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Introduction to Quantum Field Theory

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1 Introduction

Physical systems that involve an infinite number of degrees of freedom are usually described by some sort of *field theory*. Almost all systems in nature involve an extremely large number of degrees of freedom. A droplet of water contains of the order of 10^{26} molecules and while each water molecule can in many applications be described as a point particle, each molecule has itself a complicated structure which reveals itself at molecular length scales. To deal with this large number of degrees of freedom, which for all practical purposes is infinite, we regard many mechanical systems as continuous. For instance, a violin string is regarded as a continuous system and its vibrations are described by a function (called the 'displacement field') defined along the string that specifies the (transverse) displacement from equilibrium. This mechanical system is not described by giving the equations of motion directly for each atom, but instead the displacement field is used as the dynamical variable, which, being continuous, comprises an infinite number of degrees of freedom. In classical physics field theory is obviously important for continuous systems, but also for electromagnetic phenomena, as Maxwell's theory of electromagnetism is a field theory in which the electric and magnetic fields comprise the basic dynamical variables. In terms of these fields one can both understand the electromagnetic forces between charges and the phenomenon of electromagnetic radiation.

The methods of classical mechanics can be suitably formulated so that they can be used for continuous systems. However, to give a quantum-mechanical treatment of field theory is much more difficult and requires new concepts. Some of these concepts are straightforward generalizations of the quantum-mechanical treatment of systems consisting of few degrees of freedom, but others are much less obvious. At the quantum-mechanical level, the infinite number of degrees of freedom may give rise to divergences which appear when quantum operators are defined at the same point in space. These short-distance singularities require special care; a possible consequence of them is that the physical relevance of a calculated result can not always be taken for granted. Also the physical nature of the dynamical variables is not necessarily obvious.

In these lectures we introduce the concepts and methods that are used in quantum field theory. The lectures are not directly aimed at a particular application in physics, as quantum field theory plays a role in many of them, such as in condensed matter physics, nuclear physics, particle physics and string theory. But there is a certain unity in the methods that we use in all of these disciplines, although they may carry different names or they may be used in different ways depending on the context. Still, in these notes we are somewhat biased in that we will usually deal with relativistic field theories.

A central role in these lectures is played by the path integral representation of quantum field theory, which we will derive and use for both bosonic and for fermionic fields. Another topic is the use of diagrammatic representations of the path integral. We try to keep the context as simple as possible and this is the reason why we will often return to systems of a few degrees of freedom, to bring out the underlying principles as clearly as possible. For instance, we discuss quantum tunneling by means of instantons, but we will do this for a single particle, thus making contact with 'standard' quantum mechanics.

At the end of each chapter we present a number of exercises, where the student can verify whether he/she has understood the material presented in that chapter and is able to apply it in more practical situations.

Obviously, these lectures are but an introduction to the subject and the material that is covered is very incomplete. We have added a list of useful textbooks for further reading.

2 Path integrals and quantum mechanics

In quantum mechanics the time evolution of states is governed by the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\psi,t\rangle = H(P,Q)|\psi,t\rangle\,, \tag{2.1}$$

where $H(P,Q)$ is the Hamiltonian, and P and Q are the coordinate and the momentum operator (in this chapter we restrict ourselves to a single one-dimensional particle, so that we have only one coordinate and one momentum operator). The Schrödinger equations shows that there exists an evolution operator that relates states at time t to states at an earlier time t', equal to

$$U(t,t') = \exp[-\frac{i}{\hbar}H(t-t')]\,. \tag{2.2}$$

The operators P and Q satisfy the well-known Heisenberg commutation relations

$$[Q,P] = i\hbar. \tag{2.3}$$

Consider now a basis for the quantum mechanical Hilbert space consisting of states $|q\rangle$ which are eigenstates of the position operator Q with eigenvalue q. These states are time-independent and will in general not correspond to the eigenstates of the Hamiltonian (taken at some fixed time). The states $|q\rangle$ form an orthonormal set, so that

$$\begin{aligned}\langle q_1|q_2\rangle &= \delta(q_1-q_2),\\ \int dq\;|q\rangle\langle q| &= \mathbf{1}.\end{aligned} \tag{2.4}$$

Similar equations hold for the states $|p\rangle$, which are the eigenstates of the momentum operator P.

From these results it follows that the wave function of a particle with momentum p is equal to

$$\langle q|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar}pq}, \tag{2.5}$$

and the momentum operator reads $P = -i\hbar\,\partial/\partial q$. Using the ordering convention where momentum operators P are written to the left of position operators Q in the Hamilton $H(P,Q)$, we have

$$\langle p|H(P,Q)|q\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{-\frac{i}{\hbar}pq} H(p,q)\,, \tag{2.6}$$

where $H(p,q)$ is a function of p and q associated with the ordering prescription.

The above equations were defined in the so-called Schrödinger picture, where states are time-dependent while operators are in general time-independent. Alternatively, one can make use of the Heisenberg picture. Here states are time-independent and can be defined by

$$|\psi\rangle_H \equiv |\psi, t=0\rangle_S = \mathrm{e}^{\frac{i}{\hbar}Ht}\,|\psi, t\rangle_S\,, \tag{2.7}$$

(instead of $t = 0$ one may also choose some other reference time) whereas operators bare generally time-dependent and they are given by

$$A_H(t) = e^{\frac{i}{\hbar}Ht}\,A_S\,e^{-\frac{i}{\hbar}Ht}. \tag{2.8}$$

Of course, these states are determined up to phase factors, but their precise definition is of no concern. Subsequently we consider a state $|q\rangle_{t_1}$ which at $t = t_1$ is an eigenstate of the Schrödinger position operator Q with eigenvalue q. In the Schrödinger picture, this state can be written as

$$(|q\rangle_{t_1})_S = e^{-\frac{i}{\hbar}H(t-t_1)}|q\rangle, \tag{2.9}$$

while in the Heisenberg picture we have

$$(|q\rangle_{t_1})_H = e^{\frac{i}{\hbar}Ht_1}|q\rangle. \tag{2.10}$$

Observe that (2.10) is an eigenstate of $Q_H(t_1)$ with eigenvalue q. Define now the transition function between two such states,

$$W(q_2,t_2;q_1,t_1) \equiv {}_{t_2}\langle q_2|q_1\rangle_{t_1}, \tag{2.11}$$

which can be written as

$$W(q_2,t_2;q_1,t_1\rangle = \langle q_2|e^{-\frac{i}{\hbar}H(t_2-t_1)}|q_1\rangle, \tag{2.12}$$

and thus corresponds to matrix elements of the evolution operator. We now observe that W satisfies the following two properties. The first one is the product rule,

$$\int dq_2\, W(q_3,t_3;q_2,t_2)\, W(q_2,t_2;q_1,t_1) = W(q_3,t_3;q_1,t_1). \tag{2.13}$$

The second one is an initial condition,

$$W(q_2,t;q_1,t) = \delta(q_2-q_1). \tag{2.14}$$

The first result (2.13) follows directly from the completeness of the states $|q_2\rangle$, while the second result (2.14) follows from (2.12) and (2.4).

