that regime. One possible outcome is that the BH is stabilized into a "remnant," a microscopic black hole that does not radiate, similarly to electrons in atoms that do not radiate on the lowest orbit. It is plausible that the horizon area is quantized to discrete levels and that a black hole becomes stable when its horizon reaches the minimum allowed area. In this case, quanta of Hawking radiation are emitted as a result of transitions between allowed horizon levels, so the spectrum of the Hawking radiation must consist of discrete lines. This prediction of the discreteness of the spectrum of the Hawking radiation may be one of the few testable effects of quantum gravity.

Remark: cosmological consequences of BH evaporation. Black holes formed by collapse of stars have extremely small Hawking temperatures. So the Hawking effect could be observed only if astronomers discovered a black hole near the end of its life, with a very high surface temperature. However, the lifetimes of astrophysically plausible black holes are much larger than the age of the Universe which is estimated as $\sim 10^{10}$ years. To evaporate within this time, a black hole must be lighter than $\sim 10^{15}$g (see Exercise 9.3). Such black holes could not have formed as a result of stellar collapse and must be *primordial*, i.e. created at very early times when the universe was extremely dense and hot. There is currently no direct observational evidence for the existence of primordial black holes.

9.2.2 Laws of BH thermodynamics

Prior to the discovery of the BH radiation it was already known that black holes require a thermodynamical description involving a nonzero intrinsic entropy.

The entropy of a system is defined as the logarithm of the number of internal microstates of the system that are indistinguishable on the basis of macroscopically available information. Since the gravitational field of a static black hole is completely determined (both inside and outside of the horizon) by the mass M of the BH, one might expect that a black hole has only one microstate and therefore its entropy is zero. However, this conclusion is inconsistent with the second law of thermodynamics. A black hole absorbs all energy that falls onto it. If the black hole always had zero entropy, it could absorb some thermal energy and decrease the entropy of the world. This would violate the second law unless one assumes that the black hole has an intrinsic entropy that grows in the process of absorption.

Similar *gedanken* experiments involving classical general relativity and thermodynamics lead J. Bekenstein to conjecture in 1971 that a static black hole must have an intrinsic entropy S_{BH} proportional to the surface area $A = 16\pi M^2$. However, the coefficient of proportionality between S_{BH} and A could not be computed until the discovery of the Hawking radiation. The precise relation between the BH entropy and the horizon area follows from the first law of thermodynamics,

$$dE \equiv dM = T_H dS_{BH}, \tag{9.11}$$

where T_H is the Hawking temperature for a black hole of mass M. A simple calculation using Eq. (9.9) shows that

$$S_{BH} = 4\pi M^2 = \frac{1}{4}A. \tag{9.12}$$

To date, there seems to be no completely satisfactory explanation of the BH entropy. Here is an illustration of the problem. A black hole of one solar mass has the entropy $S_\odot \sim 10^{76}$. A microscopic explanation of the BH entropy would require to demonstrate that a solar-mass BH actually has $\exp(10^{76})$ indistinguishable microstates. A large number of microstates implies many internal degrees of freedom not visible from the outside. Yet, a black hole is almost all empty space, with the exception of a Planck-sized region around its center where the classical general relativity does not

apply. It is not clear how this microscopically small region could contain such a huge number of degrees of freedom. A fundamental explanation of the BH entropy probably requires a theory of quantum gravity which is not yet available.

The thermodynamical law (9.11) suggests that in certain circumstances black holes behave as objects in thermal contact with their environment. This description applies to black holes surrounded by thermal radiation and to adiabatic processes of emission and absorption of heat.

> **Remark: rotating black holes.** A static black hole has no degrees of freedom except its mass M. A more general situation is that of a rotating BH with an angular momentum J. In that case it is possible to perform work on the BH in a reversible way by making it rotate faster or slower. The first law (9.11) can be modified to include contributions to the energy in the form of work.

For a complete thermodynamical description of black holes, one needs an equation of state. This is provided by the relation

$$E(T) = M = \frac{1}{8\pi T}.$$

It follows that the heat capacity of the BH is negative,

$$C_{BH} = \frac{\partial E}{\partial T} = -\frac{1}{8\pi T^2} < 0.$$

In other words, black holes become *colder* when they absorb heat.

The second law of thermodynamics now states that the combined entropy of all existing black holes and of all ordinary thermal matter never decreases,

$$\delta S_{total} = \delta S_{matter} + \sum_k \delta S_{BH}^{(k)} \geq 0.$$

Here $S_{BH}^{(k)}$ is the entropy (9.12) of the k-th black hole.

In classical general relativity it has been established that the combined area of all BH horizons cannot decrease (this is Hawking's "area theorem"). This statement applies not only to adiabatic processes but also to strongly out-of-equilibrium situations, such as a collision of black holes with the resulting merger. It is mysterious that this theorem, derived from a purely classical theory, assumes the form of the second law of thermodynamics when one considers quantum thermal effects of black holes.

Moreover, there is a general connection between horizons and thermodynamics which has not yet been completely elucidated. The presence of a horizon in a spacetime means that a loss of information occurs, since one cannot observe events beyond the horizon. Intuitively, a loss of information entails a growth of entropy. It seems to be generally true in the theory of relativity that any event horizon behaves as a surface with a certain entropy and emits radiation with a certain temperature.[5] For instance, the Unruh effect considered in Chapter 8 can be interpreted as a thermodynamical consequence of the presence of a horizon in the Rindler spacetime.

[5] See e.g. the paper by T. Padmanabhan, *Classical and quantum thermodynamics of horizons in spherically symmetric spacetimes*, Class. Quant. Grav. **19** (2002), p. 5378.

9.2.3 Black holes in heat reservoirs

As an application of the thermodynamical description, we consider a black hole inside a reservoir of thermal energy. The simplest such reservoir is a reflecting cavity filled with radiation. Usual thermodynamical systems can be in a stable thermal equilibrium with an infinite heat reservoir. However, the behavior of black holes is different because of their negative heat capacity.

A black hole surrounded by an infinite heat bath at a lower temperature $T < T_{BH}$ would emit heat and become even hotter. The process of evaporation is not halted by the heat bath whose low temperature T remains constant. On the other hand, a black hole placed inside an infinite reservoir with a higher temperature $T > T_{BH}$ will tend to absorb radiation from the reservoir and become colder. The process of absorption will continue indefinitely. In either case, no stable equilibrium is possible. The following exercise demonstrates that a black hole can be stabilized with respect to absorption or emission of radiation only by a reservoir with a *finite* heat capacity.

Exercise 9.4

(a) Given the mass M of the black hole, find the range of heat capacities C_r of the reservoir for which the BH is in a stable equilibrium with the reservoir.

(b) Assume that the reservoir is a completely reflecting cavity of volume V filled with thermal radiation (massless fields). The energy of the radiation is $E_r = \sigma V T^4$, where the constant σ characterizes the number of degrees of freedom in the radiation fields. Determine the largest volume V for which a black hole of mass M can remain in a stable equilibrium with the surrounding radiation.

Hint: The stable equilibrium is the state with the largest total entropy.

10 The Casimir effect

Summary: Zero-point energy for a field with boundary conditions. Regularization and renormalization.

The Casimir effect is an experimentally verified prediction of QFT. It is manifested by a force of attraction between two *uncharged* conducting plates in vacuum.

This force cannot be explained except by considering the zero-point energy of the quantized electromagnetic field. The presence of the conducting plates makes the electromagnetic field vanish on the surfaces of the plates, which changes the structure of vacuum fluctuations and causes a finite shift ΔE of the zero-point energy. This energy shift depends on the distance L between the plates. As a result, it is energetically favorable for the plates to move closer together, which is manifested as the *Casimir force*

$$F(L) = -\frac{d}{dL}\Delta E(L).$$

This theoretically predicted force has been confirmed by several experiments.[1]

10.1 Vacuum energy between plates

A realistic description of the Casimir effect requires to quantize the electromagnetic field in the presence of conducting plates. To simplify the calculations, we consider a massless scalar field $\phi(t,x)$ in the flat 1+1-dimensional spacetime and impose the following boundary conditions which simulate the presence of the plates,

$$\phi(t,x)|_{x=0} = \phi(t,x)|_{x=L} = 0.$$

The equation of motion for the classical field is $\partial_t^2\phi - \partial_x^2\phi = 0$, and the general solution for the chosen boundary conditions is of the form

$$\phi(t,x) = \sum_{n=1}^{\infty} \left(A_n e^{-i\omega_n t} + B_n e^{i\omega_n t}\right) \sin\omega_n x, \quad \omega_n \equiv \frac{n\pi}{L}. \tag{10.1}$$

To quantize the field $\phi(t,x)$ in flat space, one normally uses the mode expansion

$$\hat{\phi}(t,x) = \int \frac{dk}{(2\pi)^{1/2}} \frac{1}{\sqrt{2\omega_k}} \left[\hat{a}_k^- e^{-i\omega_k t + ikx} + \hat{a}_k^+ e^{i\omega_k t - ikx}\right].$$

[1] For example, a recent measurement of the Casimir force to 1% precision is described in: U. MOHIDEEN and A. ROY, Phys. Rev. Lett. **81** (1998), p. 4549.

However, in the present case the only allowed modes are those in Eq. (10.1), so the mode expansion for $\hat{\phi}$ must be

$$\hat{\phi}(t,x) = \sqrt{\frac{2}{L}} \sum_{n=1}^{\infty} \frac{\sin \omega_n x}{\sqrt{2\omega_n}} \left[\hat{a}_n^- e^{-i\omega_n t} + \hat{a}_n^+ e^{i\omega_n t}\right]. \tag{10.2}$$

We need to compute the energy of the field only between the plates, $0 < x < L$. After some algebra, the zero-point energy per unit length is expressed as

$$\varepsilon_0 \equiv \frac{1}{L} \langle 0| \hat{H} |0\rangle = \frac{1}{2L} \sum_k \omega_k = \frac{\pi}{2L^2} \sum_{n=1}^{\infty} n. \tag{10.3}$$

Exercise 10.1
(a) Show that the normalization factor $\sqrt{2/L}$ in the mode expansion (10.2) yields the standard commutation relations $\left[\hat{a}_m^-, \hat{a}_n^+\right] = \delta_{mn}$.
(b) Derive Eq. (10.3).
Hint: Use the identities which hold for integer m, n:

$$\int_0^L dx \, \sin \frac{m\pi x}{L} \sin \frac{n\pi x}{L} = \int_0^L dx \, \cos \frac{m\pi x}{L} \cos \frac{n\pi x}{L} = \frac{L}{2}\delta_{mn}. \tag{10.4}$$

As always, the zero-point energy density ε_0 is divergent. However, in the presence of the plates the energy density diverges in a different way than in free space because $\varepsilon_0 = \varepsilon_0(L)$ depends on the distance L between the plates. The zero-point energy density in free space can be thought of as the limit of $\varepsilon_0(L)$ at $L \to \infty$,

$$\varepsilon_0^{(\text{free})} = \lim_{L\to\infty} \varepsilon_0(L).$$

When the zero-point energy is renormalized in free space, the infinite contribution $\varepsilon_0^{(\text{free})}$ is subtracted. Thus we are motivated to subtract $\varepsilon_0^{(\text{free})}$ from the energy density $\varepsilon_0(L)$ and to expect a finite difference $\Delta\varepsilon$ between these formally infinite quantities,

$$\Delta\varepsilon(L) = \varepsilon_0(L) - \varepsilon_0^{(\text{free})} = \varepsilon_0(L) - \lim_{L\to\infty} \varepsilon_0(L). \tag{10.5}$$

In the remainder of the chapter we shall calculate this energy shift $\Delta\varepsilon(L)$.

10.2 Regularization and renormalization

Taken at face value, Eq. (10.5) is meaningless because the difference between two infinite quantities is undefined. The standard way to deduce reasonable answers from infinities is a regularization followed by a renormalization. A *regularization* means introducing an extra parameter into the theory to make the divergent quantity finite unless that parameter is set to zero. Such regularization parameters or *cutoffs* can be chosen in many ways. After the regularization, one derives the asymptotic form

of the divergent quantity at small values of the cutoff. This asymptotic will usually contain divergent powers and logarithms of the cutoff as well as finite terms. *Renormalization* means removing the divergent terms and leaving only the finite terms in the expression. (Of course, a suitable justification must be provided for subtracting the divergent terms.) After renormalization, the cutoff is set to zero and the remaining terms yield the final result. If the cutoff function is chosen incorrectly, the renormalization procedure will not succeed. It is usually possible to motivate the correct choice of the cutoff by physical considerations.

We shall now apply this procedure to Eq. (10.5). As a first step, a cutoff must be introduced into the divergent expression (10.3). One possibility is to replace ε_0 by the regularized quantity

$$\varepsilon_0\left(L;\alpha\right) = \frac{\pi}{2L^2}\sum_{n=1}^{\infty} n \exp\left[-\frac{n\alpha}{L}\right], \tag{10.6}$$

where α is the cutoff parameter. The regularized series converges for $\alpha > 0$, while the original divergent expression is recovered in the limit $\alpha \to 0$.

> **Remark: choosing the cutoff function.** We regularize the series by the factor $\exp(-n\alpha/L)$ and not by $\exp(-n\alpha)$ or $\exp(-nL\alpha)$. The motivation is that the physically significant quantity is $\omega_n = \pi n/L$, therefore the cutoff factor should be a function of ω_n.

Now we need to evaluate the regularized quantity (10.6) and to analyze its asymptotic behavior at $\alpha \to 0$. A straightforward computation gives

$$\varepsilon_0\left(L;\alpha\right) = -\frac{\pi}{2L}\frac{\partial}{\partial\alpha}\sum_{n=1}^{\infty}\exp\left[-\frac{n\alpha}{L}\right] = \frac{\pi}{2L^2}\frac{\exp\left(-\frac{\alpha}{L}\right)}{\left[1-\exp\left(-\frac{\alpha}{L}\right)\right]^2}.$$

At $\alpha \to 0$ this expression is expanded in a Laurent series,

$$\varepsilon_0\left(L;\alpha\right) = \frac{\pi}{8L^2}\frac{1}{\sinh^2\frac{\alpha}{2L}} = \frac{\pi}{2\alpha^2} - \frac{\pi}{24L^2} + O\left(\alpha^2\right). \tag{10.7}$$

The series (10.7) contains the singular term $\frac{\pi}{2}\alpha^{-2}$, a finite term, and further terms that vanish as $\alpha \to 0$. The crucial fact is that the singular term in Eq. (10.7) does not depend on L. (This would not have happened if we chose the cutoff as $\exp(-n\alpha)$ or in some other way!) The limit $L \to \infty$ in Eq. (10.5) is taken *before* the limit $\alpha \to 0$, so the divergent term $\frac{\pi}{2}\alpha^{-2}$ cancels and the renormalized value of $\Delta\varepsilon$ is finite,

$$\Delta\varepsilon_{ren}(L) = \lim_{\alpha\to 0}\left[\varepsilon_0\left(L;\alpha\right) - \lim_{L\to\infty}\varepsilon_0\left(L;\alpha\right)\right] = -\frac{\pi}{24L^2}. \tag{10.8}$$

The formula (10.8) is the main result of this chapter; the zero-point energy density is nonzero in the presence of plates at $x = 0$ and $x = L$. The Casimir force between the plates is

$$F = -\frac{d}{dL}\Delta E = -\frac{d}{dL}\left(L\Delta\varepsilon_{ren}\right) = -\frac{\pi}{24L^2}.$$

Since the force is negative, the plates are pulled toward each other.

A similar calculation for a massless scalar field in 3+1 dimensions gives the Casimir force per unit area of the plates as

$$\frac{F}{A} = -\frac{\pi^2}{240} L^{-4}.$$

Remark: negative energy. Note that the zero-point energy density (10.8) is negative. Quantum field theory generally admits quantum states with a negative expectation value of energy.

10.3 Renormalization using Riemann's zeta function

An elegant way to extract information from infinities is to use Riemann's zeta (ζ) function defined by the series

$$\zeta(x) = \sum_{n=1}^{\infty} \frac{1}{n^x} \tag{10.9}$$

which converges for real $x > 1$. An analytic continuation extends this function to all (complex) x except $x = 1$ where $\zeta(x)$ has a pole.

The divergent sum $\sum_{n=1}^{\infty} n$ appearing in Eq. (10.3) is formally equivalent to the series for $\zeta(x)$ with $x = -1$. However, after an analytic continuation the ζ function has a finite value at $x = -1$ which is [2]

$$\zeta(-1) = -\frac{1}{12}.$$

This motivates us to replace the sum $\sum_{n=1}^{\infty} n$ in Eq. (10.3) by the number $-\frac{1}{12}$. After this substitution, we immediately obtain the result (10.8).

The general "recipe" of renormalization using the ζ function is the following:

1. Rewrite the divergent quantity as a series of the form $\sum_n n^{-x}$ and formally express this series through $\zeta(x)$.

2. The analytic continuation of $\zeta(x)$ to that value x is a finite number which is interpreted as the renormalized value of the originally divergent quantity.

This procedure seems to always work (*if* the calculations can be performed), although its success may appear miraculous and lacking explanation, unlike the results of other, more straightforward renormalization approaches. However, the Casimir effect and several other QFT predictions obtained by the ζ function method have been experimentally verified. Thus there are grounds to expect that the mathematical trick involving an analytic continuation of the ζ function yields correct physical results.

[2] This result requires a complicated proof. See e.g. H. BATEMAN and A. ERDELYI, *Higher transcendental functions*, vol. 1 (McGraw-Hill, New York, 1953).

Part II

Path integral methods

11 Path integral quantization

Summary: The propagator as a path integral. Path integrals with Hamiltonian and Lagrangian action.

In the first part of this book, we used *canonical quantization* which is based on replacing the canonical variables (the coordinate q and the momentum p) by Hermitian operators $\hat{q}, \hat{p}$ acting in a suitable Hilbert space. The path integral formalism provides a powerful alternative method of quantization. In this chapter we introduce path integrals by considering the evolution of simple quantum-mechanical systems.

11.1 Evolution operators. Propagators

We recall that in the Schrödinger picture of quantum mechanics, state vectors $|\psi(t)\rangle$ evolve according to the Schrödinger equation,

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle .$$

For simplicity, we focus on Hamiltonians which do not explicitly depend on time, $\hat{H} = \hat{H}(\hat{p}, \hat{q})$. Then a formal solution of the Schrödinger equation is

$$|\psi(t)\rangle = \exp\left[-\frac{i}{\hbar}(t-t_0)\hat{H}\right]|\psi_0\rangle ,$$

where $|\psi_0\rangle \equiv |\psi(t_0)\rangle$ is the initial state at time $t = t_0$.

> **Remark:** The term *formal solution* indicates that the above expression does not actually provide an explicit formula for the solution $|\psi(t)\rangle$. Moreover, the infinite series
>
> $$\exp\left[-\frac{i}{\hbar}(t-t_0)\hat{H}\right]|\psi_0\rangle \equiv |\psi_0\rangle - \frac{i(t-t_0)}{\hbar}\hat{H}|\psi_0\rangle + \frac{1}{2!}\left[-\frac{i(t-t_0)}{\hbar}\hat{H}\right]^2|\psi_0\rangle + ...$$
>
> does not necessarily converge for all $|\psi_0\rangle$. In this book we shall not discuss the subtle issue of convergence of such series.

The operator transforming $|\psi(t_0)\rangle$ into $|\psi(t)\rangle$ is called the *evolution operator*

$$\hat{U}(t, t_0) \equiv \exp\left[-\frac{i}{\hbar}(t-t_0)\hat{H}\right]. \tag{11.1}$$

This operator is unitary if $\hat{H}$ is Hermitian. It is also clear that a composition of evolution operators is equal to the evolution operator for the combined timespan, i.e.

$$\hat{U}(t_1, t_2)\hat{U}(t_2, t_3) = \hat{U}(t_1, t_3) .$$

Since $\hat{U}(t,t_0) \equiv \hat{U}(t-t_0)$ is a function only of $(t-t_0)$, we find

$$\hat{U}\left(\Delta t_1\right)\hat{U}\left(\Delta t_2\right) = \hat{U}\left(\Delta t_1 + \Delta t_2\right) = \hat{U}\left(\Delta t_2\right)\hat{U}\left(\Delta t_1\right),$$

therefore all evolution operators $\hat{U}(\Delta t)$ for all Δt commute.[1]

In the coordinate representation, the quantum state $|\psi(t)\rangle$ is described by a wavefunction $\psi(q,t)$,

$$\psi(q,t) = \langle q|\,\psi(t)\rangle; \qquad |\psi(t)\rangle = \int \psi(q,t)\,|q\rangle\,dq.$$

The evolution operator transforms an initial wavefunction $\psi\left(q,t_0\right)$ into $\psi\left(q,t\right)$ which can be expressed as

$$\begin{aligned}\psi(q,t) = \langle q|\,\psi(t)\rangle &= \int dq_0 \psi\left(q_0,t_0\right)\langle q|\,\hat{U}\left(t,t_0\right)|q_0\rangle \\ &\equiv \int dq_0 \psi\left(q_0,t_0\right) K\left(q,q_0;t,t_0\right),\end{aligned}$$

where the function $K\left(q,q_0;t,t_0\right) \equiv \langle q|\,\hat{U}\left(t,t_0\right)|q_0\rangle$, called the *propagator*, is the coordinate representation of the evolution operator. The propagator is interpreted as the quantum-mechanical amplitude of the transition between an initial state $|q_0\rangle$ at time t_0 and a final state $|q\rangle$ at time t.

11.2 Propagator as a path integral

The propagator can be expressed as an integral over all trajectories connecting the initial and the final states (a *path integral*).

To derive the path integral representation of the propagator, we consider the evolution of a quantum-mechanical system during a time interval (t_0,t_f) and choose n intermediate time moments t_1, ..., t_n, so that the range (t_0,t_f) is divided into $n+1$ subranges (t_0,t_1), ..., (t_n,t_f). For convenience, we denote $t_{n+1} \equiv t_f$. Eventually we shall take the limit $n \to \infty$ and $\Delta t_k \equiv t_{k+1} - t_k \to 0$, so it is assumed that n is large and Δt_k are small.

The evolution operator for the range (t_0,t_f) is equal to the product of evolution operators for all intermediate ranges (t_k,t_{k+1}),

$$\hat{U}\left(t_f,t_0\right) = \hat{U}\left(t_f,t_n\right)...\hat{U}\left(t_1,t_0\right) = \prod_{k=0}^{n}\hat{U}\left(t_{k+1},t_k\right).$$

Therefore the propagator

$$K\left(q_f,q_0;t_f,t_0\right) = \langle q_f|\,\hat{U}\left(t,t_0\right)|q_0\rangle = \langle q_f|\prod_{k=0}^{n}\hat{U}\left(t_{k+1},t_k\right)|q_0\rangle$$

[1] If the Hamiltonian is explicitly time-dependent, the evolution operators are not expressed by Eq. (11.1) and do not commute because $\hat{U}(t_1,t_2)$ is not a function only of $t_1 - t_2$.

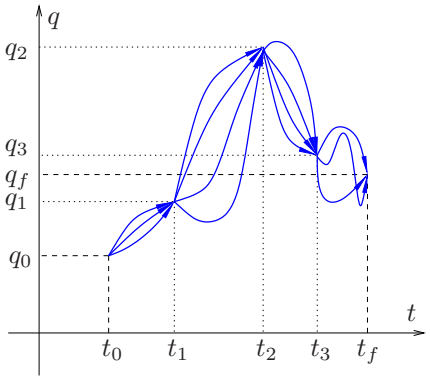


Figure 11.1: A "constrained transition" with fixed intermediate points q_1, ..., q_n. The multiple lines connecting the points q_k indicate that the motion of the quantum particle between the specified points is not described by a single classical path.

can be expressed through the propagators for the intermediate ranges by inserting n decompositions of unity of the form $\int |q\rangle \langle q| \, dq$,

$$\langle q_f| \prod_{k=0}^{n} \hat{U}\left(t_{k+1}, t_k\right) |q_0\rangle = \langle q_f| \hat{U}\left(t_{n+1}, t_n\right) \left[\int |q_n\rangle \langle q_n| \, dq_n\right] \times \hat{U}\left(t_n, t_{n-1}\right) ... \left[\int |q_1\rangle \langle q_1| \, dq_1\right] \hat{U}\left(t_1, t_0\right) |q_0\rangle ,$$

where the n auxiliary integration variables are denoted by q_n, ..., q_1. We find that the propagator is the n-fold integrated product of the propagators of all the subranges:

$$K\left(q_f, q_0; t_f, t_0\right) = \int \left(\prod_{k=1}^{n} dq_k\right) \prod_{k=0}^{n} K\left(q_{k+1}, q_k; t_{k+1}, t_k\right) . \tag{11.2}$$

The product of $(n+1)$ intermediate propagators $\prod_{k=0}^{n} K\left(q_{k+1}, q_k; t_{k+1}, t_k\right)$ is equal to the quantum-mechanical amplitude for a chain of transitions $|q_0\rangle \to |q_1\rangle \to ... \to |q_f\rangle$. This amplitude describes a certain class of "constrained transitions" for which the particle passes from q_0 to q_f while visiting the intermediate points q_k at the times t_k (see Fig. 11.1). So the formula (11.2) shows that the total amplitude for the transition from the initial state $|q_0\rangle$ to the final state $|q_f\rangle$ is found by integrating the constrained transition amplitude over all possible intermediate values q_1, ..., q_n.

The propagator $K(q_f, q_0; t_f, t_0)$ is thus reduced to propagators for short time intervals Δt_k. In the limit of small Δt_k, we can expand the evolution operator,

$$\hat{U}\left(t_{k+1}, t_k\right) = \exp\left[-\frac{i}{\hbar} \Delta t_k \hat{H}\right] = 1 - \frac{i}{\hbar} \Delta t_k \, \hat{H} + O\left(\Delta t_k^2\right) , \tag{11.3}$$

and express the short-time propagator (neglecting terms of order Δt_k^2) as

$$K\left(q', q; t_{k+1}, t_k\right) \approx \langle q'| 1 - \frac{i}{\hbar}\Delta t_k \hat{H} |q\rangle .$$

The matrix element of the Hamiltonian, $\langle q'| \hat{H} |q\rangle$, can be calculated by using the decomposition of unity in the momentum representation,

$$\langle q'| \hat{H} |q\rangle = \langle q'| \int dp \, |p\rangle \langle p| \hat{H} |q\rangle .$$

For convenience, let us reorder all operators $\hat{p}$ in the Hamiltonian to the left of all operators $\hat{q}$, so that $\hat{H}(\hat{p}, \hat{q})$ acquires the form $\hat{H} = \sum_j f_j(\hat{p}) g_j(\hat{q})$ with suitable functions f_j and g_j. The reordering must be performed using the commutation relations, e.g. the term $\hat{q}\hat{p}^2\hat{q}$ would be rewritten as $\hat{p}^2\hat{q}^2 + 2i\hbar\hat{p}\hat{q}$. When the operator ordering in the Hamiltonian is chosen in this way, we find

$$\langle p| \hat{H} |q\rangle = \sum_j f_j(p) \, g_j(q) \, \langle p|q\rangle \equiv H(p, q) \, \langle p|q\rangle ,$$

where $H(p, q)$ is the c-number function corresponding to the reordered Hamiltonian; for example, $\hat{H} = \hat{q}\hat{p}^2\hat{q}$ yields $H(p, q) = p^2q^2 + 2i\hbar pq$. The matrix element $\langle q'| \hat{H} |q\rangle$ is now computed using Eq. (2.36),

$$\langle q'| \hat{H} |q\rangle = \int dp \, \langle q'|p\rangle \langle p|q\rangle H(p, q) = \int \frac{dp}{2\pi\hbar} H(p, q) \exp \frac{i(q' - q)p}{\hbar}. \tag{11.4}$$

From Eqs. (11.3)-(11.4) we express the propagator $K\left(q_{k+1}, q_k; t_{k+1}, t_k\right)$, once again neglecting terms of order Δt_k^2, as follows,

$$\begin{aligned} K\left(q_{k+1}, q_k; t_{k+1}, t_k\right) = \langle q_{k+1}| \hat{U}\left(t_{k+1}, t_k\right) |q_k\rangle \; &\approx \; \langle q_{k+1}| 1 - \frac{i\Delta t_k}{\hbar}\hat{H} |q_k\rangle \\ &= \int \frac{dp_k}{2\pi\hbar} \left[1 - \frac{i\Delta t_k}{\hbar} H(p_k, q_k)\right] \exp \frac{i\left(q_{k+1} - q_k\right) p_k}{\hbar} \\ &\approx \int \frac{dp_k}{2\pi\hbar} \exp \left[\frac{i\Delta t_k}{\hbar} \left(\frac{q_{k+1} - q_k}{\Delta t_k} p_k - H(p_k, q_k)\right)\right] . \end{aligned}$$

For later convenience, the integration variable p was renamed to p_k.

The same calculation is repeated for each short-time propagator (setting $k = 0, ..., n$) and the results are substituted into Eq. (11.2), which yields

$$K\left(q_f, q_0; t_f, t_0\right) = \int \left[\prod_{k=1}^{n} \frac{dq_k dp_k}{2\pi\hbar}\right] \frac{dp_0}{2\pi\hbar} \exp \left[\sum_{k=0}^{n} \frac{i\Delta t_k}{\hbar} \left[\frac{q_{k+1} - q_k}{\Delta t_k} p_k - H(p_k, q_k)\right]\right] . \tag{11.5}$$

Note that Eq. (11.5) involves n integrations over q_k but $(n + 1)$ integrations over p_k.

Now we consider the limit $n \to \infty$ and $\Delta t \to 0$. When the number of intermediate points t_k becomes infinitely large, one is motivated to introduce auxiliary functions

$q(t), p(t)$ such that $q_k = q(t_k)$ and $p_k = p(t_k)$, and to replace the sum in Eq. (11.5) by an integral over t,

$$\lim_{n\to\infty} \sum_{k=0}^{n} \frac{i}{\hbar} \Delta t_k \left[\frac{q_{k+1} - q_k}{\Delta t_k} p_k - H(p_k, q_k) \right] = \int_{t_0}^{t_f} \frac{i}{\hbar} dt \left[\frac{dq(t)}{dt} p(t) - H(p(t), q(t)) \right].$$

The integration over infinitely many intermediate values q_k, p_k in Eq. (11.5) is then naturally interpreted as integration over *all functions* $q(t), p(t)$ such that $q(t_0) = q_0$, $q(t_f) = q_f$. An integral of this kind is called a *functional integral* or a *path integral*.

In the limit $n \to \infty$, the $(2n+1)$-fold integration over dp_k and dq_k becomes an infinite-dimensional integration measure which is symbolically denoted by $\mathcal{D}p\mathcal{D}q$,

$$\mathcal{D}p\mathcal{D}q \equiv \lim_{n\to\infty} \left[\prod_{k=1}^{n} \frac{dq_k dp_k}{2\pi\hbar} \right] \frac{dp_0}{2\pi\hbar}. \tag{11.6}$$

Then Eq. (11.5) is rewritten as

$$K\left(q_f, q_0; t_f, t_0\right) = \int_{q(t_0)=q_0}^{q(t_f)=q_f} \mathcal{D}p\mathcal{D}q \, \exp\left[\frac{i}{\hbar} \int_{t_0}^{t_f} \left(p\dot{q} - H(p,q) \right) dt \right]. \tag{11.7}$$

This is the propagator in the path integral formalism. Note that the expression in the exponential is the classical Hamiltonian action (2.22) and the boundary conditions for $q(t), p(t)$ are the same as those needed for the Hamiltonian action principle (Sec. 2.2.2).

The path integral is in fact a *method of quantization* since it defines[2] the quantum-mechanical amplitudes of transitions $|q_0, t_0\rangle \to |q_f, t_f\rangle$ directly through the classical Hamiltonian $H(p,q)$, without need for the Schrödinger equation or the operators $\hat{p}$, $\hat{q}$.

Remarks:

- A path integral expression always needs to be complemented by a specification of the integration measure as a limit of a suitable finite-dimensional measure, such as Eq. (11.6). Different finite-dimensional measures lead to different results in the continuous limit. Similarly, one must specify the way the action $\int (p\dot{q} - H) dt$ is represented by a finite sum (11.5). For instance, there is a difference between writing $H(p_k, q_k)$ and $H(p_k, q_{k+1})$ in Eq. (11.5).
- For systems with more than one degree of freedom, one needs to replace $p\dot{q}$ by $\sum_j p_j \dot{q}_j$ where j enumerates the generalized coordinates. If there are uncountably many degrees of freedom, the sum over j becomes itself an integral.

11.3 Lagrangian path integrals

If the Hamiltonian is a quadratic function of the momentum, e.g.

$$H\left(\hat{p}, \hat{q}\right) = \frac{\hat{p}^2}{2m} + V(\hat{q}), \tag{11.8}$$

[2] Formulating a rigorous definition of integration over all paths in Eq. (11.7) is an open mathematical problem. We shall however ignore this issue and manipulate path integrals as if they are well-defined.

the path integral has a simpler form (see Exercise 11.1). The integration over $\mathcal{D}p$ can be eliminated and the result is

$$K\left(q_f, q_0; t_f, t_0\right) = \int_{q(t_0)=q_0}^{q(t_f)=q_f} \mathcal{D}q \, \exp\left[\frac{i}{\hbar}\int_{t_0}^{t_f} L\left(\dot{q}, q\right) dt\right], \tag{11.9}$$

where $L\left(\dot{q}, q\right)$ is the Lagrangian. This was the original form of the path integral introduced by R. Feynman.

Exercise 11.1*

For the Hamiltonian (11.8), express the propagator as a path integral

$$\langle q_f | \hat{U}\left(t_f, t_0\right) | q_0 \rangle = \int_{q(t_0)=q_0}^{q(t_f)=q_f} \mathcal{D}q \, \exp\left(\frac{i}{\hbar} S\left[q; t_f, t_0\right]\right), \tag{11.10}$$

where the functional $S\left[q; t_f, t_0\right]$ is the classical Lagrangian action,

$$S\left[q; t_f, t_0\right] = \int_{t_0}^{t_f} \left[m\frac{\dot{q}^2}{2} - V(q)\right] dt,$$

and the integration measure $\mathcal{D}q$ is defined by the following limit,

$$\mathcal{D}q = \lim_{n\to\infty} \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{n+1}{2}} \prod_{k=1}^{n} dq_k, \quad \Delta t \equiv \frac{t_f - t_0}{n+1}. \tag{11.11}$$

Hint: Substitute the Hamiltonian (11.8) into the path integral derived in the chapter and explicitly evaluate the Gaussian integral over the momenta p_k using the formula

$$\int_{-\infty}^{+\infty} \exp\left[-\frac{ax^2}{2} + ibx\right] dx = \sqrt{\frac{2\pi}{a}} \exp\left[-\frac{b^2}{2a}\right].$$

(This identity holds also for complex a, b as long as the integral converges.)

If the Hamiltonian contains terms that are not quadratic in p, for example p^4, then the Lagrangian path integral (11.9) is impossible to derive. The Hamiltonian path integral formulation (11.7) is the only one available in such cases.

So far we considered only systems with time-independent Hamiltonians, but the path integral formalism also applies to time-dependent Hamiltonians.

Exercise 11.2

Derive the path integral expression for the propagator $\langle q_f | \hat{U}\left(t_f, t_0\right) | q_0 \rangle$ for an explicitly time-dependent Hamiltonian $\hat{H}(\hat{p}, \hat{q}, t)$.

Hint: Operators $\hat{H}(\hat{p}, \hat{q}, t)$ at different times t do not commute and one should manipulate them more carefully. The explicit form (11.1) of the evolution operator which holds only for time-independent Hamiltonians is not actually needed for the derivation of the path integral; only the approximation (11.3) is important.

12 Effective action

Summary: Green's functions of a harmonic oscillator. Euclidean oscillator. Euclidean path integrals. Effective action of a driven harmonic oscillator. Calculating matrix elements from path integrals. Backreaction and the effective action. Backreaction of quantum fields on the metric. Polarization of vacuum. Semiclassical gravity.

12.1 Green's functions of a harmonic oscillator

In Chapter 3 we considered an oscillator driven by an external force $J(t)$ which acts only during the time interval $0 < t < T$. The vacuum states $|0_{in}\rangle$ at $t \leq 0$ and $|0_{out}\rangle$ at $t \geq T$ are related by

$$|0_{in}\rangle = \exp\left(-\frac{1}{2}|J_0|^2 + J_0 \hat{a}^\dagger_{out}\right)|0_{out}\rangle\,,$$

where J_0 is defined by Eq. (3.5). For late times $t \geq T$, we computed the expectation value

$$\langle 0_{in}|\,\hat{q}\,(t)\,|0_{in}\rangle = \int_0^T \frac{\sin\omega(t-t')}{\omega} J(t')dt' \tag{12.1}$$

and the in-out matrix element

$$\frac{\langle 0_{out}|\,\hat{q}\,(t)\,|0_{in}\rangle}{\langle 0_{out}|0_{in}\rangle} = \frac{i}{2\omega}\int_0^T e^{-i\omega(t-t')}J(t')dt'. \tag{12.2}$$

We have related these results to Green's functions which will now be discussed in greater detail.

12.1.1 Green's functions

The standard use of Green's functions is to express solutions to inhomogeneous linear differential equations. For instance, the inhomogeneous equation describing a driven oscillator,

$$\frac{d^2}{dt^2}q\,(t) + \omega^2 q\,(t) = J\,(t)\,, \tag{12.3}$$

is solved for arbitrary $J(t)$ by the following expression,

$$q\,(t) = \int_{-\infty}^{+\infty} J\,(t')\,G\,(t,t')\,dt', \tag{12.4}$$

where $G(t,t')$ is a *Green's function* which satisfies

$$\frac{\partial^2}{\partial t^2}G(t,t') + \omega^2 G(t,t') = \delta(t-t'). \tag{12.5}$$

It is straightforward to verify that the formula (12.4) provides a solution to Eq. (12.3). The Green's function can be interpreted as the oscillator's response to a sudden jolt, that is to a force $J(t) = \delta(t-t')$ acting only at time $t = t'$ and conferring a unit of momentum to the oscillator.

Since Eq. (12.3) is second-order, its solution is specified uniquely if two conditions are imposed on the function $q(t)$. For instance, a typical problem is to compute the response of an oscillator initially at rest to a force $J(t)$ that is absent until a time $t = t_0$, i.e. $J(t) = 0$ for $t < t_0$. In that case, the relevant conditions on $q(t)$ are $q(t_0) = \dot{q}(t_0) = 0$. However, instead of specifying conditions on $q(t)$, appropriate constraints can be imposed *on the function* $G(t,t')$. In other words, the Green's function can be chosen such that the formula (12.4) will always yield solutions $q(t)$ satisfying the desired boundary conditions, for any $J(t)$. Different boundary conditions will specify different Green's functions that are appropriate in various contexts.

The response of an oscillator at rest to an external force is described by the *retarded Green's function* $G_{ret}(t,t')$ which is defined as the solution of Eq. (12.5) with the boundary condition $G_{ret}(t,t') = 0$ for all $t \leq t'$. If the driving force $J(t)$ is absent until $t = t_0$, then Eq. (12.4) with $G = G_{ret}$ yields $q(t) = 0$ for all $t \leq t_0$, i.e. the oscillator remains at rest until the force is switched on.

> **Exercise 12.1**
> Show that the retarded Green's function $G_{ret}(t,t')$ for a harmonic oscillator is
>
> $$G_{ret}(t,t') = \theta(t-t')\frac{\sin\omega(t-t')}{\omega}. \tag{12.6}$$

The *Feynman Green's function*,

$$G_F(t,t') = \frac{i}{2\omega}e^{-i\omega|t-t'|}, \tag{12.7}$$

is the solution of Eq. (12.5) which is symmetric in t and t', i.e. selected by the condition $G_F(t,t') = G_F(t',t)$.

Using these Green's functions, we may rewrite the results (12.1)-(12.2) as

$$\langle 0_{in}|\,\hat{q}\,(t)\,|0_{in}\rangle = \int_{-\infty}^{+\infty} G_{ret}(t,t')J(t')dt', \tag{12.8}$$

$$\frac{\langle 0_{out}|\,\hat{q}\,(t)\,|0_{in}\rangle}{\langle 0_{out}|0_{in}\rangle} = \int_{-\infty}^{+\infty} G_F(t,t')J(t')dt'. \tag{12.9}$$

Note that these relations hold for all t and not only for $t > T$. Other matrix elements can also be expressed through the Green's functions (see Exercise 3.4 on p. 40).

Interpretation of Green's functions

The retarded Green's function describes the familiar *causal* effect of an external force that influences the future evolution of the system but cannot change its behavior in the past. The Feynman Green's function, however, corresponds to a time-symmetric effect, namely a perturbation $\delta(t-t')$ at time $t=t'$ affects the future and the past evolution of the system in equal measure. This *acausal* relation between perturbation and response obviously does not occur in nature. If the Feynman Green's function were used to compute the influence of a force, one would arrive at an unphysical "Feynman solution" $q_F(t)$ that is affected by a force even before that force is switched on. Nevertheless, the fact that the Feynman Green's function appears in quantum-mechanical matrix elements between different states is not problematic since the "in-out" matrix elements are unobservable quantities. On the other hand, expectation values (which are observable) always involve the retarded Green's function.

12.1.2 Wick rotation. Euclidean oscillator

Many calculations in quantum field theory are easier if one performs an analytic continuation in the time variable and considers pure imaginary times $t=-i\tau$, where τ is a real parameter. This procedure is called the *Wick rotation*, and τ is called the *Euclidean time*. The picture is that of "rotating" the real axis in the complex t plane by 90 degrees to transform it into the imaginary axis. Having obtained a solution using the Euclidean time τ, one then performs the analytic continuation back to real (*Lorentzian*) time t.

The names "Euclidean time" and "Lorentzian time" are motivated by the transformation of the Lorentzian metric

$$ds^2 = dt^2 - d\mathbf{x}^2$$

under the Wick rotation. If we substitute pure imaginary times $t=-i\tau$, the metric becomes

$$ds^2 = -d\tau^2 - d\mathbf{x}^2,$$

which has a Euclidean signature (apart from an irrelevant overall sign).

The transition to complex time is motivated primarily by mathematical convenience. Complex values such as $t=-(4i)$ sec and the Euclidean time τ are introduced formally and cannot be interpreted as moments of time; only *real* values of t signify time.

In this chapter we study some basic applications of the Wick rotation, such as the construction of the Euclidean action and Euclidean path integrals. To make the underlying ideas more transparent, we shall perform all calculations for a very simple system, namely a driven harmonic oscillator with the equation of motion (in Lorentzian time)

$$\frac{d^2q}{dt^2} + \omega^2 q = J(t). \tag{12.10}$$

Assuming for the moment that the function $J(t)$ is analytic in a sufficiently large domain of the complex t plane, we can treat Eq. (12.10) as a differential equation in complex time. Then $q(t)$ and $J(t)$ become complex-valued functions that satisfy Eq. (12.10) for all complex t within the mentioned domain. Substituting pure imaginary values $t = -i\tau$ (with real τ), we thus obtain the equation of the *Euclidean driven oscillator*,

$$-\frac{d^2q(\tau)}{d\tau^2} + \omega^2 q(\tau) = J(\tau). \tag{12.11}$$

Since this equation does not explicitly involve complex numbers, one may consider only *real-valued* $J(\tau)$ and $q(\tau)$. We call a real function $q(\tau)$ a *Euclidean trajectory* or *Euclidean path*.

> **Remark:** A real-valued function $q(\tau)$ may become complex-valued after an analytic continuation back to the Lorentzian time t. Similarly, a real analytic function $q(t)$ is in general not real-valued at $t = -i\tau$. Below we shall show that a Euclidean path $q(\tau)$ *cannot* be interpreted as an analytic continuation of the physically relevant solution $q(t)$. For our purposes, the path $q(\tau)$ is a formally introduced real-valued function which will not enter the final results.

As before, we assume that the driving force $J(\tau)$ is nonzero only for a finite period of Euclidean time τ. In that case it is natural to require that the response $q(\tau)$ to that force does not grow at large $|\tau|$, i.e. that there exists a number C such that

$$|q(\tau \to \pm\infty)| < C < \infty.$$

Since at sufficiently large $|\tau|$ there is no force and the solutions of the free equation are $\exp(\pm\omega\tau)$, the only possibility for $q(\tau)$ to remain bounded is when $q(\tau) \propto \exp(\mp\omega\tau)$ for $\tau \to \pm\infty$. This is equivalent to the boundary condition

$$\lim_{\tau\to\pm\infty} q(\tau) = 0, \tag{12.12}$$

which indicates that the Euclidean oscillator is in the "vacuum state" at large $|\tau|$. Thus, Eq. (12.12) is the natural boundary condition for Euclidean trajectories.

The general solution of Eq. (12.11) can be expressed through the *Euclidean Green's function* $G_E(\tau, \tau')$,

$$q(\tau) = \int_{-\infty}^{+\infty} d\tau' G_E(\tau, \tau') J(\tau'). \tag{12.13}$$

To satisfy the boundary condition (12.12), the Euclidean Green's function must be selected by

$$\lim_{\tau\to\pm\infty} G_E(\tau, \tau') = 0.$$

This condition specifies $G_E(\tau, \tau')$ uniquely (see Exercise 12.2),

$$G_E(\tau, \tau') = \frac{1}{2\omega} e^{-\omega|\tau-\tau'|}. \tag{12.14}$$

With the above Green's function, the solution (12.13) satisfies the boundary condition (12.12) for any force $J(\tau)$ acting for only a finite period of Euclidean time.

Exercise 12.2
Derive the formula (12.14) by solving the equation

$$\left[-\frac{\partial^2}{\partial\tau^2}+\omega^2\right]G_E(\tau,\tau')=\delta(\tau-\tau') \tag{12.15}$$

with the boundary conditions $|G_E(\tau,\tau')|\to 0$ at $\tau\to\pm\infty$.

Connection between G_E and G_F

The similarity between the Euclidean and the Feynman Green's functions is apparent from a comparison of Eqs. (12.7) and (12.14). Performing the substitution $\tau = it$ in Eq. (12.13), one can verify that the analytic continuation of the solution $q(\tau)$ back to real times t yields the unphysical solution $q_F(t)$ discussed in Sec. 12.1.1 (p. 143),

$$q(\tau)=\int_{-\infty}^{+\infty}d\tau' G_E(\tau,\tau')J(\tau') \quad \xrightarrow{\tau=it} \quad q_F(t)=\int_{-\infty}^{+\infty}dt' G_F(t,t')J(t').$$

Both the Feynman and the Euclidean Green's functions are symmetric in their two arguments. One might be tempted to say that they are analytic continuations of each other, except for the fact that neither of the two Green's functions $G_E(\tau,\tau')$ and $G_F(t,t')$ are analytic in t or t'. Strictly speaking, only the restrictions of $G_F(t,t')$ to $t>t'$ or to $t<t'$ are analytic functions such that $G_F(t,t')$ for $t>t'$ is the analytic continuation of $iG_E(\tau,\tau')$ for $\tau<\tau'$ and vice versa.

Note that the retarded Green's function $G_F(t,t')$ is also not analytic. Generally, a Green's function cannot be an analytic function of t or t' in the entire complex plane. This can be explained by considering the requirements imposed on Green's functions. From physical grounds, we expect that if the force $J(t)$ is active only during a finite time interval $0<t<T$, then the influence of $J(t)$ should not grow as $|t|\to\infty$. However, there are no nonzero analytic functions that remain uniformly bounded for all complex t. Thus one has to consider only real t or only pure imaginary t and determine suitable Green's functions in each case.

12.2 Introducing effective action

Effective action is widely used in quantum field theory as a powerful method of calculation. An extensive development of the formalism and applications of effective action is far beyond the scope of this textbook. We employ effective action only as a tool to describe the interaction of quantum systems with classical external fields (backgrounds).

The method of effective action is based on Euclidean path integrals which we shall now discuss, using a driven harmonic oscillator as the main example.

12.2.1 Euclidean path integrals

In Chapter 11 we showed that the propagator for a quantized system can be written as a path integral over trajectories $q(t)$ connecting the initial and the final points,

$$K\left(q_f, q_0; t_f, t_0\right) = \int_{q(t_0)=q_0}^{q(t_f)=q_f} \mathcal{D}q\, e^{iS[q]}, \tag{12.16}$$

where $S[q]$ is the classical Lagrangian action (see Sec. 11.3). A driven harmonic oscillator is described by the action

$$S\left[q\right] = \int_{t_0}^{t_f} dt \left[\frac{1}{2}\dot{q}^2 - \frac{\omega^2}{2}q^2 + J(t)q\right]. \tag{12.17}$$

If we perform the Wick rotation $t = -i\tau$, the action (12.17) is expressed as the following functional of the Euclidean path $q(\tau)$,

$$iS\left[q(t)\right]_{t=-i\tau} = -\int_{\tau_0}^{\tau_f} d\tau \left[\frac{1}{2}\dot{q}^2 + \frac{\omega^2}{2}q^2 - J(\tau)q\right] \equiv -S_E\left[q(\tau)\right], \tag{12.18}$$

where we have denoted $\dot{q} \equiv dq/d\tau$. In a sense, the functional $S_E\left[q(\tau)\right]$ is the *analytic continuation* of the functional $\frac{1}{i}S\left[q(t)\right]$ to pure imaginary values of t; the factor $(-i)$ is introduced for convenience. One then considers the *Euclidean path integral*

$$\int_{q(\tau_0)=q_0}^{q(\tau_f)=q_f} \mathcal{D}q\, e^{-S_E[q(\tau)]}, \tag{12.19}$$

in which the integration is performed over all *real-valued* Euclidean trajectories $q(\tau)$ constrained by the specified boundary conditions at τ_0 and τ_f. The expression (12.19) can be viewed as the analytic continuation of the Lorentzian-time path integral (12.16).

One expects to obtain a useful result by computing the Euclidean path integral and performing the analytic continuation back to the real time t. However, the correspondence between the Lorentzian and the Euclidean path integrals is not a mathematical equality because normally the integration contour in Eq. (12.17) cannot be deformed from real t to the imaginary line. Also, the path integral involves trajectories $q(\tau)$ that are not necessarily analytic functions. So a straightforward analytic continuation back to the Lorentzian time cannot directly yield physical results. Below we shall see how the expressions obtained from Euclidean calculations are related to the correct answers found in Chapter 3.

> **Remark:** While the path integral (12.16) involves a rapidly oscillating exponential, its Euclidean analog (12.19) contains a rapidly decaying expression and can be expected to converge better. In fact, a mathematically rigorous definition of functional integration is currently available only for Euclidean path integrals. It is also easier in practice to perform calculations with the Euclidean action. These are the main reasons for introducing the Wick rotation.

Calculation of the Euclidean path integral

Unlike the Lorentzian action, the Euclidean action S_E is often bounded from below[1] and the minimum of the action is achieved at the classical Euclidean trajectory $q_{cl}(\tau)$. For instance, the action (12.18) of the Euclidean oscillator has a lower bound:

$$S_E[q] = \frac{1}{2}\dot{q}^2 + \frac{1}{2}\omega^2 q^2 - Jq = \frac{1}{2}\dot{q}^2 + \frac{1}{2}\left(\omega q - \frac{J}{\omega}\right)^2 - \frac{1}{2}\frac{J^2}{\omega^2} \geq -\frac{1}{2}\frac{J^2}{\omega^2}.$$

Therefore the dominant contribution to the path integral in Eq. (12.19) comes from paths $q(\tau)$ with the smallest value of the action. These are the paths near a solution $q_{cl}(\tau)$ of the classical Euclidean equation of motion,

$$\frac{\delta S_E[q]}{\delta q(\tau)} = 0.$$

Evaluating the functional derivative of the action (12.18), we obtain

$$-\frac{d^2}{d\tau^2}q_{cl} + \omega^2 q_{cl} = J(\tau). \tag{12.20}$$

This is of course the same as Eq. (12.11). We impose the natural boundary conditions (12.12),

$$\lim_{\tau\to\pm\infty} q_{cl}(\tau) = 0, \tag{12.21}$$

and then the Euclidean classical path $q_{cl}(\tau)$ is expressed by Eq. (12.13),

$$q_{cl}(\tau) = \int_{-\infty}^{+\infty} d\tau' G_E(\tau,\tau')J(\tau').$$

The path integral (12.19) contains contributions not only from $q_{cl}(\tau)$ but also from neighbor paths whose action S_E is only slightly larger than the minimum value $S_E[q_{cl}]$. To evaluate the path integral over all $q(\tau)$, it is convenient to split the function $q(\tau)$ into the sum of $q_{cl}(\tau)$ and a deviation $\tilde{q}(\tau)$,

$$q(\tau) \equiv q_{cl}(\tau) + \tilde{q}(\tau).$$

It is clear that the deviation $\tilde{q}(\tau)$ should satisfy the boundary conditions $\tilde{q}(\pm\infty) = 0$.

The path integral over all paths $q(\tau)$ can now be rewritten as an integral over all paths $\tilde{q}(\tau)$, with

$$\mathcal{D}q = \mathcal{D}[q_{cl}(\tau) + \tilde{q}(\tau)] = \mathcal{D}\tilde{q}.$$

This operation can be visualized as follows. The measure $\mathcal{D}q$ is the limit of a product of the form $dq(\tau_1)\ldots dq(\tau_n)$. Each integration variable $q(\tau_k)$ can be shifted by a *constant* amount $q_{cl}(\tau_k)$, and then

$$dq(\tau_k) = d[q_{cl}(\tau_k) + \tilde{q}(\tau_k)] = d\tilde{q}(\tau_k)$$

[1] This is not always the case. For instance, the Euclidean action for general relativity is bounded neither from below nor from above.

because $q_{cl}(\tau_k)$ is a fixed number. In other words: the function $q(\tau)$, which is the "variable" of path integration, is shifted by a fixed, q-independent function $q_{cl}(\tau)$.

Thus we can rewrite Eq. (12.19) as

$$\int_{q(-\infty)=0}^{q(+\infty)=0} \mathcal{D}q\, e^{-S_E[q(\tau)]} = \int_{\tilde{q}(-\infty)=0}^{\tilde{q}(+\infty)=0} \mathcal{D}\tilde{q}\, e^{-S_E[q_{cl}(\tau)+\tilde{q}(\tau)]}. \tag{12.22}$$

The action $S_E\left[q_{cl}(\tau)+\tilde{q}(\tau)\right]$ is then transformed using integration by parts,

$$\begin{aligned} S_E\left[q_{cl}+\tilde{q}\right] &= \int \left[\frac{1}{2}\left(\dot{q}_{cl}+\dot{\tilde{q}}\right)^2 + \frac{\omega^2}{2}\left(q_{cl}+\tilde{q}\right)^2 - \left(q_{cl}+\tilde{q}\right)J\right] d\tau \\ &= \left[\frac{1}{2}\dot{q}_{cl}q_{cl} + \dot{q}_{cl}\tilde{q}\right]_{-\infty}^{+\infty} + \frac{1}{2}\int \left(\dot{\tilde{q}}^2 + \omega^2\tilde{q}^2\right) d\tau - \int q_{cl}J d\tau \\ &\quad + \int \left(-\ddot{q}_{cl} + \omega^2 q_{cl} - J\right)\tilde{q}\, d\tau + \int \left[-\frac{1}{2}\ddot{q}_{cl}q_{cl} + \frac{\omega^2}{2}q_{cl}^2\right] d\tau \\ &= \frac{1}{2}\int \left(\dot{\tilde{q}}^2 + \omega^2\tilde{q}^2\right) d\tau - \frac{1}{2}\int q_{cl}J d\tau. \end{aligned}$$

The last line was obtained using the boundary conditions for q and $\tilde{q}$ as well as the equation of motion (12.20) to eliminate $\ddot{q}_{cl}$. The resulting expression is substituted into Eq. (12.22) which yields

$$\int_{q_0(-\infty)=0}^{q_f(+\infty)=0} \mathcal{D}q\, e^{-S_E[q(\tau)]} = \exp\left(\frac{1}{2}\int q_{cl}J d\tau\right) \int_{\tilde{q}(-\infty)=0}^{\tilde{q}(+\infty)=0} \mathcal{D}\tilde{q}\, e^{-\frac{1}{2}\int\left(\dot{\tilde{q}}^2+\omega^2\tilde{q}^2\right)d\tau}. \tag{12.23}$$

Note that the remaining path integral in Eq. (12.23) is independent of $J(\tau)$ and is a function only of ω. We shall denote that function by N_ω; an explicit expression for N_ω will not be necessary since we are interested only in the effect of the external force J on the oscillator. Therefore the final result is

$$\begin{aligned} \int_{q(-\infty)=0}^{q(+\infty)=0} \mathcal{D}q\, e^{-S_E[q(\tau)]} &= N_\omega \exp\left[\frac{1}{2}\int_{-\infty}^{+\infty} q_{cl}(\tau)J(\tau)d\tau\right] \\ &= N_\omega \exp\left[\frac{1}{2}\int J(\tau)J(\tau')G_E(\tau,\tau')d\tau d\tau'\right]. \end{aligned} \tag{12.24}$$

12.2.2 Definition of effective action

For a quantum system with a coordinate $\hat{q}$ interacting with a classical field J (the background), we define the *Euclidean effective action* as the functional $\Gamma_E\left[J(\tau)\right]$ determined by the relation

$$e^{-\Gamma_E[J(\tau)]} = \int_{q(-\infty)=0}^{q(+\infty)=0} \mathcal{D}q\, e^{-S_E[q(\tau),J(\tau)]}, \tag{12.25}$$

where $S_E[q, J]$ is the Euclidean classical action for the variable q including its interaction with the background J. Note that $\Gamma_E[J]$ is a functional of J but not of q. We shall see below that the effective action $\Gamma[J]$ indirectly describes both the influence of the background on the quantum system $\hat{q}$ and the effect of the quantum fluctuations of $\hat{q}$ on the classical field J (the *backreaction*).

The effective action for the driven oscillator can be read off from Eq. (12.24):

$$\Gamma_E[J(\tau)] = -\frac{1}{2}\int J(\tau)J(\tau')G_E(\tau,\tau')d\tau d\tau' - \ln N_\omega. \tag{12.26}$$

As we said before, a Euclidean quantity such as $q(\tau)$ has no direct relation to the observable value of $q(t)$. To obtain Lorentzian-time quantities, one needs to perform an analytic continuation that involves replacing $\tau = it$. The *Lorentzian effective action* $\Gamma_L[J(t)]$ is defined as the analytic continuation of the Euclidean effective action $\Gamma_E[J(\tau)]$ with an extra factor i:

$$\Gamma_L[J(t)] \equiv i\Gamma_E[J(\tau)]_{\tau=it}. \tag{12.27}$$

Formally, we may replace the Euclidean path integral in Eq. (12.25) by the corresponding Lorentzian one and write

$$e^{i\Gamma_L[J(t)]} = \int_{q(-\infty)=0}^{q(+\infty)=0} e^{iS[q(t),J]}\mathcal{D}q. \tag{12.28}$$

This equation should be understood merely a symbolic representation of the analytic continuation of the Euclidean path integral, since the Lorentzian path integral is ill-defined. However, it is intuitively easier to manipulate the Lorentzian path integral (12.28) directly, as if it were well-defined; for instance, we may compute functional derivatives of Γ_L or change variables in the path integral. These operations should be understood as the analogous manipulations on the Euclidean path integral, followed by the analytic continuation to the Lorentzian time. Below we shall perform such formal manipulations of Lorentzian path integrals without further comments.

To compute the Lorentzian effective action for the oscillator, we set $d\tau d\tau' = -dtdt'$ and replace the Euclidean Green's function G_E in Eq. (12.26) by its analytic continuation, $\frac{1}{i}G_F$. The result is

$$\begin{aligned}\Gamma_L[J(t)] &= \frac{1}{2}\int J(t)J(t')G_F(t,t')dtdt' - i\ln N_\omega \\ &= \frac{i}{2}|J_0|^2 + \int J(t)J(t')\frac{\sin\omega|t-t'|}{4\omega}dt\,dt' - i\ln N_\omega,\end{aligned} \tag{12.29}$$

where J_0 is defined by Eq. (3.5).

We note that the expression

$$\int_{q(-\infty)=0}^{q(+\infty)=0}\mathcal{D}q\,e^{iS[q(t),J]} \equiv \exp\left(i\Gamma_L[J]\right)$$

almost coincides with the matrix element $\langle 0_{out}|0_{in}\rangle$,

$$\langle 0_{out}|0_{in}\rangle = \exp\left(-\frac{1}{2}|J_0|^2\right),$$

up to a phase factor that can be absorbed into the definition of $|0_{out}\rangle$, and a normalization factor N_ω (which is J-independent). So we conjecture that a matrix element such as

$$\langle 0_{out}|\,\hat{q}\,(t_1)\,|0_{in}\rangle$$

might be related to the path integral

$$\int_{q(-\infty)=0}^{q(+\infty)=0} \mathcal{D}q\, q\,(t_1)\, e^{iS[q,J]}. \tag{12.30}$$

To test this conjecture, we now compute this path integral and compare the result with the known expression (12.9).

Since the external field J enters linearly into the action,

$$S\,[q,J] = S_0\,[q] + \int J(t)q(t)dt,$$

the functional derivative of S with respect to $J(t_1)$ is

$$\frac{\delta S\,[q,J]}{\delta J\,(t_1)} = q\,(t_1)\,,$$

and thus we may formally write

$$\int \mathcal{D}q\, q\,(t_1)\, e^{iS[q,J]} = \frac{1}{i}\frac{\delta}{\delta J\,(t_1)}\int \mathcal{D}q\, e^{iS[q,J]}.$$

For brevity, we shall omit the boundary conditions $q(\pm\infty) = 0$ that enter all path integrals. Substituting the definition (12.28), we find

$$\frac{\int q\,(t_1)\, e^{iS[q,J]}\mathcal{D}q}{\int e^{iS[q,J]}\mathcal{D}q} = \frac{\frac{1}{i}\frac{\delta}{\delta J(t_1)}\exp\left(i\Gamma_L\,[J]\right)}{\exp\left(i\Gamma_L\,[J]\right)} = \frac{\delta\Gamma_L\,[J]}{\delta J\,(t_1)}. \tag{12.31}$$

For the driven oscillator, Eq. (12.29) yields

$$\frac{\delta\Gamma_L\,[J]}{\delta J\,(t_1)} = \int J(t)G_F\,(t_1,t)\,dt, \tag{12.32}$$

where we used the symmetry of the Feynman Green's function, $G_F(t,t') = G_F(t',t)$. Since Eq. (12.32) coincides with Eq. (12.9), the conjecture is confirmed; the relation between the "in-out" matrix element and the Lorentzian effective action is

$$\frac{\int q\,(t_1)\, e^{iS[q,J]}\mathcal{D}q}{\int e^{iS[q,J]}\mathcal{D}q} = \frac{\delta\Gamma_L\,[J]}{\delta J\,(t_1)} = \frac{\langle 0_{out}|\,\hat{q}\,(t_1)\,|0_{in}\rangle}{\langle 0_{out}|0_{in}\rangle}. \tag{12.33}$$

Below we shall see to what extent this relation can be generalized to other matrix elements.

Effective action as a generating functional

Generating functions are a standard mathematical tool. For example, to compute statistical averages $\langle x\rangle$, $\langle x^2\rangle$, ... with respect to some probability distribution of x, one defines a *generating function* as a series in an auxiliary variable p,

$$g(p) \equiv \sum_{n=0}^{\infty} \frac{(ip)^n}{n!} \langle x^n\rangle = \left\langle e^{ipx}\right\rangle .$$

Once the generating function is computed, one can evaluate all the averages as follows,

$$\langle x\rangle = \frac{1}{i}\frac{dg}{dp}\bigg|_{p=0}, \quad ..., \quad \langle x^n\rangle = \frac{1}{i^n}\frac{d^n}{dp^n}\bigg|_{p=0} g(p).$$

In case of many variables x_i, the generating function depends on several arguments p_i, one for each x_i. For uncountably many variables x_t, where t is a continuous index, one introduces a *generating functional* that depends on a function $p_t \equiv p(t)$ and uses *functional* derivatives with respect to $p(t)$.

This method can be applied to path integrals of the form

$$\int q\left(t_1\right) q\left(t_2\right) q\left(t_3\right) ... q\left(t_n\right) e^{iS[q]} \mathcal{D}q. \tag{12.34}$$

We define the generating functional $G[J]$ by the path integral

$$G\left[J\right] \equiv \int \exp\left[iS\left[q\right] + i\int q(t)J(t)dt\right] \mathcal{D}q, \tag{12.35}$$

where $J(t)$ is an auxiliary function. Functional derivatives of $G[J]$ with respect to $J(t)$ yield the required results, e.g.

$$\int q\left(t_1\right) q\left(t_2\right) e^{iS[q]} \mathcal{D}q = \frac{1}{i}\frac{\delta}{\delta J(t_1)}\frac{1}{i}\frac{\delta}{\delta J(t_2)}\bigg|_{J(t)=0} G\left[J\right].$$

More generally, for arbitrary $J(t)$ we have

$$\int q\left(t_1\right) q\left(t_2\right) \exp\left[iS\left[q\right] + i\int q(t)J(t)dt\right] \mathcal{D}q = \frac{1}{i}\frac{\delta}{\delta J(t_1)}\frac{1}{i}\frac{\delta}{\delta J(t_2)} G\left[J\right].$$

Note that the action (12.17) of a driven oscillator is already in the form (12.35), where $J(t)$ is the external force. Thus the functional $G[J] \equiv \exp\left(i\Gamma_L\left[J\right]\right)$ can be viewed as the generating functional for path integrals of the form (12.34).

12.2.3 The effective action "recipe"

Comparing Eqs. (12.8) and (12.9), we find that the only difference between the "in-out" matrix element and the "in-in" expectation value is the presence of the retarded

Green's function G_{ret} instead of G_F. Replacing G_F by G_{ret} in the final expression for the matrix element, we get

$$\langle 0_{in}|\,\hat{q}\,(t)\,|0_{in}\rangle = \left.\frac{\delta\Gamma_L\,[J]}{\delta J\,(t)}\right|_{G_F\to G_{ret}}. \tag{12.36}$$

Note that the replacement $G_F \to G_{ret}$ is to be performed *after* computing the functional derivative. The expression (12.36) is again a functional of $J(t)$ as it should be since the expectation value of $\hat{q}$ depends on the force J. In this way the effective action $\Gamma_L[J]$ describes the influence of the external force on the quantum system $\hat{q}$, under the assumption that $\hat{q}$ is initially in the vacuum state.

We formulate our findings as a recipe for computing "in-out" matrix elements and "in-in" expectation values for a quantum system coupled to a classical background:

1. Perform the Wick rotation $t = -i\tau$ to determine the Euclidean action S_E. Compute the Euclidean effective action $\Gamma_E\,[J(\tau)]$ from Eq. (12.25). The Euclidean effective action will involve the Euclidean Green's function G_E.

2. By an analytic continuation to the Lorentzian time t according to Eq. (12.27), obtain the Lorentzian effective action

$$\Gamma_L\,[J(t)] = i\,\Gamma_E\,[J(\tau)]|_{\tau=it}\,,$$

   replacing the Euclidean Green's function G_E by the Feynman Green's function, namely $G_E \to \frac{1}{i}G_F$.

3. Using formal manipulations with the Lorentzian path integral, express the desired matrix element as a combination of functional derivatives of $\Gamma_L[J]$ with respect to J. For example, if J enters linearly into the action as $\int Jqdt$ and we need a matrix element of $\hat{q}(t_1)$, the required functional derivative is simply that in Eq. (12.33).

4. Compute the functional derivatives, keeping the Feynman Green's function G_F. The result is the "in-out" matrix element. Then replace G_F by G_{ret} to obtain the "in-in" expectation value.

> **Remark:** There is no known method to obtain expectation values directly from the effective action. Without replacing $G_F \to G_{ret}$ by hand, the analytic continuation from the Euclidean time cannot be used to produce observable quantities.

Example: correlation functions of the oscillator

To test the recipe, we now compute the correlation function

$$\langle 0_{in}|\,\hat{q}\,(t_1)\,\hat{q}\,(t_2)\,|0_{in}\rangle\,. \tag{12.37}$$

According to the effective action method, we first replace the "in-out" matrix element by a path integral and then rewrite it using functional derivatives:

$$\frac{\langle 0_{out}|\,\hat{q}\,(t_1)\,\hat{q}\,(t_2)\,|0_{in}\rangle}{\langle 0_{out}|0_{in}\rangle} \to \frac{\int q\,(t_1)\,q\,(t_2)\,e^{iS[q,J]}\mathcal{D}q}{\int e^{iS[q,J]}\mathcal{D}q} \tag{12.38}$$

$$= \exp\left(-i\Gamma_L\left[J\right]\right)\frac{1}{i}\frac{\delta}{\delta J\,(t_1)}\frac{1}{i}\frac{\delta}{\delta J\,(t_2)}\exp\left(i\Gamma_L\left[J\right]\right)$$

$$= \frac{\delta\Gamma_L}{\delta J\,(t_1)}\frac{\delta\Gamma_L}{\delta J\,(t_2)} - i\frac{\delta^2\Gamma_L}{\delta J\,(t_1)\,\delta J\,(t_2)}. \tag{12.39}$$

The functional derivatives are evaluated as in Eq. (12.32),

$$\left[\int G_F\,(t,t_1)\,J(t)dt\right]\left[\int G_F\,(t',t_2)\,J(t')dt'\right] - iG_F\,(t_1,t_2)\,. \tag{12.40}$$

However, this result does not coincide with the answer of Exercise 3.4b (see p. 40) because of the J-independent term which should be proportional to $\exp\left(-i\omega(t_1-t_2)\right)$, while we computed it as

$$-iG_F\,(t_1,t_2) = \frac{1}{2\omega}\exp\left(-i\omega\,|t_1-t_2|\right). \tag{12.41}$$

Replacing G_F by G_{ret} in Eq. (12.40), we also obtain an expression which disagrees with the "in-in" expectation value found in Exercise 3.4b in the J-independent term. However, the J-dependent terms are correct.

Exercise 12.3*

Compute the expectation value $\langle 0_{in}|\,\hat{a}^+(t)\hat{a}^-(t)\,|0_{in}\rangle$ using the path integral ratio

$$\frac{\int a^+(t)a^-(t)e^{iS[q,J]}\mathcal{D}q}{\int e^{iS[q,J]}\mathcal{D}q}$$

and the Lorentzian effective action $\Gamma_L\left[J\right]$, by following the recipe described in the text. Compare the results with Eq. (3.12).

Hint: First consider the (Lorentzian) action with two auxiliary external forces $J^{\pm}(t)$,

$$S\left[q,J^+,J^-\right] = \int\left(\frac{1}{2}\dot{q}^2 - \frac{\omega^2}{2}q^2 + J^+a^+ + J^-a^-\right)dt.$$

Here $a^{\pm}(t)$ are the variables introduced in Sec. 3.1 and $J^- = \left(J^+\right)^*$ are complex conjugates. An integration by parts transforms this action into $S\left[q,J\right]$ of this chapter with an appropriately chosen J. The J-dependent terms should coincide with the result (3.12).

Why is are the results of these calculations not entirely correct? We note that the path integral (12.38) is symmetric in t_1 and t_2, while the matrix element (12.37) cannot be a symmetric function since $\hat{q}(t_1)$ does not commute with $\hat{q}(t_2)$. Thus one cannot hope to compute the correct matrix element of a product such as $\hat{q}(t_1)\hat{q}(t_2)$ by calculating a path integral. Sometimes one even finds *divergent* spurious terms (see Exercise 12.3). However, the J-dependent terms are always correct. This phenomenon can

be informally explained as follows: The wrong terms are the result of neglecting the quantum nature of the system $\hat{q}$ manifested by the noncommuting operators. However, an interaction of $\hat{q}$ with a classical external field J cannot depend on the order of quantum operators; one may say that the classical field is "unaware" of the quantum noncommutativity. Therefore one could expect to obtain the correct J-dependent terms by this method. For the applications of the effective action considered in this book, the J-dependent terms are the only important ones.

Remark: One can show that the result of using the path integral (12.38) is the vacuum expectation value of the *time-ordered product*

$$T\hat{q}\left(t_1\right)\hat{q}\left(t_2\right) \equiv \begin{cases} \hat{q}\left(t_1\right)\hat{q}\left(t_2\right), & t_1 \geq t_2; \\ \hat{q}\left(t_2\right)\hat{q}\left(t_1\right), & t_1 \leq t_2. \end{cases}$$

The letter T signifies the ordering of time-dependent operators by decreasing time. We see from Eqs. (12.40)-(12.41) that the result obtained from the path integral calculation is indeed time-ordered, with $|t_1 - t_2|$ instead of $(t_1 - t_2)$ in the exponential. The appearance of the time-ordered product can be understood as follows. The path integral is a representation of an infinite product of propagators for infinitesimal time intervals,

$$\int e^{iS[q,J]}\mathcal{D}q = \lim_{n\to\infty}\int \langle q_f, t_f|\, q_n, t_n\rangle ... \langle q_1, t_1|q_0, t_0\rangle \, dq_1 ... dq_n . \tag{12.42}$$

It can be shown that

$$\frac{1}{i}\frac{\delta}{\delta J(t_k)}\langle q_{k+1}, t_{k+1}|q_k, t_k\rangle = \langle q_{k+1}, t_{k+1}|\hat{q}(t_k)|q_k, t_k\rangle \, .$$

Therefore, evaluating a functional derivative of both sides of Eq. (12.42) with respect to $J(t_k)$ will insert the operator $\hat{q}(t_k)$ at the k-th place in that expression,

$$\frac{1}{i}\frac{\delta e^{i\Gamma_L}}{\delta J\left(t_k\right)} = \int \langle q_f, t_f|\, q_n, t_n\rangle ... \langle q_{k+1}, t_{k+1}|\hat{q}(t_k)|q_k, t_k\rangle ... \langle q_1, t_1|q_0, t_0\rangle \, dq_1 ... dq_n .$$

A second functional derivative with respect to $J(t_l)$ inserts the operator $\hat{q}(t_l)$ at the l-th place. It is clear that if $t_k > t_l$ then $\hat{q}(t_l)$ will appear to the right of $\hat{q}(t_k)$. Now we can remove the decompositions of unity and obtain

$$\int q(t_k)q(t_l)e^{iS[q,J]}\mathcal{D}q = \frac{1}{i}\frac{\delta}{\delta J(t_k)}\frac{1}{i}\frac{\delta}{\delta J(t_l)}e^{i\Gamma_L} = \langle q_f, t_f|\, \hat{q}(t_k)\hat{q}(t_l)\,|q_0, t_0\rangle \, , \quad t_k > t_l .$$

If $t_k < t_l$, the sequence of the operators would be $\hat{q}(t_l)\hat{q}(t_k)$, in accordance with the time ordering prescription.

It follows that the effective action method applied to the correlation function (12.37) actually yields $\langle 0_{in}|\, T\hat{q}(t_1)\hat{q}(t_2)\,|0_{in}\rangle$. The difference between the time-ordered and the usual products is precisely the deviation of the answer we obtained from the correct expression.

12.3 Backreaction

As we can see from the computation of matrix elements in the previous section, the effective action allows one to compute the influence of an external classical force on

a quantum system $\hat{q}$, assuming that $\hat{q}$ is initially in the vacuum state. Another important application of the effective action is to determine the backreaction of the vacuum fluctuations of $\hat{q}$ on the classical background.

In realistic situations the background $J(t)$ is itself a dynamical field described by a classical action $S_B[J]$. In the absence of interactions between $\hat{q}$ and J, the equation of motion for the background would be

$$\frac{\delta S_B\left[J\right]}{\delta J\left(t\right)} = 0.$$

The combined classical action for the total system (q, J) is

$$S_{total} = S\left[q, J\right] + S_B\left[J\right].$$

When the subsystem q is quantized while J remains classical, the modified dynamics of J can be characterized by a "reduced action" $S_{red}[J]$ which is a functional only of J that reflects the influence of the quantum variable $\hat{q}$ (assuming that $\hat{q}$ is in the vacuum state).

If q were a classical system, the reduced action would be obtained by substituting the vacuum trajectory $q(t)$ into the total action. However, in the present case $\hat{q}$ is a quantum variable and its behavior in the vacuum state is not described by a single trajectory. Therefore we are motivated to perform a path integration of $\exp(iS[q, J])$ over appropriate paths $q(t)$ and to define the reduced action by the relation

$$\exp\left(iS_{red}\left[J\right]\right) \equiv \int \mathcal{D}q\, \exp\left(iS\left[q, J\right] + iS_B\left[J\right]\right) = \exp\left(i\Gamma_L\left[J\right] + iS_B\left[J\right]\right),$$

where $\Gamma_L[J]$ is the effective action (12.28). Then the modified equation of motion for the background is

$$\frac{\delta S_{red}\left[J\right]}{\delta J\left(t\right)} = \frac{\delta \Gamma_L\left[J\right]}{\delta J(t)}\bigg|_{G_F \to G_{ret}} + \frac{\delta S_B\left[J\right]}{\delta J(t)} = 0. \tag{12.43}$$

As explained in the previous section, the replacement $G_F \to G_{ret}$ is necessary to obtain physically meaningful results.

The new equation of motion (12.43) describes the dynamics of the background $J(t)$ influenced by the backreaction of the quantum system $\hat{q}$ in the "in" vacuum state. Note that the choice of the "in" vacuum state has been implicit in our derivation of the effective action, and the results would have to be modified if the subsystem $\hat{q}$ is in a different quantum state.

> **Remark: visualizing the backreaction.** In the case of the driven oscillator, Eq. (12.36) shows that the backreaction term in Eq. (12.43) is equal to the vacuum expectation value $\langle\hat{q}(t)\rangle$. Classically, the background J interacts with q as Jq, which means that J is the external force for the oscillator while q is the external force for the system J. Thus we may interpret the backreaction term as the vacuum expectation value of the "backreaction force" $\hat{q}$.

12.3.1 Gauge coupling

A similar picture of the backreaction holds for quantum fields interacting with classical gauge fields. For instance, a matter field ψ interacting with the $U(1)$ gauge field A_μ (the electromagnetic field) can be described by a $U(1)$-invariant action $S^{(m)}[\psi, A_\mu]$. The invariance with respect to local $U(1)$ transformations (5.12) leads to the conservation law for the classical current j^μ,

$$j^\mu_{,\mu} = 0, \quad j^\mu \equiv -\frac{\delta S^{(m)}}{\delta A_\mu}.$$

The dynamics of the electromagnetic field alone is determined by the action $S^{EM}[A_\mu]$. The functional derivative of the total classical action with respect to the field A_μ yields the Maxwell equations,

$$\frac{\delta S^{EM}}{\delta A_\mu} + \frac{\delta S^{(m)}}{\delta A_\mu} = 0 \quad \Rightarrow \quad \frac{1}{4\pi} F^{\mu\nu}_{\ \ ,\nu} + j^\mu = 0, \tag{12.44}$$

where $F_{\mu\nu} = A_{\mu,\nu} - A_{\nu,\mu}$ is the field strength tensor.

Assuming that the quantum field $\hat{\psi}$ is in the vacuum state, we can compute the effective action $\Gamma_L[A_\mu]$ and write the modified classical equation of motion as

$$\frac{\delta S^{EM}}{\delta A_\mu} + \left.\frac{\delta \Gamma_L[A_\mu]}{\delta A_\mu}\right|_{G_F \to G_{ret}} = 0 \quad \Rightarrow \quad \frac{1}{4\pi} F^{\mu\nu}_{\ \ ,\nu} + \left.\frac{\delta \Gamma_L[A_\mu]}{\delta A_\mu}\right|_{G_F \to G_{ret}} = 0.$$

At the same time, the functional derivative of the effective action is related to the vacuum expectation value of the current $\hat{j}^\mu$,

$$\begin{aligned}\langle \hat{j}^\mu(x) \rangle \equiv \langle 0_{in}| \hat{j}^\mu(x) |0_{in}\rangle &= \left. \frac{\int j^\mu(x) \exp\left(iS^{(m)}[\psi, A_\mu]\right) \mathcal{D}\psi}{\int \exp\left(iS^{(m)}[\psi, A_\mu]\right) \mathcal{D}\psi} \right|_{G_F \to G_{ret}} \\ &= \exp\left(-i\Gamma_L[A_\mu]\right) \left(-\frac{1}{i}\right) \frac{\delta}{\delta A_\mu(x)} \exp\left(i\Gamma_L[A_\mu]\right) = -\left. \frac{\delta \Gamma_L[A_\mu]}{\delta A_\mu(x)} \right|_{G_F \to G_{ret}}.\end{aligned}$$

This expectation value can be interpreted as the "effective current" contributed by the quantum field $\hat{\psi}$ due to the presence of the background A_μ; without the electromagnetic field, the expectation value of $\hat{j}^\mu$ would vanish in the vacuum state. The effective current is conserved, $\langle \hat{j}^\mu \rangle_{,\mu} = 0$, and acts as a source to the classical equation of motion (12.44) for the background field A_μ,

$$F^{\mu\nu}_{\ \ ,\nu} = -4\pi \langle \hat{j}^\mu \rangle.$$

This is the vacuum Maxwell equation modified by the backreaction of the quantum field $\hat{\psi}$. (Note that both sides of this equation involve only A_μ since $\langle \hat{j}^\mu \rangle$ is a functional of A_μ.)

12.3.2 Coupling to gravity

An important problem is to compute the backreaction of quantum fluctuations of matter fields on gravitation. For a quantum field $\hat{\phi}$ in a curved spacetime, the metric tensor $g^{\alpha\beta}$ plays the role of the classical background J. The backreaction of the field $\hat{\phi}$ on the metric may be found using the effective action $\Gamma_L\left[g_{\mu\nu}\right]$,

$$\exp\left(i\Gamma_L\left[g_{\mu\nu}\right]\right) \equiv \int \exp\left(iS^{(m)}\left[g_{\mu\nu},\phi\right]\right)\mathcal{D}\phi,$$

where $S^{(m)}[g_{\mu\nu},\phi]$ is the action for the matter field ϕ in the presence of gravitation. If $S^{\text{grav}}[g_{\mu\nu}]$ is the Einstein-Hilbert action for gravity, then the vacuum Einstein equation (5.21),

$$\frac{\delta S^{\text{grav}}}{\delta g^{\alpha\beta}} = -\frac{\sqrt{-g}}{16\pi G}\left(R_{\alpha\beta} - \frac{1}{2}g_{\alpha\beta}R\right) = 0,$$

is modified by a backreaction term in the following way,

$$\frac{\delta S^{\text{grav}}}{\delta g^{\alpha\beta}} + \frac{\delta\Gamma_L\left[g_{\mu\nu}\right]}{\delta g^{\alpha\beta}} = -\frac{\sqrt{-g}}{16\pi G}\left(R_{\alpha\beta} - \frac{1}{2}g_{\alpha\beta}R\right) + \frac{\delta\Gamma_L\left[g_{\mu\nu}\right]}{\delta g^{\alpha\beta}} = 0. \tag{12.45}$$

(Here and below the replacement of Feynman Green's functions by retarded Green's functions is implied.) Using the formula (5.23) for the classical EMT,

$$T_{\alpha\beta}(x) = \frac{2}{\sqrt{-g}}\frac{\delta S^m\left[g_{\mu\nu},\phi\right]}{\delta g^{\alpha\beta}(x)},$$

we can express the vacuum expectation value of the quantum EMT through the effective action as

$$\begin{aligned}\langle\hat{T}_{\alpha\beta}(x)\rangle &= \frac{\int T_{\alpha\beta}(x)\exp\left(iS\left[g,\phi\right]\right)\mathcal{D}\phi}{\int\exp\left(iS\left[g,\phi\right]\right)\mathcal{D}\phi} \\ &= \exp\left(-i\Gamma_L\right)\frac{2}{i\sqrt{-g}}\frac{\delta}{\delta g^{\alpha\beta}(x)}\exp\left(i\Gamma_L\right) = \frac{2}{\sqrt{-g}}\frac{\delta\Gamma_L\left[g_{\mu\nu}\right]}{\delta g^{\alpha\beta}(x)}.\end{aligned}$$

Then Eq. (12.45) is rewritten as the *semiclassical Einstein equation*,

$$R_{\alpha\beta} - \frac{1}{2}g_{\alpha\beta}R = 8\pi G\langle\hat{T}_{\alpha\beta}\rangle. \tag{12.46}$$

In other words, vacuum fluctuations of $\hat{\phi}$ contribute to gravitation by the expectation value of the quantum EMT as if it were the EMT of a classical field. The semiclassical Einstein equation approximately describes the backreaction of quantum fields on the classical metric.

12.3.3 Polarization of vacuum and semiclassical gravity

The presence of gravity changes the properties of the vacuum state of quantum fields. Whether or not particles are produced, the local field observables such as the vacuum expectation value $\langle \hat{T}_{\mu\nu}(x) \rangle$ of the EMT at a point x are different from their Minkowski values. This modification of the vacuum state due to the influence of the classical background is called the *polarization of vacuum*.

The standard measure of the vacuum polarization is the expectation value $\langle \hat{T}_{\mu\nu}(x) \rangle$ of the EMT of quantum fields. It is natural that the polarization of vacuum is described by a *local* function of spacetime. We would like to constrast this with the number density of produced particles, which is an essentially nonlocal quantity that depends on the entire history up to the present time. The concept of "particle" involves nonlocality, and it is impossible to define a generally covariant and local function of quantum fields that would correspond to the number density of particles at a point.

The expectation value of the EMT also describes the backreaction of the quantum fields on the metric via the semiclassical Einstein equation (12.46). Once the metric changes due to this backreaction, the vacuum polarization also changes. So a self-consistent theory of quantum fields in a curved spacetime may be formulated in the following way. A quantum field $\hat{\phi}$ has a nonzero vacuum expectation of the EMT induced by the metric. One computes the value of $\langle \hat{T}_{\mu\nu} \rangle$ in a fixed metric $g_{\mu\nu}(x)$ and then requires that this $g_{\mu\nu}(x)$ should satisfy the semiclassical Einstein equation sourced by the same effective EMT $\langle \hat{T}_{\mu\nu} \rangle$. The theory formulated in this way is known as *semiclassical gravity*.

Solving the self-consistent equations of semiclassical gravity is a challenging task. For instance, it is not straightforward to compute the EMT of a quantum field even in simple spacetimes.[2] Also, self-consistent solutions are not always physically relevant: there are known cases of "runaway" solutions when gravity generates a large value of $\langle \hat{T}_{\mu\nu} \rangle$ which gives rise to a more curved spacetime and to an even stronger vacuum polarization, *ad infinitum*. Semiclassical gravity is an approximate theory applicable only to weakly curved spacetimes where the vacuum polarization is small.

[2] Calculations of the EMT occupy much of the book by N. D. BIRRELL and P. C. W. DAVIES, *Quantum fields in curved space* (Cambridge University Press, 1982).

13 Functional determinants and heat kernels

Summary: Euclidean effective action as a functional determinant. Zeta functions and renormalization of determinants. Computation of ζ functions using heat kernels.

The subject of this and the following chapters is the application of the method of effective action to the description of a quantum scalar field in a gravitational background. In this chapter we introduce the formalisms of functional determinants and heat kernels, which are powerful and elegant tools used in many branches of mathematics and physics. In Chapters 14 and 15 these tools will be applied to the task of computing the generally covariant effective action.

Below we shall often work with spacetimes of dimension two and four, so for convenience we now denote the number of dimensions by 2ω. However, it will not be assumed that ω is integer. The (Greek) spacetime indices, such as μ in "$\partial_\mu\phi$", range from 0 to $2\omega - 1$.

13.1 Euclidean action for fields

We consider a scalar field ϕ described by the classical action

$$S\left[\phi, g_{\mu\nu}\right] = \frac{1}{2}\int \sqrt{-g} d^{2\omega}x \left(g^{\mu\nu}\phi_{,\mu}\phi_{,\nu} - V(x)\phi^2\right), \tag{13.1}$$

where $g_{\mu\nu}(x)$ is the spacetime metric and the potential $V(x)$ is an external field that plays the role of the effective mass of the field ϕ. (This general form of the action can represent both minimally coupled and conformally coupled fields.) We assume that the metric $g_{\mu\nu}(x)$ and the potential $V(x)$ are fixed and known functions of the spacetime.

It is convenient to rewrite the action as a quadratic functional of ϕ,

$$S\left[\phi, g_{\mu\nu}\right] = \frac{1}{2}\int \sqrt{-g} d^{2\omega}x \left[\phi(x)\hat{F}\phi(x)\right], \tag{13.2}$$

where $\hat{F}$ is a suitable differential operator. An explicit form for $\hat{F}$ is easy to derive from Eq. (13.1) using integration by parts. Assuming that $\phi(x) \to 0$ sufficiently

rapidly as $x \to \infty$, we omit the boundary terms and find

$$S[\phi, g_{\mu\nu}] = \frac{1}{2}\int d^{2\omega}x \left[\phi\left(\sqrt{-g}\, g^{\mu\nu}\phi_{,\mu}\right)_{,\nu} - \sqrt{-g}V\phi^2\right]$$
$$= \frac{1}{2}\int \sqrt{-g}d^{2\omega}x \left[\phi\left(-\Box_g - V\right)\phi\right]. \tag{13.3}$$

This form of the action is reminiscent of Eqs. (4.3) and (4.5). Thus the operator $\hat{F}$ is

$$\hat{F} = -\Box_g - V(x),$$

where the symbol $\Box_g$ denotes the covariant D'Alembert operator for scalar fields in the metric $g_{\mu\nu}$,

$$\Box_g\phi \equiv \frac{1}{\sqrt{-g}}\partial_\mu\left[\sqrt{-g}\, g^{\mu\nu}\partial_\nu\phi\right].$$

The classical equation of motion for the field $\phi(x)$ can be written as

$$\hat{F}\phi = \left[-\Box_g - V(x)\right]\phi(x) = 0.$$

13.1.1 Transition to Euclidean metric

We now perform an analytic continuation of the action (13.3) to the Euclidean time $\tau = it$. According to the general procedure outlined in Sec. 12.2.1, the Euclidean action $S_E\left[\phi^{(E)}, g^{(E)}_{\mu\nu}\right]$ is the functional of Euclidean trajectories $\phi^{(E)}(\tau, \mathbf{x})$ and $g^{(E)}_{\mu\nu}(\tau, \mathbf{x})$ defined by

$$S_E\left[\phi^{(E)}, g^{(E)}_{\mu\nu}\right] \equiv \frac{1}{i}S[\phi, g_{\mu\nu}]_{t=-i\tau}.$$

While the Euclidean scalar field ϕ^E is determined straightforwardly,

$$\phi^{(E)}(\tau, \mathbf{x}) = \phi(t, \mathbf{x})|_{t=-i\tau},$$

the metric $g_{\mu\nu}(x)$ is a tensor and must be appropriately transformed under a change of coordinates $\tau = it$. Let us examine this transformation in a little more detail. To simplify the problem, we first consider a purely real change of coordinates

$$x \equiv (t, \mathbf{x}) \to \tilde{x} \equiv \left(\tilde{t}, \mathbf{x}\right) = (\lambda t, \mathbf{x}), \tag{13.4}$$

where λ is a real constant; we shall afterwards perform an analytic continuation in λ and set $\lambda = i$, $\tilde{t} \equiv \tau$.

The transformed scalar field is

$$\tilde{\phi}\left(\tilde{t}, \mathbf{x}\right) = \phi(\lambda t, \mathbf{x}).$$

The components $g_{\mu\nu}$ of the metric tensor transform as

$$g_{\alpha\beta}(t, \mathbf{x}) = \tilde{g}_{\mu\nu}\left(\tilde{t}, \mathbf{x}\right)\frac{\partial\tilde{x}^\mu}{\partial x^\alpha}\frac{\partial\tilde{x}^\nu}{\partial x^\beta} = \begin{pmatrix} \lambda^2\tilde{g}_{00} & \lambda\tilde{g}_{01} & \lambda\tilde{g}_{02} & \lambda\tilde{g}_{03} \\ \lambda\tilde{g}_{10} & \tilde{g}_{11} & \tilde{g}_{12} & \tilde{g}_{13} \\ \lambda\tilde{g}_{20} & \tilde{g}_{21} & \tilde{g}_{22} & \tilde{g}_{23} \\ \lambda\tilde{g}_{30} & \tilde{g}_{31} & \tilde{g}_{32} & \tilde{g}_{33} \end{pmatrix}. \tag{13.5}$$

It is easy to see that the determinant $g \equiv \det g_{\mu\nu}$ changes as $g = \lambda^2 \tilde{g}$ because one row and one column of the matrix $\tilde{g}_{\mu\nu}$ are multiplied by λ. Since

$$d^{2\omega}x = \lambda^{-1} d\tilde{t}\, d^{2\omega-1}\mathbf{x} = \lambda^{-1} d^{2\omega}\tilde{x},$$

the form of the covariant volume measure $\sqrt{-g}d^{2\omega}x$ remains unchanged under the transformation (13.4),

$$\sqrt{-g}d^{2\omega}x = \lambda^{-1}\sqrt{-\lambda^2\tilde{g}}d^{2\omega}\tilde{x} = \sqrt{-\tilde{g}}d^{2\omega}\tilde{x},$$

at least for real λ. The action $S[\phi, g_{\mu\nu}]$ is a generally covariant scalar, therefore we can write

$$\tilde{S}\left[\tilde{\phi}, \tilde{g}_{\mu\nu}\right] = \frac{\lambda^{-1}}{2}\int \sqrt{-\lambda^2\tilde{g}}d^{2\omega}\tilde{x}\left[\tilde{\phi}\left(-\Box_{\tilde{g}} - V\right)\tilde{\phi}\right].$$

Setting $\lambda = i$ and denoting $\tilde{t} \equiv \tau$, $\tilde{x}_\mu \equiv x^{(E)}_\mu$, we now obtain the analytically continued Euclidean field and metric,

$$\phi^{(E)} \equiv \tilde{\phi}\Big|_{\lambda=i}, \quad g^{(E)}_{\mu\nu} \equiv \tilde{g}_{\mu\nu}|_{\lambda=i}, \quad \sqrt{-g} = \sqrt{\tilde{g}} = \sqrt{g^{(E)}}.$$

Thus the Euclidean action can be written as

$$S_E\left[\phi^{(E)}, g^{(E)}_{\mu\nu}\right] = \frac{1}{i}S\left[\phi, g_{\mu\nu}\right]_{t=-i\tau} = \frac{1}{2}\int \sqrt{g^{(E)}}d^{2\omega}x^{(E)}\left[\phi^{(E)}\left(\Box_{g^{(E)}} + V\right)\phi^{(E)}\right]. \tag{13.6}$$

The Euclidean field $\phi^{(E)}$ and the Euclidean metric $g^{(E)}_{\mu\nu}$ are now chosen to be *real-valued* functions of $x^{(E)}$ despite the fact that the transformation (13.5) of a real metric $g_{\mu\nu}$ with $\lambda = i$ will generally yield complex-valued components $\tilde{g}_{\mu\nu}$. As we already remarked in Sec. 12.1.2, the real-valued Euclidean fields do not have a direct physical interpretation. The Euclidean variables $\phi^{(E)}$ and $g^{(E)}_{\mu\nu}$ are introduced merely to obtain the analytic continuation of the *action functional* to the Euclidean domain, $S\left[...\right] = -iS_E\left[...\right]$.

Now we shall bring the Euclidean action to a more convenient form. In our sign convention, the Lorentzian metric $g_{\mu\nu}\left(x\right)$ has the signature $(+---)$, and it is evident from Eq. (13.5) that the Wick rotation transforms $g_{\mu\nu}$ to a metric $g^{(E)}_{\mu\nu}$ with the signature $(----)$. For convenience, we now change the overall sign of the metric and define a new metric variable,

$$\gamma_{\mu\nu}\left(\tau, \mathbf{x}\right) \equiv -g^{(E)}_{\mu\nu}\left(\tau, \mathbf{x}\right) = -\left.g_{\mu\nu}\left(t, \mathbf{x}\right)\right|_{t=-i\tau}.$$

The new metric $\gamma_{\mu\nu}$ is positive-definite with the standard Euclidean signature, namely $(++++)$. Under this last change of variables, we have $\gamma = g^{(E)}$ and $\Box_\gamma = -\Box_{g^{(E)}}$, so the Euclidean action (13.6) is expressed through the new metric as

$$S_E\left[\phi, \gamma_{\mu\nu}\right] = \frac{1}{2}\int \sqrt{\gamma}d^{2\omega}x^{(E)}\left[\phi^{(E)}\left(-\Box_\gamma + V(x)\right)\phi^{(E)}\right].$$

In the next two chapters, we shall perform all calculations exclusively with the Euclidean metric $\gamma_{\mu\nu}$, the field $\phi^{(E)}$ and the coordinates $x^{(E)}$. Therefore it will be convenient henceforth to denote the Euclidean quantities simply by $g_{\mu\nu}$, ϕ and x. We shall keep the symbol $\Box_g$ for the covariant Laplace operator,

$$\Box_g \phi = \frac{1}{\sqrt{g}} \partial_\mu \left[\sqrt{g}\, g^{\mu\nu} \partial_\nu \phi \right],$$

as a reminder of the analytic continuation back to the Lorentzian time that shall be eventually performed.

Thus the final form of the Euclidean action for the field ϕ is

$$S_E \left[\phi, g_{\mu\nu} \right] = \frac{1}{2} \int \sqrt{g} d^{2\omega} x \left[\phi(x) \left(-\Box_g + V(x) \right) \phi(x) \right], \tag{13.7}$$

The Euclidean field $\phi(x)$ satisfies the equation of motion

$$\left[-\Box_g + V(x) \right] \phi(x) = 0. \tag{13.8}$$

13.1.2 Euclidean action for gravity

To illustrate the construction of the Euclidean action on another example, we consider the Einstein-Hilbert action (5.18) for pure gravity,

$$S^{\text{grav}} \left[g_{\mu\nu} \right] = -\frac{1}{16\pi G} \int \left(R + 2\Lambda \right) \sqrt{-g} d^4 x.$$

Performing the transformation $x_\mu \to x_\mu^{(E)}$, $g_{\mu\nu} \to g_{\mu\nu}^{(E)}$ similarly to the previous section, we compute the Euclidean action functional as

$$S_E^{\text{grav}} \left[g_{\mu\nu}^{(E)} \right] = \frac{1}{16\pi G} \int \left(R^{(E)} + 2\Lambda \right) \sqrt{g^{(E)}} d^4 x.$$

Now we express this functional through the positive-definite Euclidean metric $\gamma_{\mu\nu} \equiv -g_{\mu\nu}^{(E)}$. When we flip the sign of the metric, the Christoffel symbol $\Gamma_{\mu\nu}^{\alpha}$ remains unchanged, while the Riemann scalar changes sign,

$$R^E \left[g_{\mu\nu}^{(E)} \right] = -R \left[\gamma_{\mu\nu} \right].$$

Hence the Euclidean action for gravity is

$$S_E^{\text{grav}} \left[\gamma_{\mu\nu} \right] = \frac{1}{16\pi G} \int \left(-R \left[\gamma \right] + 2\Lambda \right) \sqrt{\gamma} d^4 x.$$

13.2 Effective action as a functional determinant

According to Sec. 12.2, the Euclidean effective action $\Gamma_E[g_{\mu\nu}]$ is found from

$$\exp\left(-\Gamma_E\left[g_{\mu\nu}\right]\right) = \int \mathcal{D}\phi \, \exp\left(-S_E\left[\phi, g_{\mu\nu}\right]\right). \tag{13.9}$$

It is not straightforward to define a suitable measure $\mathcal{D}\phi$ in the space of functions $\phi(x)$ because the definition introduced in Sec. 11.3 is not generally covariant. One way to define a generally covariant functional measure is to use expansions in orthogonal eigenfunctions.