We will now discuss an alternative representation for W in the form of a so-called path integral. For that purpose we evaluate W by means of a limiting procedure. We first divide a time interval (t_0,t_N) into N intervals (t_i,t_{i+1}) with $t_{i+1}-t_i=\Delta$, so that $t_N-t_0=N\Delta$, and furthermore we write $q_i=q(t_i)$. Then $W(q_N,t_N;q_0,t_0)$ can be written as

$$W(q_N,t_N;q_0,t_0) = \int dq_{N-1}\cdots\int dq_1\, W(q_N,t_N;q_{N-1},t_{N-1})\cdots W(q_1,t_1;q_0,t_0). \tag{2.15}$$

For small values of Δ we may write

$$\begin{aligned} W(q_{i+1},t_i+\Delta;q_i,t_i) &= \langle q_{i+1}|e^{-\frac{i}{\hbar}H(P,Q)\Delta}|q_i\rangle \\ &= \int dp_i\,\langle q_{i+1}|p_i\rangle\langle p_i|e^{-\frac{i}{\hbar}H(P,Q)\Delta}|q_i\rangle \\ &\approx \frac{1}{2\pi\hbar}\int dp_i\,\exp\left(\frac{i}{\hbar}[p_i(q_{i+1}-q_i)-H(p_i,q_i)\Delta]\right), \end{aligned} \tag{2.16}$$

where we made use of (2.6) and of the fact that Δ is small. Substituting (2.16) into (2.15) yields

$$\begin{aligned} W(q_N,t_N;q_0,t_0) &= \int dq_{N-1}\cdots\int dq_1\int\frac{dp_0}{2\pi\hbar}\cdots\int\frac{dp_{N-1}}{2\pi\hbar} \\ &\qquad \exp\left(\frac{i}{\hbar}\Delta\sum_{i=0}^{N-1}\left[\frac{p_i(q_{i+1}-q_i)}{\Delta}-H(p_i,q_i)\right]\right). \end{aligned} \tag{2.17}$$

Observe that we have $N-1$ q_i integrals and N p_i integrals.

We now make the assumption that

$$H = \frac{P^2}{2m}+V(Q)\,, \tag{2.18}$$

and therefore $H(p_i,q_i)=\frac{p_i^2}{2m}+V(q_i)$. The exponent in (2.17) can then be written as

$$\begin{aligned} \frac{p_i(q_{i+1}-q_i)}{\Delta} &- \frac{p_i^2}{2m}-V(q_i) = \\ &- \frac{1}{2m}\left(p_i-m\frac{q_{i+1}-q_i}{\Delta}\right)^2+\frac{m}{2}\left(\frac{q_{i+1}-q_i}{\Delta}\right)^2-V(q_i). \end{aligned} \tag{2.19}$$

With this result the integrals over p_i in (2.17) are just Gaussian integrals,

$$\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}, \tag{2.20}$$

apart from the fact that a is imaginary in this case $a = i\Delta/(2m\hbar)$. Ignoring this subtlety [1] for the moment let us perform the p_i integrals by means of (2.20), so that W becomes

$$\begin{aligned} W(q_N, t_N; q_0, t_0) &= \int dq_{N-1} \cdots \int dq_1 \left(\frac{m}{2\pi i\hbar\Delta}\right)^{N/2} \\ &\quad \times \exp\left(\frac{i}{\hbar}\Delta \sum_{i=0}^{N-1} \left[\frac{m}{2}\left(\frac{q_{i+1}-q_i}{\Delta}\right)^2 - V(q_i)\right]\right). \end{aligned} \tag{2.21}$$

Taking the limit $N \to \infty$, $\Delta \to 0$, while keeping $N\Delta = t_N - t_0$ fixed, the exponent in (1.20) tends to

$$\exp\left\{\frac{i}{\hbar}\int_{t_0}^{t_N} dt' \left(\frac{m}{2}(\dot{q}(t'))^2 - V(q(t'))\right)\right\}. \tag{2.22}$$

This can be written as $\exp\left\{\frac{i}{\hbar}S[q(t)]\right\}$, where S is the (classical) action defined as the time integral of the Lagrangian $L = T - V$. Observe that the action is *not* a function, but a so-called functional, which assigns a number to each trajectory $q(t)$. Of course, by discretizing the time, as we did previously, the action can be regarded as a function of the $N+1$ variables $q_i = q(t_i)$. Furthermore, the integration over dq_i approaches an integration over *all possible functions* $q(t)$ with boundary values $q(t_{1,2}) = q_{1,2}$. Such an integral is called a *path integral* and we may write

$$W(q_2, t_2; q_1, t_1) = \int_{\substack{q(t_1)=q_1 \\ q(t_2)=q_2}} \mathcal{D}q(t)\, e^{\frac{i}{\hbar}S[q(t)]}\,. \tag{2.23}$$

This is the path integral representation of W. Observe that this representation satisfies the product rule (2.13).

In the path integral (2.23) the factor $\exp\left(\frac{i}{\hbar}S[q(t)]\right)$ thus assigns a weight to every "path" or trajectory described by the function $q(t)$. In contrast with the usual integration of functions, the path integral is an integration of functionals. It is not easy to give a general and more rigorous definition of a path integral. Such a definition depends on the class of functionals that appear in the integrand. The expression that results from the limiting procedure (cf. (1.20)) is one particular way to define a path integral. It is known as the Wiener measure, and is usually defined by the requirement that $\int dq_2\, W(q_1, t_1; q_2, t_2) = 1$ when the action is that of a free particle. Indeed, it is easy to verify that the N integrals in (1.20) over $q_0, \ldots, q_{N-1}$ yield 1 in the case that $V(q_i) = 0$. It turns out, that this definition applies also to more general functionals S that consist of a standard kinetic term and a large class of potentials V (at least, in the Euclidean theory, where one does not have the troublesome factor

[1] Observe that (2.20) still holds provided $\mathrm{Re}\, a > 0$.

of i in the exponential; see chapter 5). For this class trajectories that are not sufficiently smooth, will be suppressed in the integral.