We consider the following eigenvalue problem (in Euclidean space),

$$\left[-\Box_g + V(x)\right] \phi_n(x) = \lambda_n \phi_n(x), \tag{13.10}$$

where $\phi_n(x)$ are eigenfunctions with eigenvalues λ_n. For mathematical convenience, we impose boundary conditions on $\phi(x)$ at the boundary of a finite box, so that the spectrum of eigenvalues λ_n is discrete ($n = 0, 1, ...$) and the operator $-\Box_g + V$ is self-adjoint with respect to the natural scalar product

$$(f, g) \equiv \int \sqrt{g} d^{2\omega} x \, f(x) g(x). \tag{13.11}$$

Under natural assumptions on $g_{\mu\nu}$ and $V(x)$, one can show that the eigenvalues λ_n are bounded from below and that the set of all eigenfunctions is normalized and constitutes a complete orthonormal basis in the space of functions,

$$\int \sqrt{g} d^{2\omega} x \, \phi_m(x) \phi_n(x) = \delta_{mn}.$$

Then an arbitrary function $f(x)$ is expanded in this basis as

$$f(x) = \sum_{n=0}^{\infty} c_n \phi_n(x); \tag{13.12}$$

$$c_n = \int \sqrt{g} d^{2\omega} x \, f(x) \phi_n(x). \tag{13.13}$$

The coefficients c_n (which are real numbers) are the coordinates of the function $f(x)$ in the basis $\{\phi_n\}$. There are infinitely many coordinates since the space of functions is infinite-dimensional.

Substituting Eq. (13.12) into the action (13.7), we find a particularly simple expression,

$$S_E\left[\phi, g_{\mu\nu}\right] = \frac{1}{2} \int \sqrt{g} d^{2\omega} x \sum_{m,n} c_m c_n \lambda_m \phi_m \phi_n = \frac{1}{2} \sum_n c_n^2 \lambda_n.$$

This is to be expected since the action (13.7) is a quadratic functional of ϕ which is diagonalized in the basis of eigenfunctions $\{\phi_n\}$.

Once an orthonormal system of eigenfunctions $\{\phi_n(x)\}$ is chosen, the coefficients c_n are independent of the spacetime coordinates since Eq. (13.13) expresses c_n in terms of generally covariant integrals. The action is a function of c_n and λ_n, and the eigenvalues λ_n are also coordinate-independent quantities (eigenvalues of a generally covariant operator). Hence we are motivated to define the functional measure in the path integral (13.9) through the quantities c_n, for example $\mathcal{D}\phi = \prod_n f(c_n) dc_n$ with some function $f(c)$. The simplest choice for $f(c)$ is a constant, and a comparison with the usual path integral measure in flat space suggests the definition

$$\mathcal{D}\phi = \prod_n \frac{dc_n}{\sqrt{2\pi}}. \tag{13.14}$$

Then the path integral (13.9) is evaluated as

$$\int \exp\left(-S_E\left[\phi, g_{\mu\nu}\right]\right) \mathcal{D}\phi = \int \prod_{n=0}^{\infty} \frac{dc_n}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}\lambda_n c_n^2\right) = \left[\prod_{n=0}^{\infty} \lambda_n\right]^{-1/2}.$$

It is well known that the product of all eigenvalues $\prod_n \lambda_n$ of a *finite*-dimensional operator is equal to its determinant. Assuming that a suitable generalization of the determinant can be defined also for infinite-dimensional operators, we can formally rewrite the Euclidean effective action as

$$\Gamma_E\left[g_{\mu\nu}\right] = \frac{1}{2} \ln \prod_{n=0}^{\infty} \lambda_n = \frac{1}{2} \ln \det\left[-\Box_g + V\right]. \tag{13.15}$$

The task of computing an effective action is now reduced to the problem of calculating the determinant of a differential operator (a *functional determinant*). However, it is clear that a functional determinant is not a straightforwardly defined quantity. For a differential operator such as $-\Box_g$, the eigenvalues λ_n grow with n and their product $\prod_n \lambda_n$ diverges. A finite result can be obtained only after an appropriate regularization and renormalization of the determinant. Below by a "functional determinant" we shall always mean "a renormalized functional determinant."

13.3 Zeta functions and heat kernels

To compute the functional determinant of the operator $-\Box_g + V$, we shall first reformulate the problem in terms of linear operators in an auxiliary Hilbert space. If a Hermitian operator $\hat{M}$ acting in some Hilbert space with vectors $|\psi\rangle$ is such that its spectrum of eigenvalues $\{\tilde{\lambda}_n\}$ coincides with $\{\lambda_n\}$,

$$\hat{M}\left|\psi_n\right\rangle = \tilde{\lambda}_n \left|\psi_n\right\rangle, \quad \tilde{\lambda}_n = \lambda_n,$$

then it is clear that the determinant of $\hat{M}$ is the same as the determinant of $-\Box_g + V$.

Such a Hilbert space and an operator $\hat{M}$ can be defined as follows. We postulate an uncountable basis of "generalized vectors" $|x\rangle$, where the label x goes over the

2ω-dimensional (Euclidean) spacetime, exactly as the coordinate x in Eq. (13.10). The basis is assumed to be complete and orthonormal in the distributional sense, so that

$$\langle x|x'\rangle = \delta(x - x'),$$

where we use the ordinary, noncovariant δ function in 2ω dimensions. Vectors of the Hilbert space are, by definition, integrals of the form

$$|\psi\rangle = \int d^{2\omega}x\, \psi(x)\, |x\rangle\,.$$

The integration above is not covariant because x is simply a label. The function $\psi(x)$ specifies the coordinates of the vector $|\psi\rangle$ in the basis $\{|x\rangle\}$; it follows that $\psi(x) = \langle x|\psi\rangle$ and $\hat{1} = \int d^{2\omega}x\, |x\rangle\, \langle x|$. The "generalized vectors" $|x\rangle$ do not belong to the Hilbert space because they do not have a finite norm. This construction is completely analogous to the usual coordinate basis in the Hilbert space of quantum-mechanical wave functions.

The scalar product of vectors $|\psi_1\rangle$ and $|\psi_2\rangle$ is defined by

$$\langle\psi_1|\psi_2\rangle = \langle\psi_1| \left(\int d^{2\omega}x\, |x\rangle\, \langle x| \right) |\psi_2\rangle = \int d^{2\omega}x\, \psi_1(x)\psi_2(x). \tag{13.16}$$

Again, note the noncovariant integration.

From a comparison of Eqs. (13.11) and (13.16), one can see that the difference between the Hilbert space with vectors $|\psi\rangle$ represented by functions $\psi(x)$ and the space of functions $\phi(x)$ is only in the extra factor $\sqrt{g}$ in the scalar product. This suggests a one-to-one correspondence between functions $\phi(x)$ and vectors $|\psi\rangle$ in the auxiliary Hilbert space according to the formula

$$\phi(x) \;\leftrightarrow\; |\psi\rangle \text{ such that } \psi(x) = \langle x|\psi\rangle \equiv g^{1/4}\phi(x). \tag{13.17}$$

This mapping between functions $\phi(x)$ and vectors $|\psi\rangle$ preserves the scalar product: if $\phi_1(x)$ is mapped to $|\psi_1\rangle$ and $\phi_2(x)$ is mapped to $|\psi_2\rangle$, then $(\phi_1, \phi_2) = \langle\psi_1|\psi_2\rangle$.

Using the map (13.17), the self-adjoint differential operator $-\Box_g + V$ can be transformed into a Hermitian operator $\hat{M}$ acting in the Hilbert space. The required operator $\hat{M}$ must be such that for all vectors $|\psi\rangle$,

$$\text{if } \; |\psi\rangle \leftrightarrow \phi(x) \; \text{ then } \; \hat{M}\,|\psi\rangle \leftrightarrow (-\Box_g + V)\,\phi(x).$$

It follows from Eq. (13.17) that $\hat{M}\,|\psi\rangle$ is the vector with the coordinate function

$$\langle x|\,\hat{M}\,|\psi\rangle \equiv g^{1/4}(x)\,(-\Box_g + V)\left[g^{-1/4}\psi(x)\right]. \tag{13.18}$$

The operator $\hat{M}$ is defined by Eq. (13.18) as a certain differential operator acting on coordinate functions.

It is convenient to represent this operator by its matrix elements in the $|x\rangle$ basis:

$$\langle x|\,\hat{M}\,|x'\rangle = g^{1/4}(x)\left(-\Box_{g(x)} + V\right)\left[g^{-1/4}(x)\delta(x - x')\right]. \tag{13.19}$$

This representation is easy to derive from Eq. (13.18) if we note that the vector $|x'\rangle$ has the coordinate function $\langle x|x'\rangle = \delta(x - x')$. One may use Eq. (13.19) as a definition of the operator $\hat{M}$. (We wrote $\Box_{g(x)}$ in Eq. (13.19) with the subscript $_{g(x)}$ to show that the derivatives implied by the symbol $\Box$ are with respect to x and not x'.)

We have shown that the set of orthonormal eigenfunctions $\phi_n(x)$ of the differential operator $-\Box_g + V$ is in a one-to-one correspondence with the set of orthonormal eigenvectors $|\psi_n\rangle$ of the operator $\hat{M}$ with the same eigenvalues λ_n. Thus we replaced a problem involving a partial differential equation by an equivalent problem with linear operators in a Hilbert space.

> **Remark: Hilbert space $\neq$ quantum mechanics.** The appearance of a Hilbert space and of the Dirac notation does not mean that the vectors $|\psi\rangle$ are states of some quantum system. We use the Hilbert space formalism because it makes calculations of renormalized determinants easier. It is possible but much more cumbersome to derive the same results by direct manipulations of the equivalent partial differential equations.

13.3.1 Renormalization using zeta functions

The method of zeta (ζ) functions can be used to compute renormalized determinants of operators. For an operator $\hat{M}$ with eigenvalues λ_n, we define the *zeta function of the operator* $\hat{M}$, denoted $\zeta_M(s)$, by

$$\zeta_M(s) \equiv \sum_{n=0}^{\infty} \left(\frac{1}{\lambda_n}\right)^s . \tag{13.20}$$

The function $\zeta_M(s)$ is similar to Riemann's ζ function (10.9) except for the summation over the eigenvalues λ_n instead of the natural numbers. The sum in Eq. (13.20) converges for large enough real s, and for all other s one obtains $\zeta_M(s)$ by an analytic continuation. Usually the resulting function $\zeta_M(s)$ is well-defined for almost all complex values of s.

It follows from Eq. (13.20) that

$$\frac{d\zeta_M(s)}{ds} = \frac{d}{ds}\sum_n e^{-s\ln\lambda_n} = -\sum_n e^{-s\ln\lambda_n}\ln\lambda_n,$$

and therefore

$$\ln\det\hat{M} = \ln\prod_n \lambda_n = \sum_n \ln\lambda_n = -\left.\frac{d\zeta_M(s)}{ds}\right|_{s=0} . \tag{13.21}$$

After an analytic continuation, the function $\zeta_M(s)$ is usually regular at $s = 0$, so the derivative $d\zeta_M/ds$ exists and is finite. Then the formula (13.21) is regarded as a *definition* of the determinant $\det\hat{M}$. Of course, this definition coincides with the standard one for finite-dimensional operators.

The formula (13.21) is the main result of the ζ function method. We stress that the derivations of Eqs. (13.15) and (13.21) are *formal* (i.e. not mathematically well-defined) because we manipulated sums such as $\sum_n \ln\lambda_n$ as if these sums were finite.

Lacking a rigorous argument, one should use such formal calculations with caution as tools with an unknown domain of validity. In practice, Eq. (13.21) has a wide area of application and seems to always give physically reasonable results. In many cases, the answers obtained from the ζ function method have been verified by other, more direct regularization and renormalization procedures. For this reason the method of ζ functions is considered a valid method of renormalization of divergences in QFT.

As an example, we compute the determinant of the Laplace operator $\hat{M} = -\partial_x^2$ in one-dimensional box of length L. (The minus sign is chosen to make the eigenvalues positive.) The operator $-\partial_x^2$ is self-adjoint in the space of square-integrable functions $f(x)$ satisfying the boundary conditions $f(0) = f(L) = 0$. The eigenvalues and the eigenfunctions are

$$-\frac{\partial^2}{\partial x^2} f_n = \lambda_n f_n, \quad f_n(x) = \sin\frac{\pi n x}{L}, \quad \lambda_n = \frac{\pi^2 n^2}{L^2}, \; n = 1, 2, ...$$

The function $\zeta_M(s)$ is computed as

$$\zeta_M(s) = \sum_{n=1}^{\infty} \frac{1}{\lambda_n^s} = \frac{L^{2s}}{\pi^{2s}} \sum_{n=1}^{\infty} \frac{1}{n^{2s}} = \frac{L^{2s}}{\pi^{2s}} \zeta(2s),$$

where $\zeta(s)$ is Riemann's zeta function. Therefore

$$\det(-\partial_x^2) = -\left.\frac{d}{ds}\right|_{s=0} \zeta_M(s) = -\left.\frac{d}{ds}\right|_{s=0} \left[\frac{L^{2s}}{\pi^{2s}} \zeta(2s)\right] = \ln(2L),$$

where we have used the properties (proved in the theory of the Riemann's ζ function)

$$\zeta(0) = -\frac{1}{2}, \quad \zeta'(0) = -\frac{1}{2}\ln(2\pi).$$

> **Remark: another representation of ζ function.** If the operator $\hat{M}^{-s}$ is well-defined for some s, then the spectrum of eigenvalues of $\hat{M}^{-s}$ consists of $\{\lambda_n^{-s}\}$ and the ζ function of the operator $\hat{M}$ can be expressed through the trace of $\hat{M}^{-s}$ as
>
> $$\zeta_M(s) = \sum_n (\lambda_n)^{-s} = \mathrm{Tr}\,(\hat{M}^{-s}). \tag{13.22}$$
>
> As long as $\mathrm{Tr}\,(\hat{M}^{-s})$ is well-defined, Eq. (13.22) is equivalent to the definition (13.20).

13.3.2 Heat kernels

The definition (13.20) of the function $\zeta_M(s)$ requires one to know all eigenvalues λ_n of the operator $\hat{M}$. In practice it is more convenient to compute the ζ function using another mathematical construction called the heat kernel.

We assume that $\hat{M}$ is a Hermitian operator with positive eigenvalues λ_n and a complete basis of the corresponding orthonormal eigenvectors $|\psi_n\rangle$. The *heat kernel*

of the operator $\hat{M}$ is the operator $\hat{K}_M(\tau)$ which is a function of a scalar parameter τ, defined by

$$\hat{K}_M(\tau) \equiv \sum_n e^{-\lambda_n \tau} |\psi_n\rangle \langle\psi_n| . \tag{13.23}$$

It is easy to see that $\hat{K}_M(\tau)|_{\tau=0} = \hat{1}$ and that the operator $\hat{K}_M(\tau)$ is well-defined for $\tau > 0$. The real parameter τ is sometimes called the "proper time" but has no immediate physical significance as time. In the present context, the variable τ is purely formal and will eventually disappear from calculations.

Now we shall show that the *trace* of the heat kernel, $\mathrm{Tr}\, \hat{K}_M(\tau)$, is related to the ζ function of the operator $\hat{M}$. The trace of an operator is the same in any basis, and $\mathrm{Tr}\, \hat{K}_M(\tau)$ is most easily expressed in the basis $|\psi_n\rangle$:

$$\mathrm{Tr}\, \hat{K}_M(\tau) = \sum_n \langle\psi_n| \hat{K}_M(\tau) |\psi_n\rangle = \sum_n e^{-\lambda_n \tau}.$$

Rescaling the definition of Euler's Γ function (see Appendix A.3) by a constant λ,

$$\Gamma(s) = \int_0^\infty e^{-\tau} \tau^{s-1} d\tau = \lambda^s \int_0^\infty e^{-\lambda\tau} \tau^{s-1} d\tau, \quad \mathrm{Re}\, s > 0,$$

one obtains the following representation for the function $\zeta_M(s)$,

$$\zeta_M(s) = \sum_n (\lambda_n)^{-s} = \frac{1}{\Gamma(s)} \int_0^{+\infty} \left[\mathrm{Tr}\, \hat{K}_M(\tau)\right] \tau^{s-1} d\tau. \tag{13.24}$$

The integral converges for the same range of s for which the sum (13.20) converges. Thus the ζ function of an operator can be computed if the trace of the corresponding heat kernel is known.

At first it seems to be more difficult to compute $\hat{K}_M(\tau)$ than $\zeta_M(s)$, since Eq. (13.23) requires one to know not only all the eigenvalues λ_n but also the eigenvectors $|\psi_n\rangle$. However, the heat kernel has a useful property: it is a solution of an operator-valued differential equation. Evaluating the derivative of the heat kernel with respect to τ, one finds

$$\frac{d}{d\tau} \hat{K}_M(\tau) = -\sum_n e^{-\lambda_n \tau} \lambda_n |\psi_n\rangle \langle\psi_n| = -\hat{M}\hat{K}_M. \tag{13.25}$$

The formal solution of Eq. (13.25) with the initial condition $\hat{K}_M(0) = \hat{1}$ is

$$\hat{K}_M(\tau) = \exp(-\tau\hat{M}). \tag{13.26}$$

The trace of the heat kernel is therefore expressed as

$$\mathrm{Tr}\, \hat{K}_M(\tau) = \int d^{2\omega}x \, \langle x| \exp(-\tau\hat{M}) |x\rangle .$$

In practice it is easier to solve the differential equation (13.25) in a conveniently chosen basis than to evaluate the exponential of the operator $\hat{M}$.

As an example, we shall compute the heat kernel of the Laplace operator $\hat{M} \equiv -\Delta$ in one-dimensional space,

$$\hat{K}_M(\tau) = \exp(\tau\Delta_x) = \exp(\tau\partial_x^2).$$

The matrix element $\langle x|\, \hat{K}_M(\tau)\, |x'\rangle \equiv K(x, x', \tau)$ is a solution of

$$\frac{d}{d\tau}K(x, x', \tau) = \Delta_x K(x, x', \tau) \tag{13.27}$$

with the initial condition

$$K\ (x, x', \tau)|_{\tau=0} = \delta(x - x').$$

A Fourier transform in x,

$$K(x, x', \tau) = \int \frac{dk}{2\pi} e^{ikx} \tilde{K}(k, x', \tau); \quad \tilde{K}(k, x', \tau) = \int dx\, e^{-ikx} K(x, x', \tau),$$

yields the equation

$$\frac{d}{d\tau}\tilde{K}(k, x', \tau) = -k^2 \tilde{K}(k, x', \tau), \quad \tilde{K}\ (k, x', \tau)|_{\tau=0} = e^{-ikx'},$$

which has the solution

$$\tilde{K}(k, x', \tau) = e^{-\tau k^2 - ikx'} \quad \Rightarrow \quad K(x, x', \tau) = \frac{1}{\sqrt{4\pi\tau}} \exp\left[-\frac{(x - x')^2}{4\tau}\right].$$

The origin of the name "heat kernel" is that $\hat{K}_M(\tau)$ with $\hat{M} = -\Delta$ is a solution of the heat equation (13.27) which describes the propagation of heat in a homogeneous medium. However, the construction of the heat kernel has a much wider area of application, from quantum statistical physics to differential topology.

> **Remark: exponentials of operators.** Representations involving operator-valued exponentials, such as Eq. (13.26), do not always help to obtain explicit solutions. For instance, it is well known that the time-dependent Schrödinger equation cannot be explicitly solved for general time-independent Hamiltonians $\hat{H}$, although one always has the representation of the solution in the form
>
> $$|\psi(t)\rangle = \exp(-it\hat{H})\, |\psi(0)\rangle\,.$$
>
> Also, such representations are *formal* because the exponential of an operator is not always well-defined. The convergence of the series for $\exp \hat{M}$ is certain only for finite-dimensional spaces where all operators have bounded eigenvalues. Indeed, the operator $\exp \hat{M}$ applied to a vector $|\psi\rangle$ is equal to the series
>
> $$e^{\hat{M}}\, |\psi\rangle \equiv \sum_{n=0}^{\infty} \frac{1}{n!} \hat{M}^n\, |\psi\rangle$$
>
> which is generally not guaranteed to converge. For example, the action of the operator $\exp(-\Delta) = \exp(-\partial_x^2)$ on the function $\phi(x) = \exp\left(-x^2\right)$ is undefined. In contrast, the

action of $\exp(+\partial_x^2)$, which is the heat kernel for $\hat{M} \equiv -\partial_x^2$ evaluated at $\tau = 1$, is well-defined on $\exp\left(-x^2\right)$. Moreover, this heat kernel has an integral representation

$$\left[\hat{K}_M(\tau)\psi\right](x) = \langle x|\, \hat{K}_M(\tau) \int dy\, |y\rangle\, \psi(y) = \int \frac{\psi(y)\, dy}{\sqrt{4\pi\tau}} \exp\left[-\frac{(x-y)^2}{4\tau}\right]$$

which is well-defined for *all* (not necessarily differentiable) square-integrable functions $\psi(x)$. Thus the exponential representation $\exp(\tau\partial_x^2)$ is too restrictive for this operator.

Keeping in mind that the literal interpretation of $\exp \hat{M}$ as an infinite series may be problematic, we shall nevertheless often write expressions such as $\exp(\tau\Delta)$ as a symbolic shorthand for the heat kernel and other similar operators.

13.3.3 The zeta function "recipe"

To summarize, we arrived at the following recipe for computing the renormalized effective action $\Gamma_E[J]$ for a classical background J interacting with a free quantum field $\hat{\phi}$:

1. Write the classical Euclidean equations of motion for ϕ (at fixed J) as $\hat{F}\phi = 0$ and formulate the eigenvalue problem, $\hat{F}\phi_n(x) = \lambda_n \phi_n(x)$, with the appropriate boundary conditions.

2. Construct a Hermitian operator $\hat{M}$ with the same spectrum of eigenvalues, acting in a suitable Hilbert space.

3. Compute the heat kernel $\hat{K}_M(\tau)$ of the operator $\hat{M}$ by solving Eq. (13.25). Find the trace of the heat kernel.

4. Determine the zeta function $\zeta_M(s)$ from Eq. (13.24) and analytically continue to $s = 0$.

5. Find the Euclidean effective action from the formula

$$\Gamma_E[J] = \frac{1}{2} \ln\det \hat{M} \equiv -\frac{1}{2} \left.\frac{d\zeta_M(s)}{ds}\right|_{s=0}.$$

14 Calculation of heat kernel

Summary: Calculation of the trace of the heat kernel as a perturbative series. Comparison with the Seeley-DeWitt expansion.

We shall now perform a calculation of the heat kernel of a Euclidean scalar field in a gravitational background. This is the first step toward computing the effective action which is the subject of the next chapter. The calculation is long and will be presented in detail.

According to the method developed in Chapter 13, the effective action is expressed through the trace of the heat kernel $\hat{K}_M(\tau) \equiv \exp(-\tau \hat{M})$ of the operator $\hat{M}$ defined by Eq. (13.19),

$$\hat{M} = g^{1/4}(x)\,(-\Box_g + V(x))\,g^{-1/4}(x),$$

where $\Box_g$ is the covariant Laplace operator corresponding to the metric $g_{\mu\nu}$, and $V(x)$ is an external potential. It is difficult to compute the heat kernel $\hat{K}_M(\tau)$ for a general metric $g_{\mu\nu}(x)$ and a general potential $V(x)$. However, for small potentials $|V| \ll 1$ and for metrics $g_{\mu\nu}$ that are almost flat, the operator $\hat{M}$ is almost equal to $-\Box$, where $\Box$ is the Laplace operator in flat space (with the metric $\delta_{\mu\nu}$). The heat kernel for the flat space is easily found; below it will be denoted by $\hat{K}_0(\tau)$ and calculated explicitly. Therefore we shall consider the case when the space is almost flat (weakly curved).

In that case, there exists a coordinate system in which one can decompose $g_{\mu\nu}$ into a sum of the flat Euclidean metric $\delta_{\mu\nu}$ and a small perturbation $h_{\mu\nu}$:

$$g_{\mu\nu}(x) = \delta_{\mu\nu} + h_{\mu\nu}(x), \quad g^{\mu\nu}(x) = \delta^{\mu\nu} + h^{\mu\nu}(x). \tag{14.1}$$

Note that $h^{\mu\nu}$ is the perturbation in $g^{\mu\nu}$ which is not the same as $h_{\mu\nu}$ with raised indices, and in fact

$$g^{\mu\alpha}g_{\mu\beta} = (\delta^{\mu\alpha} + h^{\mu\alpha})(\delta_{\mu\beta} + h_{\mu\beta}) = \delta^\alpha_\beta \quad \Rightarrow \quad h^{\mu\nu} = -h_{\alpha\beta}\delta^{\mu\alpha}\delta^{\mu\beta} + O\left[(h_{\alpha\beta})^2\right].$$

The decomposition (14.1) is not generally covariant, i.e. it depends on the choice of the coordinate system: since $\delta_{\mu\nu}$ is not a tensor but a fixed matrix, the components of the perturbation $h_{\mu\nu}$ do not transform as components of a tensor under a change of coordinates. The coordinate system must be chosen so that $h_{\mu\nu}(x)$ is everywhere small; for an only slightly curved space, this choice is always possible. Assuming also that $|V| \ll 1$, we can represent the heat kernel $\hat{K}_M(\tau)$ as a sum of the flat-space kernel $\hat{K}_0(\tau)$ and progressively smaller corrections,

$$\hat{K}_M(\tau) = \hat{K}_0(\tau) + \hat{K}_1(\tau) + \hat{K}_2(\tau) + ..., \tag{14.2}$$

where $\hat{K}_n(\tau)$ are operators of n-th order in the small parameters $h_{\mu\nu}$ and V. We shall compute the heat kernel in this way (i.e. *perturbatively*).

In the leading order, the curvature of the space is proportional to second derivatives of $h_{\mu\nu}$, so the perturbative expansion is meaningful if the curvature and the potential V are small. We shall calculate only the initial term $\hat{K}_0(\tau)$ and the leading correction $\hat{K}_1(\tau)$ which is of first order in $h_{\mu\nu}$ and V. Computations of higher-order corrections are certainly possible but rapidly become extremely cumbersome.

14.1 Perturbative ansatz for the heat kernel

We begin with a calculation of the initial approximation to the heat kernel, $\hat{K}_0(\tau)$. This operator satisfies

$$\frac{d\hat{K}_0}{d\tau} = \Box\hat{K}_0, \quad \hat{K}_0(0) = \hat{1}, \tag{14.3}$$

where $\Box$ is the flat Laplace operator. The formal solution is $\hat{K}_0(\tau) = \exp(\tau\Box)$, and the matrix element of $\hat{K}_0(\tau)$ can be written as

$$\langle x|\, \hat{K}_0(\tau)\, |y\rangle = \langle x|\, e^{\tau\Box}\, |y\rangle = e^{\tau\Box_x}\delta(x-y),$$

where $\Box_x$ indicates that the Laplace operator is acting on the x argument. (Recall that $|y\rangle$ is a vector with the coordinate function $\psi(x) = \delta(x-y)$, and that the operator $\exp(\tau\Box)$ acts on coordinate functions $\psi(x)$ by differentiating with respect to x.)

Now we use the Fourier representation of the δ function in 2ω dimensions,

$$\delta(x-y) = \int \frac{d^{2\omega}k}{(2\pi)^{2\omega}} e^{ik\cdot(x-y)},$$

expand $e^{\tau\Box_x}$ in the power series and find

$$\begin{aligned}\langle x|\, \hat{K}_0(\tau)\, |y\rangle = e^{\tau\Box_x}\delta(x-y) &= \int \frac{d^{2\omega}k}{(2\pi)^{2\omega}} \left[\sum_{n=0}^{\infty} \frac{(\tau\Box_x)^n}{n!}\right] e^{ik\cdot(x-y)} \\ &= \int \frac{d^{2\omega}k}{(2\pi)^{2\omega}} \left[\sum_{n=0}^{\infty} \frac{\left(-\tau k^2\right)^n}{n!}\right] e^{ik\cdot(x-y)} = \int \frac{d^{2\omega}k}{(2\pi)^{2\omega}} e^{-\tau k^2 + ik\cdot(x-y)}.\end{aligned}$$

The resulting Gaussian integral is easily computed:

$$\langle x|\, \hat{K}_0(\tau)\, |y\rangle = \frac{1}{(4\pi\tau)^{\omega}} \exp\left[-\frac{(x-y)^2}{4\tau}\right]. \tag{14.4}$$

This expression also coincides with the Green's function of the heat equation in 2ω spatial dimensions.

Perturbative expansion for $\hat{K}_M(\tau)$

For a weakly curved space and small potentials $|V| \ll 1$, the operator $-\hat{M}$ can be represented as a sum of the flat-space Laplace operator and a small correction which we denote by $\hat{s}\,[h_{\mu\nu}, V]$:

$$-\hat{M} = \Box + \hat{s}\,[h_{\mu\nu}, V]\,.$$

The full heat kernel $\hat{K}_M = \hat{K}_0 + \hat{K}_1 + ...$ is a solution of

$$\frac{d}{d\tau}\hat{K}_M = (\Box + \hat{s})\,\hat{K}_M, \qquad \hat{K}_M(0) = \hat{1}. \tag{14.5}$$

To find the first correction $\hat{K}_1$, we substitute $\hat{K}_M(\tau) = \hat{K}_0(\tau) + \hat{K}_1(\tau)$ into Eq. (14.5), use Eq. (14.3), and get

$$\frac{d}{d\tau}\hat{K}_1 = (\Box + \hat{s})\,\hat{K}_1 + \hat{s}\hat{K}_0, \qquad \hat{K}_1(0) = 0.$$

The operator $\hat{s}$ is considered to be a small perturbation, so we can neglect the higher-order term $\hat{s}\hat{K}_1$ and thus obtain the equation that determines $\hat{K}_1(\tau)$,

$$\frac{d}{d\tau}\hat{K}_1 = \Box\hat{K}_1 + \hat{s}\hat{K}_0, \qquad \hat{K}_1(0) = 0. \tag{14.6}$$

Similarly the second-order correction $\hat{K}_2(\tau)$ can be found from

$$\frac{d}{d\tau}\hat{K}_2 = \Box\hat{K}_2 + \hat{s}\hat{K}_1, \qquad \hat{K}_2(0) = 0.$$

In this way one could in principle calculate all terms of the expansion (14.2) consecutively.

The small parameters of the perturbative expansion are $h_{\mu\nu}$ and V. For convenience, we shall denote them collectively by h, writing e.g. $O(h)$ for terms which are first-order in $h_{\mu\nu}$ and V.

Explicit form of $\hat{s}$

By combining Eqs. (13.19) and (14.1), the correction operator $\hat{s}$ can be represented as a sum of three terms,

$$\hat{s} = \hat{h} + \hat{\Gamma} + \hat{P}, \tag{14.7}$$

for which the following exercise derives the explicit formulae.

Exercise 14.1

The matrix elements of the operator $\hat{M}$ in the coordinate basis $|x\rangle$ are

$$\begin{aligned}\langle x|\,\hat{M}\,|x'\rangle &= g^{1/4}\left(-\Box_{g(x)} + V\right)\left[g^{-1/4}\delta(x-x')\right] \\ &= -g^{1/4}\frac{1}{\sqrt{g}}\frac{\partial}{\partial x^\nu}\left[g^{\mu\nu}\sqrt{g}\frac{\partial}{dx^\mu}\left(g^{-1/4}\delta(x-x')\right)\right] + V(x)\delta(x-x').\end{aligned}$$

Using the expansion (14.1) for the metric, show that the operator $\hat{M}$ may be rewritten as

$$-\hat{M} = \Box + \hat{h} + \hat{\Gamma} + \hat{P},$$

where the operators $\Box$, $\hat{h}$, $\hat{\Gamma}$, $\hat{P}$ are defined by specifying their matrix elements as follows,

$$\langle x|\,\Box\,|x'\rangle \equiv \delta^{\mu\nu}\partial_\mu\partial_\nu\delta(x-x'), \tag{14.8}$$

$$\langle x|\,\hat{h}\,|x'\rangle \equiv h^{\mu\nu}\partial_\mu\partial_\nu\delta(x-x'), \tag{14.9}$$

$$\langle x|\,\hat{\Gamma}\,|x'\rangle \equiv h^{\mu\nu}_{,\nu}\partial_\mu\delta(x-x'), \tag{14.10}$$

$$\langle x|\,\hat{P}\,|x'\rangle \equiv P(x)\delta(x-x'). \tag{14.11}$$

The partial derivatives are $\partial_\mu \equiv \partial/\partial x^\mu$ (not $\partial/\partial x'^\mu$) and the auxiliary function $P(x)$ is defined by

$$P(x) \equiv -\frac{1}{4}g^{\mu\nu}g^{\alpha\beta}h_{\alpha\beta,\mu\nu} - \frac{1}{4}g^{\mu\nu}h^{\alpha\beta}_{,\mu}h_{\alpha\beta,\nu} - \frac{1}{4}h^{\mu\nu}_{,\nu}g^{\alpha\beta}h_{\alpha\beta,\mu} - \frac{1}{16}g^{\mu\nu}g^{\alpha\beta}g^{\kappa\lambda}h_{\alpha\beta,\mu}h_{\kappa\lambda,\nu} - V.$$

Hint: Use the identity $(\ln g)_{,\mu} = g^{\alpha\beta}g_{\alpha\beta,\mu}$.

Again we note that the decomposition of $\hat{M}$ into $\Box$ and $\hat{s}$ is not covariant but depends on the coordinate system. The operators $\Box$, $\hat{h}$, $\hat{\Gamma}$, $\hat{P}$ given by Eqs. (14.8)-(14.11) are also not covariantly defined. Nevertheless, the final result will be brought to a generally covariant form.

The first correction, $\hat{K}_1(\tau)$

Since $\hat{K}_0(\tau)$ is already known, we can solve Eq. (14.6) by the standard method of variation of constants, keeping in mind that the operators $\Box$, $\hat{K}_0(\tau)$, and $\hat{s}$ do not commute. We let $\hat{K}_1(\tau) = \hat{K}_0(\tau)\hat{C}(\tau)$ where $\hat{C}(\tau)$ is an unknown function, substitute into Eq. (14.6) and find

$$\hat{K}_0(\tau)\frac{d}{d\tau}\hat{C}(\tau) = \hat{s}\hat{K}_0(\tau) \;\Rightarrow\; \hat{C}(\tau) = \int_0^\tau d\tau'\,\hat{K}_0^{-1}(\tau')\hat{s}\hat{K}_0(\tau'). \tag{14.12}$$

The integral is performed from $\tau' = 0$ to satisfy the initial condition $\hat{C}(0) = 0$. It follows from Eq. (14.3) that

$$\hat{K}_0(\tau)\hat{K}_0(\tau') = \hat{K}_0(\tau+\tau'), \quad \tau > 0,\ \tau' > 0.$$

Therefore $\hat{K}_0^{-1}(\tau) = \hat{K}_0(-\tau)$ and the solution is

$$\hat{K}_1(\tau) = \int_0^\tau d\tau'\,\hat{K}_0(\tau-\tau')\hat{s}\hat{K}_0(\tau'). \tag{14.13}$$

Remark: inverting the heat kernel. Note that Eq. (14.12) involves the inverse heat kernel $\hat{K}_0^{-1}(\tau) = \hat{K}_0(-\tau)$ which is undefined on most functions. Indeed, from Eq. (14.4) one finds that the operator $\hat{K}_0(\tau)$ with $\tau < 0$ can be applied to a function only if that function decays extremely quickly at large $|x|$. However, the potentially problematic operator $\hat{C}(\tau)$ does not enter the final formula (14.13) which contains only $\hat{K}_0(\tau-\tau')$ and $\hat{K}_0(\tau')$ with $\tau - \tau' \geq 0$ and $\tau \geq 0$.

Diagonal matrix element of $\hat{K}_1$

Our next task is to compute the trace of the operator (14.13) with $\hat{s}$ given by Eq. (14.7). Since $\hat{K}_1$ is linear in $\hat{s}$ and $\hat{s} = \hat{h} + \hat{\Gamma} + \hat{P}$, the result is also a sum that can be symbolically written as

$$\hat{K}_1 = \hat{K}_1^h + \hat{K}_1^\Gamma + \hat{K}_1^P.$$

To compute the trace of the operator $\hat{K}_1$, we need to determine the matrix element

$$\langle x|\, \hat{K}_1\, |x\rangle = \langle x|\, \hat{K}_1^h\, |x\rangle + \langle x|\, \hat{K}_1^\Gamma\, |x\rangle + \langle x|\, \hat{K}_1^P\, |x\rangle\,.$$

We start with the term $\hat{K}_1^P$ because it is the simplest one. Using Eqs. (14.4) and (14.11), one finds

$$\begin{aligned}
\langle x|\, \hat{K}_1^P\, |x\rangle &= \int_0^\tau d\tau'\, \langle x|\, \hat{K}_0(\tau-\tau')\hat{P}\hat{K}_0(\tau')\, |x\rangle \\
&= \int_0^\tau d\tau'\, \langle x|\, \hat{K}_0(\tau-\tau') \int d^{2\omega}y\, |y\rangle\, \langle y|\, \hat{P} \int d^{2\omega}z\, |z\rangle\, \langle z|\, \hat{K}_0(\tau')\, |x\rangle \\
&= \int_0^\tau d\tau' \int d^{2\omega}y\, \langle x|\, \hat{K}_0(\tau-\tau')\, |y\rangle\, P(y)\, \langle y|\, \hat{K}_0(\tau')\, |x\rangle \\
&= \int_0^\tau d\tau' \int d^{2\omega}y \frac{\exp\left[-\frac{(x-y)^2}{4(\tau-\tau')} - \frac{(x-y)^2}{4\tau'}\right]}{[4\pi(\tau-\tau')]^\omega\, [4\pi\tau']^\omega} P(y).
\end{aligned}$$

To convert the last integral to a more useful form, we use another mathematical trick. Introducing the Fourier transform of the function $P(y)$,

$$P(y) = \int \frac{d^{2\omega}k}{(2\pi)^\omega} e^{ik\cdot y} p(k),$$

we can evaluate the Gaussian integral over $d^{2\omega}y$ (see Exercise 14.2),

$$\begin{aligned}
\langle x|\, \hat{K}_1^P\, |x\rangle &= \int_0^\tau d\tau' \int \frac{d^{2\omega}k\, d^{2\omega}y}{(2\pi)^\omega} \frac{\exp\left[-\frac{(x-y)^2}{4(\tau-\tau')} - \frac{(x-y)^2}{4\tau'} + ik\cdot y\right]}{[4\pi(\tau-\tau')]^\omega\, [4\pi\tau']^\omega} p(k) \\
&= \frac{1}{(4\pi\tau)^\omega} \int_0^\tau d\tau' \int \frac{d^{2\omega}k}{(2\pi)^\omega} \exp\left[-\frac{\tau'(\tau-\tau')}{\tau} k^2 + ik\cdot x\right] p(k).
\end{aligned}$$

The result can be rewritten in an operator form which will be useful later:

$$\langle x|\, \hat{K}_1^P\, |x\rangle = \frac{1}{(4\pi\tau)^\omega} \int_0^\tau d\tau'\, \exp\left[\frac{\tau'(\tau-\tau')}{\tau} \Box_x\right] P(x). \tag{14.14}$$

As before, the flat Laplace operator $\Box_x$ contains derivatives with respect to the coordinate x. Note that the operator exponential in Eq. (14.14) is to be understood formally, i.e. as a shorthand representation of the corresponding integral operator; the function $P(x)$ does not need to be infinitely differentiable.

Exercise 14.2
Verify the following Gaussian integral over the 2ω-dimensional Euclidean space:

$$\int d^{2\omega}\mathbf{x}\, \exp\left[-A\left|\mathbf{x}-\mathbf{a}\right|^2 - B\left|\mathbf{x}-\mathbf{b}\right|^2 + 2\mathbf{c}\cdot\mathbf{x}\right] = \frac{\pi^\omega}{(A+B)^\omega}\exp\left[-\frac{AB\left|\mathbf{a}-\mathbf{b}\right|^2}{A+B} + \frac{2\mathbf{c}\cdot(A\mathbf{a}+B\mathbf{b}) + \left|\mathbf{c}\right|^2}{A+B}\right].$$

Here $A>0$, $B>0$ are constants and $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ are fixed 2ω-dimensional vectors. The scalar product of 2ω-dimensional vectors is denoted by $\mathbf{a}\cdot\mathbf{b}$.

Nondiagonal matrix element of $\hat{K}_1^P$

We shall see shortly that the remaining terms $\hat{K}_1^\Gamma$ and $\hat{K}_1^h$ can be expressed through the nondiagonal matrix element $\langle x|\,\hat{K}_1^P\,|y\rangle$. It is not difficult to compute this matrix element by the same method as we used for $\langle x|\,\hat{K}_1^P\,|x\rangle$. The calculation leading to Eq. (14.14) needs to be modified:

$$\langle x|\,\hat{K}_1^P\,|y\rangle = \int_0^\tau d\tau'\,\langle x|\,\hat{K}_0(\tau-\tau')\hat{P}\hat{K}_0(\tau')\,|y\rangle \tag{14.15}$$

$$= \int_0^\tau d\tau' \int d^{2\omega}z \frac{\exp\left[-\frac{(x-z)^2}{4(\tau-\tau')} - \frac{(z-y)^2}{4\tau'}\right]}{\left[4\pi(\tau-\tau')\right]^\omega\left[4\pi\tau'\right]^\omega}P(z)$$

$$= \frac{\exp\left[-\frac{(x-y)^2}{4\tau}\right]}{(4\pi\tau)^\omega}\int_0^\tau d\tau'\int\frac{d^{2\omega}k}{(2\pi)^\omega}\exp\left[-\frac{\tau'(\tau-\tau')}{\tau}k^2 + \frac{1}{\tau}ik\cdot(x\tau'+y(\tau-\tau'))\right]p(k). \tag{14.16}$$

In the limit $y\to x$ we recover Eq. (14.14), as expected.

Remaining terms

We now consider the term $\hat{K}_1^\Gamma$,

$$\hat{K}_1^\Gamma(\tau) \equiv \int_0^\tau d\tau'\,\hat{K}_0(\tau-\tau')\hat{\Gamma}\hat{K}_0(\tau'),$$

where the operator $\hat{\Gamma}$ is defined by Eq. (14.10). The matrix element $\langle x|\,\hat{K}_1^\Gamma(\tau)\,|y\rangle$ can be transformed as follows,

$$\langle x|\,\hat{K}_1^\Gamma(\tau)\,|y\rangle = \int_0^\tau d\tau'\int d^{2\omega}z\,\langle x|\,\hat{K}_0(\tau-\tau')\,|z\rangle\,h^{\mu\nu}_{,\nu}(z)\frac{\partial}{\partial z^\mu}\,\langle z|\,\hat{K}_0(\tau')\,|y\rangle$$

$$= -\frac{\partial}{\partial y^\mu}\int_0^\tau d\tau'\int d^{2\omega}z\,\langle x|\,\hat{K}_0(\tau-\tau')\,|z\rangle\,h^{\mu\nu}_{,\nu}(z)\,\langle z|\,\hat{K}_0(\tau')\,|y\rangle\,.$$

In the last line, we used the fact that $\langle z|\,\hat{K}_0(\tau)\,|y\rangle$ is a function only of $(z-y)$ and τ to replace the derivative ∂_z by $-\partial_y$. The formula we obtained is quite similar to the expression (14.15) for the matrix element $\langle x|\,\hat{K}_1^P(\tau)\,|y\rangle$, except for the function $h^{\mu\nu}_{,\nu}(z)$ instead of $P(z)$ inside the integral. Therefore we can use Eq. (14.16) to find

$$\begin{aligned}\langle x|\,\hat{K}_1^\Gamma(\tau)\,|x\rangle &= -\lim_{y\to x}\frac{\partial}{\partial y^\mu}\,\langle x|\,\hat{K}_1^P(\tau)\,|y\rangle\Big|_{P(z)\to h^{\mu\nu}_{,\nu}(z)}\\ &= -\frac{1}{(4\pi\tau)^\omega}\int_0^\tau d\tau'\,\exp\left[\frac{\tau'(\tau-\tau')}{\tau}\Box_x\right]\frac{\tau-\tau'}{\tau}h^{\mu\nu}_{,\mu\nu}(x).\end{aligned}$$

The diagonal matrix element of the operator $\hat{K}_1^h$ is computed in a similar way.

Exercise 14.3
Verify the following expression for the matrix element $\langle x|\,\hat{K}_1^h(\tau)\,|x\rangle$,

$$\langle x|\,\hat{K}_1^h(\tau)\,|x\rangle = \int_0^\tau d\tau'\frac{\exp\left[\frac{\tau'(\tau-\tau')}{\tau}\Box_x\right]}{(4\pi\tau)^\omega}\left\{-\frac{\delta_{\mu\nu}h^{\mu\nu}(x)}{2\tau}+\left(\frac{\tau-\tau'}{\tau}\right)^2 h^{\mu\nu}_{,\mu\nu}(x)\right\}.$$

Hint: Follow the computation of $\langle x|\,\hat{K}_1^\Gamma\,|y\rangle$ in the text.

14.2 The trace of the heat kernel

The trace of the heat kernel in the current approximation is

$$\mathrm{Tr}\,\hat{K}(\tau) = \int d^{2\omega}x\,\langle x|\left(\hat{K}_0+\hat{K}_1\right)|x\rangle + O\left(h^2\right).$$

Now the full expression for the first-order correction $\hat{K}_1$ can be put together,

$$\begin{aligned}\langle x|\,\hat{K}_1(\tau)\,|x\rangle =& \frac{1}{(4\pi\tau)^\omega}\int_0^\tau d\tau'\,\exp\left[\frac{\tau'(\tau-\tau')}{\tau}\Box_x\right]\\ &\times\left\{P(x)-\frac{1}{2\tau}\delta_{\mu\nu}h^{\mu\nu}(x)-\frac{\tau'(\tau-\tau')}{\tau^2}h^{\mu\nu}_{,\mu\nu}(x)\right\},\end{aligned}\tag{14.17}$$

where we can ignore terms of higher order in h and set

$$P(x) = \frac{1}{4}\delta_{\mu\nu}\Box h^{\mu\nu}(x) - V(x) + O\left(h^2\right).$$

The exponential is expanded in series,

$$\exp\left[\frac{\tau'(\tau-\tau')}{\tau}\Box_x\right] = \hat{1}+\sum_{n=1}^\infty\frac{1}{n!}\left(\frac{\tau'(\tau-\tau')}{\tau}\Box_x\right)^n,$$

and yields terms such as $\Box^n h^{\mu\nu}$ and $\Box^n V$ with prefactors that can be integrated term by term over $d\tau'$. After some algebra, we rewrite the expansion (14.17) as

$$\begin{aligned}\langle x|\,\hat{K}_1(\tau)\,|x\rangle &= \frac{1}{(4\pi\tau)^\omega}\left\{P(x)\tau - \frac{1}{2}\delta_{\mu\nu}h^{\mu\nu}(x) - \frac{1}{6}\tau h^{\mu\nu}_{,\mu\nu}(x)\right.\\ &\qquad\left. +\frac{\tau}{6}\Box P - \frac{\tau}{12}\delta_{\mu\nu}\Box h^{\mu\nu}(x) - \frac{\tau}{30}\Box h^{\mu\nu}_{,\mu\nu}(x) + \Box^2(\ldots)\right\}\\ &= \frac{1}{(4\pi\tau)^\omega}\left\{-\frac{1}{2}\delta_{\mu\nu}h^{\mu\nu}(x) - \tau V(x) + \frac{\tau}{6}\left[\delta_{\mu\nu}\Box h^{\mu\nu}(x) - h^{\mu\nu}_{,\mu\nu}(x)\right] + \Box(\ldots)\right\},\end{aligned}$$

where the omitted terms collected under the last Laplace operator $\Box(\ldots)$ are functions of x that contain at least a second derivative of $h^{\mu\nu}$.

The covariant volume factor $\sqrt{g}$ and the Ricci scalar R are related to $h^{\mu\nu}$ by

$$\sqrt{g} = 1 - \frac{1}{2}\delta_{\mu\nu}h^{\mu\nu} + O\left(h^2\right), \quad R = \delta_{\mu\nu}\Box h^{\mu\nu} - h^{\mu\nu}_{,\mu\nu} + O\left(h^2\right). \tag{14.18}$$

Exercise 14.4
Derive the relations (14.18) for the metric (14.1).