An important advantage of the path-integral formalism as compared to the canonical operator approach, is that it is manifestly Lorentz invariant (see chapter 4). The reason is that the action is a Lorentz scalar, at least for relativistically invariant theories. Another advantage is that the path integral can also be used in those cases where the time variable can not be globally defined. This may happen when the (field) theory is defined in a space-time of nontrivial topology.

We will now demonstrate some properties of W. First let $\{|n\rangle\}$ be a complete set of eigenstates of H: $H|n\rangle = E_n|n\rangle$. In the q representation, where $\langle q|n\rangle = \varphi_n(q)$, we then find the following expression for W

$$W(q_2,t_2;q_1,t_1) = \sum_n \varphi_n(q_2)\,\varphi_n^*(q_1)\,e^{-\frac{i}{\hbar}E_n(t_2-t_1)}\,. \tag{2.24}$$

It is easily checked that (2.13) and (2.14) are indeed valid for this representation of W, as a result of the fact that the eigenstates $|n\rangle$ form a complete orthonormal set. Observe that (2.24) is precisely the evolution operator in the Schrödinger representation, so that wave functions $\psi(q,t)$ satisfy

$$\psi(q,t) = \int dq'\; W(q,t;q',t_0)\;\psi(q',t_0). \tag{2.25}$$

Therefore W must itself satisfy the Schrödinger equation, as follows indeed from (2.24),

$$\begin{aligned} i\hbar\frac{\partial}{\partial t_2}W(q_2,t_2;q_1,t_1) &= i\hbar\sum_n\left(-\frac{i}{\hbar}E_n\right)\varphi_n(q_2)\,\varphi_n^*(q_1)\,e^{\frac{i}{\hbar}E_n(t_1-t_2)} \\ &= \sum_n H_{q_2}\varphi_n(q_2)\,\varphi_n^*(q_1)\,e^{\frac{i}{\hbar}E_n(t_1-t_2)} \\ &= H_{q_2}W(q_2,t_2;q_1,t_1)\,, \end{aligned} \tag{2.26}$$

where H_q is the Hamilton operator in the coordinate representation.

Problem 2.1 : How will (2.23) change for a system described by the Hamiltonian $H = \frac{P^2}{2m}f(Q) + V(Q)$? Show that the classical action will now contain modifications of order $\hbar$, as a result of the integrations over the p_i.

Problem 2.2 : The free relativistic particle

When a free particle travels from one point to another, the obvious relativistic invariant is the proper time, i.e. the time that it takes measured in the rest frame of the particle. During an infinitesimal amount of time dt a particle with velocity $\dot{\mathbf{q}}$ is displaced over a distance

$\mathrm{d}\mathbf{q} = \dot{\mathbf{q}}\,\mathrm{d}t$. As is well-known, the corresponding time interval is shorter in the particle rest frame, and equal to $\mathrm{d}\tau = \sqrt{1-(\dot{\mathbf{q}}/c)^2}\mathrm{d}t$, where c is the velocity of light. If we integrate the proper time during the particle motion we have a relativistic invariant. Hence we assume a Lagrangian

$$L = -mc^2\sqrt{1-(\dot{\mathbf{q}}/c)^2}\,. \tag{2.27}$$

Show that the momentum and energy are given by

$$\begin{aligned} \mathbf{p} &= \frac{\partial L}{\partial \dot{\mathbf{q}}} = \frac{m\dot{\mathbf{q}}}{\sqrt{1-(\dot{\mathbf{q}}/c)^2}}\,, \\ E &= \dot{\mathbf{q}}\cdot\mathbf{p} - L = \frac{mc^2}{\sqrt{1-(\dot{\mathbf{q}}/c)^2}}\,, \end{aligned} \tag{2.28}$$

and satisfy the relation $E^2 = \mathbf{p}^2c^2 + m^2c^4$. To study the Lorentz transformations is somewhat involved, as we are not dealing with space-time coordinates, but with trajectories $\mathbf{q}(t)$. Under Lorentz transformations both $\mathbf{q}$ and the time t transform, and an infinitesimal transformation takes the form $\mathbf{q}(t') = \mathbf{q}(t) + c\mathbf{v}\,t$ with $t' = t + c^{-1}(\mathbf{v}\cdot\mathbf{q}(t))$. This is enough to establish that $\mathrm{d}\tau$ is invariant and so is the action. On the other hand, the Hamiltonian is not invariant as $\mathbf{p}$ and E transform as a four-vector.

3 The classical limit

In the path integral one sums over all possible trajectories of a particle irrespective of whether these trajectories follow from the classical equations of motion. However, in the limit $\hbar \to 0$ one expects that the relevant contribution comes from the classical trajectory followed by the particle. To see how this comes about, consider the path integral,

$$W = \int \mathcal{D}q\; e^{\frac{i}{\hbar}S[q(t)]}\,, \tag{3.1}$$

and note that for $\hbar \to 0$ the integrand $\exp(\frac{i}{\hbar}S)$ becomes a rapidly oscillating "function" (or rather a functional) of $q(t)$. Therefore the integral (3.1) will tend to vanish. The dominant contributions to the integral come from those $q(t)$ at which S approaches an extremum: $\delta S[q(t)] = 0$. This we recognize as Hamilton's principle, according to which the *classical* path is described by that function $q_0(t)$ for which the action has an extremum (note that we are discussing paths that are all subject to the same boundary condition: $q(t_{1,2}) = q_{1,2}$). As is well known, this function must then satisfy the Euler-Lagrange equations.