The formulae (14.18) yield

$$\langle x|\,\hat{K}_1(\tau)\,|x\rangle = \frac{\sqrt{g}}{(4\pi\tau)^\omega}\left[-\tau V(x) + \frac{\tau}{6}R(x) + \Box(\ldots) + O(h^2)\right].$$

Adding the initial term $\hat{K}_0$, we compute the trace of the heat kernel to first order in h,

$$\begin{aligned}\mathrm{Tr}\,\hat{K} &= \int d^{2\omega}x\,\langle x|\left(\hat{K}_0 + \hat{K}_1\right)|x\rangle\\ &= \frac{1}{(4\pi\tau)^\omega}\int d^{2\omega}x\sqrt{g}\left[1 + \left(\frac{R}{6} - V\right)\tau + O\left(h^2\right)\right].\end{aligned} \tag{14.19}$$

The terms we denoted earlier by $\Box(\ldots)$ are total divergences and vanish after the integration over $d^{2\omega}x$. The disregarded terms $O(h^2)$ involve R^2, V^2, VR, and higher-order expressions. Equation (14.19), which has a manifestly covariant form, is the main result of this chapter.

14.3 The Seeley-DeWitt expansion

Equation (14.19) provides the first two terms of the trace of the heat kernel as an expansion in the curvature. There also exists an expansion of the heat kernel in powers of τ, called the *Seeley-DeWitt expansion* or the proper time expansion,

$$\langle x|\,\hat{K}(\tau)\,|x\rangle = \frac{\sqrt{g}}{(4\pi\tau)^\omega}\left[1 + a_1(x)\tau + a_2(x)\tau^2 + O\left(\tau^3\right)\right]. \tag{14.20}$$

Here the *Seeley-DeWitt coefficients* $a_i(x)$ are local, scalar functions of the curvature $R_{\kappa\lambda\mu\nu}$ and $V(x)$. The Seeley-DeWitt expansion is derived without assuming that the curvature is small.

Although we cannot present a derivation of Eq. (14.20) here, we note that the integrand of Eq. (14.19) coincides with the Seeley-DeWitt expansion in its first two terms; the terms $O(h^2)$ in Eq. (14.19) are also of order $O(\tau^2)$. The first Seeley-DeWitt coefficient is therefore

$$a_1(x) = \frac{1}{6}R(x) - V(x).$$

The heat kernel enters Eq. (13.24) where we need to integrate from $\tau = 0$ to $\tau = \infty$. The Seeley-DeWitt expansion (14.20) is valid only for small τ and so cannot be used to compute the zeta function. The behavior of the heat kernel at small τ corresponds to the ultraviolet limit of quantum field theory. This can be informally justified by noting that τ has dimension of x^2 and therefore small values of τ correspond to small distances. Effects of QFT at small distances, i.e. local effects, include the vacuum polarization. On the other hand, large values of τ correspond to the infrared limit which is related to particle production effects.

To obtain the infrared behavior of the heat kernel, one needs a representation valid uniformly for all τ, such as the expansion (14.19). It is possible to compute further terms of this expansion, although the formulae rapidly become complicated at higher orders. The second-order terms were found by Barvinsky and Vilkovisky.[1] We state their result without proof:

$$\begin{aligned}\operatorname{Tr}\hat{K}(\tau) = \int \frac{d^{2\omega}x\sqrt{g}}{(4\pi\tau)^\omega}\Big\{1 + \tau\left[\frac{R}{6} - V\right] \\ + \frac{\tau^2}{2}\left[V - \frac{R}{6}\right] f_1\left(-\tau\Box_g\right) V + \tau^2 V f_2\left(-\tau\Box_g\right) R \\ + \tau^2 R f_3\left(-\tau\Box_g\right) R + \tau^2 R_{\mu\nu} f_4\left(-\tau\Box_g\right) R^{\mu\nu} + O\left(R^3, V^3, ...\right)\Big\},\end{aligned} \tag{14.21}$$

where the auxiliary functions $f_i(\xi)$ are

$$f_1(\xi) \equiv \int_0^1 e^{-\xi u(1-u)} du, \qquad f_2(\xi) \equiv -\frac{f_1(\xi)}{6} - \frac{f_1(\xi) - 1}{2\xi}, \tag{14.22}$$

$$f_4(\xi) \equiv \frac{f_1(\xi) - 1 + \frac{1}{6}\xi}{\xi^2}, \qquad f_3(\xi) \equiv \frac{f_1(\xi)}{32} + \frac{f_1(\xi) - 1}{8\xi} - \frac{f_4(\xi)}{8}. \tag{14.23}$$

Since the functions $f_i(\xi)$ are analytic and have Taylor expansions that converge uniformly for all $\xi \geq 0$, the application of functions $f_i(\xi)$ to operators, such as $f_i(-\tau\Box_g)$, is well-defined. Expressions such as $f_i(-\tau\Box_g)V(x)$ can be also rewritten as certain integrals of $V(x)$, but we shall not need explicit forms of these nonlocal expressions.

Note that nonlocal terms such as $f_1(-\tau\Box_g)V$ contain all (nonnegative) powers of τ. The Seeley-DeWitt coefficients can be reproduced by expanding these terms in τ,

[1] A. O. Barvinsky and G. A. Vilkovisky, Nucl. Phys. **B333** (1990), p. 471.

up to total derivative terms which vanish under the integration over all x. Neglecting the terms of order $O(\tau^3)$, one finds

$$\begin{aligned}\mathrm{Tr}\,\hat{K}(\tau) = &\int \frac{d^{2\omega}x\sqrt{g}}{(4\pi\tau)^\omega}\Bigg\{1+\tau\left[\frac{R}{6}-V\right]\\ &+\tau^2\left[\frac{1}{2}V^2-\frac{1}{6}VR+\frac{1}{120}R^2+\frac{1}{60}R_{\mu\nu}R^{\mu\nu}\right]+O\left(\tau^3,R^3,V^3,...\right)\Bigg\}. \quad (14.24)\end{aligned}$$

This agrees with the second-order Seeley-DeWitt expansion, up to a total divergence.

Exercise 14.5

To derive the coefficients at τ^2 in the above formula, show that

$$f_1(0)=1, \quad f_2(0)=-\frac{1}{12}, \quad f_3(0)=\frac{1}{120}, \quad f_4(0)=\frac{1}{60}$$

for the functions (14.22)-(14.23).

15 Results from effective action

Summary: Divergences in the effective action. Renormalization of constants. Nonlocal terms in the renormalized action. Polyakov action in 1+1 dimensions. Conformal anomaly.

The goal of this final chapter of the book is to complete the calculation of the effective action for a scalar field in a weakly curved background and to interpret the results. As we have seen in Chapter 12, the effective action describes both the influence of gravity on the quantum field (the polarization of vacuum, characterized by the expectation value $\langle \hat{T}_{\mu\nu} \rangle$) and the backreaction of the vacuum fluctuations on the metric. We shall explore both effects after we learn how to remove the divergences that appear in the effective action.

15.1 Renormalization of effective action

In the previous chapter we computed the trace of the heat kernel $\mathrm{Tr}\, \hat{K}_M(\tau)$ as a perturbative expansion in the curvature. According to the method of Chapter 13, the renormalized effective action is obtained by an analytic continuation of the suitable zeta function,

$$\Gamma_E\left[g_{\mu\nu}\right] = -\frac{1}{2}\left.\frac{d}{ds}\right|_{s=0} \zeta_M\left(s\right),$$
$$\zeta_M\left(s\right) \equiv \frac{1}{\Gamma\left(s\right)} \int_0^\infty \tau^{s-1} \mathrm{Tr}\, \hat{K}_M\left(\tau\right) d\tau. \tag{15.1}$$

Without analytic continuation, the above integral diverges at $s = 0$. The procedure of analytic continuation provides a finite value for the effective action but does not justify the removal of the divergences.

In this section we present a qualitative analysis of the divergent parts of the effective action and motivate the procedure of renormalization. More rigorous treatments are possible but require much more cumbersome computations.

15.1.1 Leading divergences

To be specific, we consider a minimally coupled massless field ($V = 0$) in the four-dimensional Euclidean space ($\omega = 2$). The zeta function is obtained by substituting the expression (14.21) into Eq. (15.1). The large-τ behavior of the heat kernel is such that the integral (15.1) converges at the upper limit; thus the divergences are found

only at $\tau \to 0$. The small-τ (ultraviolet) behavior of the integral can be analyzed with help of the simpler Seeley-DeWitt expansion (14.24) which is valid only for small τ, instead of using the full expression (14.21). To perform this analysis, we artificially truncate the integral at large τ by a cutoff at $\tau = \tau_1$ and find at $s = 0$ the following expression,

$$\begin{aligned}\zeta(s) =& \frac{1}{(4\pi)^2\Gamma(s)} \int d^4x\sqrt{g} \left[\int_0^{\tau_1} \tau^{s-3} d\tau + \frac{R}{6} \int_0^{\tau_1} \tau^{s-2} d\tau \right. \\ & \left. + \left(\frac{1}{120} R^2 + \frac{1}{60} R_{\mu\nu} R^{\mu\nu} \right) \int_0^{\tau_1} \tau^{s-1} d\tau + (\text{finite terms}) \right]. \end{aligned} \tag{15.2}$$

The divergences we can study at this point arise at the $\tau = 0$ limit of integration when we set $s = 0$. Further terms of the expansion in τ contain τ^{s+n} with $n \geq 0$ and are finite at $\tau = 0$.

To examine the behavior of the divergences in Eq. (15.2), we introduce a cutoff $\tau = \tau_0$ at the lower limit and denote the resulting integrals for brevity by

$$A(\tau_0) \equiv \int_{\tau_0}^{\tau_1} \tau^{s-3} d\tau, \; B(\tau_0) \equiv \int_{\tau_0}^{\tau_1} \tau^{s-2} d\tau, \; C(\tau_0) \equiv \int_{\tau_0}^{\tau_1} \tau^{s-1} d\tau.$$

The leading divergences of the ζ function at $\tau_0 \to 0$ are

$$\begin{aligned}\zeta(s) =& \frac{1}{\Gamma(s)} \int \frac{d^4x\sqrt{g}}{(4\pi)^2} \left[A(\tau_0) + \frac{R}{6} B(\tau_0) \right. \\ & \left. + \left(\frac{1}{120} R^2 + \frac{1}{60} R_{\mu\nu} R^{\mu\nu} \right) C(\tau_0) + (\text{finite terms}) \right]. \end{aligned}$$

The leading behavior of the auxiliary functions A, B, C at $s = 0$ and $\tau_0 \to 0$ is easily derived,

$$A(\tau_0) \sim \frac{1}{2}\tau_0^{-2}, \quad B(\tau_0) \sim \tau_0^{-1}, \quad C(\tau_0) \sim |\ln \tau_0| .$$

The Γ function factor at $s = 0$ has the expansion (A.25),

$$\frac{1}{\Gamma(s)} = s + O\left(s^2\right).$$

Therefore the effective action can be written as

$$\begin{aligned}\Gamma_E[g_{\mu\nu}] =& -\frac{1}{2} \left. \frac{d\zeta}{ds} \right|_{s=0} = -\int \frac{d^4x\sqrt{g}}{32\pi^2} \left[\frac{1}{2\tau_0^2} + \frac{1}{6\tau_0} R \right. \\ & \left. + \left(\frac{1}{120} R^2 + \frac{1}{60} R_{\mu\nu} R^{\mu\nu} \right) |\ln \tau_0| + (\text{finite terms}) \right]. \end{aligned} \tag{15.3}$$

This is a regularized form of the effective action that becomes infinite if the cutoff parameter τ_0 is set to 0.

The divergent terms in the Lorentzian effective action $\Gamma_L[g_{\mu\nu}]$ are a straightforward analytic continuation of Eq. (15.3). Since no Green's functions are present in the divergent terms, we only need to replace $\sqrt{g}$ by $\sqrt{-g}$.

15.1.2 Renormalization of constants

The backreaction of the quantum field on the gravitational background causes a modification of the Einstein equation. The total action for the gravitational background is a sum of the free gravitational action (5.18) and the (Lorentzian) effective action $\Gamma_L[g_{\mu\nu}]$ induced by the quantum field. However, the effective action is divergent and we need to renormalize it to obtain a finite total action.

The free action of general relativity, $S^{\text{grav}}[g_{\mu\nu}]$, contains the cosmological constant term Λ and the curvature term R that are similar to the divergent terms from Eq. (15.3). One possibility of renormalization is to assume that the free gravitational action contains certain infinite terms that cancel the infinities in the effective action, so that the total action is finite. This renormalization procedure is implemented as follows.

We postulate that the free gravitational action (without backreaction of quantum fields) has different constants and contains terms quadratic in the curvature,

$$S^{\text{grav}}_{\text{bare}}[g_{\mu\nu}] = \int d^4x\sqrt{-g}\left[-\frac{R+2\Lambda_B}{16\pi G_B} + \alpha_B\left(\frac{R^2}{120} + \frac{R_{\mu\nu}R^{\mu\nu}}{60}\right)\right]. \tag{15.4}$$

Here Λ_B, G_B, and α_B are called the *bare coupling constants* of the theory; these constants are never observable since the quantum field is always present and its backreaction cannot be "switched off." The modified action for gravity is the sum of the free action and the effective action,

$$S^{\text{grav}}_{\text{bare}}[g_{\mu\nu}] + \Gamma_L[g_{\mu\nu}] = \int d^4x\sqrt{-g}\left\{\left[-\frac{\Lambda_B}{8\pi G_B} - \frac{A(\tau_0)}{32\pi^2}\right]\right.$$
$$\left. - \left[\frac{1}{16\pi G_B} + \frac{B(\tau_0)}{192\pi^2}\right]R + \left[\alpha_B - \frac{C(\tau_0)}{32\pi^2}\right]\left[\frac{R^2}{120} + \frac{R_{\mu\nu}R^{\mu\nu}}{60}\right] + (\text{finite terms})\right\}.$$

If the bare constants were finite, the presence of the divergent factors $A(\tau_0)$, $B(\tau_0)$, and $C(\tau_0)$ would make the total action infinite in the limit $\tau_0 = 0$. The renormalization procedure postulates that the bare constants are *functions of* τ_0 chosen to cancel the divergences in the effective action, so that the remaining terms coincide with the usual action (5.18). It is easy to see that with the choices

$$\frac{\Lambda_B}{8\pi G_B} = \frac{\Lambda}{8\pi G} - \frac{A(\tau_0)}{32\pi^2}, \quad \frac{1}{16\pi G_B} = \frac{1}{16\pi G} - \frac{B(\tau_0)}{192\pi^2}, \quad \alpha_B = \frac{C(\tau_0)}{32\pi^2},$$

we obtain a finite total gravitational action at $\tau_0 = 0$. After setting $\tau_0 = 0$ (removing the cutoff), the renormalized constants are equal to the observed cosmological constant Λ and Newton's constant G.

The "bare" gravitational action (15.4) differs from the standard Einstein-Hilbert action (5.18) by two extra terms that are quadratic in the curvature. These terms are necessary to renormalize the backreaction of matter fields on gravity. If the curvature is small, $R \ll 1$ (in Planck units), the extra terms are insignificant in comparison with S^{grav} which is linear in R. In this limit Einstein's general relativity is a good approximation that agrees with the available experiments. When the curvature is

large, $R \gtrsim 1$, the extra terms may become significant. However, we expect that in that regime some as yet unknown effects of quantum gravity dominate and the theory of quantum fields in classical spacetime breaks down.

> **Remark: "bare" constants and renormalization.** The terms "bare constants" and "bare action" are motivated by the following consideration. The free gravitational action $S^{\text{grav}}_{\text{bare}}[g_{\mu\nu}]$ describes the gravitational field that does not interact with any other fields. However, vacuum fluctuations of various quantum fields are always present and their backreaction on the gravitational background cannot be suppressed. Hence, the observed gravitational field is always determined by the total ("dressed") action and not by the "bare" action. So the bare constants can have arbitrary values or be arbitrary functions of the cutoff parameter as long as the dressed constants agree with the experimental data.
>
> The backreaction of the quantum field on the metric is described by the effective action $\Gamma_L[g_{\mu\nu}]$ which has divergences. Therefore the theory needs to be renormalized. One starts with a Lagrangian containing bare coupling constants and introduces a cutoff parameter to make the interesting quantities finite (*regularization*). The cutoff becomes a parameter of the theory. The bare coupling constants are not directly observable, so one postulates that the bare constants are certain functions of the cutoff. These functions are chosen to cancel the divergences appearing in the results (*renormalization*), so that the cutoff may be removed. The renormalized ("dressed") values of the coupling constants are fixed by the experimental data.
>
> A field theory that does not lead to divergent quantities and does not involve cutoffs would be more satisfying; however, such a theory is presently unavailable. Currently, the most successful theory of fundamental interactions is QFT combined with renormalization.

The divergences found in Eq. (15.3) result from the backreaction of one scalar field. Other fields will give similar contributions, differing only in the numerical coefficients at the terms R^2 and $R_{\mu\nu}R^{\mu\nu}$. Therefore in general we need to introduce four independent bare constants into the bare gravitational action, controlling the terms 1, R, R^2, and $R_{\mu\nu}R^{\mu\nu}$.

In dimensions other than four, the divergences contain other powers of τ_0; the leading divergence is

$$\int_{\tau_0}^{\tau_1} \frac{d\tau}{(4\pi\tau)^\omega} \tau^{s-1}\Big|_{s=0} \sim \tau_0^{-\omega}$$

and therefore in 2ω dimensions we expect to find $\omega + 1$ divergent terms: $\tau_0^{-\omega}$, ..., τ_0^{-1}, and $|\ln \tau_0|$.

15.2 Finite terms in the effective action

We have found that the theory of quantum fields in a classical curved spacetime includes a formally infinite backreaction of the quantum fields in their vacuum state. This divergent backreaction would be present even in an almost flat spacetime such as the one we live in. It is clear that the divergence must be removed to obtain physically relevant results. To make the divergences disappear, we introduced some extra terms into the bare gravitational action and renormalized the coupling constants. The

resulting renormalized action is the standard Einstein-Hilbert action with some additional finite terms that describe the actually observable backreaction. In the previous section we have studied the structure of the divergences, and now we examine the finite terms.

15.2.1 Nonlocal terms

The Seeley-DeWitt expansion is not adequate for extracting the finite terms because it is not valid for large τ. Therefore we employ the expansion (14.21) with $V = 0$ and find

$$\zeta(s) = \frac{1}{(4\pi)^\omega \Gamma(s)} \int d^{2\omega}x\sqrt{g} \left\{ \int_0^\tau d\tau\, \tau^{s-1-\omega} \left[1 + \frac{\tau}{6}R \right.\right. \\ \left.\left. + \tau^2 R f_3\left(-\tau\Box_g\right) R + \tau^2 R_{\mu\nu} f_4\left(-\tau\Box_g\right) R^{\mu\nu} \right] \right\}. \tag{15.5}$$

First we consider the two-dimensional spacetime ($\omega = 1$). In two dimensions, the Ricci tensor is always proportional to the metric:

$$R_{\mu\nu} = \frac{1}{2} g_{\mu\nu} R. \tag{15.6}$$

> **Remark:** The Einstein equation (in vacuum) is identically satisfied in two dimensions due to Eq. (15.6). To obtain a nontrivial theory of gravity, the Einstein-Hilbert action needs to be modified. The renormalized effective action provides one such modification.

We have seen that the renormalization of the effective action has the effect of removing the first two terms in Eq. (15.5). Simplifying the resulting expression with help of Eq. (15.6), we get

$$\zeta(s) = \frac{1}{4\pi\Gamma(s)} \int d^2x\sqrt{g} \int_0^\infty d\tau\, \tau^s R \left[f_3\left(-\tau\Box_g\right) + \frac{1}{2} f_4\left(-\tau\Box_g\right) \right] R.$$

The renormalized effective action is then found as

$$\Gamma_E\left[g_{\mu\nu}\right] = -\frac{1}{2}\left.\frac{d\zeta}{ds}\right|_{s=0} \\ = -\frac{1}{8\pi} \int d^2x\sqrt{g}\, R \int_0^\infty d\tau \left[f_3\left(-\tau\Box_g\right) + \frac{1}{2} f_4\left(-\tau\Box_g\right) \right] R.$$

To compute the integral, we formally change the variable τ to $\xi = -\tau\Box_g$ and obtain[1] the following expression,

$$\Gamma_E\left[g_{\mu\nu}\right] = \frac{1}{8\pi} I_0 \int d^2x\sqrt{g} R\, \Box_g^{-1} R,$$

[1] This rather unorthodox "change of the variable" can be justified by a more rigorous calculation which we omit.

where I_0 is a constant computed in Exercise 15.1,

$$I_0 \equiv \int_0^\infty d\xi \left[f_3(\xi) + \frac{1}{2} f_4(\xi) \right] = \frac{1}{12}.$$

The resulting functional is called the *Polyakov action*:

$$\begin{aligned} \Gamma_E [g_{\mu\nu}] &= \frac{1}{96\pi} \int d^2x \sqrt{g} R \Box_g^{-1} R \\ &\equiv \frac{1}{96\pi} \int d^2x \sqrt{g(x)}\, d^2y \sqrt{g(y)} R(x) R(y) G_E(x,y), \end{aligned} \tag{15.7}$$

where G_E is the (Euclidean) Green's function of the Laplace operator $\Box_g$. Since $\Box_g^{-1}$ is an integral operator, the Polyakov action is a *nonlocal* functional of $g_{\mu\nu}(x)$.

Exercise 15.1*

Verify the definite integral

$$I_0 \equiv \int_0^\infty d\xi \left[f_3(\xi) + \frac{1}{2} f_4(\xi) \right] = \frac{1}{12},$$

where the auxiliary functions $f_3(\xi)$ and $f_4(\xi)$ are defined by Eqs. (14.22)-(14.23).

Hint: Rewrite I_0 as a double integral over ξ and u, regularize the integral over ξ by the factor $\exp(-a\xi)$ with $a > 0$, exchange the order of integration and take the limit $a \to 0$ at the end of calculation.

Remark: the four-dimensional result. In the four-dimensional case ($\omega = 2$), we omit the calculations and only quote the result,

$$\Gamma_E [g_{\mu\nu}] \sim \int d^4x \sqrt{g}\, R \ln\left(\frac{-\Box_g}{\mu^2}\right) R + \text{terms with } R_{\mu\nu} \ln\left(\frac{-\Box_g}{\mu^2}\right) R^{\mu\nu},$$

where μ is a mass scale introduced for dimensional reasons (the operator $\Box_g$ has dimension m^2). The logarithm of the Laplace operator is defined by

$$\ln\left(\frac{-\Box_g}{\mu^2}\right) = \int_0^{+\infty} d\left(m^2\right) \left[\frac{1}{\mu^2 + m^2} - \frac{1}{-\Box_g + m^2} \right],$$

where the second term in the brackets is the Green's function of the operator $-\Box_g + m^2$.

Note that the parameter μ is introduced formally for dimensional reasons. A change in the parameter μ, for example $\mu \to \tilde{\mu} = \mu/b$, would add a term $(\ln b) R^2$ to the action. However, the bare action already contains the R^2 term with a bare coupling constant fixed by the renormalization of the action. A different choice of the parameter μ can be compensated by adding a finite term to this bare constant to remain in agreement with the observable ("dressed") value of the coupling constant. The actual value of μ needed to obtain specific predictions in this theory must be found from an experiment measuring the coefficient at R^2 at a certain energy.

15.2.2 EMT from the Polyakov action

Using the effective action (15.7), we can compute the vacuum expectation value of the energy-momentum tensor of the quantum field.

The general procedure is to perform the analytic continuation of $\Gamma_E[g_{\mu\nu}]$ back to the Lorentzian time and to substitute the Feynman Green's function instead of the Euclidean one. The result will be the Lorentzian effective action $\Gamma_L[g_{\mu\nu}]$. After this, the vacuum expectation value of the EMT will be expressed as

$$\langle 0_{in}|\,\hat{T}_{\mu\nu}(x)\,|0_{in}\rangle = \frac{2}{\sqrt{-g(x)}}\,\frac{\delta\Gamma_L}{\delta g^{\mu\nu}(x)}\bigg|_{G_F\to G_{ret}}.$$

Before showing the detailed calculations, we quote the final expression,[2]

$$\begin{aligned}\langle 0_{in}|\,\hat{T}_{\mu\nu}\,|0_{in}\rangle =& \frac{1}{48\pi}\Big\{-2\nabla_\mu\nabla_\nu\left(\Box_g^{-1}R\right)+\nabla_\mu\left(\Box_g^{-1}R\right)\nabla_\nu\left(\Box_g^{-1}R\right)\\ &+\left[2R-\frac{1}{2}\nabla^\lambda\left(\Box_g^{-1}R\right)\nabla_\lambda\left(\Box_g^{-1}R\right)\right]g_{\mu\nu}\Big\}. \qquad (15.8)\end{aligned}$$

In the above equation, the operator $\Box_g^{-1}$ represents the *retarded* Green's function $G_{ret}(x,y)$, so that for any scalar $f(x)$

$$\left(\Box_g^{-1}f\right)(x) \equiv \int d^2y\sqrt{-g}\,f(y)G_{ret}(x,y).$$

The expression (15.8) is nonlocal and contains information about particle production as well as the complete description of the vacuum polarization at all points. A similar technique has been applied to study spherically symmetric modes of the Hawking radiation.[3]

Derivation of Eq. (15.8)

First we need to convert the Euclidean effective action $\Gamma_E\,[g_{\mu\nu}]$ to the Lorentzian one, $\Gamma_L\,[g_{\mu\nu}]$. We recall that the Euclidean metric $g_{\mu\nu}$ entering the effective action $\Gamma_E[g_{\mu\nu}]$ is, in the notation of Sec. 13.1.1, the positive-definite metric $\gamma_{\mu\nu}$ related to the Lorentzian metric by an analytic continuation with an additional sign change:

$$\gamma_{\mu\nu} = -g^{(E)}_{\mu\nu} = -\,g_{\mu\nu}|_{t\to -i\tau}\,.$$

Therefore we need to return to the original Euclidean variable $g^{(E)}_{\mu\nu}$ before performing the analytic continuation. The replacement $\gamma_{\mu\nu} = -g^{(E)}_{\mu\nu}$ entails

$$\sqrt{\gamma} = \sqrt{g^{(E)}}, \quad R[\gamma] = -R[g^{(E)}], \quad \Box_\gamma = -\Box_{g^{(E)}}, \qquad (15.9)$$

[2] This expression agrees with the Barvinsky-Vilkovisky paper but the derivation in Sec. 15.3 produces an extra minus sign. The reason for this mismatch is not yet clear to the authors!

[3] See the paper by V. F. MUKHANOV, A. WIPF, and A. I. ZEL'NIKOV, Phys. Lett. **B332** (1994), p. 283. This method originates from the paper by A. O. BARVINSKY and G. A. VILKOVISKY, Nucl. Phys. **B333** (1990), p. 471.

and it is easy to see that the action (15.7) also changes the sign,

$$\begin{aligned}\Gamma_E[\gamma_{\mu\nu}] &= \frac{1}{96\pi}\int d^2x\sqrt{\gamma}R[\gamma]\,\Box_\gamma^{-1}R[\gamma] \\ &= -\frac{1}{96\pi}\int d^2x^{(E)}\sqrt{g^{(E)}}R[g^{(E)}]\Box_{g^{(E)}}^{-1}R[g^{(E)}].\end{aligned}$$

After the analytic continuation we have $d^2x^{(E)} = id^2x$ and $\sqrt{g^{(E)}} = \sqrt{-g}$, where x and $g_{\mu\nu}$ are now the Lorentzian quantities. Following the recipe outlined in Sec. 12.2.3, we replace the Euclidean Green's function G_E by the Feynman function $\frac{1}{i}G_F$ and obtain the Lorentzian effective action,

$$\begin{aligned}\Gamma_L[g_{\mu\nu}] &= i\Gamma_E\left[g^{(E)}_{\mu\nu}\right]_{\tau=it} \\ &= -i\frac{1}{96\pi}\int id^2x_1\int id^2x_2\sqrt{-g(x_1)}R(x_1)\frac{1}{i}G_F(x_1,x_2)\sqrt{-g(x_2)}R(x_2) \\ &= \frac{1}{96\pi}\int d^2x\sqrt{-g}R\,\Box_g^{-1}R, \qquad (15.10)\end{aligned}$$

where the symbol $\Box_g^{-1}$ in the last line involves the Feynman Green's function G_F of the D'Alembert operator in the Lorentzian metric $g_{\mu\nu}$.

It remains to compute the variation of the Lorentzian effective action (15.10) with respect to the metric $g_{\mu\nu}$. The following exercises provide a derivation of the result (15.8).

Exercise 15.2*

(a) Verify the formula for the variation of the Christoffel symbol,

$$\delta\Gamma^\alpha_{\mu\nu} = \frac{1}{2}g^{\alpha\beta}\left(\nabla_\mu\delta g_{\beta\nu} + \nabla_\nu\delta g_{\beta\mu} - \nabla_\beta\delta g_{\mu\nu}\right).$$

(b) Show that the variation of $\Box_g\phi$, where ϕ is a scalar function, is

$$\delta\Box_g\phi = (\delta g^{\mu\nu})\,\nabla_\mu\nabla_\nu\phi - g^{\mu\nu}\left(\delta\Gamma^\alpha_{\mu\nu}\right)\nabla_\alpha\phi,$$

while the variation of the inverse D'Alembert operator is

$$\delta\Box_g^{-1}\phi = -\Box_g^{-1}\left(\delta\Box_g\right)\Box_g^{-1}\phi. \qquad (15.11)$$

(c) Derive the variation of the Riemann tensor in the form

$$\delta R^\alpha{}_{\beta\mu\nu} = \nabla_\mu\delta\Gamma^\alpha_{\beta\nu} - \nabla_\nu\delta\Gamma^\alpha_{\mu\beta}. \qquad (15.12)$$

Hint: perform all calculations in a locally inertial frame where $\Gamma^\alpha_{\mu\nu} = 0$, and then generalize to arbitrary coordinates.

Exercise 15.3*

Compute the variation of the Polyakov action (15.10) with respect to $g^{\mu\nu}$ and derive Eq. (15.8).

15.3 Conformal anomaly

Although the trace of the EMT vanishes for a classical conformally coupled field, $T_{\mu\nu}g^{\mu\nu} = 0$, the vacuum expectation value of the trace $\langle\hat{T}_{\mu\nu}\rangle g^{\mu\nu}$ for a quantum field is in general nonzero. This phenomenon is called the *conformal anomaly* or *trace anomaly*.

Trace of the classical EMT

For any classical field with a conformally invariant action, e.g. for conformally coupled scalar fields or for the electromagnetic field, the trace of the EMT identically vanishes, $g^{\mu\nu}T_{\mu\nu} \equiv 0$.

This can be shown by a simple calculation. If the action $S[\phi, g_{\mu\nu}]$ of a generally covariant theory is invariant under conformal transformations,

$$S[\phi, g_{\mu\nu}] = S[\phi, \tilde{g}_{\mu\nu}], \qquad g_{\mu\nu}(x) \to \tilde{g}_{\mu\nu}(x) = \Omega^2(x) g_{\mu\nu}(x),$$

where $\Omega(x) \neq 0$ is an arbitrary smooth function, then the variation of the action with respect to an infinitesimal conformal transformation must vanish. An infinitesimal conformal transformation with $\Omega(x) = 1 + \delta\Omega(x)$ yields

$$\delta g_{\mu\nu}(x) = 2 g_{\mu\nu}(x)\delta\Omega(x). \tag{15.13}$$

Using Eq. (5.23), we find

$$0 = \delta S = \int d^{2\omega}x \frac{\delta S}{\delta g^{\mu\nu}(x)} \delta g^{\mu\nu}(x) = \int d^{2\omega}x \sqrt{-g} T_{\mu\nu} g^{\mu\nu} \delta\Omega. \tag{15.14}$$

This relation should hold for arbitrary functions $\delta\Omega(x)$, therefore the integrand must vanish for all x,

$$T^{\mu}_{\mu}(x) \equiv T_{\mu\nu}(x) g^{\mu\nu}(x) \equiv 0.$$

The conclusion holds for any classical generally covariant and conformally invariant field theory, but (as a rule) fails for quantum fields.

Trace of the quantum EMT

Now we compute the vacuum expectation value of the trace of the EMT of a quantum field.

For simplicity, we work in two dimensions ($\omega = 1$). First, we can obtain the vacuum expectation value $\langle 0_{in}| g^{\mu\nu}\hat{T}_{\mu\nu} |0_{in}\rangle$ directly from Eq. (15.8) . Using the identities

$$g^{\mu\nu}\nabla_\mu\nabla_\nu \left(\Box_g^{-1} R\right) = \Box_g \left(\Box_g^{-1} R\right) = R,$$
$$g^{\mu\nu} g_{\mu\nu} = 2\omega = 2,$$

one finds

$$\langle 0| g^{\mu\nu}\hat{T}_{\mu\nu}(x) |0\rangle = -\frac{R(x)}{24\pi} = -\frac{a_1(x)}{4\pi}, \tag{15.15}$$

where a_1 is the first Seeley-DeWitt coefficient.[4] It is clear that the trace of the EMT does not vanish if $R \neq 0$.

> **Remark:** The reason for conformal symmetry to be broken can be understood from the path integral formulation of QFT. The quantum theory would be conformally invariant if a path integral such as
>
> $$\int \mathcal{D}\phi \, e^{-S_E[\phi, g_{\mu\nu}]}$$
>
> were invariant under conformal transformations. However, this is impossible because one cannot choose the integration measure $\mathcal{D}\phi$ to be conformally invariant and at the same time generally covariant. For instance, the generally covariant integration measure (13.14) is not conformally invariant since the eigenvalues and the eigenfunctions are not preserved by conformal transformations.

We conclude this chapter by presenting a more detailed derivation of the conformal anomaly in two dimensions. The idea is to compute the variation of the effective action under an infinitesimal conformal transformation (15.13) and to show that the result is related to the expectation value of $\hat{T}_{\mu\nu} g^{\mu\nu}$.

We shall perform all calculations with Euclidean quantities and convert the result to the Lorentzian time at the end. The effective action is expressed through the zeta function $\zeta_g(s)$ of the operator $\hat{M}_g$,

$$\Gamma_E[g_{\mu\nu}] = -\frac{1}{2} \left. \frac{d\zeta_g}{ds} \right|_{s=0} .$$

The operator $\hat{M}_g$ and its zeta function are given by Eqs. (13.18) and (13.22),

$$\begin{aligned} \hat{M}_g |\psi\rangle &= g^{-1/4} \partial_\mu \left[\sqrt{g} g^{\mu\nu} \left(\partial_\nu g^{-1/4} |\psi\rangle \right) \right] , \\ \zeta_g(s) &= \mathrm{Tr} \left[\hat{M}_g^{-s} \right] . \end{aligned}$$

Under an infinitesimal conformal transformation (15.13), the combination $\sqrt{g} g^{\mu\nu}$ is invariant (see Eq. (8.11) on p. 106) while the operator $\hat{M}_g$ becomes $\hat{M}_{\Omega^2 g}$:

$$\begin{aligned} \hat{M}_{\Omega^2 g} &= \Omega^{-1} \hat{M}_g \Omega^{-1} = (1 - \delta\Omega) \hat{M}_g (1 - \delta\Omega) + O\left(\delta\Omega^2\right) \\ &= \hat{M}_g - \delta\Omega \hat{M}_g - \hat{M}_g \delta\Omega + O\left(\delta\Omega^2\right) . \end{aligned}$$

The transformed zeta function is, up to terms $O\left(\delta\Omega^2\right)$,

$$\begin{aligned} \zeta_{g+\delta g}(s) &= \mathrm{Tr} \left[\left(\hat{M}_g - \delta\Omega \hat{M}_g - \hat{M}_g \delta\Omega \right)^{-s} \right] \\ &= \mathrm{Tr} \left[\hat{M}_g^{-s} + s \hat{M}_g^{-s-1} \left(\delta\Omega \hat{M}_g + \hat{M}_g \delta\Omega \right) \right] = \mathrm{Tr} \hat{M}_g^{-s} + 2s \mathrm{Tr} \left[\delta\Omega \hat{M}_g^{-s} \right] . \end{aligned}$$

[4] The connection with the Seeley-DeWitt coefficients is notable because in four dimensions the trace anomaly involves the second coefficient a_2.

(The order of operators can be cyclically permuted under the trace, as long as all the traces are finite.) Therefore the transformed effective action is

$$\Gamma_E\left[g_{\mu\nu}+\delta g_{\mu\nu}\right]=-\frac{1}{2}\left.\frac{d\zeta_{g+\delta g}}{ds}\right|_{s=0}=-\lim_{s\to 0}\mathrm{Tr}\left(\delta\Omega\hat{M}^{-s}\right)+\Gamma_E\left[g_{\mu\nu}\right].$$

Note that the limit $s\to 0$ is be evaluated *after* computing the trace. We use the coordinate representation of operators to get

$$\begin{aligned}\mathrm{Tr}\left(\delta\Omega\hat{M}^{-s}\right)&=\int d^2x\,d^2y\,\langle x|\,\delta\Omega\,|y\rangle\,\langle y|\,\hat{M}^{-s}\,|x\rangle\\&=\int d^2x\,\delta\Omega(x)\,\langle x|\,\hat{M}^{-s}\,|x\rangle\,.\end{aligned}$$

The matrix element is computed with the help of the Seeley-DeWitt expansion (14.20),

$$\begin{aligned}\langle x|\,\hat{M}^{-s}\,|x\rangle&=\frac{1}{\Gamma(s)}\int_0^{+\infty}d\tau\,\tau^{s-1}\,\langle x|\,\hat{K}(\tau)\,|x\rangle\\&=\frac{\sqrt{g}}{4\pi\Gamma(s)}\int_0^{+\infty}d\tau\,\tau^{s-2}\left[1+a_1(x)\tau+a_2(x)\tau^2+O\left(\tau^3\right)\right].\end{aligned}\qquad(15.16)$$

At first glance, the integral in Eq. (15.16) diverges at both the upper and the lower limits. However, the upper limit divergence is spurious. The Seeley-DeWitt expansion is only valid for small τ and does not show that in fact the heat kernel decays at large τ and that the integral converges at $\tau\to+\infty$. The most important contributions to the integral come from small τ, so the Seeley-DeWitt expansion actually provides enough information to obtain the results. To simulate the correct behavior of the integrand, we artificially truncate the integration at large τ. Thus the procedure is to multiply the integrand by $\exp(-\alpha\tau)$ with $\alpha>0$, compute the limit $s\to 0$ at fixed α, and then set $\alpha\to 0$. The divergences at $\tau=0$ are renormalized by the analytic continuation in s using the gamma function, namely we replace

$$\int_0^{\infty}d\tau\,\tau^{s-2}e^{-\alpha\tau}\to\alpha^{1-s}\Gamma(s-1).$$

Then the terms of the expansion are

$$\begin{aligned}\frac{1}{\Gamma(s)}\int_0^{+\infty}d\tau\,\tau^{s-2}e^{-\alpha\tau}&=\frac{\alpha^{1-s}\Gamma(s-1)}{\Gamma(s)}=\frac{\alpha^{1-s}}{s-1};\\\frac{a_1}{\Gamma(s)}\int_0^{+\infty}d\tau\,\tau^{s-1}e^{-\alpha\tau}&=a_1\alpha^{-s};\\\frac{a_2}{\Gamma(s)}\int_0^{+\infty}d\tau\,\tau^{s}e^{-\alpha\tau}&=a_2 s\alpha^{-s-1}.\end{aligned}$$

When $s\to 0$ at fixed $\alpha>0$, only the first two terms in Eq. (15.16) give nonvanishing contributions. Of these, the first term is proportional to α^{1-s} and vanishes as $\alpha\to 0$.

Hence

$$\lim_{\alpha\to+0}\left(\lim_{s\to+0}\langle x|\,\hat{M}^{-s}\,|x\rangle\right)=\frac{1}{4\pi}\sqrt{g}\,a_1(x)=\frac{\sqrt{g}}{24\pi}R\,[g]\,,$$

where $R[g]$ is the Ricci scalar corresponding to the (Euclidean) metric $g_{\mu\nu}$.

The final result is that the variation of the effective action after an infinitesimal conformal transformation is

$$\delta\Gamma_E=\Gamma_E\,[g_{\mu\nu}+\delta g_{\mu\nu}]-\Gamma_E\,[g_{\mu\nu}]=-\frac{1}{24\pi}\int d^2x\sqrt{g}\,\delta\Omega(x)R(x). \tag{15.17}$$

Since Eq. (15.17) does not contain any Green's functions, the analytic continuation to the Lorentzian regime is straightforward. Thus the variation of the *Lorentzian* effective action under a conformal transformation is

$$\delta\Gamma_L=-\frac{1}{24\pi}\int d^2x\sqrt{-g}\delta\Omega(x)R(x). \tag{15.18}$$

On the other hand, the expectation value of the EMT is related to $\delta\Gamma_L$ by

$$\delta\Gamma_L=\int d^2x\frac{\delta\Gamma_L}{\delta g^{\mu\nu}(x)}\delta g^{\mu\nu}(x)=\int d^2x\sqrt{-g}\langle\hat{T}^\mu_\mu\rangle\delta\Omega(x). \tag{15.19}$$

Comparing Eqs. (15.18) and (15.19), we obtain the result (15.15),

$$\langle\hat{T}^\mu_\mu\rangle=-\frac{R}{24\pi}.$$

Appendices

A Mathematical supplement

A.1 Functionals and distributions (generalized functions)

This appendix is an informal introduction to functionals and distributions.

Functionals

A *functional* is a map from a space of functions into numbers. If a functional S maps a function $q(t)$ into a number a, we write $S[q] = a$ or $S[q(t)] = a$. This notation is intended to show that the value $S[q]$ depends on the behavior of $q(t)$ at all t, not only at one particular t.

Some functionals can be written as integrals,

$$A[q(t)] = \int_{t_1}^{t_2} F(q(t))\, dt,$$

where $F(q)$ is an ordinary function applied to the value of q. For example, the functional

$$A[q(t)] = \int_0^1 [q(t)]^2\, dt$$

yields $A[t^n] = (2n+1)^{-1}$ and $A[\sin t] = \frac{1}{2} - \frac{1}{4}\sin 2$.

A functional may not be well-defined on all functions. For example, the above functional $A[q]$ can be applied only to functions $q(t)$ that are square-integrable on the interval $[0,1]$. Together with a functional one always implies a suitable space of functions on which the functional is well-defined. Functions from this space are called *base functions* of a given functional.

Distributions

Not all functionals are expressible in the form of an integral. For example, the *delta function* denoted by $\delta(t-t_0)$ is by definition a functional that returns the value of a function at the point t_0, i.e.

$$\delta(t-t_0)[f(t)] \equiv f(t_0).$$

This functional cannot be written as an integral because there exists no function $F(t,f)$ such that for any continuous function $f(t)$,

$$f(t_0) = \int F(t, f(t))\, dt.$$

However, it is very convenient to be able to represent such functionals as integrals. So one writes

$$\delta\left(t-t_0\right)\left[f(t)\right]=f\left(t_0\right)\equiv\int_{-\infty}^{+\infty}f(t)\delta\left(t-t_0\right)dt \tag{A.1}$$

even though $\delta(t-t_0)$ is not a function with numeric values (it is a "generalized function") and the integration is purely symbolic. This notation is a convenient shorthand because one can manipulate expressions linear in the δ function as if they were normal functions; for instance,

$$\int\left[a_1\delta\left(x-x_1\right)+a_2\delta\left(x-x_2\right)\right]f\left(x\right)dx=a_1f\left(x_1\right)+a_2f\left(x_2\right).$$

However, expressions such as $\sqrt{\delta(t)}$ or $\exp\left[\delta(t)\right]$ are undefined.

Note that the functional $\delta\left(t-t_0\right)$ is well-defined only on functions that are continuous at $t=t_0$. If we need to work with these functionals, we usually restrict the base functions to be everywhere continuous.

As an example, consider the functional

$$B\left[q(t)\right]\equiv3\sqrt{q(1)}+\sin\left[q(2)\right],$$

where $q(1)$ and $q(2)$ are the values of the function $q(t)$. This functional depends only on the values of $q(t)$ at $t=1$ and $t=2$ and can be written in an integral form as

$$\begin{aligned}B\left[q(t)\right]&=3\sqrt{q(1)}+\sin\left[q(2)\right]\\&=\int_{-\infty}^{+\infty}dt\left\{3\delta(t-1)\sqrt{q(t)}+\delta(t-2)\sin\left[q(t)\right]\right\}.\end{aligned} \tag{A.2}$$

Generalized function and *distribution* are other names for "a linear functional on a suitable space of functions." A functional is *linear* if

$$S\left[f(t)+cg(t)\right]=S\left[f\right]+cS\left[g\right]$$

for arbitrary base functions f, g and an arbitrary constant c. It is straightforward to verify that $\delta\left(t-t_0\right)$ is a linear functional.

The application of a linear functional A to a function $f(x)$ is written symbolically as an integral

$$A\left[f\right]\equiv\int f(x)A(x)dx, \tag{A.3}$$

where $A(x)$ is the *integration kernel* which represents the functional. Note that there may be no actual integration in Eq. (A.3) because $A(x)$ is not necessarily an ordinary function. For instance, there is no real integration performed in Eqs. (A.1) and (A.2).

> **Remark:** The δ function is sometimes "defined" by the conditions $\delta(x)=0$ for $x\neq0$ and $\delta(0)=+\infty$, while $\int\delta(x)dx=1$. However, these contradictory requirements cannot be satisfied by any function with numeric values. It is more consistent to say that $\delta\left(x-x_0\right)$ is not really a function of x and to treat Eq. (A.1) as a purely symbolic relation.

Distributions defined on a certain space of base functions build a linear space. An ordinary function $a(x)$ naturally defines a functional

$$a\left[f(x)\right] \equiv \int a(x)f(x)dx$$

and thus also belongs to the space of distributions if the integral converges for all base functions $f(x)$. For example, the function $a(x) \equiv 1$ defines a distribution on the base space of integrable functions on $[-\infty, +\infty]$, although $a(x)$ itself does not belong to the base space.

Distributions can be multiplied by ordinary functions, and the result is a distribution. For example, suppose $A(x)$ is a distribution and $a(x)$ is an ordinary function, then the action of Aa on a base function $f(x)$ is

$$A(x)a(x)\left[f\right] \equiv \int A(x)a(x)f(x)dx \equiv A(x)\left[af\right].$$

Sometimes two distributions can be multiplied, e.g. $\delta(x-x_0)\delta(y-y_0)$ is defined on continuous functions $f(x,y)$ and yields the value $f(x_0,y_0)$.

Two distributions are equal when they give equal results for all base functions. For instance, one can easily show that in the space of distributions $(x-x_0)\,\delta\left(x-x_0\right)=0$ when applied to continuous base functions.

Derivatives of the δ function are defined as functionals that yield the value of the derivative of a function at a fixed point. If $\delta(x-x_0)$ were a normal function, one would expect the following identity to hold,

$$\int f(x)\delta'\left(x-x_0\right)dx = -\int f'(x)\delta\left(x-x_0\right)dx = -f'\left(x_0\right).$$

Therefore one *defines* the distribution $\delta'(x-x_0)$ as the functional

$$\delta'\left(x-x_0\right)\left[f(x)\right] \equiv -f'(x_0).$$

More generally,

$$\frac{d^n\delta\left(x-x_0\right)}{dx^n}\left[f\right] = (-1)^n\left.\frac{d^nf}{dx^n}\right|_{x=x_0}.$$

Derivatives of the δ function are functionals defined on sufficiently smooth base functions.

Principal value integrals

Not all distributions arise from combinations of δ functions. Another important example is the principal value integral.

If the space of base functions includes all continuous functions, then the distribution

$$a(x) = \frac{1}{x-x_0}$$

is undefined on some base functions because the integral with a function $f(x)$ diverges at the pole $x = x_0$ if $f(x_0) \neq 0$. The Cauchy principal value prescription helps to define $a[f]$ in such cases.

Definition

For integrals $\int_A^B F(x)dx$ where $F(x)$ has a pole at $x = x_0$ within the interval (A, B), one defines the *principal value* denoted by $\mathcal{P}\int$ as

$$\mathcal{P}\int_A^B F(x)dx \equiv \lim_{\varepsilon\to+0}\left[\int_A^{x_0-\varepsilon} F(x)dx + \int_{x_0+\varepsilon}^B F(x)dx\right],$$

when the limit exists. The idea is to cut out a neighborhood of the pole symmetrically at both sides. If the integrand contains several poles, the same limit procedure is applied to each pole separately; if there are no poles, the usual integration is performed. For example,

$$\mathcal{P}\int_{-\infty}^{+\infty}\frac{dx}{x^3} = 0; \quad \mathcal{P}\int_0^M \frac{dx}{x^2-1} = \frac{1}{2}\ln\frac{M-1}{M+1},\ M > 1.$$

We write

$$\mathcal{P}\frac{1}{x-x_0}$$

to denote the distribution that acts by applying the principal value prescription to the integral, i.e.

$$\left(\mathcal{P}\frac{1}{x-x_0}\right)[f(x)] \equiv \mathcal{P}\int_A^B \frac{f(x)dx}{x-x_0}.$$

This integral converges in a neighborhood of $x = x_0$ if $f(x)$ is continuous there.