The fact that we are dealing with a functional, rather than a function, makes our manipulations more involved, and we will have functional derivatives, rather than ordinary derivatives. Normally a derivative of a function $f(x)$ is generated by a displacement $x \to x + \delta x$, so that $\delta f(x) = f'(x)\,\delta x$. For a functional $F[f(x)]$ the *functional derivative* is generated by $f(x) \to f(x) + \delta f(x)$ and the variation of F takes the form,

$$\delta F[f] = \int \mathrm{d}x\, \frac{\partial F[f]}{\partial f(x)}\, \delta f(x)\,. \tag{3.2}$$

This defines the functional derivative. Alternative the functional derivative can be understood by discretizing x into N parameters $f_i \equiv f(x_i)$, so that $F[f]$ becomes a function $F(x_i)$ of N variables. The integral in (3.2) is then replaced by a sum: $\delta F = \sum_i (\partial F/\partial f_i)\,\delta f_i$. We have already used this approach in the previous chapter. Let us now return to the path integral (3.1)

In quantum mechanics the classical path is somewhat smeared out; the deviations of the classical path are expected to be of order $\sqrt{\hbar}$. To study the quantum-mechanical corrections, let us expand the action about some solution $q_0(t)$ of the equation of motion,

$$\begin{aligned} S[q(t)] &= S[q_0(t)] \\ &+ \frac{1}{2}\int dt_1' dt_2'\, \frac{\delta^2 S[q(t)]}{\delta q(t_1')\delta q(t_2')}\Big|_{q=q_0} (q(t_1') - q_0(t_1'))(q(t_2') - q_0(t_2')) \\ &+ \frac{1}{6}\int dt_1' dt_2' dt_3'\, \frac{\delta^3 S[q(t)]}{\delta q(t_1')\delta q(t_2')\delta q(t_3')}\Big|_{q=q_0} (q(t_1') - q_0(t_1'))(q(t_2') - q_0(t_2'))(q(t_3') - q_0(t_3')) \\ &+ \cdots . \end{aligned} \tag{3.3}$$

Note that we suppressed the term proportional to $\delta S[q(t)]/\delta q(t_1')$ because q_0 is a solution of the equation of motion, so that $\delta S[q_0(t)] = 0$. Substituting (3.3) into (3.1), W becomes

$$\begin{aligned} W &= \exp\Big(\frac{i}{\hbar} S[q_0(t)]\Big) \\ &\times \int \mathcal{D}q \exp\Big\{\frac{i}{2\hbar}\int dt_1' dt_2'\, \frac{\delta^2 S[q(t)]}{\delta q(t_1')\delta q(t_2')}\Big|_{q=q_0} (q(t_1') - q_0(t_1'))(q(t_2') - q_0(t_2')) + \cdots\Big\}, \end{aligned} \tag{3.4}$$

where the terms in parentheses represent the quantum-mechanical corrections. It is convenient to replace the integration variables $q(t)$ by $q_0(t) + \sqrt{\hbar} q(t)$, so that, up to an irrelevant normalization factor which can be absorbed into the integration measure,

$$\begin{aligned} W \propto \int \mathcal{D}q \exp\Big(\frac{i}{\hbar}\Big\{ & S[q_0(t)] \\ & + \frac{\hbar}{2}\int dt_1' dt_2'\, \frac{\delta^2 S[q(t)]}{\delta q(t_1')\delta q(t_2')}\Big|_{q=q_0} q(t_1')\, q(t_2') \\ & + \frac{\hbar^{3/2}}{6}\int dt_1' dt_2' dt_3'\, \frac{\delta^3 S[q(t)]}{\delta q(t_1')\delta q(t_2')\delta q(t_3')}\Big|_{q=q_0} q(t_1')\, q(t_2')\, q(t_3') + \cdots \Big\}\Big). \end{aligned} \tag{3.5}$$

Observe that the new integration variable $q(t)$ satisfies the boundary conditions $q(t_{1,2}) = 0$. The functional derivatives of the action are taken at the classical solution and are therefore not affected by the change of variables.

Let us now recall the following equalities,

$$\int_{-\infty}^{\infty} dx_1 \cdots dx_n \, e^{-(x,Ax)} = \pi^{n/2} (\det A)^{-\frac{1}{2}}, \tag{3.6}$$

$$\det A = e^{\ln \det A} = e^{\mathrm{Tr}\, \ln A}, \tag{3.7}$$

where A is an $n \times n$ matrix and

$$(x, Ax) \equiv \sum_{i,j} x_i A_{ij} x_j. \tag{3.8}$$

It is possible to use analogous expressions for functions. One replaces the continuous time variable by a finite number of discrete points, just as in the limiting procedure employed in the previous chapter. Integrals then take the form of sums and, for instance, the term containing $\delta^2 S/\delta q(t_1')\delta q(t_2')$ in (3.4) can be written as (q, Sq), where S_{ij} is a matrix proportional to $\delta^2 S/\delta q(t_i')\delta q(t_j')$ and $q_i \equiv q(t_i')$. Using the analogue of (3.6-3.7), W can be written as

$$W \propto \exp\Big(\frac{i}{\hbar}\Big\{S[q_0(t)] + \tfrac{1}{2} i\hbar\, \delta(0) \int dt_1' dt_2' \, \delta(t_1' - t_2') \, \ln \frac{\delta^2 S[q(t)]}{\delta q(t_1')\delta q(t_2')}\Big|_{q=q_0} + \mathcal{O}(\hbar^2)\Big\}\Big), \tag{3.9}$$

where $\delta(t_1' - t_2')$ establishes that the trace is taken; $\delta(0)$ represents the inverse separation distance between the discrete time points before taking the continuum limit. In this limit we thus encounter a divergence. In practice we will try to avoid expressions like these and try to rewrite determinants as much as possible in terms of Gaussian integrals. (Observe that in this result we have absorbed certain q_0-independent multiplicative terms in the path integral.) Of course, we can also write the above formula as

$$W \propto \Big[\det\Big(\frac{\delta^2 S[q(t)]}{\delta q(t_1')\delta q(t_2')}\Big|_{q=q_0}\Big)\Big]^{-1/2} \exp\Big(\frac{i}{\hbar}\Big\{S[q_0(t)] + \mathcal{O}(\hbar^2)\Big\}\Big), \tag{3.10}$$

where we have introduced the determinant of a functional differential operator (subject to the appropriate boundary conditions; therefore this operator usually has a discrete eigenvalue spectrum).