It is almost always the case that one cannot use the ordinary function $1/x$ as a distribution and *must* use $\mathcal{P}\frac{1}{x}$ instead, because the base functions are typically such that the ordinary integral $\int \frac{dx}{x} f(x)$ would diverge.

Example calculation with residues

A typical example is the principal value integral

$$\mathcal{P}\int_{-\infty}^{+\infty}\frac{e^{-ikx}}{x}dx \equiv \lim_{\varepsilon\to+0}\left[\int_{-\infty}^{-\varepsilon}\frac{e^{-ikx}}{x}dx + \int_{\varepsilon}^{+\infty}\frac{e^{-ikx}}{x}dx\right]. \tag{A.4}$$

Since the indefinite integral

$$\int\frac{e^{-ikx}}{x}dx \tag{A.5}$$

cannot be computed, we need to use the method of residues. First we assume that $\mathrm{Re}\, k > 0$ and consider the contour C in the complex x plane that goes around the pole

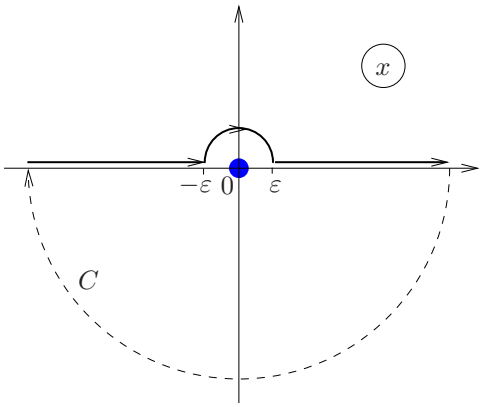


Figure A.1: The integration contour C for Eq. (A.4).

at $x = 0$ along a semicircle of radius ε (see Fig. A.1). The contour may be closed in the lower half-plane since $\operatorname{Re} k > 0$. The integral around the contour C is found from the residue at $x = 0$ which is equal to 1, so

$$\oint_C \frac{e^{-ikx}}{x} dx = -2\pi i.$$

This integral differs from that of Eq. (A.4) only by the contribution of the semicircle. The function near the pole is nearly equal to $1/x$ and one can easily show by an explicit calculation that in the limit $\varepsilon \to +0$ the integral around the semicircle is equal to $-\pi i$ times the residue (a half of the integral over the full circle). Therefore,

$$\mathcal{P}\int_{-\infty}^{+\infty} \frac{e^{-ikx}}{x} dx = -2\pi i - (-\pi i) = -\pi i, \quad \operatorname{Re} k > 0.$$

Analogous calculations give the opposite sign for $k < 0$ and the final result is

$$\mathcal{P}\int_{-\infty}^{+\infty} \frac{e^{-ikx}}{x} dx = -i\pi \operatorname{sign} k.$$

We could have chosen another contour instead of C; a very similar calculation yields the same answer for the contour with the semicircle in the opposite direction. We would like to emphasize that the choice of a contour is a purely technical issue inherent in the method of residues. The principal value integral is well-defined regardless of any integration in the complex plane; one would not need to choose any contours if we could compute the indefinite integral (A.5) or if there existed another method for evaluating the two integrals in Eq. (A.4) separately.

Convergence in the distributional sense

The δ function may be approximated by certain sequences of functions, for example (here $n = 1, 2, ...$)

$$\begin{aligned} f_n(x) &= \begin{cases} 0, & |x| > \frac{1}{2n}, \\ n, & |x| < \frac{1}{2n}; \end{cases} \\ g_n(x) &= \sqrt{\frac{n}{\pi}} \exp\left[-nx^2\right]; \\ h_n(x) &= \frac{1}{\pi} \frac{\sin nx}{x}. \end{aligned}$$

The sequences f_n and g_n converge pointwise to zero at $x \neq 0$, while the sequence h_n does not have any finite pointwise limit at any x. At first sight these three sequences may appear to be very different. However, one can show that for any integrable function $q(x)$ continuous at $x = 0$, the identity

$$\lim_{n\to\infty} \int_{-\infty}^{+\infty} dx\, f_n(x) q(x) = q(0)$$

and the analogous identities for $g_n(x)$ and $h_n(x)$ hold. This statement suggests that all three sequences in fact converge to $\delta(x)$. The mathematical term is *convergence in the sense of distributions*.

A sequence of functionals F_n, $n = 1, 2, ...$, converges in the distributional sense if the limit

$$\lim_{n\to\infty} F_n[q]$$

exists for all base functions $q(x)$. It is clear from our example that a sequence of functions may converge in the distributional sense even if it has no pointwise limits.

Various statements concerning the δ function can (and should) be verified by calculations with explicit sequences of ordinary functions that converge to the δ function in the distributional sense.

The Sokhotsky formula

Another example of convergence to a distribution is the family of functions

$$a_\varepsilon(x) \equiv \frac{1}{x + i\varepsilon}, \quad \varepsilon > 0.$$

As $\varepsilon \to 0$, the functions $a_\varepsilon(x)$ converge pointwise to $1/x$ everywhere except at $x = 0$.

The Sokhotsky formula is the limit (understood in the distributional sense)

$$\lim_{\varepsilon\to+0} \frac{1}{x + i\varepsilon} = -i\pi\delta(x) + \mathcal{P}\frac{1}{x}. \tag{A.6}$$

This formula is derived by integrating $a_\varepsilon(x)f(x)$, where $f(x)$ is an arbitrary continuous base function,

$$\int_{-\infty}^{+\infty} \frac{1}{x+i\varepsilon} f(x)dx = \int_{-\infty}^{+\infty} \frac{xf(x)dx}{x^2+\varepsilon^2} - i\int_{-\infty}^{+\infty} \frac{\varepsilon\, f(x)dx}{x^2+\varepsilon^2}, \tag{A.7}$$

and showing that in the limit $\varepsilon \to 0$ the two terms in the RHS converge to

$$\mathcal{P}\int_{-\infty}^{+\infty} \frac{f(x)}{x}dx - i\pi f(0).$$

We omit the detailed proof.

Distributional convergence of integrals

The concept of convergence in the distributional sense applies also to integrals. For example, consider the ordinarily divergent integral

$$a(x) \equiv \int_0^{+\infty} dk\, \sin kx. \tag{A.8}$$

If we take Eq. (A.8) at face value as an equality of functions, then $a(x)$ would be undefined for any x except $x = 0$ where $a(0) = 0$. However, if we interpret Eq. (A.8) in the distributional sense, it yields a certain well-defined distribution $a(x)$.

To demonstrate this, we attempt to define the functional

$$a\,[f] \equiv \int dx\, f(x)a(x) = \int dx\, f\,(x) \int_0^{+\infty} dk\, \sin kx.$$

This expression is meaningless because of the divergent integral over k. If we now formally reverse the order of integrations, we get a meaningful formula

$$a\,[f] \equiv \int_0^{+\infty} dk \int dx\, f(x) \sin kx. \tag{A.9}$$

The integrations performed in this order do converge as long as $f(x)$ is sufficiently well-behaved (continuous and decaying at infinity). Therefore it is reasonable to *define* the functional $a[f]$ by Eq. (A.9).

We can now reduce the well-defined functional $a[f]$ to a simpler form. To transform the expression (A.9), it is useful to be able to interchange the order of integrations. However, this can be done for uniformly convergent integrals, while the double integral (A.9) converges non-uniformly. Therefore we temporarily introduce a cutoff into the integral over dk at the upper limit (large k). At the end of the calculation we shall remove the cutoff and obtain the final result. Now we show the details of this procedure for the functional (A.9).

A simple way to introduce a cutoff is to multiply the integrand by $\exp(-\alpha k)$ where $\alpha > 0$ is a real parameter; the original integral is restored when $\alpha = 0$. It is clear that for any sufficiently well-behaved function $f(x)$,

$$\lim_{\alpha\to+0}\int_0^{+\infty} dk \int dx\, f(x)e^{-\alpha k}\sin kx = \int_0^{+\infty} dk \int dx\, f(x)\sin kx \equiv a\,[f]\,.$$

The double integral

$$\int_0^{+\infty} dk \int dx\, f(x)e^{-\alpha k}\sin kx$$

converges uniformly in k and x, so we can reverse the order of integrations *before* evaluating the limit $\alpha \to 0$. In the inner integral we obtain the family of functions

$$a_\alpha(x) \equiv \int_0^{+\infty} dk\, \sin kx\, \exp(-\alpha k) = \frac{x}{\alpha^2 + x^2}.$$

At this point we can impose the limit $\alpha \to 0$, use Eqs. (A.6)-(A.7) and find

$$a\,[f] = \lim_{\alpha\to+0}\int dx\, a_\alpha(x) f(x) = \lim_{\alpha\to+0}\int \frac{x f(x) dx}{x^2+\alpha^2} = \mathcal{P}\int dx \frac{f(x)}{x}.$$

This holds for any base function $f(x)$, therefore we obtain the following equality of distributions,

$$a(x) \equiv \int_0^{+\infty} dk\, \sin kx = \lim_{\alpha\to+0} a_\alpha(x) = \mathcal{P}\frac{1}{x}. \tag{A.10}$$

We may say that the integral (A.8) diverges in the usual sense but converges in the distributional sense.

The distributional limit of a divergent integral is usually found by regularizing the integral with a convenient factor such as $\exp(-\alpha k)$ and by removing the cutoff after the integration. The way to introduce the cutoff in k is of course not unique. For instance, we could multiply the integrand by $\exp\left(-\alpha k^2\right)$ or simply replace the infinite upper limit in Eq. (A.8) by a parameter $k_{\max}$ and then evaluate the limit $k_{\max} \to +\infty$. The calculations are somewhat less transparent in that case but the result is the same. We are free to choose a cutoff in any form, as long as the cutoff allows us to reverse the order of integration.

> **Remark:** We should keep in mind that there must be some base functions $f(x)$ to which both sides of Eq. (A.10) are applied as linear functionals. Only then the manipulations with the artificial cutoff become well-defined operations in the space of distributions. Although it is tempting to treat $a(x)$ as an ordinary function equal to $1/x$, it would be an abuse of notation since e.g.
>
> $$a(2) = \int_0^{+\infty} dk\, \sin 2k = \frac{1}{2} \quad ???$$
>
> is a meaningless statement. Expressions such as Eq. (A.8) usually appear as inner integrals in calculations, for example,
>
> $$\int_{-\infty}^{+\infty} dx \int_0^{+\infty} dk\, x e^{-x^2}\sin kx,$$

which looks like an application of the distribution $a(x)$ to the base function xe^{-x^2}. In such cases we are justified to treat the inner integral as the distribution (A.10).

Fourier representations of distributions

A well-known integral representation of the δ function is

$$\delta(x - x_0) = \int_{-\infty}^{+\infty} \frac{dk}{2\pi} e^{ik(x-x_0)}. \tag{A.11}$$

The integral in Eq. (A.11) diverges for all x and must be understood in the distributional sense, similarly to the integral (A.8).

Distributions often turn up in calculations when we use Fourier transforms. If $\tilde{f}(k)$ is a Fourier transform of $f(x)$, so that

$$f(x) = \int \tilde{f}(k) e^{ikx} dk,$$

then $\tilde{f}(k)$ may well be a distribution since the only way it is connected with real functions is through integration. We shall see examples of this in Appendix A.2.

Solving equations for distributions

Distributions may be added together, multiplied by ordinary functions, or differentiated to yield other distributions. For example, the distribution $\mathcal{P}\frac{1}{x^2}$ multiplied by the function $2x$ yields the distribution $\mathcal{P}\frac{2}{x}$. Although such calculations are in most cases intuitively obvious, they need to be verified more formally by analyzing explicit distributional limits.

A curious phenomenon occurs when solving algebraic equations that involve distributions, e.g.

$$(x - x_0)\, a(x) = 1. \tag{A.12}$$

Note that $(x - x_0)\,\delta(x - x_0) = 0$. So the solution of Eq. (A.12) in terms of distributions is

$$a(x) = \mathcal{P}\frac{1}{x - x_0} + A\delta(x - x_0),$$

where the constant A is an arbitrary number. This shows that one should be careful when doing arithmetic with distributions. For instance, dividing a distribution by x is possible but the result contains the term $A\delta(x)$ with an arbitrary constant A.

A.2 Green's functions, boundary conditions, and contours

Green's functions are used to solve linear differential equations. The typical problem involves a linear differential operator $\hat{L}_x$ such as

$$\hat{L}_x = \frac{d^2}{dx^2} + a^2. \tag{A.13}$$

A *Green's function* of the operator $\hat{L}$ is a distribution $G(x, x')$ that solves the equation

$$\hat{L}_x G(x, x') = \delta(x - x'). \tag{A.14}$$

Because of this relation which can be symbolically represented by $\hat{L}_x \hat{G} = \hat{1}$, the Green's function is frequently written as the "inverse" of the operator $\hat{L}_x$, i.e. $\hat{G} = \hat{L}_x^{-1}$. However, one should keep in mind that this notation is symbolic and the operator such as $\hat{L}_x$ does not actually have an inverse operator.

The Green's function must also satisfy a set of boundary conditions imposed usually at $|x| = \infty$ or perhaps at some finite boundary points, according to the particular problem. For example, the causal boundary condition in one dimension (real x) is

$$G_{ret}(x, x') = 0 \text{ for } x < x'. \tag{A.15}$$

This condition specifies the retarded Green's function.

Green's functions can be used to solve equations of the form

$$\hat{L}_x f(x) = s(x),$$

where $s(x)$ is a known "source" function. The general solution of the above equation can be written as

$$f(x) = f_0(x) + \int G(x, x') s(x') dx',$$

where $f_0(x)$ is a general solution of the homogeneous equation, $\hat{L} f_0 = 0$.

Equation (A.14) defines a Green's function only up to a solution of the homogeneous equation. Boundary conditions are needed to fix the Green's function uniquely. Green's functions obtained with different boundary conditions differ by a solution of the homogeneous equation.

Using Fourier transforms

To find a Green's function, it is often convenient to use Fourier transforms, especially when $G(x, x') = G(x - x')$. In that case we can use the Fourier representation in n dimensions,

$$G(x - x') \equiv G(\Delta x) = \int \frac{d^n k}{(2\pi)^n} g(k) e^{ik \cdot \Delta x}. \tag{A.16}$$

However, it often turns out that the Fourier transform of a Green's function is a *distribution* and not an ordinary function.

As an example, we consider the Green's function $G(x-x')$ of the one-dimensional operator (A.13). The Fourier image $g(k)$ of $G(\Delta x)$ defined by Eq. (A.16) satisfies

$$\left(a^2-k^2\right)g(k)=1. \tag{A.17}$$

Here we are forced to treat $g(k)$ as a distribution because the ordinary solution

$$G(\Delta x)=\int_{-\infty}^{+\infty}\frac{dk}{2\pi}\frac{1}{a^2-k^2}e^{ik\Delta x} \quad ???$$

involves a meaningless divergent integral. In the space of distributions, the general solution of Eq. (A.17) is

$$g(k)=\mathcal{P}\frac{1}{a^2-k^2}+g_1\delta(k-a)+g_2\delta(k+a), \tag{A.18}$$

with arbitrary complex constants $g_{1,2}$. Then the general form of the Green's function is found from Eq. (A.16) with $n=1$,

$$G(\Delta x)=\mathcal{P}\int_{-\infty}^{+\infty}\frac{dk}{2\pi}\frac{e^{ik\Delta x}}{a^2-k^2}+\frac{g_1}{2\pi}e^{ia\Delta x}+\frac{g_2}{2\pi}e^{-ia\Delta x}.$$

The constants $g_{1,2}$ describe the general solution of the homogeneous equation,

$$\hat{L}_x\left(g_1e^{ia\Delta x}+g_2e^{-ia\Delta x}\right)=0.$$

These constants can be found from the particular boundary conditions after computing the principal value integral. We find, for instance, that the boundary conditions (A.15) require

$$g_{1,2}=\pm\frac{\pi}{2ia} \tag{A.19}$$

(see Eq. (D.31) in the solution to Exercise 12.2) and the retarded Green's function is expressed by Eq. (D.32).

Contour integration and boundary conditions

We have shown that the boundary condition for $G(x,x')$ determines the choice of the constants $g_{1,2}$ which parametrize the general solution of the homogeneous oscillator equation, while the nontrivial part of Green's function (a special solution of the inhomogeneous equation) is equal to a certain principal value integral. Instead of using the principal value prescription, we could select a contour C in the complex k plane and express the Green's function as

$$G(\Delta x)=\int_C\frac{dk}{2\pi}\frac{e^{ik\Delta x}}{a^2-k^2}+\frac{\tilde{g}_1}{2\pi}e^{ia\Delta x}+\frac{\tilde{g}_2}{2\pi}e^{-ia\Delta x}. \tag{A.20}$$

In effect we replaced the principal value prescription $\mathcal{P}\int$ by a certain choice of the contour. This alternative prescription adds some residue terms at the poles $k = \pm a$, so the constants $\tilde{g}_{1,2}$ differ from those in Eq. (A.19). The resulting Green's function is of course the same because the change in the constants $g_{1,2} \to \tilde{g}_{1,2}$ cancels the extra residue terms.

Example calculation with a contour

Let us select the contour C shown in Fig. A.2, where both semicircles are *arbitrarily* chosen to lie in the upper half-plane. The contour C must be closed in the lower half-plane if $\Delta x < 0$ and in the upper half-plane if $\Delta x > 0$. The integral along each semicircle is equal to $-\pi i$ times the residue at the corresponding pole. Therefore the integral along the contour C is

$$\int_C \frac{e^{ik\Delta x}}{a^2 - k^2} dk = \begin{cases} 0, & \Delta x > 0; \\ \frac{2\pi}{a} \sin(a\Delta x), & \Delta x < 0. \end{cases}$$

To satisfy the boundary conditions (A.15), we must choose the constants as

$$g_{1,2} = \pm \frac{\pi}{ia}.$$

Note that this differs from Eq. (A.19). The resulting Green's function is

$$G_{ret}(\Delta x) = \theta(x - x') \frac{\sin a\Delta x}{a},$$

which coincides with Eq. (D.32). The same result is obtained from any other choice of the contour in Eq. (A.20) when the constants $g_{1,2}$ are chosen correctly.

Choosing the contour as in Fig. A.2 is equivalent to considering the limit

$$\lim_{\varepsilon \to +0} \int_{-\infty}^{+\infty} \frac{dk\, e^{ik\Delta x}}{a^2 - k^2 - ik\varepsilon},$$

since a replacement $k \to k + \frac{1}{2} i\varepsilon$ under the integral corresponds to shifting the integration line upwards.

We could choose the contour of integration in a clever way to make $g_{1,2} = 0$. This is achieved if both semicircles in Fig. A.2 are turned upside-down. This is the calculation often presented in textbooks, where one is instructed to rewrite the integral as

$$\lim_{\varepsilon \to +0} \int_{-\infty}^{+\infty} \frac{dk\, e^{ik\Delta x}}{a^2 - k^2 \pm i\varepsilon} \quad \text{or} \quad \lim_{\varepsilon \to +0} \int_{-\infty}^{+\infty} \frac{dk\, e^{ik\Delta x}}{a^2 - k^2 \pm ik\varepsilon} \tag{A.21}$$

with small real $\varepsilon > 0$ and to take the limit $\varepsilon \to +0$. As we have seen, such limits with a prescription for inserting ε into the denominator are equivalent to particular choices of contours in the complex k plane. It is difficult to remember the correct prescription of the contour or the specific ansatz with ε that one needs for each operator $\hat{L}_x$ and for each set of boundary conditions. These tricks are unnecessary if one treats the

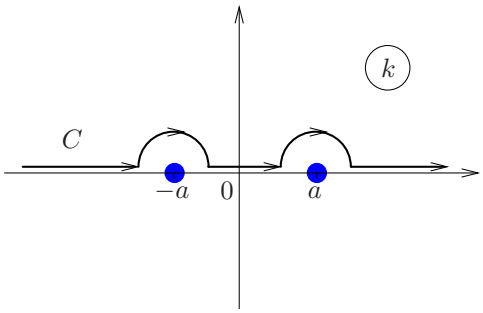


Figure A.2: Alternative integration contour for Green's function, Eq. (A.20).

Fourier image $g(k)$ as a distribution with unknown constants, as in Eq. (A.18). One is then free to choose either a principal value prescription or an arbitrary contour in the complex k plane, as long as one determines the relevant constants from boundary conditions.

So far we considered only one-dimensional examples. In higher-dimensional spaces, one often obtains integrals such as

$$\int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{k^2 - m^2}$$

in which the kernel $1/(k^2 - m^2)$ must be understood as a distribution and rewritten as

$$\text{“}\frac{1}{k^2 - m^2}\text{”} = \mathcal{P}\frac{1}{k^2 - m^2} + h\left(\mathbf{k}\right)\delta\left(k^2 - m^2\right),$$

where $h\left(\mathbf{k}\right)$ is an arbitrary function of the vector $\mathbf{k}$. To obtain an explicit principal value formulation of such integrals, one first separates the divergent integration over a scalar variable (in this case over dk),

$$\mathcal{P}\int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{k^2 - m^2} = \int_0^\pi d\theta \sin\theta\, \mathcal{P}\int_0^{+\infty} \frac{k^2 dk}{(2\pi)^2} \frac{e^{ikx\cos\theta}}{k^2 - m^2},$$

and then uses the principal value prescription. (In this particular case the integration over $d\theta$ can be performed first.) The relevant arbitrary parameters such as $h\left(\mathbf{k}\right)$ must be determined from the appropriate boundary conditions.

A.3 Euler's gamma function and analytic continuations

Euler's gamma function $\Gamma(x)$ is a transcendental function that generalizes the factorial $n!$ from natural n to complex numbers. We shall now summarize some of its standard properties.

The usual definition is

$$\Gamma(x) = \int_0^{+\infty} t^{x-1} e^{-t} dt. \tag{A.22}$$

The integral (A.22) converges for real $x > 0$ (and also for complex x such that $\operatorname{Re} x > 0$) and defines an analytic function. It is easy to check that $\Gamma(n) = (n-1)!$ for integer $n \geq 1$; in particular, $\Gamma(1) = 1$. The gamma function can be analytically continued to all complex x.

Analytic continuations

If an analytic function $f(x)$ is defined only for some x, an analytic continuation can be used to obtain values for other x.

A familiar case of analytic continuation is the geometric series,

$$f(x) = \sum_{n=0}^{\infty} x^n, \quad |x| < 1.$$

The series converges only for $|x| < 1$. One can manipulate this series and derive the formula

$$f(x) = \frac{1}{1-x}, \quad |x| < 1, \tag{A.23}$$

which defines the function $f(x)$ for all $x \neq 1$ and coincides with the old definition for $|x| < 1$. Therefore, Eq. (A.23) provides the analytic continuation of $f(x)$ to the entire complex plane (except for the pole at $x = 1$).

If a function $f(x)$ is defined by an integral relation such as

$$f(x) = \int F(x, y) dy,$$

where the integral converges only for some x, one might be able to transform the specific integral until one obtains some other formula for $f(x)$ that is valid for a wider range of x. According to a standard theorem of complex calculus, two analytic functions that coincide in some region of the complex plane must coincide in the entire plane (perhaps after branch cuts). Therefore any formula for $f(x)$ defines the same analytic function. The hard part is to obtain a better formula out of the original definition. Unfortunately, there is no general method to perform the analytic continuation. One has to apply tricks that are suitable to the problem at hand.

The gamma function for all x

The analytic continuation of $\Gamma(x)$ can be performed as follows. Integrating Eq. (A.22) by parts, one obtains the identity

$$x\Gamma(x) = \Gamma(x+1), \quad x > 0. \tag{A.24}$$

This formula determines $\Gamma(x)$ for $\mathrm{Re}\, x > -1$, because $\Gamma(x+1)$ is well-defined and one can write

$$\Gamma(x) \equiv \frac{\Gamma(x+1)}{x}, \quad \mathrm{Re}\, x > -1.$$

The point $x = 0$ is clearly a pole of $\Gamma(x)$, but at $x \neq 0$ the function is finite. Subsequently we define $\Gamma(x)$ for $\mathrm{Re}\, x > -2$ by

$$\Gamma(x) \equiv \frac{\Gamma(x+2)}{x(x+1)}, \quad \mathrm{Re}\, x > -2,$$

for $\mathrm{Re}\, x > -3$ and so on. (Thus $\Gamma(x)$ has poles at $x = 0, -1, -2, ...$) The resulting analytic function coincides with the original integral for $\mathrm{Re}\, x > 0$.

Series expansions

One can expand the gamma function in power series as

$$\Gamma(1+\varepsilon) = 1 - \gamma\varepsilon + O\left(\varepsilon^2\right),$$

where

$$\gamma \equiv -\int_0^{+\infty} dt\, e^{-t} \ln t \approx 0.5772$$

is Euler's constant. From the above series it is easy to deduce the asymptotic behavior at the poles, for instance

$$\Gamma(x \to 0) = \frac{\Gamma(x+1)}{x} = \frac{1}{x} - \gamma + O(x). \tag{A.25}$$

Product identity

A convenient identity connects $\Gamma(x)$ and $\Gamma(1-x)$:

$$\Gamma(x)\Gamma(1-x) = \frac{\pi}{\sin \pi x}. \tag{A.26}$$

This identity holds for all (complex) x; for instance, it follows that $\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$. One can also obtain the formula

$$\Gamma(ix)\Gamma(-ix) = |\Gamma(ix)|^2 = \frac{\pi}{x \sinh \pi x}. \tag{A.27}$$

Finally, Eq. (A.26) allows one to express $\Gamma(x)$ for $\mathrm{Re}\, x \leq 0$ through $\Gamma(1-x)$, which is another way to define the analytic continuation of $\Gamma(x)$ to all complex x.

Derivation of Eq. (A.26). We first derive the identity for $0 < \mathrm{Re}\, x < 1$. Using Eq. (A.22), we have

$$\Gamma(x)\Gamma(1-x) = \int_0^{+\infty} ds \int_0^{+\infty} dt\, s^{x-1} t^{-x} e^{-(s+t)},$$

where the integrals are convergent if $0 < \mathrm{Re}\, x < 1$. After a change of the variables $(s,t) \to (u,v)$,

$$u \equiv s+t,\ v \equiv \ln \frac{s}{t}, \quad ds\, dt = \frac{u e^v}{(e^v+1)^2} du\, dv,$$

where $0 < u < +\infty$ and $-\infty < v < +\infty$, the integral over u is elementary and we get

$$\Gamma(x)\Gamma(1-x) = \int_{-\infty}^{+\infty} \frac{e^{vx} dv}{e^v + 1}.$$

The integral converges for $0 < \mathrm{Re}\, x < 1$ and is evaluated using residues by shifting the contour to $v = 2\pi i + \tilde{v}$ which multiplies the integral by $\exp(2\pi i x)$. The residue at $v = i\pi$ is equal to $-\exp(i\pi x)$. We find

$$\left(1 - e^{2\pi i x}\right) \Gamma(x)\Gamma(1-x) = -2\pi i e^{\pi i x},$$

from which Eq. (A.26) follows for $0 < \mathrm{Re}\, x < 1$.

To show that the identity holds for all x, we use Eq. (A.24) to find for integer $n \geq 1$

$$\begin{aligned}\Gamma(x-n)\Gamma\left(1-(x-n)\right) &= \frac{\Gamma(x)\Gamma(1-x)}{(x-1)...(x-n)}(1-x)...(n-x) \\ &= (-1)^n \frac{\pi}{\sin \pi x} = \frac{\pi}{\sin \pi(x-n)}, \quad 0 < \mathrm{Re}\, x < 1.\end{aligned}$$

Expressing integrals through the gamma function

Some transcendental integrals such as

$$\int_0^{+\infty} x^{s-1} e^{-bx} dx \tag{A.28}$$

are expressed through the gamma function after a change of variable $y = bx$,

$$\int_0^{+\infty} x^{s-1} e^{-bx} dx = b^{-s}\Gamma(s).$$

However, complications arise when s and b are complex numbers, because of the ambiguity of the phase of b. For example, i^i is an inherently ambiguous expression since one may write

$$i^i = \left[\exp\left(\frac{i\pi}{2} + 2\pi i n\right)\right]^i = \exp\left(-\frac{\pi}{2} - 2\pi n\right), \quad n \in \mathbb{Z}.$$

We consider Eq. (A.28) with a complex b such that $\operatorname{Re} b > 0$. (The integral diverges if $\operatorname{Re} b < 0$, converges conditionally when $\operatorname{Re} b = 0$, $b \neq 0$, and $0 < \operatorname{Re} s < 1$, while for other s the limit $\operatorname{Re} b \to +0$ may be taken only in the distributional sense.) The integrand is rewritten as

$$x^{s-1}e^{-bx} = \exp\left[-bx + (s-1)\ln x\right].$$

The contour of integration may be rotated to the half-line $x = e^{i\phi}y$, with a fixed angle $|\phi| < \frac{\pi}{2}$, and y varying in the interval $0 < y < +\infty$. Therefore, if $\operatorname{Re} s > 0$ we can change the variable $bx \equiv y$ as long as $\operatorname{Re} b > 0$. Then we should select the branch of the complex logarithm function covering the region $-\frac{\pi}{2} < \phi < \frac{\pi}{2}$,

$$\ln(A + iB) \equiv \ln|A + iB| + i\,(\operatorname{sign} B)\arctan\frac{|B|}{A}, \quad A > 0. \tag{A.29}$$

With this definition of the logarithm, the integral (A.28) is transformed to

$$\int_0^{+\infty} x^{s-1}e^{-bx}dx = b^{-s}\int_0^{+\infty} y^{s-1}e^{-y}dy = \exp(-s\ln b)\Gamma(s). \tag{A.30}$$

In the calculations for the Unruh effect (Sec. 8.2.4) we encountered the following integral,

$$F(\omega,\Omega) \equiv \int_{-\infty}^{+\infty}\frac{du}{2\pi}\exp\left(i\Omega u + i\frac{\omega}{a}e^{-au}\right).$$

This integral can be expressed through the gamma function. Changing the variable to $x \equiv e^{-au}$, we obtain

$$F(\omega,\Omega) = \frac{1}{2\pi a}\int_0^{+\infty} dx\, x^{-\frac{i\Omega}{a}-1}e^{\frac{i\omega}{a}x} \tag{A.31}$$

which is of the form (A.28) with

$$b = -\frac{i\omega}{a}, \quad s = -\frac{i\Omega}{a}.$$

Since $\operatorname{Re} s = 0$, the integral in Eq. (A.31) diverges at $x = 0$. To obtain the distributional limit of this integral, we need to take the limit of s having a vanishing positive real part. Since b also must satisfy $\operatorname{Re} b > 0$, we choose

$$b = -\frac{i\omega}{a} + \varepsilon, \;\; s = -\frac{i\Omega}{a} + \varepsilon, \quad \varepsilon > 0,$$

and take the limit of $\varepsilon \to +0$. Then we can use Eq. (A.30) in which we must evaluate

$$\ln b = \lim_{\varepsilon\to+0}\ln\left(-\frac{i\omega}{a} + \varepsilon\right) = \ln\left|\frac{\omega}{a}\right| - i\frac{\pi}{2}\operatorname{sign}\left(\frac{\omega}{a}\right).$$

Substituting into Eq. (A.30), we find

$$F(\omega,\Omega) = \frac{1}{2\pi a}\exp\left[\frac{i\Omega}{a}\ln\left|\frac{\omega}{a}\right| + \frac{\pi\Omega}{2a}\operatorname{sign}\left(\frac{\omega}{a}\right)\right]\Gamma\left(-\frac{i\Omega}{a}\right).$$

Now it is straightforward to obtain the relation

$$F(\omega,\Omega) = F(-\omega,\Omega)\exp\left(\frac{\pi\Omega}{a}\right), \quad \omega > 0,\ \Omega > 0.$$

Finally, we derive an explicit formula for the quantity

$$|\beta_{\omega\Omega}|^2 = \frac{\Omega}{\omega}\,|F(-\omega,\Omega)|^2$$

which is related to the mean particle number by Eq. (8.28). Using Eq. (A.27), we get

$$|\beta_{\omega\Omega}|^2 = \frac{\Omega}{4\pi^2 a^2 \omega}\exp\left(-\frac{\pi\Omega}{a}\right)\left|\Gamma\left(-\frac{i\Omega}{a}\right)\right|^2 = \frac{1}{2\pi\omega a}\left[\exp\left(\frac{2\pi\Omega}{a}\right) - 1\right]^{-1}.$$

B Adiabatic approximation for Bogolyubov coefficients

In this Appendix we present a method for computing the Bogolyubov coefficients in the adiabatic approximation. This method has been widely used in calculations of particle production by classical fields. We shall use the notation of Chapter 6.

The mode function $v(\eta)$ for a mode $\chi_{\mathbf{k}}$ of a quantum field is a solution of Eq. (6.18),

$$v''(\eta) + \omega^2(\eta) v(\eta) = 0, \tag{B.1}$$

where for brevity we omitted the index k in v_k and ω_k. The adiabatic approximation can be applied to Eq. (B.1) if the effective frequency $\omega(\eta)$ is a slowly-changing function, i.e. when the adiabaticity condition (6.45) holds,

$$|\omega'(\eta)| \ll |\omega(\eta)|^2 . \tag{B.2}$$

We shall assume that the function $\omega(\eta)$ satisfies this condition. In that case, the mode function $v_1(\eta)$ describing the adiabatic vacuum at a time $\eta = \eta_1$ is approximately expressed by the WKB ansatz (6.44),

$$v_1(\eta) \approx \frac{1}{\sqrt{\omega(\eta)}} \exp\left[i \int_{\eta_1}^{\eta} \omega(\eta) d\eta \right] . \tag{B.3}$$

The problem at hand is to compute the Bogolyubov coefficients relating the adiabatic vacua defined at two different times $\eta = \eta_1$ and $\eta = \eta_2$.

First we shall try to use the WKB approximation (B.3). The adiabatic vacuum $|_{\eta_1} 0_{ad}\rangle$ at $\eta = \eta_1$ is described by the mode function $v_1(\eta)$ satisfying the conditions

$$v_1(\eta_1) = \frac{1}{\sqrt{\omega(\eta_1)}}, \qquad \left.\frac{dv_1}{d\eta}\right|_{\eta=\eta_1} = \left.\frac{1}{\sqrt{\omega}}\left(i\omega - \frac{1}{2}\frac{\omega'}{\omega} \right)\right|_{\eta=\eta_1} ,$$

and a similar set of conditions specifies the mode function $v_2(\eta)$ of the vacuum $|_{\eta_2} 0_{ad}\rangle$. However, the ansatz (B.3) exactly satisfies both conditions. Therefore both mode functions $v_1(\eta)$ and $v_2(\eta)$ are expressed by the same formula (B.3) within the accuracy of the WKB approximation. Since in fact $v_1(\eta) \neq v_2(\eta)$, we conclude that the WKB approximation is insufficiently precise to distinguish between the vacua $|_{\eta_1} 0_{ad}\rangle$ and $|_{\eta_2} 0_{ad}\rangle$. It can be also shown that the Bogolyubov coefficients relating the *instantaneous* vacua $|_{\eta_1} 0\rangle$ and $|_{\eta_2} 0\rangle$ cannot be correctly computed using Eq. (B.3).

A more accurate approximation is based on perturbation theory. We shall consider a simpler problem of computing the Bogolyubov coefficients between the instantaneous vacua $|_{\eta_1} 0\rangle$ and $|_{\eta_2} 0\rangle$. Essentially the same calculation can be applied also to adiabatic vacua.

As we have seen in Sec. 6.2.2, the instantaneous vacuum $|_\eta 0\rangle$ defined at an intermediate time $\eta > \eta_1$ is a squeezed state with respect to $|_{\eta_1} 0\rangle$. Let the functions $\alpha(\eta)$ and $\beta(\eta)$ be the "instantaneous Bogolyubov coefficients" relating the initial vacuum $|_{\eta_1} 0\rangle$ and the state $|_\eta 0\rangle$. These coefficients can be expressed through $v(\eta)$ using Eq. (6.30) where we need to replace $\omega_k \equiv \omega$, $v_{\mathbf{k}} \equiv v(\eta)$, and choose $u_{\mathbf{k}}(\eta)$ according to the conditions (6.40) for the mode function at time η. After some algebra we find

$$\alpha(\eta) = \frac{-v^{*\prime} + i\omega v^*}{2i\sqrt{\omega}}, \qquad \beta(\eta) = \frac{v^{*\prime} + i\omega v^*}{2i\sqrt{\omega}}.$$

It is convenient to introduce the function $\zeta(\eta)$ instead of $v(\eta)$ as follows,

$$\zeta(\eta) \equiv \frac{\beta^*(\eta)}{\alpha^*(\eta)} = -\frac{v'(\eta) - i\omega(\eta)v(\eta)}{v'(\eta) + i\omega(\eta)v(\eta)}.$$

The function $\zeta(\eta)$ satisfies the first-order equation

$$\frac{d\zeta}{d\eta} + 2i\omega\zeta = \left(1 - \zeta^2\right)\frac{\omega'}{2\omega} \tag{B.4}$$

which straightforwardly follows from Eq. (B.1). Since $v'(\eta_1) = i\omega(\eta_1)v(\eta_1)$, the initial condition is $\zeta(\eta_1) = 0$ and then it can be shown using Eqs. (B.2) and (B.4) that $\zeta(\eta)$ always remains small (of order ω'/ω^2). The advantage of introducing the variable ζ is that its smallness facilitates applying perturbation theory to Eq. (B.4). To a first approximation we may replace $1 - \zeta^2$ by 1 and obtain the equation

$$\frac{d\zeta_{(1)}}{d\eta} + 2i\omega\zeta_{(1)} = \frac{\omega'}{2\omega}, \quad \zeta_{(1)}\big|_{\eta=\eta_1} = 0,$$

which can be solved in the form of an integral

$$\zeta_{(1)}(\eta) = \int_{\eta_1}^{\eta} d\eta' \frac{1}{2\omega(\eta')}\frac{d\omega(\eta')}{d\eta'} \exp\left[-2i\int_{\eta'}^{\eta}\omega(\eta'')d\eta''\right].$$

Further approximations are computed similarly, for example $\zeta_{(2)}(\eta)$ is the solution of

$$\frac{d\zeta_{(2)}}{d\eta} + 2i\omega\zeta_{(2)} = \left(1 - \zeta_{(1)}^2\right)\frac{\omega'}{2\omega}, \quad \zeta_{(2)}\big|_{\eta=\eta_1} = 0.$$

The first approximation, $\zeta_{(1)}(\eta)$, is usually sufficiently precise in the adiabatic regime.

Using Eq. (6.25), the Bogolyubov coefficients are expressed through $\zeta(\eta)$ as

$$\beta(\eta) = \frac{\zeta^*(\eta)}{\sqrt{1 - |\zeta(\eta)|^2}}, \quad \alpha(\eta) = \frac{1}{\sqrt{1 - |\zeta(\eta)|^2}}.$$

This is the result of using the method of adiabatic approximation.

C Mode expansions cheat sheet

We present a list of formulae relevant to mode expansions of free, real scalar fields. This should help resolve any confusion about the signs $\mathbf{k}$ and $-\mathbf{k}$ or similar technicalities.

All equations (except commutation relations) hold for operators as well as for classical quantities. The formulae for a field quantized in a box are obtained by replacing the factors $(2\pi)^3$ in the denominators with the volume V of the box. (Note that this replacement changes the physical dimension of the modes $\phi_{\mathbf{k}}$.)

$$\phi(\mathbf{x},t) = \int \frac{d^3\mathbf{k}\, e^{i\mathbf{k}\cdot\mathbf{x}}}{(2\pi)^{3/2}}\phi_{\mathbf{k}}(t); \quad \phi_{\mathbf{k}}(t) = \int \frac{d^3\mathbf{x}\, e^{-i\mathbf{k}\cdot\mathbf{x}}}{(2\pi)^{3/2}}\phi(\mathbf{x},t)$$

$$a^-_{\mathbf{k}}(t) = \sqrt{\frac{\omega_k}{2}}[\phi_{\mathbf{k}} + \frac{i}{\omega_k}\pi_{\mathbf{k}}]; \quad a^+_{\mathbf{k}}(t) = \sqrt{\frac{\omega_k}{2}}[\phi_{-\mathbf{k}} - \frac{i}{\omega_k}\pi_{-\mathbf{k}}]$$

$$\phi_{\mathbf{k}}(t) = \frac{a^-_{\mathbf{k}}(t) + a^+_{-\mathbf{k}}(t)}{\sqrt{2\omega_k}}; \quad \pi_{\mathbf{k}}(t) = \sqrt{\frac{\omega_k}{2}}\frac{a^-_{\mathbf{k}}(t) - a^+_{-\mathbf{k}}(t)}{i}$$

Time-independent creation and annihilation operators $\hat{a}^{\pm}_{\mathbf{k}}$ are defined by

$$\hat{a}^{\pm}_{\mathbf{k}}(t) \equiv \hat{a}^{\pm}_{\mathbf{k}} \exp(\pm i\omega_k t)$$

Note that all $a^{\pm}_{\mathbf{k}}$ below are time-independent.

$$\phi^\dagger(x) = \phi(x); \quad (\phi_{\mathbf{k}})^\dagger = \phi_{-\mathbf{k}}; \quad \left(a^-_{\mathbf{k}}\right)^\dagger = a^+_{\mathbf{k}}$$

$$\pi(\mathbf{x},t) = \frac{d}{dt}\phi(\mathbf{x},t); \quad \pi_{\mathbf{k}}(t) = \frac{d}{dt}\phi_{\mathbf{k}}(t)$$

$$\left[\hat{\phi}(\mathbf{x},t),\, \hat{\pi}(\mathbf{x}',t)\right] = i\delta(\mathbf{x}-\mathbf{x}')$$
$$\left[\hat{\phi}_{\mathbf{k}}(t),\, \hat{\pi}_{\mathbf{k}'}(t)\right] = i\delta(\mathbf{k}+\mathbf{k}')$$
$$\left[\hat{a}^-_{\mathbf{k}},\, \hat{a}^+_{\mathbf{k}'}\right] = \delta(\mathbf{k}-\mathbf{k}')$$

$$\hat{\phi}(\mathbf{x},t) = \int \frac{d^3\mathbf{k}}{(2\pi)^{3/2}}\frac{1}{\sqrt{2\omega_k}}\left[\hat{a}^-_{\mathbf{k}} e^{-i\omega_k t + i\mathbf{k}\cdot\mathbf{x}} + \hat{a}^+_{\mathbf{k}} e^{i\omega_k t - i\mathbf{k}\cdot\mathbf{x}}\right]$$

Mode expansions may use anisotropic mode functions $v_{\mathbf{k}}(t)$. Isotropic mode expansions use scalar k instead of vector $\mathbf{k}$ because $v_{\mathbf{k}} \equiv v_k$ for all $|\mathbf{k}| = k$.

$$\hat{\phi}(\mathbf{x},t) = \int \frac{d^3\mathbf{k}}{(2\pi)^{3/2}}\frac{1}{\sqrt{2}}\left[\hat{a}^-_{\mathbf{k}} v^*_{\mathbf{k}}(t) e^{i\mathbf{k}\cdot\mathbf{x}} + \hat{a}^+_{\mathbf{k}} v_{\mathbf{k}}(t) e^{-i\mathbf{k}\cdot\mathbf{x}}\right]$$

(Note: the factor $\sqrt{2}$ and the choice of $v^*_{\mathbf{k}}$ instead of $v_{\mathbf{k}}$ are for consistency with literature. This could have been chosen differently.)

$$v_{-\mathbf{k}} = v_{\mathbf{k}} \neq v^*_{\mathbf{k}}; \quad \ddot{v}_{\mathbf{k}} + \omega_k^2(t) v_{\mathbf{k}} = 0; \quad \dot{v}_{\mathbf{k}} v^*_{\mathbf{k}} - v_{\mathbf{k}} \dot{v}^*_{\mathbf{k}} = 2i$$

$$\phi_{\mathbf{k}}(t) = \frac{1}{\sqrt{2}} \left[a^-_{\mathbf{k}} v^*_{\mathbf{k}}(t) + a^+_{-\mathbf{k}} v_{\mathbf{k}}(t) \right]; \quad \pi_{\mathbf{k}}(t) = \frac{1}{\sqrt{2}} \left[a^-_{\mathbf{k}} \dot{v}^*_{\mathbf{k}}(t) + a^+_{-\mathbf{k}} \dot{v}_{\mathbf{k}}(t) \right]$$

Here the $a^\pm_{\mathbf{k}}$ are time-independent although $v_{\mathbf{k}}$ and $\phi_{\mathbf{k}}$, $\pi_{\mathbf{k}}$ depend on time:

$$a^-_{\mathbf{k}} = \frac{1}{i\sqrt{2}} \left[\dot{v}_{\mathbf{k}}(t) \phi_{\mathbf{k}}(t) - v_{\mathbf{k}}(t) \pi_{\mathbf{k}}(t) \right]; \quad a^+_{\mathbf{k}} = \frac{i}{\sqrt{2}} \left[\dot{v}^*_{\mathbf{k}}(t) \phi_{-\mathbf{k}}(t) - v^*_{\mathbf{k}}(t) \pi_{-\mathbf{k}}(t) \right]$$

Free scalar field mode functions in the flat space:

$$v_k(t) = \frac{1}{\sqrt{\omega_k}} e^{i\omega_k t}.$$

Bogolyubov transformations

Note: $\hat{a}^\pm_{\mathbf{k}}$ are defined by $v_{\mathbf{k}}(\eta)$ and $\hat{b}^\pm_{\mathbf{k}}$ are defined by $u_{\mathbf{k}}(\eta)$.

$$v^*_{\mathbf{k}}(\eta) = \alpha_{\mathbf{k}} u^*_{\mathbf{k}}(\eta) + \beta_{\mathbf{k}} u_{\mathbf{k}}(\eta); \quad |\alpha_{\mathbf{k}}|^2 - |\beta_{\mathbf{k}}|^2 = 1$$

$$\hat{b}^-_{\mathbf{k}} = \alpha_{\mathbf{k}} \hat{a}^-_{\mathbf{k}} + \beta^*_{\mathbf{k}} \hat{a}^+_{-\mathbf{k}}, \quad \hat{b}^+_{\mathbf{k}} = \alpha^*_{\mathbf{k}} \hat{a}^+_{\mathbf{k}} + \beta_{\mathbf{k}} \hat{a}^-_{-\mathbf{k}}$$

$$\alpha_{\mathbf{k}} = \alpha_{-\mathbf{k}}, \quad \beta_{\mathbf{k}} = \beta_{-\mathbf{k}}$$

$$\hat{a}^-_{\mathbf{k}} = \alpha^*_{\mathbf{k}} \hat{b}^-_{\mathbf{k}} - \beta^*_{\mathbf{k}} \hat{b}^+_{-\mathbf{k}}, \quad \hat{a}^+_{\mathbf{k}} = \alpha_{\mathbf{k}} \hat{b}^+_{\mathbf{k}} - \beta_{\mathbf{k}} \hat{b}^-_{-\mathbf{k}}$$

D Solutions to exercises

Chapter 1

Exercise 1.1 (p. 6)

Given $\phi(x)$, the mode $\phi_{\mathbf{k}}$ is

$$\phi_{\mathbf{k}} = \int \frac{d^3\mathbf{x}}{(2\pi)^{3/2}} e^{-i\mathbf{k}\cdot\mathbf{x}} \phi(\mathbf{x}).$$

Substituting into Eq. (1.9), we get

$$I = \int \frac{d^3\mathbf{x} d^3\mathbf{y} d^3\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot(\mathbf{y}-\mathbf{x})} \phi(\mathbf{x}) \phi(\mathbf{y}) \sqrt{k^2+m^2}.$$

Therefore

$$K(\mathbf{x},\mathbf{y}) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot(\mathbf{y}-\mathbf{x})} \sqrt{k^2+m^2}.$$

This integral does not converge and should be understood in the distributional sense (see Appendix A.1). Compare

$$\int \frac{d^3\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{x}} = \delta(\mathbf{x}); \quad \int \frac{d^3\mathbf{k}}{(2\pi)^3} \mathbf{k} e^{i\mathbf{k}\cdot\mathbf{x}} = -i\nabla\delta(\mathbf{x}).$$

Exercise 1.2 (p. 7)

We substitute the Fourier transform of $\phi(\mathbf{x})$ into the integral over the cube-shaped region,

$$\phi_L = \frac{1}{L^3}\int_{L^3} \phi(\mathbf{x})\, d^3\mathbf{x} = \frac{1}{L^3}\int_{L^3} d^3\mathbf{x} \int \frac{d^3\mathbf{k}}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot\mathbf{x}} \phi_{\mathbf{k}}.$$

The integral over $d^3\mathbf{x}$ can be performed explicitly using the formula

$$\int_{-L/2}^{L/2} dx\, e^{ik_x x} = \frac{2}{k_x L} \sin\frac{k_x L}{2} \equiv f(k_x).$$

Then the expectation value of ϕ_L^2 is

$$\left\langle \phi_L^2 \right\rangle = \int \frac{d^3\mathbf{k} d^3\mathbf{k}'}{(2\pi)^3} \left\langle \phi_{\mathbf{k}} \phi_{\mathbf{k}'} \right\rangle f(k_x) f(k_y) f(k_z) f(k_x') f\left(k_y'\right) f(k_z'). \tag{D.1}$$

If $\delta\phi_{\mathbf{k}}$ is the given typical amplitude of fluctuations in the mode $\phi_{\mathbf{k}}$, then the expectation value of $\langle\phi_{\mathbf{k}}\phi_{\mathbf{k}'}\rangle$ in the vacuum state is

$$\langle\phi_{\mathbf{k}}\phi_{\mathbf{k}'}\rangle = (\delta\phi_{\mathbf{k}})^2\,\delta(\mathbf{k}+\mathbf{k}')\,.$$

So the integral over $\mathbf{k}, \mathbf{k}'$ in Eq. (D.1) reduces to a single integral over $\mathbf{k}$,

$$\langle\phi_L^2\rangle = \int \frac{d^3\mathbf{k}}{(2\pi)^3}\,(\delta\phi_{\mathbf{k}})^2\,[f(k_x)\,f(k_y)\,f(k_z)]^2\,. \tag{D.2}$$

The function $f(k)$ is of order 1 for $|kL| \lesssim 1$ but very small for $|kL| \gg 1$. Therefore the integration in Eq. (D.2) selects the vector values $\mathbf{k}$ of magnitude $|\mathbf{k}| \lesssim L^{-1}$ in all directions. As a qualitative estimate, we may take $\delta\phi_{\mathbf{k}}$ to be constant throughout the effective region of integration in $\mathbf{k}$ and obtain

$$\langle\phi_L^2\rangle \sim \int_{|\mathbf{k}|<L^{-1}} d^3\mathbf{k}\,(\delta\phi_{\mathbf{k}})^2 \sim k^3\,(\delta\phi_{\mathbf{k}})^2\Big|_{k=L^{-1}}\,.$$

Exercise 1.3 (p. 10)

The problem is similar to the Schrödinger equation with a step-like potential barrier between two free regions. The general solution in the tunneling region $0 < t < T$ is

$$q(t) = A\cosh\Omega_0 t + B\sinh\Omega_0 t. \tag{D.3}$$

The matching condition at $t = 0$ selects $A = 0$ and $B = q_1\omega_0/\Omega_0$. The general solution in the region $t > T$ is

$$q(t) = q_2\sin[\omega_0(t-T)+\alpha]\,.$$

The constant q_2 is determined by the matching conditions at $t = T$. The values $q(T)$, $\dot{q}(T)$ must match $q_2\sin\alpha$ and $q_2\omega_0\cos\alpha$. Therefore we can find q_2 from

$$q_2^2 = [q(T)]^2 + \left[\frac{\dot{q}(T)}{\omega_0}\right]^2.$$

Substituting the values from Eq. (D.3), we find

$$q_2^2 = q_1^2\left[1 + \left(1+\frac{\omega_0^2}{\Omega_0^2}\right)\sinh^2\Omega_0 T\right]. \tag{D.4}$$

For $\Omega_0 T \gg 1$ we can approximate this exact answer by

$$q_2 \approx q_1\frac{\exp(\Omega_0 T)}{2}\sqrt{1+\frac{\omega_0^2}{\Omega_0^2}}.$$

Exercise 1.4 (p. 10)

The "number of particles" is formally estimated using the energy of the oscillator. A state with an amplitude q_0 has energy $E = \frac{1}{2}\left(\dot{q}^2 + \omega_0^2 q^2\right) = \frac{1}{2} q_0^2 \omega_0^2$. Therefore the number of particles is related to the amplitude by

$$n = \frac{q_0^2 \omega_0 - 1}{2}. \tag{D.5}$$

If the oscillator was initially in the ground state, then $q_1 = \omega_0^{-1/2}$ and Eq. (D.4) gives

$$n = \frac{1}{2}\left(1 + \frac{\omega_0^2}{\Omega_0^2}\right) \sinh^2 \Omega_0 T.$$

There are no produced particles if $T = 0$; the number of particles is exponentially large in $\Omega_0 T$.