Let us now derive the following useful result. If the action is at most quadratic in $q(t)$, we only have the second-order term proportional to $\delta^2 S[q(t)]/\delta q(t_1')\delta q(t_2')$ in (3.5), which is independent of q_1 and q_2. Furthermore the boundary condition ($q(t_{1,2}) = 0$) in the path integral (3.5) does not refer to $q_{1,2}$ either. Therefore the full dependence on $q_{1,2}$ is contained in the classical result $S_{cl} \equiv S[q_0]$, so that W reduces to

$$W(q_2, t_2; q_1, t_1) = f(t_1, t_2) \exp\left(\frac{i}{\hbar} S_{cl}\right). \tag{3.11}$$

In most theories the Lagrangian does not depend explicitly on the time. In that case the path integral depends only on the difference $t_2 - t_1$. This conclusion is in accord with the representation (2.24). Hence we may write

$$W(q_2, t_2; q_1, t_1) = f(t_2 - t_1) \exp\left(\frac{i}{\hbar} S_{cl}\right) . \tag{3.12}$$

The function f can be determined by various methods. Either one imposes the product rule (2.13) (although this may lead to technical difficulties in view of the factor i in the exponent) or one derives a first-order differential equation for f which follows from the Schrödinger equation (2.26), in which case one needs (2.14) to fix the overall normalization of f. If one of the eigenfunctions of the Schrödinger equation is explicitly known, one may also determine f from (2.25).

We will now describe the transition from classical mechanics to quantum mechanics in a more formal manner (which was first proposed by Dirac). In classical mechanics, the equations of motion follow from Hamilton's principle, according to which the classical trajectory is the one for which the action acquires an extremum,

$$\delta S[q(t)] = 0, \tag{3.13}$$

where

$$S[q(t)] = \int dt \; L(q, \dot{q}) \tag{3.14}$$

is the action, and $L(q(t), \dot{q}(t))$ is the Lagrangian of the system. The conjugate momentum is defined by

$$p \equiv \frac{\partial L}{\partial \dot{q}} . \tag{3.15}$$

and the differential equation corresponding to (3.13) is the Euler-Lagrange equation

$$\frac{\mathrm{d}}{\mathrm{d}t} p = \frac{\partial L}{\partial q} . \tag{3.16}$$

The Hamiltonian is given by

$$H(p, q) \equiv p\, \dot{q} - L(q, \dot{q}) . \tag{3.17}$$

Note that the Hamiltonian is a function of the phase-space variables p and q. From $\delta H = \partial H/\partial q\, \delta q + \partial H/\partial p\, \delta p = \delta p\, \dot{q} + (p - \partial L/\partial \dot{q})\delta \dot{q} - \partial L/\partial q\, \delta q$, we deduce that the Euler-lagrange equations can be expressed in terms of Hamilton's equations

$$\dot{q} = \frac{\partial H}{\partial p} , \qquad \dot{p} = -\frac{\partial H}{\partial q} . \tag{3.18}$$

This equation can be rewritten with the help of so-called Poisson brackets,

$$\frac{dq}{dt} = (q, H), \qquad \frac{dp}{dt} = (p, H), \tag{3.19}$$

where the Poisson bracket for two functions $A(p, q)$ and $B(p, q)$ is defined as

$$(A, B) \equiv \frac{\partial A}{\partial q}\frac{\partial B}{\partial p} - \frac{\partial A}{\partial p}\frac{\partial B}{\partial q}. \tag{3.20}$$

Note that

$$(q, p) = 1\,, \tag{3.21}$$

and that the time evolution of some function u of the coordinate and momentum, $u(q(t), p(t); t)$, is given by

$$\frac{du}{dt} = (u, H) + \frac{\partial u}{\partial t}. \tag{3.22}$$

In quantum mechanics the coordinates and momenta become operators and the Poisson brackets are replaced by $(i\hbar)^{-1}$ times the commutator. Therefore in the Heisenberg picture we obtain

$$[Q(t), P(t')]_{t=t'} = i\hbar \tag{3.23}$$

and

$$\frac{dU}{dt} = \frac{1}{i\hbar}[U, H] + \frac{\partial U}{\partial t}, \tag{3.24}$$

where U is some operator depending on $Q(t)$, $P(t)$ and t. This result is in one-to-one correspondence with the classical result (3.22). This feature is the motivation for using the Heisenberg picture in field theory.

The Feynman path integral leads to an alternative description of quantum mechanics, where the time evolution is encoded in the transition function,

$$W(q_2, t_2; q_1, t_1) = \int \mathcal{D}q\ \exp\left(\frac{i}{\hbar}S[q(t)]\right). \tag{3.25}$$

Problem 3.1 : The free particle

The Lagrangian is given by

$$L = \tfrac{1}{2}m\dot{q}^2. \tag{3.26}$$

The equation of motion implies that the velocity must be constant. Therefore the velocity equals

$$\dot{q} = \frac{q_2 - q_1}{t_2 - t_1}.$$

It is now easy to calculate the action for a solution of the equation of motion subject to the proper boundary conditions,

$$S_{cl} = \int_{t_1}^{t_2} dt' \, \frac{m}{2} \left(\frac{q_2 - q_1}{t_2 - t_1} \right)^2 = \frac{m}{2(t_2 - t_1)} (q_2 - q_1)^2. \tag{3.27}$$

According to (3.12) the path integral takes the form

$$W = f(t_2 - t_1) \exp \left\{ \frac{im}{2\hbar} \frac{(q_2 - q_1)^2}{t_2 - t_1} \right\},$$

where f can be determined by imposing the Schrödinger equation (2.26). This leads to the following differential equation for f,

$$\frac{\partial f}{\partial t_2} + \frac{f}{2(t_2 - t_1)} = 0\,.$$

Show that, up to a multiplicative constant, this leads to

$$W(q_2, t_2; q_1, t_1) = \sqrt{\frac{m}{2\pi i\hbar (t_2 - t_1)}} \exp \left\{ \frac{im}{2\hbar} \frac{(q_2 - q_1)^2}{t_2 - t_1} \right\}. \tag{3.28}$$

Problem 3.2 : Check by using (2.14) that (3.28) is properly normalized and verify the product rule (2.13).