Exercise 1.5 (p. 11)

To find the strongest currently available electric field, one can perform an Internet search for descriptions of Schwinger effect experiments. The electric field of strongest lasers available in 2003 was $\sim 10^{11}\mathrm{V/m}$. There is a proposed X-ray laser experiment where the radiation is focused, yielding peak fields of order 10^{17}–$10^{18}\mathrm{V/m}$. (See A. Ringwald, Phys. Lett. **B510** (2001), p. 107; also `arxiv.org/abs/hep-ph/0103185` on the Web.)

Rewriting Eq. (1.13) in the SI units, we get

$$P = \exp\left(-\frac{m_e c^3}{\hbar e E}\right).$$

The result for the electric field of a laser, $E = 10^{11}\mathrm{V/m}$, is

$$P \approx \exp\left(-\frac{\left(9.11 \cdot 10^{-31}\right)^2 \left(3.00 \cdot 10^8\right)^3}{\left(1.05 \cdot 10^{-34}\right)\left(1.60 \cdot 10^{-19}\right)\left(10^{11}\right)}\right) \sim e^{-10^7}.$$

Thus, even a strong laser field gives no measurable particle production. For the proposed focusing experiment, P is between 10^{-11} and 10^{-2}, and some electrons could be observed.

Exercise 1.6 (p. 12)

We need to express all quantities in the SI units. The equation $T = a/(2\pi)$ becomes

$$kT = \frac{\hbar}{c}\frac{a}{2\pi}.$$

Here $k \approx 1.38 \cdot 10^{-23}\mathrm{J/K}$ is Boltzmann's constant. The boiling point of water is $T = 373\mathrm{K}$. The required acceleration is $a \sim 10^{22}\mathrm{m/s^2}$ which is clearly beyond any practical possibility.

Chapter 2

Exercise 2.1 (p. 14)

We choose the general solution of Eq. (2.7) as

$$q(t) = A\cos\omega\left(t-t_1\right) + B\sin\omega\left(t-t_1\right).$$

The initial condition at $t = t_1$ gives $A = q_1$. The final condition at $t = t_2$ gives

$$B = \frac{q_2 - q_1\cos\omega\left(t_2-t_1\right)}{\sin\omega\left(t_2-t_1\right)}.$$

The classical trajectory exists and is unique if $\sin\omega\left(t_2-t_1\right) \neq 0$. Otherwise we need to consider two possibilities: either $q_1 = q_2$ or not. If $q_1 \neq q_2$, the value of B is formally infinite; this indicates that the action does not have a minimum (there is no classical trajectory). If $q_1 = q_2$, the value of B remains undetermined (there are infinitely many classical trajectories).

Exercise 2.2 (p. 17)

The first functional derivative is

$$\frac{\delta S}{\delta q\left(t_1\right)} = \frac{\partial L}{\partial q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}}\bigg|_{q(t_1)} = -\left[\ddot{q}\left(t_1\right) + \omega^2 q\left(t_1\right)\right]. \tag{D.6}$$

As expected, it vanishes on-shell. To evaluate the second functional derivative, we need to rewrite Eq. (D.6) as an integral of some function over time, e.g.

$$\ddot{q}\left(t_1\right) + \omega^2 q\left(t_1\right) = \int \left[\ddot{q}(t) + \omega^2 q(t)\right]\delta\left(t-t_1\right)dt. \tag{D.7}$$

For an expression of the form $\int q(t)f(t)dt$, the functional derivative with respect to $q\left(t_2\right)$ is $f\left(t_2\right)$. We can rewrite Eq. (D.7) in this form:

$$\ddot{q}\left(t_1\right) + \omega^2 q\left(t_1\right) = \int \left[\delta''\left(t-t_1\right) + \omega^2\delta\left(t-t_1\right)\right]q(t)dt.$$

Therefore

$$\frac{\delta^2 S}{\delta q\left(t_1\right)\delta q\left(t_2\right)} = -\delta''\left(t_2-t_1\right) - \omega^2\delta\left(t_2-t_1\right).$$

Exercise 2.3 (p. 20)

a) The Hamilton action functional

$$S\left[q(t),p(t)\right] = \int \left[p\dot{q} - H(p,q)\right]dt$$

is extremized when

$$\frac{\delta S}{\delta q(t)} = 0, \quad \frac{\delta S}{\delta p(t)} = 0.$$

Computing the functional derivatives, we obtain the Hamilton equations [Eq. (2.19)].

When computing $\delta S/\delta p(t)$ we did not have to integrate by parts because S does not depend on $\dot{p}$. Therefore the variation $\delta p(t)$ is not constrained. However, to compute $\delta S/\delta q(t)$ we need to integrate by parts and we obtain a boundary term

$$p(t)\delta q(t)|_{t_1}^{t_2},$$

which must vanish. Therefore the appropriate extremization problem is to specify either $q(t_1)$ and $q(t_2)$ without restricting $p(t)$, or to specify $p(t_1) = 0$ and fix $q(t_2)$, or vice versa.

b) A simple calculation using Eq. (2.19) gives

$$\frac{dH}{dt} = \frac{\partial H}{\partial q}\dot{q} + \frac{\partial H}{\partial p}\dot{p} = 0.$$

c) The Hamiltonian H is defined as $p\dot{q} - L$ where $\dot{q}$ is replaced by a function of p that follows from Eq. (2.13). This equation is equivalent to the first of the Hamilton equations (2.19). Therefore the function $p\dot{q} - H$ is equal to L on the classical paths.

Exercise 2.4 (p. 21)

We use the identity

$$[A, BC] = B[A, C] + [A, B]C. \tag{D.8}$$

Compute first the commutator

$$\left[\hat{q}, \hat{p}^2\right] = [\hat{q}, \hat{p}]\,\hat{p} + \hat{p}\,[\hat{q}, \hat{p}] = 2i\hbar\hat{p}.$$

Then we obtain

$$\hat{q}\hat{p}^2\hat{q} - \hat{p}^2\hat{q}^2 = \left[\hat{q}, \hat{p}^2\right]\hat{q} = 2i\hbar\hat{p}\hat{q}.$$

Exercise 2.5 (p. 21)

a) See the solution for Exercise 2.4. First we find that

$$[\hat{q}, \hat{p}^n] = i\hbar\hat{p}^{n-1} + \hat{p}\left[\hat{q}, \hat{p}^{n-1}\right].$$

Then we use induction to prove that

$$[\hat{q}, \hat{p}^n] = i\hbar n\hat{p}^{n-1}$$

for $n = 1, 2, ...$ The statement of the problem follows since $[\hat{q}, \hat{q}^m] = 0$.

The analogous relation with $\hat{p}$ is obtained automatically if we switch $\hat{q} \leftrightarrow \hat{p}$ and change the sign of the commutator ($i\hbar$ to $-i\hbar$).

b) We can generalize the result of part a) to terms of the form $\hat{q}^a\hat{p}^b\hat{q}^c$ by using Eq. (D.8),

$$\left[\hat{q}, \hat{q}^a\hat{p}^b\hat{q}^c\right] = i\hbar b\hat{q}^a\hat{p}^{b-1}\hat{q}^c \equiv i\hbar\frac{\partial}{\partial p}\hat{q}^a\hat{p}^b\hat{q}^c. \tag{D.9}$$

Here we imply that the derivative $\partial/\partial p$ should act only on $\hat{p}$ where it appears in the expression; the operator ordering should remain unchanged. To prove Eq. (D.9), it is enough to demonstrate that for any two terms $f(\hat{p},\hat{q})$ and $g(\hat{p},\hat{q})$ of this form that already satisfy Eq. (2.27), the product fg also satisfies this equation.

An analytic function $f(p,q)$ is expanded into a sum of terms of the form $...\hat{q}^a\hat{p}^b\hat{q}^c\hat{p}^d...$ and the relation of Eq. (D.9) can be generalized to terms of this form. Each term of the expansion of $f(\hat{p},\hat{q})$ satisfies the relation; therefore the sum will also satisfy the relation.

Exercise 2.6 (p. 22)

Note that $\hat{q}$ does not commute with $d\hat{q}/dt$ (coordinates cannot be measured together with velocities). So the time derivative of e.g. $\hat{q}^3$ must be written as

$$\frac{d}{dt}\hat{q}^3 = \hat{q}^2\dot{\hat{q}} + \hat{q}\dot{\hat{q}}\hat{q} + \dot{\hat{q}}\hat{q}^2.$$

It is easy to show that for any operators $\hat{A}$, $\hat{B}$, $\hat{H}$ (not necessarily Hermitian) that satisfy

$$\frac{\partial}{\partial t}\hat{A} = [\hat{A},\hat{H}], \quad \frac{\partial}{\partial t}\hat{B} = [\hat{B},\hat{H}],$$

it follows that

$$\frac{\partial}{\partial t}(\hat{A}+\hat{B}) = [\hat{A}+\hat{B},\hat{H}]; \quad \frac{\partial}{\partial t}(\hat{A}\hat{B}) = \frac{\partial\hat{A}}{\partial t}\hat{B} + \hat{A}\frac{\partial\hat{B}}{\partial t} = [\hat{A}\hat{B},\hat{H}].$$

By induction, starting from $\hat{p}$ and $\hat{q}$, we prove the same property for arbitrary terms of the form $...\hat{q}^a\hat{p}^b\hat{q}^c\hat{p}^d...$ and their linear combinations. Any observable $A(p,q)$ that can be approximated by such polynomial terms will satisfy the same equation [Eq. (2.28)].

Exercise 2.7 (p. 30)

We insert the decomposition of unity, $\int |q\rangle\langle q|\,dq$, into the normalization condition $\langle p_1|p_2\rangle = \delta(p_1-p_2)$ and obtain

$$\delta(p_1-p_2) = \int \langle p_1|q\rangle\langle q|p_2\rangle\,dq. \tag{D.10}$$

Since from our earlier calculations we know that

$$\langle p|q\rangle = C\exp\left(\frac{ipq}{\hbar}\right),$$

we now substitute this into Eq. (D.10) and find the condition for C,

$$\begin{aligned}\delta\left(p_1-p_2\right) &= |C|^2 \int_{-\infty}^{+\infty} dq\, \exp\left[\frac{i\left(p_1-p_2\right)q}{\hbar}\right] \\ &= 2\pi\hbar\,|C|^2\,\delta\left(p_1-p_2\right).\end{aligned}$$

From this we obtain $|C| = (2\pi\hbar)^{-1/2}$. Note that C is defined up to an irrelevant phase factor.

Chapter 3

Exercise 3.1 (p. 34)

The differential equation

$$\frac{dy}{dx} = f(x)y + g(x)$$

with the initial condition $y\left(x_0\right) = y_0$ has the following solution,

$$y(x) = y_0 \exp\left(\int_{x_0}^{x} f(x')dx'\right) + \int_{x_0}^{x} dx' g(x') \exp\left(\int_{x'}^{x} f(x'')dx''\right).$$

The solution for the driven harmonic oscillator is a special case of this formula with $f(x) = -i\omega$ and $g(x) = J$.

Exercise 3.2 (p. 34)

The result follows by simple algebra.

More generally, if $\hat{A}(t)$ and $\hat{B}(t)$ are operators satisfying the equation

$$\frac{d}{dt}\hat{A} = [\hat{A}, \hat{B}]$$

and $\hat{A}\left(t_0\right)$ is a c-number, i.e. $\hat{A}\left(t_0\right) = A_0\hat{1}$, then $\hat{A}(t) = A_0\hat{1}$ for all other t. [This follows because all derivatives $d^n\hat{A}/dt^n$, $n \geq 1$, vanish at $t = t_0$.] Therefore it is enough to compute the commutator $[\hat{a}^-(t), \hat{a}^+(t)]$ at one value of t.

Exercise 3.3 (p. 37)

Compute the matrix element

$$0 = \langle n_{out}|\,\hat{a}^-_{in}\,|0_{in}\rangle = \langle n_{out}|\,\hat{a}^-_{in}\left(\sum_{k=0}^{\infty}\Lambda_k\,|k_{out}\rangle\right);$$

since $\hat{a}^-_{in} = \hat{a}^-_{out} - C$ and $\hat{a}^-_{out}\,|k_{out}\rangle = \sqrt{k}\,|k-1_{out}\rangle$, we obtain

$$0 = -C\Lambda_n + \sqrt{n+1}\Lambda_{n+1}.$$

Exercise 3.4 (p. 40)

(a) Expanding $\hat{q}(t_1)$ for $t_1 \geq T$ in the "in" creation and annihilation operators $\hat{a}^{\pm}_{in}$, we find

$$\hat{q}(t_1) = \frac{1}{\sqrt{2\omega}} \left(\hat{a}^{-}_{in} e^{-i\omega t_1} + \hat{a}^{-}_{in} e^{-i\omega t_1} + 2Re\left(J_0 e^{-i\omega t_1} \right) \right)$$

and then we obtain

$$\langle 0_{in}| \hat{q}(t_1) \hat{q}(t_2) |0_{in}\rangle = \frac{1}{2\omega} e^{i\omega(t_2 - t_1)} + \frac{2}{\omega} Re\left(J_0 e^{-i\omega t_1} \right) Re\left(J_0 e^{-i\omega t_2} \right).$$

The first term is the expectation value without the external force. The second term can be written as a double integral of $J(t)$ as required, since

$$J_0 = \frac{i}{\sqrt{2\omega}} \int_0^T e^{i\omega t} J(t) dt.$$

(b) To compute this matrix element, we expand $\hat{q}(t_1)$ in the "out" operators $\hat{a}^{\pm}_{out}$ and $\hat{q}(t_2)$ in the "in" operators. Then we need to compute the following matrix elements:

$$\langle 0_{out}| \hat{a}^{-}_{out} |0_{in}\rangle = J_0 \langle 0_{out}|0_{in}\rangle,$$
$$\langle 0_{out}| \hat{a}^{-}_{out} \hat{a}^{+}_{in} |0_{in}\rangle = \left(1 - |J_0|^2\right) \langle 0_{out}|0_{in}\rangle.$$

The final result is

$$\frac{\langle 0_{out}| \hat{q}(t_1) \hat{q}(t_2) |0_{in}\rangle}{\langle 0_{out}|0_{in}\rangle} = \frac{1}{2\omega} e^{i\omega(t_2 - t_1)} + \frac{1}{2\omega} J_0^2 e^{-i\omega(t_1 + t_2)}.$$

Again, the last term

$$\frac{1}{2\omega} J_0^2 e^{-i\omega(t_1 + t_2)}$$

is rewritten as a double integral as required.

Chapter 4

Exercise 4.1 (p. 41)

From linear algebra it is known that a positive-definite symmetric matrix M_{ij} can be diagonalized using an orthogonal basis v^i_α with positive eigenvalues ω^2_α, $\alpha = 1, ..., N$. In other words, there exists a nondegenerate matrix $v_{i\alpha}$ such that

$$\sum_i M_{ij} v_{i\alpha} = \omega_\alpha v_{j\alpha}, \quad \sum_i v_{i\alpha} v_{i\beta} = \delta_{\alpha\beta}.$$

Here we do not use the Einstein summation convention but write all sums explicitly.

Transforming q_i into a new set of variables $\tilde{q}_\alpha$ by

$$q_i \equiv \sum_\alpha v_{i\alpha} \tilde{q}_\alpha,$$

we find that the quadratic form in the action becomes

$$\sum_{ij} q_i M_{ij} q_j = \sum_{\alpha\beta ij} \tilde{q}_\alpha v_{i\alpha} M_{ij} v_{j\beta} \tilde{q}_\beta = \sum_{\alpha\beta} \omega_\beta \delta_{\alpha\beta} \tilde{q}_\alpha \tilde{q}_\beta = \sum_\alpha \omega_\alpha \tilde{q}_\alpha^2.$$

This provides the required diagonalized form of the action.

Exercise 4.2 (p. 43)

We compute the action of the transformed field $\tilde{\phi}(x)$ after a Lorentz transformation with a matrix Λ^μ_ν. Since the determinant of Λ is equal to 1, we may change the variables of integration d^4x to the transformed variables $d^4\tilde{x}$ and the Jacobian is 1. The action [Eq. (4.4)] has two terms, one with ϕ^2 and the other with derivatives of ϕ. The field values $\phi(\mathbf{x})$ do not change, therefore the integral over $d^4\tilde{x}$ of $\tilde{\phi}^2$ is the same as the integral in the old coordinates. But the field derivatives $\partial_\mu \phi$ change,

$$\partial_\mu \phi \to \Lambda^\nu_\mu \partial_\nu \phi.$$

The action contains the scalar term $m^2\phi^2$ that does not change, and also the term

$$\eta^{\mu\nu} (\partial_\mu \phi) (\partial_\nu \phi)$$

that transforms according to the Lorentz transformation of the field derivatives,

$$\eta^{\mu\nu} (\partial_\mu \phi) (\partial_\nu \phi) \to \eta^{\mu\nu} \Lambda^{\mu'}_\mu (\partial_{\mu'} \phi) \Lambda^{\nu'}_\nu (\partial_{\nu'} \phi).$$

But the Lorentz transformation leaves the metric unchanged [see Eq. (4.6)]. Therefore this term in the action is unchanged as well. We obtain the invariance of the action under Lorentz transformations.

Exercise 4.3 (p. 43)

Solution with explicit variation. From the action of Eq. (4.4) we obtain the variation δS with respect to a small change $\delta\phi(x)$ of the field, assuming that $\delta\phi$ vanishes at spatial and temporal infinities:

$$\begin{aligned} \delta S &= \int d^4x \left[\eta^{\mu\nu} (\partial_\mu \phi) (\partial_\nu \delta\phi) - m^2 \phi \delta\phi\right] \\ &= \int d^4x \left[-\eta^{\mu\nu} (\partial_\nu \partial_\mu \phi) - m^2 \phi\right] \delta\phi \end{aligned}$$

(the second line follows by Gauss's theorem). The expression in square brackets must vanish for the action to be extremized, so the equation of motion is

$$-\eta^{\mu\nu} (\partial_\nu \partial_\mu \phi) - m^2 \phi = -\ddot{\phi} + \Delta\phi - m^2 \phi = 0.$$

Solution with functional derivatives. The equation of motion is $\delta S/\delta\phi = 0$. To compute the functional derivative, we rewrite the action in an explicit integral form with some function $M(x,y)$,

$$S[\phi] = \frac{1}{2}\int d^4x d^4y \phi(x)\phi(y)M(x,y). \tag{D.11}$$

(The factor $1/2$ is for convenience.) Integrating by parts, we find

$$M(x,y) = -m^2\delta(x-y) + \eta^{\mu\nu}\frac{\partial}{\partial x^\mu}\frac{\partial}{\partial y^\nu}\delta(x-y). \tag{D.12}$$

The functional derivative of the action (D.11) is

$$\frac{\delta S}{\delta\phi(x)} = \int d^4y \phi(y)M(x,y).$$

Substituting M from Eq. (D.12), we find

$$\frac{\delta S}{\delta\phi(x)} = -m^2\phi(x) - \eta^{\mu\nu}\frac{\partial^2}{\partial x^\mu \partial x^\nu}\phi(x)$$

as required.

Exercise 4.4 (p. 44)

If $\phi(\mathbf{x})$ is a real function, then

$$(\phi_{\mathbf{k}})^* = \int \frac{d^3\mathbf{x}}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot\mathbf{x}}\phi(\mathbf{x}) = \phi_{-\mathbf{k}}.$$

Exercise 4.5 (p. 46)

We use the relations

$$\hat{\phi}_{\mathbf{k}} = \frac{1}{\sqrt{2\omega_k}}\left(\hat{a}^-_{\mathbf{k}}e^{-i\omega_k t} + \hat{a}^+_{-\mathbf{k}}e^{i\omega_k t}\right),\ \hat{\pi}_{\mathbf{k}} = i\sqrt{\frac{\omega_k}{2}}\left(\hat{a}^+_{-\mathbf{k}}e^{i\omega_k t} - \hat{a}^-_{\mathbf{k}}e^{-i\omega_k t}\right).$$

(Here $\hat{a}^\pm_{\mathbf{k}}$ are time-independent operators.) Then we find

$$\frac{1}{2}\left(\hat{\pi}_{\mathbf{k}}\hat{\pi}_{-\mathbf{k}} + \omega_k^2\hat{\phi}_{\mathbf{k}}\hat{\phi}_{-\mathbf{k}}\right) = \frac{\omega_k}{2}\left(\hat{a}^-_{\mathbf{k}}\hat{a}^+_{\mathbf{k}} + \hat{a}^+_{-\mathbf{k}}\hat{a}^-_{-\mathbf{k}}\right).$$

When we integrate over all $\mathbf{k}$, the terms with $-\mathbf{k}$ give the same result as the terms with $\mathbf{k}$. Therefore

$$\hat{H} = \int d^3\mathbf{k}\frac{\omega_k}{2}\left(\hat{a}^+_{\mathbf{k}}\hat{a}^-_{\mathbf{k}} + \hat{a}^-_{\mathbf{k}}\hat{a}^+_{\mathbf{k}}\right).$$

Chapter 5

Exercise 5.1 (p. 59)

The computation is split into three parts: (1) the variation of the determinant $\sqrt{-g}$ with respect to $g^{\alpha\beta}$; (2) the variation of the action with respect to $\Gamma^{\lambda}_{\rho\sigma}$; (3) the variation of the action with respect to $g^{\alpha\beta}$.

1. To find the variation of the determinant $\sqrt{-g}$, we need to compute the derivative of $g \equiv \det g_{\alpha\beta}$ with respect to a parameter. We can use the matrix identity (for finite-dimensional matrices A)

$$\det A = \exp\left(\mathrm{Tr}\ln A\right).$$

Choosing $A \equiv A(s)$ as a matrix that depends on some parameter s, we get

$$\frac{d}{ds}\det A = \frac{d}{ds}\exp\left(\mathrm{Tr}\ln A\right) = (\det A)\mathrm{Tr}\left(A^{-1}\frac{dA}{ds}\right).$$

Here A^{-1} is the inverse matrix. We now set $A \equiv g_{\mu\nu}$ (the covariant metric tensor in some basis) and $s \equiv g_{\alpha\beta}$ with *fixed* α and β. Then

$$\frac{\partial g}{\partial s} \equiv \frac{\partial g}{\partial g_{\alpha\beta}} = g\, g^{\mu\nu}\frac{\partial g_{\mu\nu}}{\partial g_{\alpha\beta}} = g\, g^{\mu\nu}\delta^{\alpha}_{\mu}\delta^{\beta}_{\nu} = g\, g^{\alpha\beta}.$$

The derivative with respect to components of the inverse matrix $g^{\mu\nu}$ is computed quickly if we recall that the determinant of $g^{\mu\nu}$ is g^{-1}:

$$\frac{\partial g}{\partial g^{\alpha\beta}} = -g\, g_{\alpha\beta}; \quad \frac{\partial\sqrt{-g}}{\partial g^{\alpha\beta}} = -\frac{1}{2}\sqrt{-g}g_{\alpha\beta}. \tag{D.13}$$

(Note that $\sqrt{-g}\sqrt{-g} = -g > 0$.) We may also consider $\sqrt{-g(x')}$ with fixed x' to be a functional of $g^{\alpha\beta}(x)$. Its functional derivative is

$$\frac{\delta\sqrt{-g(x')}}{\delta g^{\alpha\beta}(x)} = \frac{\partial\sqrt{-g}}{\partial g^{\alpha\beta}}\delta(x-x') = -\frac{\sqrt{-g}}{2}g_{\alpha\beta}\delta(x-x').$$

As a by-product, we also find the spatial derivatives of the determinant:

$$\partial_\mu g = g\, g_{\alpha\beta,\mu}g^{\alpha\beta}; \quad \partial_\mu\sqrt{-g} = \frac{\sqrt{-g}}{2}g^{\alpha\beta}g_{\alpha\beta,\mu}. \tag{D.14}$$

2. To compute $\delta S/\delta\Gamma^{\lambda}_{\rho\sigma}$, we rewrite the action as an integral of $\Gamma^{\lambda}_{\rho\sigma}$ times some function. This requires some reshuffling of indices and integrations by parts. For example,

$$\int\sqrt{-g}d^4x\, g^{\alpha\beta}\Gamma^{\mu}_{\alpha\beta,\mu} = -\int d^4x\Gamma^{\lambda}_{\rho\sigma}\left(\sqrt{-g}g^{\rho\sigma}\right)_{,\lambda},$$
$$-\int\sqrt{-g}d^4x\, g^{\alpha\beta}\Gamma^{\mu}_{\alpha\mu,\beta} = \int d^4x\Gamma^{\lambda}_{\rho\sigma}(\sqrt{-g}g^{\rho\beta}\delta^{\sigma}_{\lambda})_{,\beta}.$$

The functional derivatives of these terms with respect to $\Gamma^\lambda_{\rho\sigma}$ is read off from these integrals. The terms bilinear in Γ need to be rewritten twice, with $\Gamma^\lambda_{\rho\sigma}$ at the first place or at the second place:

$$\Gamma^\mu_{\alpha\beta}\Gamma^\nu_{\mu\nu} = \Gamma^\lambda_{\rho\sigma}\Gamma^\nu_{\lambda\nu}\delta^\rho_\alpha\delta^\sigma_\beta = \Gamma^\rho_{\alpha\beta}\Gamma^\lambda_{\rho\sigma}\delta^\sigma_\lambda,$$
$$\Gamma^\nu_{\alpha\mu}\Gamma^\mu_{\beta\nu} = \Gamma^\lambda_{\rho\sigma}\Gamma^\sigma_{\beta\lambda}\delta^\rho_\alpha = \Gamma^\sigma_{\alpha\lambda}\Gamma^\lambda_{\rho\sigma}\delta^\rho_\beta.$$

The functional derivatives of these terms are then computed by omitting $\Gamma^\lambda_{\rho\sigma}$ from the above expressions:

$$\frac{\delta}{\delta\Gamma^\lambda_{\rho\sigma}}\left(\int \Gamma^\mu_{\alpha\beta}\Gamma^\nu_{\mu\nu}\sqrt{-g}g^{\alpha\beta}d^4x\right) = \sqrt{-g}g^{\alpha\beta}\left(\Gamma^\nu_{\lambda\nu}\delta^\rho_\alpha\delta^\sigma_\beta + \Gamma^\rho_{\alpha\beta}\delta^\sigma_\lambda\right),$$
$$\frac{\delta}{\delta\Gamma^\lambda_{\rho\sigma}}\left(-\int \Gamma^\nu_{\alpha\mu}\Gamma^\mu_{\beta\nu}\sqrt{-g}g^{\alpha\beta}d^4x\right) = -\sqrt{-g}g^{\alpha\beta}\left(\Gamma^\sigma_{\beta\lambda}\delta^\rho_\alpha + \Gamma^\sigma_{\alpha\lambda}\delta^\rho_\beta\right).$$

Therefore the equation of motion for $\Gamma^\lambda_{\rho\sigma}$ is

$$0 = \frac{\delta S}{\delta\Gamma^\lambda_{\rho\sigma}} = -\left(\sqrt{-g}g^{\rho\sigma}\right)_{,\lambda} + \left(\sqrt{-g}g^{\rho\beta}\delta^\sigma_\lambda\right)_{,\beta}$$
$$+\left(\Gamma^\nu_{\lambda\nu}g^{\rho\sigma} + \Gamma^\rho_{\alpha\beta}g^{\alpha\beta}\delta^\sigma_\lambda - \Gamma^\rho_{\alpha\lambda}g^{\sigma\alpha} - \Gamma^\sigma_{\alpha\lambda}g^{\rho\alpha}\right)\sqrt{-g}.$$

It is now convenient to convert the upper indices ρ, σ into lower indices μ, ν by multiplying both parts by $g_{\mu\rho}g_{\nu\sigma}$ (before doing this, we rename the mute index ν above into α). The derivatives of $\sqrt{-g}$ are found in Eq. (D.14). The common factor $\sqrt{-g}$ cancels. We obtain the following equation for $\Gamma^\mu_{\alpha\beta}$:

$$\Gamma^\alpha_{\lambda\alpha}g_{\mu\nu} + \Gamma^\rho_{\alpha\beta}g_{\mu\rho}g_{\lambda\nu}g^{\alpha\beta} - \Gamma^\rho_{\nu\lambda}g_{\mu\rho} - \Gamma^\sigma_{\mu\lambda}g_{\nu\sigma}$$
$$= \frac{1}{2}g_{\lambda\nu}g^{\alpha\beta}\left(2g_{\alpha\mu,\beta} - g_{\alpha\beta,\mu}\right) + \frac{1}{2}g_{\mu\nu}g^{\alpha\beta}g_{\alpha\beta,\lambda} - g_{\mu\nu,\lambda}.$$

This is a complicated (although linear) equation that needs to be solved for Γ. One way is to separate the terms on both sides by their index symmetry and by their dependence on $g_{\alpha\beta}$. To make the symmetry in the indices easier to use, we lower the index μ in $\Gamma^\mu_{\alpha\beta}$ to obtain the auxiliary quantity $\Gamma_{\mu.\alpha\beta}$ defined by

$$\Gamma^\mu_{\alpha\beta} \equiv g^{\mu\nu}\Gamma_{\nu.\alpha\beta}$$

(the period after ν is merely a typographical separator). Then we find

$$g_{\lambda\nu}g^{\alpha\beta}\Gamma_{\mu.\alpha\beta} + g_{\mu\nu}g^{\alpha\beta}\Gamma_{\beta.\lambda\alpha} - \left(\Gamma_{\mu.\nu\lambda} + \Gamma_{\nu.\mu\lambda}\right)$$
$$= \frac{1}{2}g_{\lambda\nu}g^{\alpha\beta}\left(2g_{\alpha\mu,\beta} - g_{\alpha\beta,\mu}\right) + \frac{1}{2}g_{\mu\nu}g^{\alpha\beta}g_{\alpha\beta,\lambda} - g_{\mu\nu,\lambda}. \qquad \text{(D.15)}$$

Now we note that there are three pairs of terms at each side: terms with free $g_{\lambda\nu}$, terms with free $g_{\mu\nu}$, and terms without any free (undifferentiated) g. We notice that

the second and the third pair of terms are symmetric in μ, ν. Therefore the first pair of terms, which is not symmetric under $\mu \leftrightarrow \nu$, must match separately:

$$g_{\lambda\nu} g^{\alpha\beta} \Gamma_{\mu.\alpha\beta} = \frac{1}{2} g_{\lambda\nu} g^{\alpha\beta} \left(2 g_{\alpha\mu,\beta} - g_{\alpha\beta,\mu}\right).$$

This equation is obviously solved by

$$\Gamma_{\mu.\alpha\beta} = \frac{1}{2} \left(g_{\alpha\mu,\beta} + g_{\beta\mu,\alpha} - g_{\alpha\beta,\mu}\right), \tag{D.16}$$

and this is equivalent to Eq. (5.20). [Here we identically rewrote

$$2 g^{\alpha\beta} g_{\alpha\mu,\beta} = g^{\alpha\beta} \left(g_{\alpha\mu,\beta} + g_{\beta\mu,\alpha}\right),$$

to make $\Gamma_{\mu.\alpha\beta}$ symmetric in α, β.] Then we need to check that the other two pairs of terms also cancel. With the above choice of $\Gamma_{\mu.\alpha\beta}$ we find

$$\begin{aligned} \Gamma_{\mu.\nu\lambda} + \Gamma_{\nu.\mu\lambda} &= g_{\mu\nu,\lambda}, \\ g^{\alpha\beta} \Gamma_{\beta.\lambda\alpha} &= \frac{1}{2} g^{\alpha\beta} g_{\alpha\beta,\lambda}. \end{aligned}$$

Therefore Eq. (5.20) is a solution.

Finally, we must show that this solution is unique. If there are two solutions $\Gamma_{\mu.\alpha\beta}$ and $\Gamma'_{\mu.\alpha\beta}$, their difference $D_{\mu.\alpha\beta}$ satisfies the homogeneous equation

$$g_{\lambda\nu} g^{\alpha\beta} D_{\mu.\alpha\beta} + g_{\mu\nu} g^{\alpha\beta} D_{\beta.\lambda\alpha} - \left(D_{\mu.\nu\lambda} + D_{\nu.\mu\lambda}\right) = 0. \tag{D.17}$$

We need to show that this equation has no solutions except $D_{\mu.\alpha\beta} = 0$ when $g_{\alpha\beta}$ is a non-degenerate matrix. First we antisymmetrize in μ, ν and find $g_{\lambda[\nu} D_{\mu].\alpha\beta} g^{\alpha\beta} = 0$. If we define $d_\mu \equiv D_{\mu.\alpha\beta} g^{\alpha\beta}$ and raise the index λ, we find that d_μ satisfies $\delta^\lambda_\nu d_\mu = \delta^\lambda_\mu d_\nu$. The only solution of this is $d_\mu = 0$ (take $\nu = \lambda \neq \mu$ to prove this). So the first term of Eq. (D.17) vanishes. Then we contract Eq. (D.17) with $g^{\mu\nu}$ and find $g^{\alpha\beta} D_{\beta.\lambda\alpha} = 0$. Therefore Eq. (D.17) is reduced to $D_{\mu.\nu\lambda} + D_{\nu.\mu\lambda} = 0$. But a tensor $D_{\mu.\nu\lambda}$ which is antisymmetric in the first two indices but symmetric in the last two indices must necessarily vanish. Therefore the solution $\Gamma_{\mu.\alpha\beta}$ of Eq. (D.15) is unique.

3. The variation of $R\sqrt{-g}$ with respect to $g^{\alpha\beta}$ is now easy to find. We write

$$R\sqrt{-g} = g^{\mu\nu} R_{\mu\nu} \sqrt{-g},$$

where $R_{\mu\nu}$ is treated as independent of $g^{\alpha\beta}$ since it is a combination of the Γ symbols. Then

$$\begin{aligned} &\frac{\delta}{\delta g^{\alpha\beta}} \left(\int g^{\mu\nu} R_{\mu\nu} \sqrt{-g} d^4x \right) \\ &= R_{\alpha\beta} \sqrt{-g} + \int g^{\mu\nu} R_{\mu\nu} \frac{\delta \sqrt{-g(x')}}{\delta g^{\alpha\beta}(x)} d^4x' = \left(R_{\alpha\beta} - \frac{1}{2} g_{\alpha\beta} R \right) \sqrt{-g}. \end{aligned}$$

The last line gives the required expression.

> **Remark: other solutions.** Here we solved for $\Gamma^{\mu}_{\alpha\beta}$ straightforwardly by extremizing the action, without choosing a special coordinate system. Another way to obtain the Einstein equation is to vary the action directly with respect to $g^{\mu\nu}$; calculations are very cumbersome unless one uses a locally inertial coordinate system.

Chapter 6

Exercise 6.1 (p. 64)

Since $a(\eta)$ depends only on time, $\Delta a(\eta) = 0$ and

$$a\left(\phi'' + 2\frac{a'}{a}\phi'\right) = (a\phi)'' - a''\phi = \chi'' - \frac{a''}{a}\chi.$$

The required equation follows.

Exercise 6.2 (p. 64)

We use the spacetime coordinates $(\mathbf{x}, \eta)$ and note that $\sqrt{-g} = a^4$ and $g^{\alpha\beta} = a^{-2}\eta^{\alpha\beta}$. Then

$$\sqrt{-g}\, m^2\phi^2 = m^2 a^2 \chi^2,$$
$$\sqrt{-g}\, g^{\alpha\beta}\phi_{,\alpha}\phi_{,\beta} = a^2\left(\phi'^2 - (\nabla\phi)^2\right).$$

Substituting $\phi = \chi/a$, we get

$$a^2\phi'^2 = \chi'^2 - 2\chi\chi'\frac{a'}{a} + \chi^2\left(\frac{a'}{a}\right)^2 = \chi'^2 + \chi^2\frac{a''}{a} - \left[\chi^2\frac{a'}{a}\right]'.$$

The total time derivative term can be omitted from the action, and we obtain the required expression.

Exercise 6.3 (p. 65)

The standard result $dW/dt = 0$ follows if we use the oscillator equation to express $\ddot{x}_{1,2}$ through $x_{1,2}$,

$$\frac{d}{dt}\left(\dot{x}_1 x_2 - x_1\dot{x}_2\right) = \ddot{x}_1 x_2 - x_1\ddot{x}_2 = \omega^2 x_1 x_2 - x_1\omega^2 x_2 = 0.$$

The solutions $x_1(t)$ and $x_2(t)$ are linearly *dependent* if there exists a constant λ such that $x_2(t) = \lambda x_1(t)$ for all t. It immediately follows that $W[x_1, x_2] = \dot{x}_1\lambda x_1 - x_1\lambda\dot{x}_1 = 0$. Conversely, $W[x_1, x_2] = 0$ means that the matrix

$$\begin{pmatrix} \dot{x}_1(t) & x_1(t) \\ \dot{x}_2(t) & x_2(t) \end{pmatrix}$$

is degenerate for each t. Thus, at a fixed time $t = t_0$ there exists λ_0 such that $x_2(t_0) = \lambda_0 x_1(t_0)$ and $\dot{x}_2(t_0) = \lambda_0 \dot{x}_1(t_0)$. The solution of the Cauchy problem with initial conditions $x(t_0) = \lambda_0 x_1(t_0)$, $\dot{x}(t_0) = \lambda_0 \dot{x}_1(t_0)$ is unique, one such solution is $x_2(t)$ and another is $\lambda_0 x_1(t)$, therefore $x_2(t) = \lambda_0 x_1(t)$ for all t.

Exercise 6.4 (p. 68)

We compute the commutation relations between $\hat{\chi}(\mathbf{x}, \eta)$ and $\hat{\pi}(\mathbf{x}, \eta)$ using the mode expansion of Eq. (6.31) and the commutation relations for $\hat{a}^{\pm}_{\mathbf{k}}$, to find

$$[\hat{\chi}(\mathbf{x}, \eta), \hat{\pi}(\mathbf{y}, \eta)] = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{v'_{\mathbf{k}} v^*_{\mathbf{k}} - v_{\mathbf{k}} v'^*_{\mathbf{k}}}{2} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}.$$

From the known relation

$$\delta(\mathbf{x} - \mathbf{y}) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}$$

it follows that Eq. (6.22) must hold for all $\mathbf{k}$.

Exercise 6.5 (p. 69)

We suppress the index k for brevity and write the normalization condition for $u(\eta)$,

$$u^* u' - u u'^* = 2i.$$

Expressing u through v as given, we obtain

$$\left(|\alpha|^2 - |\beta|^2\right)(v^* v' - v v'^*) = 2i.$$

The required relation follows from the normalization of $v(\eta)$.

Exercise 6.6 (p. 70)

The relation between the mode functions is

$$v^*_{\mathbf{k}} = \alpha_{\mathbf{k}} u^*_{\mathbf{k}} + \beta_{\mathbf{k}} u_{\mathbf{k}}.$$

From the identities $v_{\mathbf{k}} = v_{-\mathbf{k}}$, $u_{\mathbf{k}} = u_{-\mathbf{k}}$ one has $\alpha_{-\mathbf{k}} = \alpha_{\mathbf{k}}$, $\beta_{-\mathbf{k}} = \beta_{\mathbf{k}}$. We use the relations $\left(\hat{a}^-_{\mathbf{k}}\right)^\dagger = \hat{a}^+_{\mathbf{k}}$, $\alpha_{-\mathbf{k}} = \alpha_{\mathbf{k}}$, $\beta_{-\mathbf{k}} = \beta_{\mathbf{k}}$ and rewrite the Bogolyubov transformations as

$$\hat{b}^-_{\mathbf{k}} = \alpha_{\mathbf{k}} \hat{a}^-_{\mathbf{k}} + \beta^*_{\mathbf{k}} \hat{a}^+_{-\mathbf{k}}, \qquad \hat{b}^+_{-\mathbf{k}} = \beta_{\mathbf{k}} \hat{a}^-_{\mathbf{k}} + \alpha^*_{\mathbf{k}} \hat{a}^+_{-\mathbf{k}}.$$

Now we solve this system of equations for $\hat{a}^-_{\mathbf{k}}$. Using $|\alpha_{\mathbf{k}}|^2 - |\beta_{\mathbf{k}}|^2 = 1$, we find

$$\hat{a}^-_{\mathbf{k}} = \alpha^*_{\mathbf{k}} \hat{b}^-_{\mathbf{k}} - \beta^*_{\mathbf{k}} \hat{b}^+_{-\mathbf{k}}.$$

Exercise 6.7 (p. 70)

First we consider the quantum state of one mode $\hat{\phi}_{\mathbf{k}}$. The b-vacuum $\left|{}_{(b)}0_{\mathbf{k},-\mathbf{k}}\right\rangle$ is expanded as the linear combination

$$\left|{}_{(b)}0_{\mathbf{k},-\mathbf{k}}\right\rangle = \sum_{m,n=0}^{\infty} c_{mn} \left|{}_{(a)}m_{\mathbf{k}}, n_{-\mathbf{k}}\right\rangle, \tag{D.18}$$

where the state $\left|{}_{(a)}m_{\mathbf{k}}, n_{-\mathbf{k}}\right\rangle$ is the result of acting on the a-vacuum state with m creation operators $\hat{a}^{+}_{\mathbf{k}}$ and n creation operators $\hat{a}^{+}_{-\mathbf{k}}$,

$$\left|{}_{(a)}m_{\mathbf{k}}, n_{-\mathbf{k}}\right\rangle = \frac{\left(\hat{a}^{+}_{\mathbf{k}}\right)^{m}\left(\hat{a}^{+}_{-\mathbf{k}}\right)^{n}}{\sqrt{m!n!}} \left|{}_{(a)}0_{\mathbf{k},-\mathbf{k}}\right\rangle. \tag{D.19}$$

The unknown coefficients c_{mn} may be found after a somewhat long calculation by substituting Eq. (D.18) into

$$\left.\begin{array}{l} \left(\alpha_{\mathbf{k}}\hat{a}^{-}_{\mathbf{k}} + \beta^{*}_{\mathbf{k}}\hat{a}^{+}_{-\mathbf{k}}\right)\left|{}_{(b)}0_{\mathbf{k},-\mathbf{k}}\right\rangle = 0, \\ \left(\alpha_{\mathbf{k}}\hat{a}^{-}_{-\mathbf{k}} + \beta^{*}_{\mathbf{k}}\hat{a}^{+}_{\mathbf{k}}\right)\left|{}_{(b)}0_{\mathbf{k},-\mathbf{k}}\right\rangle = 0. \end{array}\right\} \tag{D.20}$$

Here is a faster and more elegant method. Equation (D.19) implies that the b-vacuum state is a result of acting on the a-vacuum by a combination of the creation operators. We denote this combination by $f\left(\hat{a}^{+}_{\mathbf{k}}, \hat{a}^{+}_{-\mathbf{k}}\right)$ where $f(x,y)$ is an unknown function. Then from Eq. (D.20) we get two equations for $\hat{f}$,

$$\left(\alpha_{\mathbf{k}}\hat{a}^{-}_{\mathbf{k}} + \beta^{*}_{\mathbf{k}}\hat{a}^{+}_{-\mathbf{k}}\right)\hat{f}\left|{}_{(a)}0_{\mathbf{k},-\mathbf{k}}\right\rangle = 0, \tag{D.21}$$

$$\left(\alpha_{\mathbf{k}}\hat{a}^{-}_{-\mathbf{k}} + \beta^{*}_{\mathbf{k}}\hat{a}^{+}_{\mathbf{k}}\right)\hat{f}\left|{}_{(a)}0_{\mathbf{k},-\mathbf{k}}\right\rangle = 0. \tag{D.22}$$

We know from Exercise 2.5b (p. 21) that the commutator $\left[\hat{a}^{-}_{\mathbf{k}}, \hat{f}\right]$ is equal to the derivative of $\hat{f}$ with respect to $\hat{a}^{+}_{\mathbf{k}}$. Therefore Eq. (D.21) gives

$$\left(\alpha_{\mathbf{k}}\frac{\partial\hat{f}}{\partial a^{+}_{\mathbf{k}}} + \beta^{*}_{\mathbf{k}}\hat{a}^{+}_{-\mathbf{k}}\hat{f}\right)\left|{}_{(a)}0_{\mathbf{k},-\mathbf{k}}\right\rangle = 0.$$

Since the function $\hat{f}$ contains only creation operators, it must satisfy

$$\alpha_{\mathbf{k}}\frac{\partial\hat{f}}{\partial a^{+}_{\mathbf{k}}} + \beta^{*}_{\mathbf{k}}\hat{a}^{+}_{-\mathbf{k}}\hat{f} = 0.$$

This differential equation has the general solution

$$f\left(\hat{a}^{+}_{\mathbf{k}}, \hat{a}^{+}_{-\mathbf{k}}\right) = C\left(\hat{a}^{+}_{-\mathbf{k}}\right)\exp\left(-\frac{\beta^{*}_{\mathbf{k}}}{\alpha_{\mathbf{k}}}\hat{a}^{+}_{\mathbf{k}}\hat{a}^{+}_{-\mathbf{k}}\right),$$

where C is an arbitrary function of $\hat{a}^+_{-\mathbf{k}}$. To determine this function, we use Eq. (D.22) to derive the analogous relation for $\partial f/\partial a^+_{-\mathbf{k}}$ and find that C must be a constant. Therefore the b-vacuum is expressed as

$$\left|{}_{(b)}0_{\mathbf{k},-\mathbf{k}}\right\rangle = C\sum_{n=0}^{\infty}\left(-\frac{\beta^*_{\mathbf{k}}}{\alpha_{\mathbf{k}}}\right)^n \left|{}_{(a)}n_{\mathbf{k}}, n_{-\mathbf{k}}\right\rangle .$$

The value of C is fixed by normalization,

$$\left\langle{}_{(b)}0_{\mathbf{k},-\mathbf{k}}\right|\left.{}_{(b)}0_{\mathbf{k},-\mathbf{k}}\right\rangle = 1 \;\Rightarrow\; C = \sqrt{1-\frac{|\beta_{\mathbf{k}}|^2}{|\alpha_{\mathbf{k}}|^2}} = \frac{1}{|\alpha_{\mathbf{k}}|}.$$

Since $|\beta_{\mathbf{k}}| < |\alpha_{\mathbf{k}}|$, the value of C as given above is always real and nonzero. The final expression for the b-vacuum state is

$$\left|{}_{(b)}0_{\mathbf{k},-\mathbf{k}}\right\rangle = \frac{1}{|\alpha_{\mathbf{k}}|}\sum_{n=0}^{\infty}\left(-\frac{\beta^*_{\mathbf{k}}}{\alpha_{\mathbf{k}}}\right)^n \left|{}_{(a)}n_{\mathbf{k}}, n_{-\mathbf{k}}\right\rangle .$$

The vacuum state $\left|{}_{(b)}0\right\rangle$ is the tensor product of the vacuum states $\left|{}_{(b)}0_{\mathbf{k},-\mathbf{k}}\right\rangle$ of all modes. Since each pair $\hat{\phi}_{\mathbf{k}}, \hat{\phi}_{-\mathbf{k}}$ is counted twice in the product over all $\mathbf{k}$, we need to take the square root of the whole expression:

$$\begin{aligned}|0\rangle &= \left[\prod_{\mathbf{k}}\frac{1}{|\alpha_{\mathbf{k}}|}\sum_{n=0}^{\infty}\left(-\frac{\beta^*_{\mathbf{k}}}{\alpha_{\mathbf{k}}}\right)^n\frac{\left(\hat{a}^+_{\mathbf{k}}\hat{a}^+_{-\mathbf{k}}\right)^n}{n!}\right]^{1/2}|0\rangle \\ &= \prod_{\mathbf{k}}\frac{1}{\sqrt{|\alpha_{\mathbf{k}}|}a}\exp\left(-\frac{\beta^*_{\mathbf{k}}}{2\alpha_{\mathbf{k}}}\hat{a}^+_{\mathbf{k}}\hat{a}^+_{-\mathbf{k}}\right)|0\rangle .\end{aligned}$$

Exercise 6.8 (p. 73)

Similarly to the calculation in Sec. 4.2, we perform a Fourier transform to find

$$\hat{H} = \frac{1}{2}\int d^3\mathbf{k}\left(\hat{\chi}'_{\mathbf{k}}\hat{\chi}'_{-\mathbf{k}} + \omega_k^2(\eta)\hat{\chi}_{\mathbf{k}}\hat{\chi}_{-\mathbf{k}}\right).$$

Now we expand the operators $\hat{\chi}_{\mathbf{k}}$ through the mode functions and use the identity $v_{\mathbf{k}}(\eta) = v_{-\mathbf{k}}(\eta)$ and Eq. (6.31). For example, the term $\hat{\chi}'_{\mathbf{k}}\hat{\chi}'_{-\mathbf{k}}$ gives

$$\begin{aligned}\frac{1}{2}\int d^3\mathbf{k}\hat{\chi}'_{\mathbf{k}}\hat{\chi}'_{-\mathbf{k}} &= \int\frac{d^3\mathbf{k}}{4}\left(v'^*_{\mathbf{k}}\hat{a}^-_{\mathbf{k}} + v'_{\mathbf{k}}\hat{a}^+_{-\mathbf{k}}\right)\left(v'^*_{\mathbf{k}}\hat{a}^-_{-\mathbf{k}} + v'_{\mathbf{k}}\hat{a}^+_{\mathbf{k}}\right) \\ = \int\frac{d^3\mathbf{k}}{4}&\left[v'^2_{\mathbf{k}}\hat{a}^+_{\mathbf{k}}\hat{a}^+_{-\mathbf{k}} + \left(v'^*_{\mathbf{k}}\right)^2\hat{a}^-_{\mathbf{k}}\hat{a}^-_{-\mathbf{k}} + |v'_{\mathbf{k}}|^2\left(\hat{a}^-_{\mathbf{k}}\hat{a}^+_{\mathbf{k}} + \hat{a}^+_{-\mathbf{k}}\hat{a}^-_{-\mathbf{k}}\right)\right].\end{aligned}$$

Since we are integrating over all $\mathbf{k}$, we may exchange $\mathbf{k}$ and $-\mathbf{k}$ in the integrand. After some straightforward algebra we obtain the required result.

Chapter 7

Exercise 7.1 (p. 81)

Using the mode expansion and the commutation relations for $\hat{a}^{\pm}_{\mathbf{k}}$, we find

$$\langle 0|\,\hat{\chi}\,(\mathbf{x},\eta)\,\hat{\chi}\,(\mathbf{y},\eta)\,|0\rangle = \langle 0|\int \frac{d^3\mathbf{k}}{(2\pi)^3}\frac{1}{2}e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}v_k^* v_k\,|0\rangle$$
$$= \int_0^\infty \frac{k^2 dk}{4\pi^2}\int_{-1}^{1} d(\cos\theta)e^{ikL\cos\theta}\frac{|v_k(\eta)|^2}{2} = \frac{1}{4\pi^2}\int_0^\infty k^2 dk\,|v_k(\eta)|^2\,\frac{\sin kL}{kL}.$$

Exercise 7.2 (p. 86)

We need to compute the mode function $v_k^{(in)}(\eta)$ at $\eta > \eta_1$ and represent it as a sum of $v_k^{(out)}$ and $v_k^{(out)*}$. To simplify the notation, we rename $v_k^{(in)} \equiv v_k$ and $v_k^{(out)} \equiv u_k$. The mode function and its derivative v_k, v_k' need to be matched at points $\eta = 0$ and $\eta = \eta_1$. To simplify the matching, we use the ansatz

$$f(t) = A\cos\omega\,(t-t_0) + \frac{B}{\omega}\sin\omega\,(t-t_0)$$

to match $f\,(t_0) = A$, $f'\,(t_0) = B$. We find for $0 < \eta < \eta_1$,

$$v_k(\eta) = \frac{1}{\sqrt{\omega_k}}\cos\Omega_k\eta + \frac{i\sqrt{\omega_k}}{\Omega_k}\sin\Omega_k\eta.$$

Then the conditions at $\eta = \eta_1$ are

$$v_k\,(\eta_1) = \frac{1}{\sqrt{\omega_k}}\cos\Omega_k\eta_1 + \frac{i\sqrt{\omega_k}}{\Omega_k}\sin\Omega_k\eta_1,$$
$$v_k'\,(\eta_1) = -\frac{\Omega_k}{\sqrt{\omega_k}}\sin\Omega_k\eta_1 + i\sqrt{\omega_k}\cos\Omega_k\eta_1.$$

So for $\eta > \eta_1$ the mode function is

$$v_k(\eta) = \frac{e^{i\omega_k(\eta-\eta_1)}}{\sqrt{\omega_k}}\left[\cos\Omega_k\eta_1 + \frac{i}{2}\left(\frac{\omega_k}{\Omega_k}+\frac{\Omega_k}{\omega_k}\right)\sin\Omega_k\eta_1\right]$$
$$+ \frac{e^{-i\omega_k(\eta-\eta_1)}}{\sqrt{\omega_k}}\left(\frac{\omega_k}{\Omega_k}-\frac{\Omega_k}{\omega_k}\right)\frac{i\sin\Omega_k\eta_1}{2}$$
$$= \alpha_k^*\frac{e^{i\omega_k(\eta-\eta_1)}}{\sqrt{\omega_k}} + \beta_k^*\frac{e^{-i\omega_k(\eta-\eta_1)}}{\sqrt{\omega_k}}.$$

The required expressions for α_k and β_k follow after a regrouping of the complex exponentials.

Exercise 7.3 (p. 88)

The energy density is given by the integral

$$\varepsilon_0 = m_0^4 \int_0^{k_{\max}} 4\pi k^2 dk \sqrt{m_0^2 + k^2} \frac{\left|\sin \eta_1 \sqrt{k^2 - m_0^2}\right|^2}{|k^4 - m_0^4|}.$$

For convenience, we introduce the dimensionless variable $s \equiv k/m_0$ and obtain

$$\frac{\varepsilon_0}{m_0^4} = 4\pi \int_0^{s_{\max}} s^2 ds \frac{\left|\sin A\sqrt{s^2-1}\right|^2}{|s^2-1|\sqrt{1+s^2}}, \tag{D.23}$$

where $A \equiv m_0\eta_1 \gg 1$ is a dimensionless parameter. The integral in Eq. (D.23) contains the contributions from the intervals $0 < s < 1$ and from $1 < s < s_{\max}$,

$$\frac{\varepsilon_0}{m_0^4} = 4\pi \int_0^1 s^2 ds \frac{\sinh^2 A\sqrt{1-s^2}}{(1-s^2)\sqrt{1+s^2}} + 4\pi \int_1^{s_{\max}} s^2 ds \frac{\sin^2 A\sqrt{s^2-1}}{(s^2-1)\sqrt{1+s^2}}. \tag{D.24}$$

The integrand in the first term in Eq. (D.24) is exponentially large for most s,

$$\sinh^2 A \approx \frac{1}{4}\exp(2A),$$

while the second term gives only a power-law growth in A,

$$\frac{\sin^2 A\sqrt{s^2-1}}{s^2-1} \leq A^2, \quad s \geq 1.$$

(Note that $\left|\frac{\sin x}{x}\right| \leq 1$ for all $x \geq 0$.) This suggests that the first term is the asymptotically dominant one for $A \gg 1$. Now we consider the two integrals in Eq. (D.24) in more detail and obtain their asymptotics for $A \to \infty$.

1) The first integral in Eq. (D.24) can be asymptotically estimated in the following way. We rewrite the integrand as a product of quickly-varying and slowly-varying functions,

$$\begin{aligned} &4\pi \int_0^1 s^2 ds \frac{\sinh^2 A\sqrt{1-s^2}}{(1-s^2)\sqrt{1+s^2}} \\ &= \pi \int_0^1 ds \left[s^2 e^{2A\sqrt{1-s^2}}\right] \frac{1 - 2e^{-2A\sqrt{1-s^2}} + e^{-4A\sqrt{1-s^2}}}{(1-s^2)\sqrt{1+s^2}}. \end{aligned} \tag{D.25}$$

The quickly-varying expression in the square brackets has the maximum at $s = s_0$ where

$$s_0^2 A = \sqrt{1-s_0^2} \;\Rightarrow\; s_0 \approx \frac{1}{\sqrt{A}} \ll 1.$$

This maximum gives the dominant contribution to the integral. Near $s = s_0$ the slowly-varying factor is of order $1 + O\left(A^{-1}\right)$ and can be neglected in the calculation

of the leading asymptotic. By changing the variable $s\sqrt{A} = u$ we find

$$\int_0^1 s^2 ds\, \exp\left(2A\sqrt{1-s^2}\right) = e^{2A}\int_0^1 s^2 ds\, e^{-As^2+O(s^4)}$$
$$= A^{-3/2}e^{2A}\int_0^{\sqrt{A}} u^2 e^{-u^2} du\,\left(1+O\left(A^{-1}\right)\right) = \frac{\sqrt{\pi}}{4}A^{-3/2}e^{2A}\left(1+O\left(A^{-1}\right)\right).$$

In the last integral we have approximated

$$\int_0^{\sqrt{A}} u^2 e^{-u^2} du \approx \int_0^{\infty} u^2 e^{-u^2} du = \frac{\sqrt{\pi}}{4},$$

since the difference is exponentially small, of order $\exp\left(-\frac{\text{const}}{A}\right)$, whereas we have already neglected terms of order A^{-1}. Therefore the first contribution to ε_0 is

$$\frac{m_0^4}{4}\left(\frac{\pi}{m_0\eta_1}\right)^{3/2} e^{2m_0\eta_1}\left(1+O\left(\frac{1}{m_0\eta_1}\right)\right).$$

2) It remains to prove that the first integral in Eq. (D.24) gives the dominant contribution for $A \gg 1$. This can be shown by finding an upper bound for the second integral. We split the range $1 < s < s_{\max}$ into two ranges $1 < s < s_1$ and $s_1 < s < s_{\max}$, where s_1 is the first point after $s = 1$ where

$$\sin A\sqrt{s_1^2-1} = 0.$$

Then

$$s_1 = \sqrt{1+\frac{\pi^2}{4A^2}} \approx 1+\frac{\pi^2}{8A^2},$$

and the integrand can be bounded from above on each of the ranges using

$$\frac{\sin^2 A\sqrt{s^2-1}}{s^2-1} \le A^2, \quad \frac{s^2}{\sqrt{1+s^2}} < 1 \quad \text{for } 0 \le s \le s_1,$$
$$\sin^2 A\sqrt{s^2-1} \le 1, \quad \frac{s^2}{s^2-1} < 1+\frac{4A^2}{\pi^2} \quad \text{for } s \ge s_1.$$

So the integral satisfies the inequalities

$$\int_1^{s_{\max}} s^2 ds \frac{\sin^2 A\sqrt{s^2-1}}{(s^2-1)\sqrt{1+s^2}} < A^2\int_1^{s_1} ds + \left(1+\frac{4A^2}{\pi^2}\right)\int_{s_1}^{s_{\max}} \frac{ds}{\sqrt{1+s^2}}$$
$$= A^2(s_1-1) + \left(1+\frac{4A^2}{\pi^2}\right)\left(\sinh^{-1} s_{\max} - \sinh^{-1} s_1\right)$$
$$< \frac{\pi^2}{8} + \left(1+\frac{4A^2}{\pi^2}\right)\ln\left(s_{\max}+\sqrt{s_{\max}^2+1}\right) \sim A^2 \ln s_{\max}, \quad A \gg 1.$$

Therefore at large A and fixed $s_{\max}$ the contribution of the second integral is subdominant to that of the first integral.

Exercise 7.4 (p. 92)

We change the variable $k|\eta| = s$ and express the mode function through the new function $f(s)$ by

$$v_k(\eta) \equiv \sqrt{s} f(s) = \sqrt{k|\eta|} f(k|\eta|).$$

Then the equation for $f(s)$ is the Bessel equation,

$$s^2 f'' + s f' + \left(s^2 - n^2\right) f = 0, \quad n \equiv \sqrt{\frac{9}{4} - \frac{m^2}{H^2}},$$

with the general solution $f(s) = AJ_n(s) + BY_n(s)$, where A and B are arbitrary constants and J_n, Y_n are the Bessel functions. Therefore the mode function $v_k(\eta)$ is

$$v_k(\eta) = \sqrt{k|\eta|}\left[AJ_n(k|\eta|) + BY_n(k|\eta|)\right]. \tag{D.26}$$

The asymptotics of the Bessel functions are known; see e.g. *The Handbook of Mathematical functions*, ed. by M. ABRAMOWITZ and I. STEGUN (National Bureau of Standards, Washington D.C., 1974):

$$J_n(s) \sim \begin{cases} \frac{1}{\Gamma(n+1)}\left(\frac{s}{2}\right)^n, & s \to 0, \\ \sqrt{\frac{2}{\pi s}}\cos\left(s - \frac{n\pi}{2} - \frac{\pi}{4}\right), & s \to \infty; \end{cases}$$

$$Y_n(s) \sim \begin{cases} -\frac{1}{\pi}\Gamma(n)\left(\frac{2}{s}\right)^n, & s \to 0, \\ \sqrt{\frac{2}{\pi s}}\sin\left(s - \frac{n\pi}{2} - \frac{\pi}{4}\right), & s \to \infty. \end{cases}$$

Since by assumption $m \ll H$, the parameter n is real and $n > 0$. So the mode function $v_k(\eta)$ defined by Eq. (D.26) has the following asymptotics:

$$v_k(\eta) \sim \begin{cases} B\frac{1}{\pi}2^n\Gamma(n)(k|\eta|)^{\frac{1}{2}-n}, & k|\eta| \to 0, \\ \sqrt{\frac{2}{\pi}}\left[A\cos\lambda + B\sin\lambda\right], & k|\eta| \to +\infty. \end{cases}$$

Here we denoted

$$\lambda \equiv k|\eta| - \frac{n\pi}{2} - \frac{\pi}{4}.$$

It is clear that the choice

$$A = \sqrt{\frac{\pi}{2k}}, \quad B = -iA$$

will result in the asymptotic at early times $k|\eta| \to \infty$ of the form

$$v_k(\eta) = \frac{1}{\sqrt{k}}\exp\left(ik\eta + \frac{in\pi}{2} + \frac{i\pi}{4}\right).$$

This coincides with the Minkowski mode function (up to a phase).

Chapter 8

Exercise 8.1 (p. 104)

The coordinates are transformed so that we get the 1-forms

$$dt = d\tau(1 + a\xi)\cosh a\tau + d\xi \sinh a\tau,$$
$$dx = d\tau(1 + a\xi)\sinh a\tau + d\xi \cosh a\tau.$$

Then we obtain Eq. (8.8) after straightforward algebra.

Exercise 8.2 (p. 111)

We substitute the expression for $\hat{b}^{\pm}_{\Omega}$ into the commutation relation and find

$$\begin{aligned}
\delta(\Omega - \Omega') &= \left[\hat{b}^{-}_{\Omega},\, \hat{b}^{+}_{\Omega'}\right] \\
&= \left[\int d\omega \left(\alpha_{\omega\Omega}\hat{a}^{-}_{\omega} + \beta_{\omega\Omega}\hat{a}^{+}_{\omega}\right),\, \int d\omega' \left(\alpha^{*}_{\omega'\Omega'}\hat{a}^{+}_{\omega'} + \beta^{*}_{\omega'\Omega'}\hat{a}^{-}_{\omega'}\right)\right] \\
&= \int d\omega d\omega' \left(\alpha_{\omega\Omega}\alpha^{*}_{\omega'\Omega'}\delta(\omega - \omega') - \beta_{\omega\Omega}\beta^{*}_{\omega'\Omega'}\delta(\omega - \omega')\right) \\
&= \int d\omega \left(\alpha_{\omega\Omega}\alpha^{*}_{\omega\Omega'} - \beta_{\omega\Omega}\beta^{*}_{\omega\Omega'}\right).
\end{aligned}$$

Exercise 8.3 (p. 112)

The function $F(\omega, \Omega)$ is reduced to Euler's Γ function by changing the variable $u \to t$,

$$t \equiv -\frac{i\omega}{a}e^{-au}.$$

The result is

$$F(\omega, \Omega) = \frac{1}{2\pi a}\exp\left(i\frac{\Omega}{a}\ln\frac{\omega}{a} + \frac{\pi\Omega}{2a}\right)\Gamma\left(-\frac{i\Omega}{a}\right), \quad \omega > 0,\ a > 0.$$

We now need to transform this expression taking $\omega \to -\omega$, but it is not clear whether to take $\ln(-\omega) = \ln\omega + i\pi$ or some other phase instead of $i\pi$. To resolve this question, we need to analyze the required analytic continuation of the Γ function (a detailed calculation is given in Appendix A.3).

A more direct approach (without using the Γ function) is to deform the contour of integration in Eq. (8.21). The contour can be shifted downwards by $-i\pi a^{-1}$ into the line $u = -i\pi a^{-1} + t$, where t is real, $-\infty < t < +\infty$ (see Fig. D.1). Then $e^{-au} = -e^{-at}$ and we obtain

$$\begin{aligned}
F(\omega, \Omega) &= \int_{-\infty}^{+\infty}\frac{dt}{2\pi}\exp\left(i\Omega t + \frac{\pi\Omega}{a} - \frac{i\omega}{a}e^{-at}\right) \\
&= F(-\omega, \Omega)\exp\left(\frac{\pi\Omega}{a}\right).
\end{aligned}$$

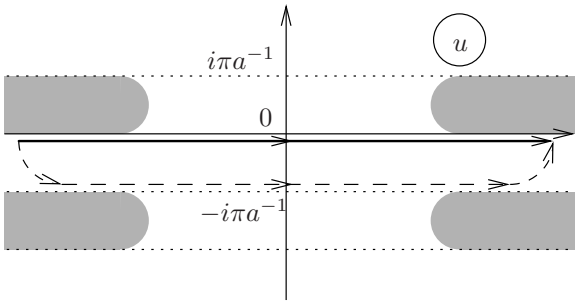


Figure D.1: The original and the shifted contours of integration for Eq. (D.28) are shown by solid and dashed lines. The shaded regions cannot be crossed when deforming the contour at infinity.

It remains to justify the shift of the contour. The integrand has no singularities and, since the lateral lines have a limited length, it is enough to show that the integrand vanishes at $u \to \pm\infty - i\alpha$ for $0 < \alpha < \pi a^{-1}$. At $u = M - i\alpha$ and $M \to -\infty$ the integrand vanishes since

$$\lim_{u\to-\infty-i\alpha} Re\left(\frac{i\omega}{a}e^{-au}\right) = -\lim_{t\to-\infty}\frac{\omega}{a}e^{-at}\sin\alpha a = -\infty. \tag{D.27}$$

At $u \to +\infty - i\alpha$ the integral does not actually converge and must be regularized, e.g. by inserting a convergence factor $\exp\left(-bu^2\right)$ with $b > 0$:

$$F(\omega,\Omega) = \lim_{b\to+0}\int_{-\infty}^{+\infty}\frac{du}{2\pi}\exp\left(-bu^2 + i\Omega u + i\frac{\omega}{a}e^{-au}\right). \tag{D.28}$$

With this (or another) regularization, the integrand vanishes at $u \to +\infty - i\alpha$ as well. Therefore the contour may be shifted and our result is justified in the sense of distributions.

Note that we cannot shift the contour to $u = -i(\pi + 2\pi n)a^{-1} + t$ with any $n \neq 0$ because Eq. (D.27) will not hold. Also, with $\omega < 0$ we will be unable to move the contour in the negative imaginary direction. The shift of the contour we used is the only one possible.

Chapter 9

Exercise 9.1 (p. 122)

We need to insert the correct combination of the constants c, G, $\hbar$, and k into the equation. The temperature is derived from the relation of the type $\omega = a/(2\pi)$ where $a = (4M)^{-1}$ is the proper acceleration of the observer and ω the frequency of field

modes. This relation becomes $\omega = a/(2\pi c)$ in the SI units. The relation between a and M contains only the constants c and G since it is a classical and not a quantum-mechanical relation. The Planck constant $\hbar$ enters only as the combination $\hbar\omega$ and the Boltzmann constant k enters as kT. Therefore we find

$$a = \frac{c^4}{4GM}, \quad kT = \hbar\omega = \frac{\hbar a}{2\pi c} \;\Rightarrow\; T = \frac{\hbar c^3}{Gk}\frac{1}{8\pi M}.$$

The relation between temperature in degrees and mass in kilograms is

$$\frac{T}{1^\circ K} \approx \frac{\left(1.05\cdot 10^{-34}\right)\left(3.00\cdot 10^{8}\right)^3}{\left(6.67\cdot 10^{-11}\right)\left(1.38\cdot 10^{-23}\right)8\pi}\left(\frac{1\text{kg}}{M}\right) = \frac{1.23\cdot 10^{23}\text{kg}}{M}.$$

Another way to convert the units is to use the Planck units explicitly: the Planck mass M_{Pl} and the Planck temperature T_{Pl} are defined by

$$M_{Pl} = \sqrt{\frac{\hbar c}{G}}, \quad kT_{Pl} = M_{Pl}c^2.$$

Then we write

$$\frac{T}{T_{Pl}} = \frac{1}{8\pi}\frac{M_{Pl}}{M}$$

and obtain the above expression for T.

Numerical evaluation gives: $T \approx 6\cdot 10^{-8}$K for $M = M_\odot = 2\cdot 10^{30}$kg; $T \approx 10^{11}$K for $M = 10^{15}$g; and $T \approx 10^{31}$K for $M = 10^{-5}$g.

Exercise 9.2 (p. 122)

(a) The Schwarzschild radius in the SI units is expressed by the formula

$$R = \frac{2GM}{c^2}.$$

The typical wavelength of a photon is

$$\lambda = \frac{2\pi}{\omega}c = \frac{(2\pi c)^2}{a} = \frac{16\pi^2 GM}{c^2}.$$

Note that the ratio of λ to R is independent of M (this can be seen already in the Planck units):

$$\frac{\lambda}{R} = 8\pi^2.$$

(b) The Compton wavelength of a proton is

$$\lambda = \frac{2\pi\hbar}{m_p c}.$$

The proton mass is $m_p \approx 1.67 \cdot 10^{-27}$kg. Protons are produced efficiently if the typical energy of an emitted particle,

$$kT = \hbar\omega = \frac{\hbar c^3}{8\pi GM},$$

is larger than the rest energy of the proton, $m_p c^2 = \hbar\omega$. The required mass of the BH is

$$M = \frac{\hbar c}{8\pi G m_p} \approx 1.1 \cdot 10^{10}\text{kg}.$$

The ratio of the Compton wavelength λ to R is (we now use the Planck units, but the dimensionless ratio is independent of units)

$$\frac{\lambda}{R} = \frac{2\pi}{m_p} 4\pi T = 8\pi^2.$$

Note that this ratio is the same for the massless particles. So the required size of the black hole is significantly smaller than the size of a proton.

Exercise 9.3 (p. 125)

The loss of energy due to Hawking radiation can be written as

$$\frac{dM}{dt} = -\frac{1}{BM^2},$$

where B is a constant. Then the lifetime of a black hole of initial mass M_0 is

$$t_L = \frac{BM_0^3}{3}.$$

In the SI units, this formula becomes

$$t_L = \frac{G^2}{\hbar c^4}\frac{BM_0^3}{3}.$$

The dimensionless coefficient B depends on γ, the number of available degrees of freedom in quantum fields. The order of magnitude of B is estimated as

$$B = \frac{15360\pi}{\gamma} \sim 10^4.$$

We find $t_L \sim 10^{74}$s for $M = M_\odot$; $t_L \sim 10^{19}$s for $M = 10^{15}$g; $t_L \sim 10^{-41}$s for $M = 10^{-5}$g. For comparison, the age of the Universe is of order $\sim 10^{10}$ years or $\sim 3 \cdot 10^{17}$s; the Planck time is $t_{Pl} \approx 5.4 \cdot 10^{-44}$s.

Exercise 9.4 (p. 128)

(a) Here we consider the black hole as a thermodynamical system with a peculiar equation of state. The results are essentially independent of the details of the Hawking radiation, of the kinds of particles emitted by the black hole, and of the nature of the reservoir.

Solution 1: elementary consideration of equilibrium. The equilibrium of a black hole with a reservoir is stable if any small heat exchange causes a reverse exchange. It is intuitively clear that in the equilibrium state the temperatures of the black hole T_{BH} and of the reservoir T_r must be equal. Suppose that initially $T_r = T_{BH}$ and the black hole absorbs an infinitesimal quantity of heat, $\delta Q > 0$, from the reservoir. Then the mass M of the black hole will increase by $\delta M = \delta Q$ and the temperatures will change according to

$$\delta T_r = -\frac{1}{C_r}\delta Q, \quad \delta T_{BH} = \delta\frac{1}{8\pi M} = -\frac{\delta Q}{8\pi M^2} + O\left(\delta Q^2\right).$$

This creates a temperature difference

$$T_{BH} - T_r = \left(\frac{1}{C_r} - \frac{1}{8\pi M^2}\right)\delta Q + O\left(\delta Q^2\right).$$

If $0 < C_r < 8\pi M^2$, then $T_{BH} > T_r$ and the black hole will subsequently tend to give heat to the reservoir, restoring the balance. However, for $C_r > 8\pi M^2$ the created temperature difference is negative, $T_{BH} - T_r < 0$, and the situation is further destabilized since the BH will tend to absorb even more heat.

Similarly, if $\delta Q < 0$ (heat initially lost by the BH), the resulting temperature difference will stabilize the system when $C_r < 8\pi M^2$. Therefore a BH of mass M can be in a stable equilibrium with the reservoir at $T_{BH} = T_r$ only if the heat capacity C_r of the reservoir is positive and not too large, $0 < C_r < 8\pi M^2$.

Solution 2: maximizing the entropy. This is a more rigorous thermodynamical consideration. If a black hole is placed inside a closed reservoir, the total energy of the system is constant and the stable equilibrium is the state of maximum entropy. Let the heat capacity of the reservoir be $C_r\left(T_r\right)$, a known function of the reservoir temperature T_r. We shall determine the energy E_r and the entropy S_r of the reservoir which maximize the entropy.

If the reservoir absorbs an infinitesimal quantity of heat δQ, the first law of thermodynamics yields

$$\delta Q = dE_r = C_r\left(T_r\right)dT_r = T_r dS_r.$$

Therefore

$$E_r\left(T_r\right) = \int_0^{T_r} C_r(T)dT, \quad S_r\left(T_r\right) = \int_0^{T_r}\frac{C_r(T)}{T}dT.$$

The entropy of a black hole with mass M is

$$S_{BH} = 4\pi M^2 = \frac{1}{16\pi T_{BH}^2}$$

and the energy of the BH is equal to its mass,

$$E_{BH} = M = \frac{1}{8\pi T_{BH}}.$$

This indicates a negative heat capacity,

$$C_{BH}(T) = \frac{dE_{BH}}{dT} = -\frac{1}{8\pi T^2}.$$

Now we have the following thermodynamical situation: two systems with temperatures T_1 and T_2 and heat capacities $C_1(T_1)$ and $C_2(T_2)$ are in thermal contact and the combined energy is constant, $E_1(T_1) + E_2(T_2) = \text{const}$. We need to find the state which maximizes the combined entropy $S = S_1(T_1) + S_2(T_2)$. This problem is solved by standard variational methods. The energy constraint gives T_2 as a function of T_1 such that

$$\frac{dT_2(T_1)}{dT_1} = -\frac{C_1(T_1)}{C_2(T_2)}.$$

The extremum condition $dS/dT_1 = 0$ gives

$$\frac{dS}{dT_1} = \frac{C_1(T_1)}{T_1} + \frac{C_2(T_2)}{T_2}\frac{dT_2}{dT_1} = \left(\frac{1}{T_1} - \frac{1}{T_2}\right) C_1(T_1) = 0.$$

Therefore $T_1 = T_2$ is a necessary condition for the equilibrium. The equilibrium is stable if $d^2S/dT_1^2 < 0$ which yields the condition

$$\left.\frac{d^2S}{dT_1^2}\right|_{T_1=T_2} = \frac{d}{dT_1}\left(\frac{1}{T_1} - \frac{1}{T_2}\right) C_1(T_1) = -\frac{C_1}{C_2}\frac{C_1 + C_2}{T_1^2} < 0.$$

Usually heat capacities are positive and the thermal equilibrium is stable. However, in our case $C_1 = C_{BH} < 0$. Therefore the equilibrium is stable if and only if $0 < C_2 = C_r < |C_{BH}|$. The condition for this is

$$0 < C_r < \frac{1}{8\pi T_{BH}^2} = 8\pi M^2.$$

We find that the equilibrium is stable only if the reservoir has a certain finite heat capacity. A combination of a BH and a sufficiently large reservoir is unstable.

(b) The heat capacity of a radiation-filled cavity of volume V is

$$C_r(T_r) = 4\sigma V T_r^3.$$

In equilibrium, $T_r = T_{BH} = T$. The stability condition gives

$$C_r = 4\sigma V T^3 < \frac{1}{8\pi T^2} \;\Rightarrow\; V < V_{\max} = \frac{1}{32\pi\sigma T^5}.$$

A black hole cannot be in a stable equilibrium with a reservoir of volume V larger than $V_{\max}$.

Chapter 10

Exercise 10.1 (p. 130)

a) We start with the normalization factor $\sqrt{2/L}$ in the mode expansion and derive the commutation relation. We integrate the mode expansion over x and use the identity of Eq. (10.4) to get

$$\int_0^L dx\, \hat{\phi}(x,t) \sin\omega_n x = \frac{1}{2}\sqrt{\frac{L}{\omega_n}}\left[\hat{a}_n^- e^{-i\omega_n t} + \hat{a}_n^+ e^{i\omega_n t}\right].$$

Then we differentiate this with respect to t and obtain

$$\int_0^L dx'\, \hat{\pi}(y,t) \sin\omega_n x' = \frac{i}{2}\sqrt{L\omega_n}\left[-\hat{a}_n^- e^{-i\omega_n t} + \hat{a}_n^+ e^{i\omega_n t}\right].$$

Now we can evaluate the commutator

$$\left[\int_0^L dx\, \hat{\phi}(x,t)\sin\omega_n x,\ \int_0^L dy\, \frac{d}{dt}\hat{\phi}(x',t)\sin\omega_{n'}x'\right] = i\frac{L}{2}\left[\hat{a}_n^-, \hat{a}_{n'}^+\right]$$
$$= \int_0^L dx \int_0^L dx'\, \sin\frac{n\pi x}{L}\sin\frac{n'\pi x'}{L} i\delta(x-x') = i\frac{L}{2}\delta_{nn'}.$$

In the second line we used $\left[\hat{\phi}(x,t), \hat{\pi}(x',t)\right] = i\delta(x-x')$. Therefore the standard commutation relations hold for $\hat{a}_n^{\pm}$.

b) The Hamiltonian for the field between the plates is

$$\hat{H} = \frac{1}{2}\int_0^L dx \left[\left(\frac{\partial\hat{\phi}(x,t)}{\partial t}\right)^2 + \left(\frac{\partial\hat{\phi}(x,t)}{\partial x}\right)^2\right].$$

The expression $\langle 0|\,\hat{H}\,|0\rangle$ is evaluated using the mode expansion above and the relations

$$\langle 0|\,\hat{a}_m^-\hat{a}_n^+\,|0\rangle = \delta_{mn}, \quad \langle 0|\,\hat{a}_m^+\hat{a}_n^+\,|0\rangle = \langle 0|\,\hat{a}_m^-\hat{a}_n^-\,|0\rangle = \langle 0|\,\hat{a}_m^+\hat{a}_n^-\,|0\rangle = 0.$$

The first term in the Hamiltonian yields

$$\langle 0|\,\frac{1}{2}\int_0^L dx \left(\frac{\partial\hat{\phi}(x,t)}{\partial t}\right)^2 |0\rangle$$
$$= \langle 0|\,\frac{1}{2}\int_0^L dx \left[\sqrt{\frac{2}{L}}\sum_{n=1}^{\infty}\frac{\sin\omega_n x}{\sqrt{2\omega_n}} i\omega_n\left(-\hat{a}_n^- e^{-i\omega_n t} + \hat{a}_n^+ e^{i\omega_n t}\right)\right]^2 |0\rangle$$
$$= \frac{1}{L}\int_0^L dx \sum_{n=1}^{\infty}\frac{(\sin\omega_n x)^2}{2\omega_n}\omega_n^2 = \frac{1}{4}\sum_n \omega_n.$$

The second term gives the same result, and we find

$$\langle 0|\,\hat{H}\,|0\rangle = \frac{1}{2}\sum_{n=1}^{\infty}\omega_n.$$

Chapter 11

Exercise 11.1 (p. 140)

The propagator was found in the text to be

$$K\left(q_f,q_0;t_f-t_0\right) = \lim_{\Delta t\to 0}\int \frac{dp_f}{2\pi\hbar}\prod_{k=1}^{n}\frac{dp_k dq_k}{2\pi\hbar}$$
$$\times\exp\left[\frac{i\Delta t}{\hbar}\sum_{k=0}^{n}\left(p_{k+1}\frac{q_{k+1}-q_k}{\Delta t}-H\left(p_{k+1},q_k\right)\right)\right].$$

When $H(p,q)$ is of the form (11.8), we can integrate separately over each p_{k+1} using the given Gaussian formula in which we set $a\equiv i\Delta t/m\hbar$ and $b=\left(q_{k+1}-q_k\right)/\hbar$:

$$\int\frac{dp_{k+1}}{2\pi\hbar}\exp\left[\frac{i\Delta t}{\hbar}\left(p_{k+1}\frac{q_{k+1}-q_k}{\Delta t}-H\left(p_{k+1},q_k\right)\right)\right]$$
$$=\frac{\sqrt{m}}{\sqrt{2\pi i\hbar\Delta t}}\exp\left[-\frac{i\Delta t}{\hbar}V\left(q_k\right)-m\frac{\left(q_{k+1}-q_k\right)^2}{2i\hbar\Delta t}\right].$$

This integration is performed $(n+1)$ times over p_{k+1} for $k=0$, ..., n. Replacing

$$\frac{\left(q_{k+1}-q_k\right)^2}{\Delta t}=\dot{q}^2\Delta t+O\left(\Delta t^2\right),$$

we get the following expression under the exponential,

$$\frac{i}{\hbar}\left(\frac{m}{2}\dot{q}^2-V(q)\right)\Delta t.$$

Therefore we obtain the required path integral (11.10) and the measure (11.11).

Exercise 11.2 (p. 140)

In the case of a time-dependent Hamiltonian, the evolution operator $\hat{U}\left(t_f,t_0\right)$ can still be expressed as a product of evolution operators for time intervals,

$$\hat{U}\left(t_f,t_0\right)=\hat{U}\left(t_f,t_n\right)\hat{U}\left(t_n,t_{n-1}\right)...\hat{U}\left(t_1,t_0\right),$$

although these operators do not commute. The propagator can be rewritten as an n-fold integration over q_k as in Eq. (11.2). The evolution throughout a short time interval Δt_k is approximated as

$$\hat{U}\left(t_{k+1}, t_k\right) = 1 - \frac{i\Delta t_k}{\hbar}\hat{H}\left(\hat{p}, \hat{q}, t_k\right) + O\left(\Delta t_k^2\right),$$

since any corrections due to time dependence of $\hat{H}$ will be of higher order in Δt. Then the derivation of the path integral proceeds as in the chapter.

Chapter 12

Exercise 12.1 (p. 142)

The general solution of an inhomogeneous equation such as Eq. (12.5) is a sum of a particular solution and the general solution of the homogeneous equation. We need to use the boundary conditions to select the correct solution.

Elementary solution. For $t \neq t'$, i.e. separately in the two domains $t > t'$ and $t < t'$, the Green's function satisfies the homogeneous equation

$$\left(\frac{\partial^2}{\partial t^2} + \omega^2\right) G_{ret}(t, t') = 0.$$

The general solution is

$$G_{ret}(t, t') = A \sin\omega(t - \alpha),$$

where A and α are constants that are different for $t > t'$ and for $t < t'$. So we may write

$$G_{ret}(t, t') = \begin{cases} A_- \sin\omega\left(t - \alpha_-\right), & t < t' \\ A_+ \sin\omega\left(t - \alpha_+\right), & t > t' \end{cases}$$
$$= A_- \sin\omega\left(t - \alpha_-\right)\theta(t' - t) + A_+ \sin\omega\left(t - \alpha_+\right)\theta(t - t').$$

The boundary condition $G_{ret}(t, t') = 0$ for $t < t'$ forces $A_- = 0$. Therefore by continuity $G_{ret}(t', t') = 0$ and $\alpha_+ = t'$. To find A_+, we integrate Eq. (12.5) over a small interval of t around t' and obtain:

$$\int_{t'-\Delta t}^{t'+\Delta t}\left[\frac{\partial^2 G_{ret}}{\partial t^2} + \omega^2 G_{ret}\right] dt = \int_{t'-\Delta t}^{t'+\Delta t}\delta(t - t')dt = 1.$$

For small $\Delta t \to 0$ this gives

$$\lim_{t\to t'+0}\frac{\partial G}{\partial t} - \lim_{t\to t'-0}\frac{\partial G}{\partial t} = 1.$$

Therefore $A_+ = \omega^{-1}$ and we find the required solution.

Solution using Fourier transforms. A Fourier transform of Eq. (12.5) gives the Fourier image $g(\Omega)$,

$$g(\Omega) = \int_{-\infty}^{+\infty} dt\, G_{ret}(t,t')e^{-i\Omega(t-t')}.$$

The function $g(\Omega)$ must satisfy the equation

$$g(\Omega)\left(\omega^2 - \Omega^2\right) = 1. \tag{D.29}$$

Here $g(\Omega)$ should be treated as a distribution (see Appendix A.1). The general solution of Eq. (D.29) in the space of distributions is

$$g(\Omega) = \mathcal{P}\frac{1}{\omega^2 - \Omega^2} + a_+\delta(\omega - \Omega) + a_-\delta(\omega + \Omega), \tag{D.30}$$

where $\mathcal{P}$ denotes the Cauchy principal value and $a_\pm$ are unknown constants.

The general form of Green's function with arbitrary constants corresponds to the freedom of choosing a solution of the homogeneous equation. The values $a_\pm$ must be determined from the boundary condition $G_{ret}(t,t') = 0$ for $t < t'$. The inverse Fourier transform of Eq. (D.30) gives

$$G_{ret}(t,t') = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\Omega e^{i\Omega(t-t')}g(\Omega)$$
$$= \frac{1}{2\pi}\left[\mathcal{P}\int_{-\infty}^{+\infty}\frac{e^{i\Omega(t-t')}}{\omega^2-\Omega^2}d\Omega + a_+e^{i\omega(t-t')} + a_-e^{-i\omega(t-t')}\right].$$

This expression confirms our expectation that the terms with $a_\pm$ represent the as-yet unspecified solution of the homogeneous oscillator equation. Now the principal value integral is computed using contour integration. For $t < t'$ the contour must be deformed into the lower half-plane $Im\,\Omega < 0$ while for $t > t'$ one must use the upper half-plane. We find

$$\frac{1}{2\pi}\mathcal{P}\int_{-\infty}^{+\infty}\frac{e^{i\Omega(t-t')}}{\omega^2-\Omega^2}d\Omega = \mathrm{sign}(t-t')\frac{\sin\omega(t-t')}{2\omega} = \frac{1}{2\omega}\sin\omega\,|t-t'|\,.$$

To satisfy the boundary conditions, the constants must be chosen as

$$a_\pm = \pm\frac{\pi}{2i\omega} \tag{D.31}$$

and then we obtain

$$G_{ret}(t,t') = \theta(t-t')\frac{\sin\omega(t-t')}{\omega}. \tag{D.32}$$

Exercise 12.2 (p. 145)

An elementary solution (without using Fourier transforms) can be found similarly to Exercise 12.1.

Solution using Fourier transforms. Performing a Fourier transform of Eq. (12.15), we obtain the equation

$$g(\Omega)\left(\omega^2+\Omega^2\right)=1$$

for the Fourier image $g(\Omega)$ defined by

$$g(\Omega)=\int_{-\infty}^{+\infty} d\tau\, G_E(\tau,\tau')e^{-i\Omega(\tau-\tau')}. \tag{D.33}$$

Here we have *already assumed* that the Green's function $G_E(\tau,\tau')$ tends to zero at large $|\tau|$ because otherwise the Fourier transform (D.33) would not exist. We obtain

$$g(\Omega)=\frac{1}{\Omega^2+\omega^2}$$

and the inverse Fourier transform presents no special problems since there are no poles on the real Ω line,

$$G_E(\tau,\tau')=\frac{1}{2\pi}\int_{-\infty}^{+\infty} d\Omega e^{i\Omega(\tau-\tau')}g(\Omega)=\frac{1}{2\pi}\int_{-\infty}^{+\infty} d\Omega\frac{e^{i\Omega(\tau-\tau')}}{\Omega^2+\omega^2}.$$

The integral is evaluated using contour integration and yields the answer (12.14). The boundary condition $G_E(\tau\to\pm\infty,\tau')=0$ is satisfied automatically.

Exercise 12.3 (p. 153)

According to the approach explained in the text, we expect to find the in-out matrix element by considering the ratio of the path integrals

$$\frac{\int a^+(t)a^-(t)e^{iS[q,J]}\mathcal{D}q}{\int e^{iS[q,J]}\mathcal{D}q} \tag{D.34}$$

and by replacing the Feynman Green's function $G_F(t,t')$ by the retarded Green's function $G_{ret}(t,t')$ in the effective action. To compute the path integrals in Eq. (D.34), consider the action

$$S\left[q,J^+,J^-\right]=\int\left(\frac{1}{2}\dot{q}^2-\frac{\omega^2}{2}q^2+J^+a^++J^-a^-\right)dt,$$

where $J^+(t)$ and $J^-(t)$ are two external forces. This action is real-valued since $J^-=(J^+)^*$. The Lorentzian effective action is

$$\exp\left(i\Gamma_L\left[J^+,J^-\right]\right)=\int\mathcal{D}q\, e^{iS\left[q,J^+,J^-\right]},$$

where the integration is over all paths $q(t)$ satisfying $q(t\to\pm\infty)=0$, as in the text. If we compute this effective action, the path integral ratio of Eq. (D.34) will be

$$\exp\left[-i\Gamma_L\right]\frac{\delta}{i\delta J^+(t)}\frac{\delta}{i\delta J^-(t)}\exp\left[i\Gamma_L\right]. \tag{D.35}$$

We express $a^{\pm}$ through q and $\dot{q}$ as

$$a^{+}(t)=\sqrt{\frac{\omega}{2}}\left(q(t)-\frac{i}{\omega}\dot{q}(t)\right),$$
$$a^{-}(t)=\sqrt{\frac{\omega}{2}}\left(q(t)+\frac{i}{\omega}\dot{q}(t)\right).$$

Then after integrations by parts we obtain

$$\int\left(J^{+}a^{+}-J^{-}a^{-}\right)dt=\int\sqrt{\frac{\omega}{2}}\left(J^{+}+\frac{i}{\omega}\frac{dJ^{+}}{dt}+J^{-}-\frac{i}{\omega}\frac{dJ^{-}}{dt}\right)q(t)dt,$$

and therefore the Lorentzian effective action can be copied from the text,

$$\Gamma_{L}\left[J\right]=\frac{1}{2}\iint J\left(t_{1}\right)J\left(t_{2}\right)G_{F}\left(t_{1},t_{2}\right)dt_{1}dt_{2}, \tag{D.36}$$

if we use for $J(t)$ the expression

$$J(t)=\sqrt{\frac{\omega}{2}}\left(J^{+}+\frac{i}{\omega}\frac{dJ^{+}}{dt}+J^{-}-\frac{i}{\omega}\frac{dJ^{-}}{dt}\right). \tag{D.37}$$

Now we should substitute Eq. (D.36) into Eq. (D.35), using $J(t)$ given by Eq. (D.37), and then replace G_F by G_{ret}. Then we will find the required matrix element according to the recipe presented in the text.

First, the expression (D.35) is simplified to

$$\frac{\delta\Gamma_{L}}{\delta J^{+}(t)}\frac{\delta\Gamma_{L}}{\delta J^{-}(t')}-i\frac{\delta^{2}\Gamma_{L}}{\delta J^{+}(t)\delta J^{-}(t')}.$$

The functional derivatives are evaluated like this,

$$\frac{\delta\Gamma_{L}}{\delta J^{+}(t)}=\int d\tilde{t}\frac{\delta\Gamma_{L}\left[J\right]}{\delta J\left(\tilde{t}\right)}\frac{\delta J\left(\tilde{t}\right)}{\delta J^{+}(t)}.$$

Using Eq. (D.36) and the fact that $G_F(t,t')$ is a symmetric function of t and t', we find

$$\frac{\delta\Gamma_{L}}{\delta J(t)}=\int J\left(t_{1}\right)G_{F}\left(t,t_{1}\right)dt_{1}.$$

To compute the functional derivative $\delta J/\delta J^{+}$, we write J as a functional of J^{+} in an integral form:

$$J\left(\tilde{t}\right)=\int J^{+}(t)\sqrt{\frac{\omega}{2}}\left[\delta\left(t-\tilde{t}\right)-\frac{i}{\omega}\delta'\left(t-\tilde{t}\right)\right]dt+c.c.$$

where we denoted the complex conjugate terms with $J^{-}=\left(J^{+}\right)^{*}$ by "$c.c.$". Then

$$\frac{\delta J\left(\tilde{t}\right)}{\delta J^{+}(t)}=\sqrt{\frac{\omega}{2}}\left[\delta\left(t-\tilde{t}\right)-\frac{i}{\omega}\delta'\left(t-\tilde{t}\right)\right],$$

and we obtain

$$\frac{\delta\Gamma_L}{\delta J^+(t)} = \sqrt{\frac{\omega}{2}} \int dt_1 J(t_1) \left[G_F(t,t_1) - \frac{i}{\omega}\frac{\partial}{\partial t} G_F(t,t_1) \right].$$

Now replacing G_F by G_{ret} and simplifying

$$G_{ret}(t,t_1) - \frac{i}{\omega}\frac{\partial}{\partial t} G_{ret}(t,t_1) = \theta(t-t_1)\frac{e^{i\omega(t-t_1)}}{i\omega},$$

we get

$$\frac{\delta\Gamma_L}{\delta J^+(t)} = -\frac{i}{\sqrt{2\omega}} \int_0^T dt_1 J(t_1) e^{i\omega t_1} \equiv -J_0.$$

The functional derivative $\delta\Gamma_L/\delta J^-(t)$ is the complex conjugate of this expression, so

$$\frac{\delta\Gamma_L}{\delta J^+(t)}\frac{\delta\Gamma_L}{\delta J^-(t)} = |J_0|^2.$$

The second functional derivative

$$\frac{\delta^2\Gamma_L}{\delta J^+(t_1)\,\delta J^-(t_2)}$$

gives terms independent of J because $\Gamma_L[J]$ is a quadratic functional of J. But the expectation value we are computing cannot have any terms independent of J since it should be equal to 0 when $J \equiv 0$. Therefore any terms we get from this functional derivative are spurious and we ignore them. Note that one of the ignored terms is proportional to $\delta(t_1 - t_2)$ and would diverge for $t_1 = t_2$.