Problem 3.3 : The harmonic oscillator

From the Lagrangian

$$L = \tfrac{1}{2} m \dot{q}^2 - \tfrac{1}{2} m \omega^2 q^2, \tag{3.29}$$

one easily proves the following results. The classical solution for $q(t)$ is given by

$$q(t) = \frac{1}{\sin \omega (t_2 - t_1)} \Big(q_2 \sin \omega (t - t_1) - q_1 \sin \omega (t - t_2) \Big), \tag{3.30}$$

whereas the corresponding classical action equals

$$S_{cl} = \frac{m\omega}{2 \sin \omega (t_2 - t_1)} \Big\{ (q_1^2 + q_2^2) \cos \omega (t_2 - t_1) - 2 q_1 q_2 \Big\}\,. \tag{3.31}$$

The path integral is again of the form (3.12). Show that it satisfies the Schrödinger equation when

$$f(t_2 - t_1) = \sqrt{\frac{m\omega}{2\pi i\hbar \sin \omega (t_2 - t_1)}},$$

so that

$$W(q_2,t_2;q_1,t_1) = \sqrt{\frac{m\omega}{2\pi i\hbar\sin\omega(t_2-t_1)}} \times \exp\left\{\frac{im\omega}{2\hbar\sin\omega(t_2-t_1)}\left[(q_1^2+q_2^2)\cos\omega(t_2-t_1)-2q_1q_2\right]\right\}. \quad (3.32)$$

Explain the singularities that arise when $t_2-t_1=n\pi/\omega$.

Problem 3.4 : The evolution operator

Verify the validity of (2.25) for the harmonic oscillator with $\psi(q,t)$ the groundstate wave function, using (3.32),

$$\psi(q,t)=\varphi_0(q)\exp(-\tfrac{1}{2}i\omega t)=\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\exp\left(-\frac{m\omega}{2\hbar}q^2-\tfrac{1}{2}i\omega t\right).$$

This confirms that W is thus the evolution operator in the coordinate representation.

Problem 3.5 : The Gel'fand-Yaglom method

From (3.5) it follows that the transition function for a particle on a line with potential energy $V(q)$ can be approximated by (semi-classical approximation),

$$W\simeq F(t_N,t_0)\exp\left\{\frac{i}{\hbar}S[q_0(t)]\right\},$$

where the prefactor is given by the path integral

$$F(t_N,t_0)=\int dq_{N-1}\ldots\int dq_1 \quad \left(\frac{m}{2\pi i\hbar\Delta}\right)^{N/2}\hbar^{(N-1)/2} \times\exp\left\{i\Delta\sum_{i=0}^{N-1}\left[\frac{m}{2}\frac{(q_{i+1}-q_i)^2}{\Delta^2}-\frac{m}{2}\omega_i^2q_i^2\right]\right\}, \quad (3.33)$$

with $q_N=q_0=0$ and $m\omega^2(t)\equiv d^2V(q)/dq^2|_{q(t)=q_0(t)}$. To calculate such path integrals there exists a general method due to Gel'fand and Yaglom. Their method is as follows.

Show that the exponent in the integrand can be written as

$$\frac{im}{2\Delta}\,q_i\,A_{ij}(\omega)\,q_j\,,$$

where q_i are the components of an $(N-1)$-component vector $(q_{N-1},\ldots,q_1)$ and $A_{ij}(\omega)$ are the elements of an $(N-1)\times(N-1)$ matrix equal to

$$A_{N-1}(\omega)=\begin{pmatrix} 2-\Delta^2\omega_{N-1}^2 & -1 & 0 & \cdot \\ -1 & 2-\Delta^2\omega_{N-2}^2 & -1 & \cdot \\ 0 & -1 & 2-\Delta^2\omega_{N-3}^2 & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{pmatrix}.$$

Performing the integrations we thus find the result

$$F(t_N, t_0) = \lim_{N\to\infty} \sqrt{\frac{m}{2\pi i\hbar\Delta}}\,(\det A_N(\omega))^{-\frac{1}{2}}.$$

We now introduce

$$\Psi_N \equiv \Delta\ \det A_N(\omega)\,.$$

Show that Ψ_N obeys the difference equation

$$\Psi_N = (2 - \Delta^2\omega_N^2)\,\Psi_{N-1} - \Psi_{N-2}\,,$$

with $\Psi_1 = \Delta(2 - \Delta^2\omega_1^2)$ and $\Psi_2 = \Psi_1 + \Delta + O(\Delta^3)$. In the continuum limit we therefore obtain

$$\frac{d^2\Psi(t,t_0)}{dt^2} = -\omega^2(t)\Psi(t,t_0)\,.$$

with the initial conditions $\Psi(t,t_0) = 0$ and $d\Psi(t,t_0)/dt = 1$ for $t = t_0$. Moreover, the desired expression for $\Delta\det A(\omega)$ then equals $\Psi(t_N)$, thus

$$F(t_N, t_0) = \sqrt{\frac{m}{2\pi i\hbar\Psi(t_N,t_0)}}\,.$$

Problem 3.6 : Show that the Gel'fand-Yaglom method leads also to the results (3.28) and (3.32) in the case $\omega(t) = 0$ or $\omega(t) = \omega$, respectively.

Problem 3.7: Verify the correctness of (3.10) by uniformly scaling the operator $\delta^2 S/\delta q(t_1')\delta q(t_2')$ by a constant. Evaluate the effect of this scaling both directly and by returning to the corresponding term in (3.5). To obtain agreement, it is important to regard the various quantities as (infinite-dimensional) matrices.

Problem 3.8 : The path integral in phase space

Consider the transition function $W(q_N, t_N; q_0, t_0) \equiv {}_{t_N}\langle q_N|q_0\rangle_{t_0}$ for a particle on a line. According to (2.17) it can be written as a path integral over phase space. In this path integral, we are dealing with N p-integrations, but only $N-1$ q-integrations. Therefore it is natural to consider instead the transition function $W(p_N, t_N; q_0, t_0) \equiv {}_{t_N}\langle p_N|q_0\rangle_{t_0}$, which can be obtained by making use of (2.5).

i) From (2.17) derive a discrete expression for $W(p_N, t_N; q_0, t_0)$ and subsequently take the continuum limit $N \to \infty$ to obtain a phase-space path integral based on two paths, $p(t)$ and $q(t)$. Specify the boundary conditions for both these paths.