Finally, we obtain

$$\langle 0_{in}|\, \hat{a}^+(t)\hat{a}^-(t)\, |0_{in}\rangle = |J_0|^2.$$

This agrees with the answer obtained in Eq. (3.12).

Chapter 14

Exercise 14.1 (p. 173)

We omit the trivial term $-V(x)\delta(x-x')$ from $\hat{M}$, compute the generalized function $g^{1/4}\Box_{g(x)}g^{-1/4}\delta(x-x')$ and substitute $g_{\alpha\beta} = \delta_{\alpha\beta} + h_{\alpha\beta}$ into the result. Denoting $\partial_\mu \equiv \partial/\partial x^\mu$ and suppressing the arguments of $\delta(x-x')$ for brevity, we find

$$\begin{aligned}
\partial_\mu\left(g^{-1/4}\delta\right) =& g^{-1/4}\left(\delta_{,\mu} - \frac{1}{4}(\ln g)_{,\mu}\delta\right), \\
g^{-1/4}\partial_\nu\left[g^{\mu\nu}\sqrt{g}\partial_\mu\left(g^{-1/4}\delta\right)\right] =& g^{\mu\nu}\left(\delta_{,\mu} - \frac{1}{4}(\ln g)_{,\mu}\delta\right)_{,\nu} \\
&+ \left(g^{\mu\nu}_{\ ,\nu} + \frac{1}{4}g^{\mu\nu}(\ln g)_{,\nu}\right)\left(\delta_{,\mu} - \frac{1}{4}(\ln g)_{,\mu}\delta\right).
\end{aligned}$$

This expression splits into terms with different orders of derivatives of $\delta(x-x')$. The derivatives of $g_{\alpha\beta}$ are replaced with the derivatives of $h_{\alpha\beta}$, but otherwise we keep $g_{\alpha\beta}$. (Therefore we do not actually need to make any approximations in this calculation and in particular do not need to assume that $h_{\alpha\beta}$ is small.) The term with the second derivative is

$$g^{\mu\nu}\delta_{,\mu\nu} = \delta^{\mu\nu}\partial_\mu\partial_\nu\delta(x-x') + h^{\mu\nu}\partial_\mu\partial_\nu\delta(x-x').$$

This corresponds to the operator expression $\Box + \hat{h}$. The term with the first derivative of δ is

$$-\frac{1}{4}g^{\mu\nu}(\ln g)_{,\mu}\delta_{,\nu} + g^{\mu\nu}_{,\nu}\delta_{,\mu} + \frac{1}{4}g^{\mu\nu}(\ln g)_{,\nu}\delta_{,\mu} = h^{\mu\nu}_{,\mu}\delta_{,\nu}.$$

This corresponds to the operator $\hat{\Gamma}$. Finally, the term without derivatives of $\delta(x-x')$ is $P(x)\delta(x-x')$, where

$$\begin{aligned} P(x) =& -\frac{1}{4}g^{\mu\nu}(\ln g)_{,\mu\nu} - \frac{1}{4}\left(g^{\mu\nu}_{,\nu} + \frac{1}{4}g^{\mu\nu}(\ln g)_{,\nu}\right)(\ln g)_{,\mu} \\ =& -\frac{1}{4}g^{\mu\nu}g^{\alpha\beta}h_{\alpha\beta,\mu\nu} - \frac{1}{4}g^{\mu\nu}h^{\alpha\beta}_{,\mu}h_{\alpha\beta,\nu} \\ & -\frac{1}{4}h^{\mu\nu}_{,\nu}g^{\alpha\beta}h_{\alpha\beta,\mu} - \frac{1}{16}g^{\mu\nu}g^{\alpha\beta}g^{\kappa\lambda}h_{\alpha\beta,\mu}h_{\kappa\lambda,\nu}. \end{aligned}$$

Here we substituted

$$(\ln g)_{,\mu} = g^{\alpha\beta}g_{\alpha\beta,\mu} = g^{\alpha\beta}h_{\alpha\beta,\mu}.$$

It remains to add the omitted term $-V(x)\delta(x-x')$ to $\hat{P}$ to obtain the required result.

Exercise 14.2 (p. 176)

Rewrite the argument of the exponential as a complete square,

$$\begin{aligned} & -A\left|\mathbf{x}-\mathbf{a}\right|^2 - B\left|\mathbf{x}-\mathbf{b}\right|^2 + 2\mathbf{c}\cdot\mathbf{x} \\ & \quad = -(A+B)\left|\mathbf{x}\right|^2 + 2\mathbf{x}\cdot(A\mathbf{a}+B\mathbf{b}+\mathbf{c}) - \left(Aa^2+Bb^2\right) \\ & \quad \equiv -(A+B)\left|\mathbf{x}-\mathbf{p}\right|^2 + Q. \end{aligned}$$

Here we introduced the auxiliary vector $\mathbf{p}$ and the constant Q:

$$\mathbf{p} \equiv \frac{A\mathbf{a}+B\mathbf{b}+\mathbf{c}}{A+B}, \quad Q \equiv (A+B)p^2 - \left(Aa^2+Bb^2\right).$$

The Gaussian integration yields the required expression:

$$\int d^{2\omega}\mathbf{x}\,\exp\left[-(A+B)\left|\mathbf{x}-\mathbf{p}\right|^2 + Q\right] = \frac{\pi^\omega\exp\left[Q\right]}{(A+B)^\omega},$$

$$Q = -\frac{AB}{A+B}\left|\mathbf{a}-\mathbf{b}\right|^2 + 2\mathbf{c}\cdot\frac{A\mathbf{a}+B\mathbf{b}}{A+B} + \frac{\left|\mathbf{c}\right|^2}{A+B}.$$

Exercise 14.3 (p. 177)

Following the method used in the text for the calculation of $\langle x|\, \hat{K}_1^{\Gamma}\, |y\rangle$, we find

$$\langle x|\, \hat{K}_1^{h}(\tau)\, |y\rangle = \frac{\partial^2}{\partial y^\mu \partial y^\nu} \langle x|\, \hat{K}_1^{P}(\tau)\, |y\rangle \Big|_{P(z)\to h^{\mu\nu}(z)}.$$

Now we use Eq. (14.16) to evaluate the second derivative and then substitute $y = x$. We find

$$\frac{\partial^2}{\partial y^\mu \partial y^\nu}\Big|_{y=x} \exp\left[-\frac{(x-y)^2}{4\tau}\right] = -\frac{\delta_{\mu\nu}}{2\tau},$$
$$\frac{\partial^2}{\partial y^\mu \partial y^\nu}\Big|_{y=x} h^{\mu\nu}\left(x + \frac{\tau-\tau'}{\tau}(y-x)\right) = \left(\frac{\tau-\tau'}{\tau}\right)^2 h^{\mu\nu}_{,\mu\nu}.$$

The terms with first derivatives are proportional to $(x^\mu - y^\mu)$ and vanish in the limit $y \to x$. Therefore we obtain the required expression.

Exercise 14.4 (p. 178)

Note that $h^{\mu\nu} = -h_{\alpha\beta}g^{\mu\alpha}g^{\nu\beta} + O(h^2)$ and since we may omit terms of order $O(h^2)$, we can convert covariant components $h_{\mu\nu}$ to contravariant $h^{\mu\nu}$ by a change of sign.

The first required identity is derived by

$$\frac{\partial\sqrt{g}}{\partial g^{\mu\nu}} = -\frac{1}{2}\sqrt{g}g_{\mu\nu} \;\Rightarrow\; \sqrt{\det\left(\delta_{\mu\nu} + h_{\mu\nu}\right)} = 1 - \frac{1}{2}\delta_{\mu\nu}h^{\mu\nu} + O\left(h^2\right).$$

Expanding the metric according to Eq. (14.1), we get

$$\Gamma^\nu_{\alpha\beta} = \frac{1}{2}g^{\mu\nu}\left(h_{\alpha\mu,\beta} + h_{\beta\mu,\alpha} - h_{\alpha\beta,\mu}\right),$$
$$g^{\alpha\beta}\partial_\nu\Gamma^\nu_{\alpha\beta} = \delta^{\alpha\beta}\delta^{\mu\nu}\left(h_{\alpha\mu,\beta\nu} - \frac{1}{2}h_{\alpha\beta,\mu\nu}\right) + O(h^2),$$
$$g^{\alpha\beta}\partial_\beta\Gamma^\nu_{\alpha\nu} = \frac{1}{2}\delta^{\alpha\beta}\delta^{\mu\nu}h_{\mu\nu,\alpha\beta} + O(h^2).$$

Using Eq. (5.19), we compute the scalar curvature as

$$\begin{aligned} R &= g^{\alpha\beta}\partial_\nu\Gamma^\nu_{\alpha\beta} - g^{\alpha\beta}\partial_\beta\Gamma^\nu_{\alpha\nu} + O(h^2) \\ &= \delta^{\alpha\beta}\delta^{\mu\nu}\left(h_{\alpha\mu,\beta\nu} - h_{\alpha\beta,\mu\nu}\right) + O(h^2) \\ &= -\delta_{\alpha\beta}\delta_{\mu\nu}\left(h^{\alpha\mu,\beta\nu} - h^{\alpha\beta,\mu\nu}\right) + O(h^2) \\ &= \delta_{\alpha\beta}\Box h^{\alpha\beta} - h^{\mu\nu}_{,\mu\nu} + O(h^2). \end{aligned}$$

Here we have used the relation $g^{\alpha\beta} = \delta^{\alpha\beta} + O(h)$.

Exercise 14.5 (p. 180)

The required values are found by computing the following limits:

$$f_1(0) = \lim_{\xi\to 0}\int_0^1 e^{-\xi u(1-u)}du = 1;$$
$$\lim_{\xi\to 0}\frac{f_1(\xi)-1}{\xi} = \left.\frac{df_1}{d\xi}\right|_{\xi=0} = -\int_0^1 u(1-u)du = -\frac{1}{6};$$
$$\lim_{\xi\to 0}\frac{f_1(\xi)-1+\frac{1}{6}\xi}{\xi^2} = \frac{1}{2}\left.\frac{d^2f_1}{d\xi^2}\right|_{\xi=0} = \frac{1}{2}\int_0^1 u^2(1-u)^2du = \frac{1}{60}.$$

Chapter 15

Exercise 15.1 (p. 186)

The task is to compute the integral

$$I_0 \equiv \frac{1}{32}\int_0^\infty dx\left(f_1(x) + 4\frac{f_1(x)-1}{x} + 12\frac{f_1(x)-1+\frac{1}{6}x}{x^2}\right) = \frac{1}{12},$$

where the function $f_1(x)$ is defined by

$$f_1(x) \equiv \int_0^1 dt\, e^{-xt(1-t)}.$$

Since

$$\int_0^1 t(1-t)dt = \frac{1}{6},$$

we may rewrite I_0 as

$$I_0 = \frac{1}{32}\int_0^\infty dx\int_0^1 dt\left(e^{-xt(1-t)} + 4\frac{e^{-xt(1-t)}-1}{x} + 12\frac{e^{-xt(1-t)}-1+xt(1-t)}{x^2}\right).$$

It is impossible to exchange the order of integration because of the nonuniform convergence of the double integral at large x. Therefore we add a regularization factor e^{-ax} with $a > 0$ and evaluate the limit $a \to 0$ at the end of the calculation,

$$I_0 = \lim_{a\to 0}\frac{1}{32}\int_0^1 dt\int_0^\infty dx\, e^{-ax}\left(e^{-xt(1-t)} + 4\frac{e^{-xt(1-t)}-1}{x}\right.$$
$$\left.+12\frac{e^{-xt(1-t)}-1+xt(1-t)}{x^2}\right).$$

Denote $q \equiv t(1-t)$. The integration over x can be performed using the auxiliary integrals

$$I_1(a,q) \equiv \int_0^\infty dx\, e^{-ax} \frac{e^{-qx}-1}{x} = \ln\frac{a}{a+q},$$
$$I_2(a,q) \equiv \int_0^\infty dx\, e^{-ax} \frac{e^{-qx}-1+qx}{x^2} = -q-(a+q)\ln\frac{a}{a+q}.$$

The functions $I_{1,2}(a,q)$ are easily found by integrating the equations

$$\frac{\partial I_1}{\partial q} = -\frac{1}{a+q}, \quad I_1(a, q=0) = 0;$$
$$\frac{\partial I_2}{\partial q} = -I_1(a,q), \quad I_2(a, q=0) = 0.$$

Then we express the integral I_0 as

$$I_0 = \frac{1}{32}\lim_{a\to 0}\int_0^1 dt \left(\frac{1}{a+t(1-t)} + 4\ln\frac{a}{a+t(1-t)} \right.$$
$$\left. +12\,(a+t(1-t))\ln\frac{a}{a+t(1-t)} - 12t(1-t)\right).$$

The last integral is elementary although rather cumbersome to compute. While performing this last calculation, it helps to decompose

$$a+t(1-t) = (a_1-t)\,(t-a_2), \quad a_{1,2} \equiv \frac{1}{2} \pm \sqrt{\frac{1}{4}+a}.$$

The limit $a \to 0$ should be performed after evaluating the integral. The result is

$$I_0 = \frac{1}{32}\lim_{a\to 0}\left[\frac{8}{3} - 16a - 32a^2\ln a + o\left(a^2\right)\right] = \frac{1}{12}.$$

Exercise 15.2 (p. 188)

In this and the following exercise, the symbol $\delta g^{\mu\nu}$ stands for the variation of the contravariant metric $g^{\mu\nu}$. Since $g_{\alpha\nu}g^{\alpha\mu} = \delta^\mu_\nu$, we have

$$0 = \delta\left(g_{\alpha\nu}g^{\alpha\mu}\right) = g_{\alpha\nu}\delta g^{\alpha\mu} + g^{\alpha\mu}\delta g_{\alpha\nu}.$$

Thus the variation $\delta g_{\mu\nu}$ of the covariant tensor $g_{\mu\nu}$ is

$$\delta g_{\mu\nu} = -g_{\alpha\mu}g_{\beta\nu}\delta g^{\alpha\beta}.$$

(a) First we prove that the variation $\delta\Gamma^\alpha_{\mu\nu}$ of the Christoffel symbol is a tensor quantity even though $\Gamma^\alpha_{\mu\nu}$ itself is not a tensor. Indeed, the components

$$\Gamma^\alpha_{\mu\nu} = \frac{1}{2}g^{\alpha\beta}\left(\partial_\mu g_{\beta\nu} + \partial_\nu g_{\beta\mu} - \partial_\beta g_{\mu\nu}\right)$$

change under a coordinate transformation according to a non-tensor law

$$\Gamma'^{\alpha}_{\mu\nu} = \frac{\partial x'^{\alpha}}{\partial x^{\beta}} \frac{\partial x^{\rho}}{\partial x'^{\mu}} \frac{\partial x^{\sigma}}{\partial x'^{\nu}} \Gamma^{\beta}_{\rho\sigma} + \frac{\partial x'^{\alpha}}{\partial x^{\beta}} \frac{\partial^2 x^{\beta}}{\partial x'^{\mu} \partial x'^{\nu}}. \tag{D.38}$$

However, it follows from Eq. (D.38) that the variation $\delta\Gamma^{\alpha}_{\mu\nu}$ transforms as

$$\delta\Gamma'^{\alpha}_{\mu\nu} = \frac{\partial x'^{\alpha}}{\partial x^{\beta}} \frac{\partial x^{\rho}}{\partial x'^{\mu}} \frac{\partial x^{\sigma}}{\partial x'^{\nu}} \delta\Gamma^{\beta}_{\rho\sigma}$$

and is therefore a third rank tensor.

We can always choose a locally inertial frame such that $\tilde{\Gamma}^{\alpha}_{\mu\nu}(x) = 0$ at a given spacetime point x. In that frame, the covariant derivative coincides with the ordinary derivative, i.e. $\tilde{\nabla}_{\mu} = \tilde{\partial}_{\mu}$, where the tilde means that the quantities are computed in the locally inertial frame at point x. Then the variation of the Christoffel symbol $\tilde{\Gamma}^{\alpha}_{\mu\nu}$ is

$$\begin{aligned} \delta\tilde{\Gamma}^{\alpha}_{\mu\nu} &= \frac{1}{2}\delta\tilde{g}^{\alpha\beta}\left(\tilde{\partial}_{\mu}\tilde{g}_{\beta\nu} + \tilde{\partial}_{\nu}\tilde{g}_{\beta\mu} - \tilde{\partial}_{\beta}\tilde{g}_{\mu\nu}\right) + \frac{1}{2}g^{\alpha\beta}\left(\tilde{\partial}_{\mu}\delta\tilde{g}_{\beta\nu} + \tilde{\partial}_{\nu}\delta\tilde{g}_{\beta\mu} - \tilde{\partial}_{\beta}\delta\tilde{g}_{\mu\nu}\right) \\ &= \frac{1}{2}g^{\alpha\beta}\left(\tilde{\partial}_{\mu}\delta\tilde{g}_{\beta\nu} + \tilde{\partial}_{\nu}\delta\tilde{g}_{\beta\mu} - \tilde{\partial}_{\beta}\delta\tilde{g}_{\mu\nu}\right) = \frac{1}{2}\left(\tilde{\nabla}_{\mu}\delta\tilde{g}_{\beta\nu} + \tilde{\nabla}_{\nu}\delta\tilde{g}_{\beta\mu} - \tilde{\nabla}_{\beta}\delta\tilde{g}_{\mu\nu}\right) \end{aligned} \tag{D.39}$$

because in the locally inertial frame we have

$$\tilde{\partial}_{\mu}\tilde{g}_{\beta\nu} + \tilde{\partial}_{\nu}\tilde{g}_{\beta\mu} - \tilde{\partial}_{\beta}\tilde{g}_{\mu\nu} = \tilde{\Gamma}^{\alpha}_{\mu\nu}\tilde{g}_{\alpha\beta} = 0.$$

Since the last expression in Eq. (D.39) involves explicitly tensorial quantities, the tensor $\delta\Gamma^{\alpha}_{\mu\nu}$ is equal to

$$\delta\Gamma^{\alpha}_{\mu\nu} = \frac{g^{\alpha\beta}}{2}\left(\nabla_{\mu}\delta g_{\beta\nu} + \nabla_{\nu}\delta g_{\beta\mu} - \nabla_{\beta}\delta g_{\mu\nu}\right) \equiv \frac{g^{\alpha\beta}}{2}\left(\delta g_{\beta\mu;\nu} + \delta g_{\beta\nu;\mu} - \delta g_{\mu\nu;\beta}\right) \tag{D.40}$$

in *all* coordinate systems. (Here is a more rigorous argument: We first consider the tensor (D.40) which happens to coincide with Eq. (D.39) in a particular coordinate system and only at the point x. However, two tensors cannot coincide in one coordinate frame but differ in another frame. Therefore the tensor $\delta\Gamma^{\alpha}_{\mu\nu}(x)$ is given by Eq. (D.40) in all coordinate systems. Since the construction is independent of the chosen point x, it follows that the formula (D.40) is valid for all x.)

Note that an explicit formula for the covariant derivative $\nabla_{\beta}\delta g_{\mu\nu}$ is

$$\nabla_{\beta}\delta g_{\mu\nu} = \partial_{\beta}\delta g_{\mu\nu} - \Gamma^{\alpha}_{\beta\nu}\delta g_{\alpha\mu} - \Gamma^{\alpha}_{\beta\mu}\delta g_{\alpha\nu}.$$

The trick of choosing a locally inertial frame helps us avoid cumbersome computations with such expressions.

(b) Since

$$\Box_g \Box_g^{-1} = \hat{1},$$

we have

$$0 = \delta\left(\Box_g \Box_g^{-1}\right) = \Box_g\left(\delta\Box_g^{-1}\right) + (\delta\Box_g)\,\Box_g^{-1}$$

and hence

$$\delta\left(\Box_g^{-1}\right) = -\Box_g^{-1}\,(\delta\Box_g)\,\Box_g^{-1}. \tag{D.41}$$

The covariant Laplace operator $\Box_g$ acting on a scalar function $\phi(x)$ is

$$\Box_g\phi \equiv g^{\mu\nu}\nabla_\mu\nabla_\nu\phi = g^{\mu\nu}\phi_{;\mu\nu} = g^{\mu\nu}\left(\phi_{,\mu\nu} - \Gamma^\alpha_{\mu\nu}\phi_{,\alpha}\right).$$

The variation of this expression with respect to $\delta g^{\mu\nu}$ is

$$\delta\Box_g\phi = (\delta g^{\mu\nu})\,\phi_{;\mu\nu} + g^{\mu\nu}\delta\left[\phi_{,\mu\nu} - \Gamma^\alpha_{\mu\nu}\phi_{,\alpha}\right] = (\delta g^{\mu\nu})\,\phi_{;\mu\nu} - g^{\mu\nu}\left(\delta\Gamma^\alpha_{\mu\nu}\right)\phi_{,\alpha}.$$

This can be rewritten as an operator identity

$$\delta\Box_g = (\delta g^{\mu\nu})\,\nabla_\mu\nabla_\nu - g^{\mu\nu}\left(\delta\Gamma^\alpha_{\mu\nu}\right)\nabla_\alpha. \tag{D.42}$$

We emphasize that this identity holds only when the operators act on a *scalar* function $\phi(x)$. For vector- or tensor-valued functions, the formula would have to be modified.

(c) To derive

$$\delta R^\alpha{}_{\beta\mu\nu} = \nabla_\mu\delta\Gamma^\alpha_{\beta\nu} - \nabla_\nu\delta\Gamma^\alpha_{\mu\beta}, \tag{D.43}$$

we again pass to a locally inertial frame in which $\tilde\Gamma^\alpha_{\mu\nu} = 0$ and $\tilde\nabla_\mu = \tilde\partial_\mu$. Then the Riemann tensor (in the Landau-Lifshitz sign convention) is

$$\tilde R^\alpha{}_{\beta\mu\nu} = \tilde\partial_\mu\tilde\Gamma^\alpha_{\beta\nu} - \tilde\partial_\nu\tilde\Gamma^\alpha_{\mu\beta}. \tag{D.44}$$

Note that the RHS of this expression is not a tensor. Varying both hand sides of the relation (D.44), we obtain

$$\delta\tilde R^\alpha{}_{\beta\mu\nu} = \tilde\partial_\mu\delta\tilde\Gamma^\alpha_{\beta\nu} - \tilde\partial_\nu\delta\tilde\Gamma^\alpha_{\mu\beta} = \tilde\nabla_\mu\delta\tilde\Gamma^\alpha_{\beta\nu} - \tilde\nabla_\nu\delta\tilde\Gamma^\alpha_{\mu\beta}. \tag{D.45}$$

Note that both sides of Eq. (D.45) are written in an explicitly covariant form and are tensors. Therefore Eq. (D.45) holds in all coordinate systems and Eq. (D.43) follows.

Exercise 15.3 (p. 188)

Here we derive the energy-momentum tensor

$$\langle T_{\mu\nu}\rangle = \frac{2}{\sqrt{-g}}\frac{\delta\Gamma_L}{\delta g^{\mu\nu}}$$

corresponding to the (Lorentzian) Polyakov effective action

$$\begin{aligned}\Gamma_L[g_{\mu\nu}] &= \frac{1}{96\pi}\int d^2x\sqrt{-g}R\,\Box_g^{-1}R \\ &\equiv \frac{1}{96\pi}\int d^2x\sqrt{-g(x)}\int d^2y\sqrt{-g(y)}R(x)G_g(x,y)R(y),\end{aligned} \tag{D.46}$$

where $G_g(x,y)$ is the (retarded) Green's function of the Laplace operator $\Box_g$. Recall that we have

$$\left(\Box_g^{-1}\Phi\right)(x) \equiv \int d^2y\sqrt{-g(y)}G_g(x,y)\Phi(y),$$

where Φ is a scalar field, and the Green's function satisfies

$$^x\Box_g G_g(x,y) = \frac{1}{\sqrt{-g(x)}}\delta(x-y).$$

The variation of $\sqrt{-g}R\,\Box_g^{-1}R$ can be written as

$$\frac{1}{\sqrt{-g}}\delta\left(\sqrt{-g}R\,\Box_g^{-1}R\right) = \frac{\delta\sqrt{-g}}{\sqrt{-g}}R\Box_g^{-1}R + (\delta R)\,\Box_g^{-1}R + R\Box_g^{-1}(\delta R) + R\left(\delta\Box_g^{-1}\right)R$$

(we have introduced the prefactor $1/\sqrt{-g}$ for convenience). This expression is integrated over d^2x, while the operator $\Box_g^{-1}$ is self-adjoint, which entails

$$\int d^2x\sqrt{-g}\,(\delta R)\,\Box_g^{-1}R = \int d^2x\sqrt{-g}R\,\Box_g^{-1}(\delta R)\,.$$

Thus for our purposes it is sufficient to compute the auxiliary quantity

$$\delta I \equiv \frac{\delta\sqrt{-g}}{\sqrt{-g}}R\Box_g^{-1}R + 2\,(\delta R)\,\Box_g^{-1}R + R\left(\delta\Box_g^{-1}\right)R. \tag{D.47}$$

The EMT is expressed through δI using

$$\int d^2x\sqrt{-g}\,\langle T_{\mu\nu}\rangle\,\delta g^{\mu\nu} = \frac{1}{48\pi\sqrt{-g}}\int d^2x\sqrt{-g}\,\delta I\,(x)\,. \tag{D.48}$$

Now we shall evaluate the expression (D.47) term by term. The variation of $\sqrt{-g}$ is (see Eq. D.13 on p. 227)

$$\frac{\delta\sqrt{-g}}{\sqrt{-g}} = -\frac{1}{2}g_{\mu\nu}\delta g^{\mu\nu}. \tag{D.49}$$

In two dimensions, the Ricci tensor $R_{\mu\nu} \equiv R^{\alpha}{}_{\mu\alpha\nu}$ is related to the Ricci scalar as

$$R_{\mu\nu} = \frac{1}{2}g_{\mu\nu}R,$$

therefore with help of Eq. (D.43) we get

$$\delta R = R_{\mu\nu}\delta g^{\mu\nu} + g^{\mu\nu}\delta R_{\mu\nu} = \frac{1}{2}Rg_{\mu\nu}\delta g^{\mu\nu} + \nabla_\alpha\left(g^{\mu\nu}\delta\Gamma^\alpha_{\mu\nu} - g^{\mu\alpha}\delta\Gamma^\nu_{\mu\nu}\right). \tag{D.50}$$

Using the formula (D.40) and the relation $g^{\alpha\beta}\delta g_{\beta\gamma} = -g_{\beta\gamma}\delta g^{\alpha\beta}$, we derive the necessary expressions

$$g^{\mu\nu}\delta\Gamma^\alpha_{\mu\nu} = -\nabla_\mu\delta g^{\alpha\mu} + \frac{1}{2}g_{\mu\nu}\nabla^\alpha\delta g^{\mu\nu},$$
$$g^{\mu\alpha}\delta\Gamma^\nu_{\mu\nu} = -\frac{1}{2}g_{\mu\nu}\nabla^\alpha\delta g^{\mu\nu}.$$

Thus the variation δR is reduced to

$$\begin{aligned}\delta R &= \frac{1}{2}Rg_{\mu\nu}\delta g^{\mu\nu} + \nabla_\alpha\left(-\nabla_\mu\delta g^{\alpha\mu} + \frac{1}{2}g_{\mu\nu}\nabla^\alpha\delta g^{\mu\nu} + \frac{1}{2}g_{\mu\nu}\nabla^\alpha\delta g^{\mu\nu}\right)\\ &= \left(\frac{1}{2}Rg_{\mu\nu} - \nabla_\mu\nabla_\nu + g_{\mu\nu}\Box_g\right)\delta g^{\mu\nu},\end{aligned}$$

while the variation of the Laplace operator becomes

$$\delta\Box_g = \left(\delta g^{\mu\nu}\right)\nabla_\mu\nabla_\nu + \left(\delta g^{\alpha\mu}_{\ \ ;\mu} - \frac{1}{2}g_{\mu\nu}\delta g^{\mu\nu;\alpha}\right)\nabla_\alpha.$$

Now we can put all terms in δI together,

$$\begin{aligned}\delta I = &-\frac{1}{2}g_{\mu\nu}\delta g^{\mu\nu}R\,\Box_g^{-1}R + 2\left(\frac{1}{2}Rg_{\mu\nu}\delta g^{\mu\nu} - \delta g^{\mu\nu}_{\ \ ;\mu\nu} + g_{\mu\nu}\Box_g\delta g^{\mu\nu}\right)\Box_g^{-1}R\\ &- R\,\Box_g^{-1}\left[\delta g^{\mu\nu}\nabla_\mu\nabla_\nu\Box_g^{-1}R + \left(\delta g^{\alpha\mu}_{\ \ ;\mu} - \frac{1}{2}g_{\mu\nu}\delta g^{\mu\nu;\alpha}\right)\nabla_\alpha\Box_g^{-1}R\right].\end{aligned}$$

It is now straightforward to compute the functional derivative (D.48). Keeping in mind that for arbitrary scalar functions $A(x)$ and $B(x)$ we have

$$\int d^2x\sqrt{-g}A\,\Box_g^{-1}B = \int d^2x\sqrt{-g}B\,\Box_g^{-1}A,$$

and that integration by parts yields for arbitrary tensors X and Y the formula

$$\int d^2x\sqrt{-g}X\nabla_\alpha Y = -\int d^2x\sqrt{-g}Y\nabla_\alpha X,$$

we compute (up to a total divergence)

$$\begin{aligned}\frac{\delta I}{\delta g^{\mu\nu}} =&\frac{1}{2}g_{\mu\nu}R\,\Box_g^{-1}R - 2\left(\Box_g^{-1}R\right)_{;\mu\nu} + 2g_{\mu\nu}R\\ &- \left(\Box_g^{-1}R\right)\left(\Box_g^{-1}R\right)_{;\mu\nu} + \left(\left(\Box_g^{-1}R\right)_{;\nu}\Box_g^{-1}R\right)_{;\mu} - \frac{1}{2}g_{\mu\nu}\left(\left(\Box_g^{-1}R\right)_{;\alpha}\Box_g^{-1}R\right)^{;\alpha}\\ =&-2\left(\Box_g^{-1}R\right)_{;\mu\nu} + 2g_{\mu\nu}R + \left(\Box_g^{-1}R\right)_{;\mu}\left(\Box_g^{-1}R\right)_{;\nu} - \frac{1}{2}g_{\mu\nu}\left(\Box_g^{-1}R\right)_{;\alpha}\left(\Box_g^{-1}R\right)^{;\alpha}.\end{aligned}$$

Thus the final result is

$$\begin{aligned}\langle T_{\mu\nu}\rangle =&\frac{1}{48\pi}\Big\{-2\nabla_\mu\nabla_\nu\Box_g^{-1}R + \left[\nabla_\nu\Box_g^{-1}R\right]\left[\nabla_\mu\Box_g^{-1}R\right]\\ &+ 2g_{\mu\nu}R - \frac{1}{2}g_{\mu\nu}\left(\nabla_\alpha\Box_g^{-1}R\right)\left(\nabla^\alpha\Box_g^{-1}R\right)\Big\},\end{aligned}$$

which coincides with Eq. (15.8).

Detailed chapter outlines

This section is intended to provide the lecturer with a snapshot of the key ideas of each chapter.

Part I: Canonical quantization

Chapter 1: Overview. A taste of quantum fields

This first chapter is an introduction and overview. The material of this chapter will be covered in much more detail later in the text.

The quantum theory of a free field is mathematically equivalent to a theory of infinitely many harmonic oscillators (field modes). Quantized fields fluctuate in the vacuum state and have a nonvanishing energy (zero-point energy). Using the oscillator analogy, we estimate the amplitude of zero-point fluctuations of a scalar field on a given scale. Vacuum fluctuations of quantum fields have observable, experimentally verified consequences, such as the spontaneous emission in hydrogen, the Lamb shift, and the Casimir effect.

In quantum field theory, particles are represented by excited quantum states of field modes. Particle production is a change of occupation numbers in the modes. "Traditional" QFT considers interacting field theories and requires complicated calculations. The focus of this book is on quantum fields interacting only with strong classical fields (backgrounds) but not with other quantum fields. The main problem of interest to us is to understand the behavior of quantum fields in a gravitational background. Examples of particle production by the gravitational field are the Unruh effect and the Hawking radiation of black holes.

Chapter 2: Reminder. Classical and quantum mechanics

In classical mechanics, equations of motion are obtained by evaluating functional derivatives of the action. (We introduce the notion of functional derivative.) Both the Lagrangian and the Hamiltonian formalisms are reviewed. The Legendre transform is explained.

Canonical quantization in the Heisenberg picture is applied to a Hamiltonian system to yield quantum equations of motion that govern the evolution of quantum observables such as the coordinate $\hat{q}(t)$ and the momentum $\hat{p}(t)$. The commutation relation between the operators $\hat{q}$ and $\hat{p}$ is the central postulate of canonical quantization.

Quantum operators act on vectors in a Hilbert space. We explain the Dirac notation ("bra-ket") and introduce the notion of separable Hilbert space by formalizing the intuitive idea of a basis in an infinite-dimensional vector space. We consider the basis $\{|q\rangle\}$ of the generalized eigenvectors of the position operator, the analogous basis $\{|p\rangle\}$ for the momentum operator, and compute the matrix elements $\langle q|\,\hat{p}\,|q'\rangle$ and $\langle p|\,q\rangle$ using only the canonical commutation relations.

The Schrödinger picture of quantum mechanics involves time-dependent states and time-independent observables. We note that the Schrödinger equation is not particular to the nonrelativistic quantum mechanics and in principle can be used to describe relativistic quantum fields.

Chapter 3: Quantizing a driven harmonic oscillator

We compute the classical trajectory $x(t)$ of a harmonic oscillator driven by an external force $J(t)$. Quantization is conveniently performed using the creation and annihilation operators. For an external force acting only during a finite time interval, we define the "in" and the "out" regimes and the corresponding creation and annihilation operators and particle states. The "in" and "out" vacuum states are different due to particle production by the external force. We derive the expansion of the "in" vacuum state through the "out" excited states and perform direct computations of matrix elements of various operators with respect to the "in" and "out" vacua.

Chapter 4: From harmonic oscillators to fields

A free field can be viewed as a collection of infinitely many harmonic oscillators. In classical mechanics, a system of linearly coupled harmonic oscillators is decoupled by a decomposition into proper oscillation modes. We use this analogy to represent a scalar field $\phi(\mathbf{x}, t)$ by a set of modes $\phi_{\mathbf{k}}(t)$ that obey the harmonic oscillator equations with frequencies ω_k.

Each mode $\phi_{\mathbf{k}}$ is quantized using creation and annihilation operators. We derive the commutation relations and introduce the mode expansion for a free real scalar field. The vacuum state and the excited states are defined using the annihilation and creation operators. We compute the zero-point energy of the field. This energy diverges for two reasons: First, it contains the infinite volume of space manifested by the factor $\delta^{(3)}(0)$. After separating this factor, we obtain the zero-point energy density which is still infinite due to the ultraviolet divergence. This divergence is removed by normal ordering.

Finally, we show how a quantum field can be described by a wave functional satisfying the functional Schrödinger equation.

Chapter 5: Overview of classical field theory

Action functionals for a classical field theory must satisfy several requirements such as locality, Lorentz invariance, and general covariance. We derive the Euler-Lagrange equations of motion from a Lagrangian of the form $\mathcal{L}(\phi, \partial_\mu \phi)$.

As an example, we consider a real scalar field in the flat (Minkowski) spacetime with a Poincaré-invariant action. To make the action generally covariant, one needs to introduce covariant derivatives and the covariant volume element into the action. The resulting action describes a scalar field with a minimal coupling to gravity. An example of nonminimal coupling is the Lagrangian for a conformally coupled scalar field.

Gauge fields arise when a global symmetry is localized. Using the example of a complex scalar field with the global $U(1)$ gauge symmetry, we introduce the gauge field A_μ and the gauge-covariant derivatives D_μ into the action. The result is the action for a scalar field with the minimal gauge coupling. The action for the gauge field itself can be built using the Yang-Mills term $F_{\mu\nu}F^{\mu\nu}$, where $F_{\mu\nu}$ is the field strength tensor. We show that the action for the electromagnetic field is conformally invariant.

Einstein's general relativity is described by the Einstein-Hilbert action. The Einstein equations are derived in an exercise.

Finally, we show that the classical energy-momentum tensor (EMT) of matter in generally covariant field theories can be defined through the functional derivative of the action with respect to the metric $g^{\mu\nu}$. The EMT defined in this way is conserved in a generally covariant sense.

Chapter 6: Quantum fields in expanding universe

We consider a homogeneous FRW universe with flat spatial sections and define a coordinate system $(\eta, \mathbf{x})$ in which the metric is conformally flat. A free, minimally coupled, massive scalar field $\phi(\eta, \mathbf{x})$ in this spacetime is quantized using a mode expansion. The modes $\phi_{\mathbf{k}}(\eta)$ are solutions of harmonic oscillator equations with time-dependent frequencies $\omega_k(\eta)$. We define mode functions $v_k(\eta)$ as suitable complex-valued solutions of these oscillator equations. The choice of the mode functions $v_k(\eta)$ is not unique unless the frequencies ω_k are time-independent.

For a given set of mode functions $v_k(\eta)$, we define the creation and annihilation operators $\hat{a}^{\pm}_{\mathbf{k}}$. Different choices of the mode functions yield different sets $\hat{a}^{\pm}_{\mathbf{k}}$ which are related by Bogolyubov transformations. The vacuum state is annihilated by $a^{-}_{\mathbf{k}}$ and is thus determined by the choice of the mode functions. We derive equations relating the Bogolyubov coefficients to the values of mode functions.

Excited states of modes are interpreted as states containing particles, and the expectation value of the particle number density in a mode $\phi_{\mathbf{k}}$ is determined by the Bogolyubov coefficient, $n_k = |\beta_k|^2$.

In a general spacetime, the vacuum state is not uniquely defined. One prescription for the vacuum state is to minimize the instantaneous energy. The instantaneous lowest-energy state exists if $\omega_k^2 > 0$ and the corresponding mode functions are specified by appropriate initial conditions. We discuss the physical interpretation of the ambiguity in the choice of the vacuum state and the approximate nature of the concept of particles. The vacuum state can be defined for high-energy modes and, separately, in spacetimes with a slowly changing metric (the adiabatic vacuum).

Chapter 7: Fields in de Sitter spacetime

Besides the particle interpretation of fields, we are interested in field observables such as $\langle 0|\, \hat{\phi}(x)\hat{\phi}(y)\, |0\rangle$. Such correlation functions are related to the amplitude of quantum fluctuations of the field $\hat{\phi}$. We introduce the formalism of window functions and use it to define the amplitude of fluctuations on a scale L. A general formula for the fluctuation amplitude in vacuum is derived as a function of L.

As an illustrative example, we choose a FRW spacetime with a special scale factor $a(\eta)$ such that the effective frequency $\omega\,(\eta)$ is a simple step-like function of the conformal time η. We compute the "in" and "out" mode functions, the Bogolyubov coefficients, the density of produced particles, and the spectrum of quantum fluctuations.

Then we consider a massive scalar field in the de Sitter spacetime. We derive the metric of the de Sitter spacetime and demonstrate the presence of horizons. The field is quantized using a suitable mode expansion. We construct the mode functions and compute their asymptotic forms in the far past and far future.

The effective frequency $\omega_k(\eta)$ for any given k becomes imaginary at late times when the wavelength of the mode exceeds the de Sitter horizon length H^{-1}. This precludes a particle interpretation of the superhorizon modes of the field. However, at early times the frequencies ω_k are approximately constant for all modes (a strongly adiabatic regime), which allows one to define the Bunch-Davies vacuum.

Assuming the Bunch-Davies vacuum state, we study the evolution of quantum fluctuations as a function of the time η and the scale L. We express this function through the physical length $L_p = a(\eta)L$ and find that the spectrum of fluctuations is approximately scale-independent, in contrast with the sharply falling spectrum in the flat spacetime.

Chapter 8: The Unruh effect

We explicitly build a system of reference moving with a uniform acceleration a (the Rindler frame). The Rindler spacetime is defined as the domain of the Minkowski spacetime seen by an accelerated observer.

Then we consider a massless scalar field in a 1+1-dimensional section of the Rindler spacetime. The formalism of mode expansions in the lightcone coordinates helps to quantize the field more conveniently. We describe the natural vacua in the Minkowski (inertial) and the Rindler (accelerated) frames of reference and argue that the correct choice is the Minkowski vacuum. The Bogolyubov coefficients relating the two vacua and the density of observed particles are computed. The particle energies obey the Bose-Einstein thermal distribution with the Unruh temperature $T = a/(2\pi)$.

Chapter 9: The Hawking effect. Thermodynamics of black holes

To derive the Hawking effect, we draw on a formal analogy with the Unruh effect studied in the previous chapter. We consider a 1+1-dimensional section of the Schwarzschild spacetime with coordinates (t, r), and we introduce two coordinate

systems: the "tortoise" coordinates corresponding to static observers far away from the black hole (BH) and the Kruskal coordinates that describe observers freely falling into the BH. The two coordinate systems naturally define two vacuum states. The relation between the coordinate systems is formally the same as that between the Rindler and the Minkowski frames. Therefore the mode expansions and the Bogolyubov coefficients are found directly from the results of the previous chapter, with the substitution $a = (4M)^{-1}$. We obtain the Hawking temperature $T_H = (8\pi M)^{-1}$, discuss physical interpretations of the Hawking radiation, and remark on other derivations.

Black holes can be described thermodynamically using the temperature T_H and the entropy $S_{BH} = \frac{1}{4}A$, where A is the horizon area (in Planck units). The heat capacity of a black hole is negative. We consider adiabatic interactions between black holes and heat reservoirs to show that a black hole cannot be in a stable equilibrium with a heat bath unless the latter has a sufficiently small size.

Chapter 10: The Casimir effect

We consider a simplified version of the Casimir effect involving a massless scalar field $\phi(x,t)$ in 1+1-dimensional spacetime. The plates are modeled by the boundary conditions $\phi|_{x=0} = \phi|_{x=L} = 0$. We find that the zero-point energy of the quantum field diverges in a different way than in the free (boundless) space. To quantify this difference, we introduce a regularization and perform a renormalization by subtracting the zero-point energy in free space. The result is a finite and negative energy density in the vacuum state. The energy density grows with the distance L, which indicates a force of attraction between the plates.

The same result can be obtained by using the analytic continuation of Riemann's ζ function instead of the renormalization procedure. (This introduces the ζ function method which will be also used in Part II.)

Part II: Path integral methods

Chapter 11: Path integral quantization

Evolution of quantum states in the Schrödinger picture can be expressed as the action of an evolution operator on the initial state. The propagator is the coordinate representation of the evolution operator. We derive the path integral representation of the propagator. The path integral involves the Hamiltonian action and is performed over all paths $q(t)$, $p(t)$ in the phase space. For Hamiltonians that are quadratic in the momentum, the path integral is simplified to an integral of $\exp(iS[q])$ over configuration space paths $q(t)$, where $S[q]$ is the Lagrangian action.

Chapter 12: Effective action

We derive the retarded (G_{ret}) and the Feynman (G_F) Green's functions of a harmonic oscillator. The analytic continuation to imaginary time (the Wick rotation) yields the

corresponding Euclidean equation of motion and the Euclidean Green's function G_E.

We define and compute the Euclidean analog of the path integral for a driven oscillator $q(t)$ with an external force $J(t)$. The Euclidean effective action $\Gamma_E[J]$ is defined through the path integral over Euclidean trajectories $q(\tau)$ connecting the vacuum states $q = 0$ at $\tau \to \pm\infty$. The Lorentzian effective action $\Gamma_L[J(t)]$ is the analytic continuation of $\Gamma_E[J(\tau)]$ back to the real time t. We find that the "in-out" matrix elements computed in Chapter 3 are related to the functional derivatives of $\Gamma_L[J]$ with respect to J. The "in-in" matrix elements can be obtained by replacing G_F by G_{ret} after evaluating the functional derivatives. This motivates a "recipe" for computing matrix elements through the effective action.

Besides describing the influence of a classical background on a quantum system, the effective action characterizes the backreaction of the quantum system on the background. The classical equations of motion for the background $J(t)$ acquire an extra term—the functional derivative $\delta\Gamma_L/\delta J(t)$ of the effective action $\Gamma_L[J]$. For the driven oscillator, this term is the expectation value of the quantum variable $\langle q(t)\rangle$.

Another important application is to quantum field theory in a curved spacetime where the gravitational field is treated as the classical background. The backreaction of a quantum field on the gravitational background is described by the functional derivative term $\delta\Gamma_L/\delta g^{\mu\nu}$ which is related to the expectation value of the energy-momentum tensor of the quantum field; this term is added to the Einstein equation. The same term describes the influence of gravity on the vacuum state of quantum fields (the polarization of vacuum). In this way one can formulate a self-consistent theory of classical gravity coupled to quantum fields (semiclassical gravity).

Chapter 13: Functional determinants and heat kernels

We consider the Euclidean effective action for a free scalar field in a gravitational background. The Euclidean action is a quadratic functional of the field and the Gaussian path integral can be evaluated in terms of the determinant of a differential operator (a functional determinant). Such determinants are always divergent and need to be renormalized.

We introduce the method of zeta (ζ) function for computing renormalized functional determinants. We define the function $\zeta_M(s)$ for an operator $\hat{M}$. The functional determinant is expressed through the derivative of $\zeta_M(s)$ at $s = 0$ which is finite after analytic continuation.

The method of heat kernels can be used to determine the ζ function. We define the heat kernel $\hat{K}_M(\tau)$ of an operator $\hat{M}$ and show how the trace of $\hat{K}_M(\tau)$ is related to the ζ function of the same operator. We formulate a "recipe" to calculate the effective action for a quantum field in a classical background. The recipe involves a ζ function computed through the trace of a certain heat kernel.

Chapter 14: Calculation of heat kernel

We perform a detailed calculation of the heat kernel for a scalar field in a weakly curved 3+1-dimensional spacetime. The result is a (nonlocal) perturbative expan-

sion in the curvature R. This expansion can be used to compute the ζ function of the Laplace operator perturbatively. We compare this expansion with the standard Seeley-DeWitt expansion of the heat kernel in powers of τ and find agreement of the computed terms. We derive the first-order terms and quote the second-order terms of both expansions *without derivation*.

Chapter 15: Results from effective action

This final chapter builds upon the results of the entire Part II of this book.

We finish the computation of the effective action for a scalar field in a weakly curved background, using the method of ζ functions. Before the analytic continuation, the method produces a divergent result. We analyze the structure of the divergent terms in the effective action. These divergences are removed by renormalizing the cosmological constant (zero-point energy), the gravitational constant, and the coupling constant at the R^2 term. The "bare" action for pure gravity can be chosen to cancel all divergences, and the resulting action describes the standard Einstein dynamics of gravity modified by the backreaction of the quantum field.

Then we analyze the finite terms in this modified action. In 1+1 dimensions, the extra term in the gravitational action is the Polyakov action. (This is derived from the *second-order* terms of the nonlocal expansion.) We quote the corresponding result in 3+1 dimensions.

Finally, we consider the energy-momentum tensor (EMT) of the quantum field which characterizes the vacuum polarization. From the Polyakov action, we derive a nonlocal formula for the polarization of vacuum in 1+1 dimensions. We use that formula to compute the trace of the EMT for a massless conformally coupled field. Unlike the prediction of the classical theory, the trace of the EMT does not vanish ("conformal anomaly"). Another derivation of the conformal anomaly in 1+1 dimensions is also presented, based on the ζ function method and the *first-order* term of the Seeley-DeWitt expansion.

Appendices

Appendix A: Mathematical supplement

This appendix contains a tutorial exposition of some mathematical constructions used in the text.

Appendix A.1: Functionals and distributions (generalized functions)

We define functionals as maps from a function space into numbers. "Generalized functions" or "distributions" are linear functionals. We define the frequently used distributions: the Dirac δ function and its derivatives, and the principal value integrals such as $\mathcal{P}\frac{1}{x}$. The notion of convergence in the distributional sense provides a

rigorous basis for formulae such as

$$\int_0^{+\infty} dx\ \sin kx = \frac{1}{k}.$$

Appendix A.2: Green's functions, boundary conditions, and contours

We define Green's functions and consider the frequently used calculation with Fourier transforms where one obtains an integral with poles. We use the formalism of distributions and principal value integrals to show how to compute the Green's function for particular boundary conditions.

Appendix A.3: Euler's gamma function and analytic continuations

Euler's gamma function is defined and some of its elementary properties are derived. In particular, we justify the analytic continuation of the gamma function which was mentioned in Sec. 8.2.4.

Appendix B: Adiabatic approximation for Bogolyubov coefficients

First we show that the WKB approximation is insufficiently precise to yield the Bogolyubov coefficients relating two vacua (instantaneous or adiabatic) defined at two different moments of time. Then we present a method of computing the Bogolyubov coefficients in spacetimes with a slowly changing metric, using the adiabatic perturbation theory. This is a well-known method which is more accurate than the WKB approximation.

Appendix C: Mode expansions cheat sheet

This is a collection of formulae related to mode expansions and commutation relations.

Appendix D: Solutions to exercises

Detailed solutions are given to each exercise appearing in the text.

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