From here you are supposed to only make use of the continuum expressions for the transition function. This expression is very similar to that for the fermionic path integral, which we will introduce in a later chapter. Note, in particular, that the action contains a boundary term and is only linear in time derivatives.

ii) Determine the 'action' $S[p(t), q(t)]$ that appears in the exponent of the integrand of the path-integral representation for $W(p', t'; q, t)$. Don't forget the boundary term.

iii) Show, using the previous result, that the classical limit $\hbar \to 0$ gives rise to Hamilton's equations with corresponding boundary conditions for $p(t)$ en $q(t)$.

iv) Express the transition function $W(p'', t''; q, t)$ in terms of the transition functions $W(p'', t''; q', t')$ and $W(p', t'; q, t)$ with $t'' > t' > t$. Make use of the completeness of the states $\{|p\rangle\}$ and $\{|q\rangle\}$.

v) Derive from $W(p', t'; q, t)$ (or again from (2.17)) a path integral expression for $W(q', t'; p, t) \equiv {}_{t'}\langle q|p\rangle_t$. Extract again the relevant action and specify the the boundary conditions for the path integrations over $p(t)$ and $q(t)$.

vi) Prove by means of the above action that the classical limit $\hbar \to 0$ gives rise to Hamilton's equations with corresponding boundary conditions for $p(t)$ and $q(t)$.

vii) Finally, prove that the evolution operator is unitary. (Note: this requires to prove the relation $[W(p', t'; q, t)]^* = W(q, t; p', t')$.)

Problem 3.9 : Jacobi identity for Poisson brackets and commutators
In eq:poisson-bracket we introduced the Poisson bracket. Show that it satisfies the jacobi identity,

$$(A, (B, C)) + (B, (C, A)) + (C, (A, B)) = 0\,. \qquad (3.34)$$

Subsequently show that the same identity is satisfied for commutators of matrices.

4 Continuous systems

Until now we have discussed a system with a finite number of degrees of freedom. The transition to an infinite number of degrees of freedom is necessary for the treatment of continuous systems, such as a vibrating solid, since their motion is described by specifying the position coordinates of all points of the solid. The continuum case can be understood as the appropriate limit of a system with a finite number of discrete coordinates. (The text below is taken from De Wit & Smith).

We illustrate this procedure for an elastic rod of fixed length l, undergoing small longitudinal vibrations. The continuous rod can be approximated by a set of discrete coordinates representing a long chain of n equal mass particles spaced a distance a apart and connected by uniform massless springs having force constants k. The total length of the system equals $l = (n+1)a$. If the displacement of the i-th particle from its equilibrium position is measured by the quantity ϕ_l then the kinetic energy of this one-dimensional lattice is

$$T = \tfrac{1}{2} \sum_{i=1}^{n} m \dot{\phi}_i^2 \,, \tag{4.1}$$

where m is the mass of each particle. The potential energy is the sum of $n + 1$ potential energies of each spring as the result of being stretched or compressed from its equilibrium length (note that $\phi_0 = \phi_{n+1} = 0$),

$$V = \tfrac{1}{2} \sum_{i=0}^{n} k(\phi_{i+1} - \phi_i)^2 \,, \tag{4.2}$$

where k is some constant. The force on the ith particle follows from the potential via $F_i = -\partial V/\partial \phi_i$:

$$F_i = k(\phi_{i+1} - \phi_i) - k(\phi_i - \phi_{i-1}) = k(\phi_{i+1} + \phi_{i-1} - 2\phi_i) \,.$$

The force thus decomposes into two parts; the force exerted by the spring on the right of the ith particle, equal to $k(\phi_{i+1} - \phi_i)$, and the force exerted by the spring on the left, equal to $k(\phi_i - \phi_{i-1})$. Combining (4.1) and (4.2) gives the Lagrangian

$$L = T - V = \tfrac{1}{2} \sum_{i=1}^{n} m \dot{\phi}_i^2 - \tfrac{1}{2} \sum_{i=0}^{n} k(\phi_{i+1} - \phi_i)^2 \,. \tag{4.3}$$

The corresponding Euler-Lagrange equations yield Newton's law $m\ddot{\phi}_i = F_i$.

In order to describe the elastic rod we must take the continuum limit of the system discussed above. Hence we increase the number of particles to infinity ($n \to \infty$) keeping the total length $l = (n + 1)a$, and the mass per unit length $\mu = m/a$ fixed. Furthermore $Y = ka$ must be kept fixed as well; this follows from Hooke's law, which tells us that the extension of the rod per unit length is directly proportional to the force exerted on the rod, with Young's modulus being the constant of proportionality. In the discrete case the force between two particles is $F = k(\phi_{i+1} - \phi_i)$, and the extension of the interparticle spacing per unit length is $(\phi_{i+1} - \phi_i)/a$; hence we identify $Y = ka$ as Young's modulus which should be kept constant in the continuum limit.

Rewriting the Lagrangian (4.3) as

$$L = \tfrac{1}{2}\sum_{i=1}^{n} a\Big(\frac{m}{a}\dot{\phi}_i^2\Big) - \tfrac{1}{2}\sum_{i=0}^{n} a(ka)\Big(\frac{\phi_{i+1}-\phi_i}{a}\Big)^2 , \tag{4.4}$$

it is straightforward to take the limit $a \to 0$, $n \to \infty$ with $l = (n+1)a$, $\mu = m/a$ and $Y = ka$ fixed. The continuous position coordinate x now replaces the label i, and ϕ_i becomes a function of x, i.e. $\phi_l \to \phi(x)$. Hence the Lagrangian becomes an integral over the length of the rod

$$L = \tfrac{1}{2}\int_0^l \mathrm{d}x\,[\mu\dot{\phi}^2 - Y(\partial_x\phi)^2] , \tag{4.5}$$

where we have used

$$\lim_{a\to 0}\frac{\phi_{i+1}-\phi_i}{a}\lim_{a\to 0}\frac{\phi(x+a)-\phi(x)}{a} = \frac{\partial\phi}{\partial x} \equiv \partial_x\phi\,.$$

Also the equation of motion for the coordinate ϕ_i can be obtained by this limiting procedure. Starting from

$$\frac{m}{a}\ddot{\phi}_i - ka\frac{\phi_{i+1}+\phi_{i-1}-2\phi_i}{a^2} = 0\,, \tag{4.6}$$

and using

$$\lim_{a\to 0}\frac{\phi_{i+1}+\phi_{i-1}-2\phi_i}{a^2} = \frac{\partial^2\phi}{\partial x^2} \equiv \partial_{xx}\phi\,,$$

the equation of motion becomes

$$\mu\ddot{\phi} - Y\partial_{xx}\phi = 0\,. \tag{4.7}$$

We see from this example that x is a continuous variable replacing the discrete label i. Just as there is a generalized coordinate ϕ_i for each i, there is a generalized coordinate $\phi(x)$ for each x, i.e. the finite number of coordinates ϕ_i has been replaced by a function of x. In fact ϕ depends also on time, so we are dealing with a function of two variables. This function $\phi(x,t)$ is called the *displacement field*, and $\dot{\phi} = \partial_t\phi$ and $\partial_x\phi$ are its partial derivatives with respect to time and position.

The Lagrangian (4.5) appears as an integral over x of

$$\mathcal{L} = \tfrac{1}{2}\mu\dot{\phi}^2 - \tfrac{1}{2}Y(\partial_x\phi)^2\,, \tag{4.8}$$

which is called the Lagrangian density. In this case it is a function of $\phi(x,t)$ and its first-order derivatives $\partial_t\phi(x,t)$ and $\partial_x\phi(x,t)$, but one can easily envisage further generalizations.

It has become common practice in field theory to simply call the Lagrangian density the Lagrangian, as the space integral of the Lagrangian density will no longer play a role. What is relevant is the action, which can now be written as an integral over both space and time, i.e.

$$S[\phi(x,t)] = \int_{t_1}^{t_2} \mathrm{d}t \int_0^l \mathrm{d}x \mathcal{L}(\phi(x,t), \dot{\phi}(x,t), \partial_x \phi(x,t)) \,. \tag{4.9}$$

It is a functional of $\phi(x,t)$, i.e. it assigns a number to any function of space and time.

It is possible to obtain the equations of motion for $\phi(x,t)$ directly from Hamilton's principle by following the same arguments as in the previous chapter. One then investigates the change in the action under an infinitesimal change in the fields

$$\begin{aligned} \phi(x,t) &\to \phi(x,t) + \delta\phi(x,t) \,, \\ \partial_t \phi(x,t) &\to \partial_t \phi(x,t) + \frac{\partial}{\partial t}\delta\phi(x,t) \,, \\ \partial_x \phi(x,t) &\to \partial_x \phi(x,t) + \frac{\partial}{\partial x}\delta\phi(x,t) \,, \end{aligned} \tag{4.10}$$

leading to

$$\begin{aligned} \delta S[\phi(x,t)] &= S[\phi(x,t) + \delta\phi(x,t)] - S[\phi(x,t)] \\ &= \int_{t_1}^{t_2} \mathrm{d}t \int_0^l \mathrm{d}x \Big\{ \frac{\partial \mathcal{L}}{\partial \phi(x,t)} \delta\phi(x,t) + \frac{\partial \mathcal{L}}{\partial(\partial_t \phi(x,t))} \frac{\partial}{\partial t}\delta\phi(x,t) \\ &\qquad + \frac{\partial \mathcal{L}}{\partial(\partial_x \phi(x,t))} \frac{\partial}{\partial x}\delta\phi(x,t) \Big\} \,. \end{aligned} \tag{4.11}$$

Integrating the second and third terms by parts

$$\begin{aligned} \int_{t_1}^{t_2} \mathrm{d}t \frac{\partial \mathcal{L}}{\partial(\partial_t \phi)} \frac{\partial}{\partial t}\delta\phi &= \frac{\partial \mathcal{L}}{\partial(\partial_t \phi)} \delta\phi\Big|_{t_1}^{t_2} - \int_{t_1}^{t_2} \mathrm{d}t \frac{\partial}{\partial t}\Big(\frac{\partial \mathcal{L}}{\partial(\partial_t \phi)}\Big)\delta\phi \,, \\ \int_0^l \mathrm{d}x \frac{\partial \mathcal{L}}{\partial(\partial_x \phi)} \frac{\partial}{\partial x}\delta\phi &= \frac{\partial \mathcal{L}}{\partial(\partial_x \phi)} \delta\phi\Big|_{t_1}^{t_2} - \int_0^l \mathrm{d}x \frac{\partial}{\partial x}\Big(\frac{\partial \mathcal{L}}{\partial(\partial_x \phi)}\Big)\delta\phi \,, \end{aligned}$$

leads to

$$\begin{aligned} \delta S[\phi(x,t)] &= \int_{t_1}^{t_2} \mathrm{d}t \int_0^1 \mathrm{d}x \, \delta\phi \Big\{ \frac{\partial \mathcal{L}}{\partial \phi} - \frac{\partial}{\partial t}\Big(\frac{\partial \mathcal{L}}{\partial(\partial_t \phi)}\Big) - \frac{\partial}{\partial x}\Big(\frac{\partial \mathcal{L}}{\partial(\partial_x \phi)}\Big) \Big\} \\ &\quad + \int_0^l \mathrm{d}x \frac{\partial \mathcal{L}}{\partial(\partial_t \phi)} \delta\phi\Big|_{t=t_1}^{t=t_2} + \int_{t_1}^{t_2} \mathrm{d}t \frac{\partial \mathcal{L}}{\partial(\partial_x \phi)} \delta\phi\Big|_{x=0}^{x=l} \,. \end{aligned} \tag{4.12}$$

Hamilton's principle requires that the action be stationary with respect to infinitesimal variations of the fields that leave the field values at the initial and final time unaffected, i.e. $\phi(x,t_1) = \phi_1(x)$ and $\phi(x,t_2) = \phi_2(x)$. Therefore we have $\delta\phi(t_1,x) = \delta\phi(t_2,x) = 0$. On the other hand, because the rod is clamped, the displacement at the endpoints must be zero, i.e. $\delta\phi(x,t) = 0$ for $x = 0$ and $x = l$. Under these circumstances the last two terms in (4.12) vanish, and Hamilton's principle gives

$$\frac{\partial}{\partial t}\Big(\frac{\partial \mathcal{L}}{\partial(\partial_t\phi)}\Big) + \frac{\partial}{\partial x}\Big(\frac{\partial \mathcal{L}}{\partial(\partial_x\phi)}\Big) - \frac{\partial \mathcal{L}}{\partial\phi} = 0 \tag{4.13}$$

This is the Euler-Lagrange equation for a continuous system. As a check one can insert the Lagrangian (4.8) into (4.13) to derive the equation of motion, which indeed gives (4.7). Note that with a suitable choice of units we can write the Lagrangian (4.8) as

$$\mathcal{L} = -\tfrac{1}{2}(\partial_x\phi)^2 + \tfrac{1}{2}(\partial_t\phi)^2\,. \tag{4.14}$$

The generalization to continuous systems in more space dimensions is now straightforward, and one can simply extend the definitions of the Lagrangian and the Euler-Lagrange equations. For example, in two dimensions one may start with a two-dimensional system of springs. The displacement of the particle at the site labelled by (i,j) is measured by the quantity $\phi_{ij}(t)$, which is a two-dimensional vector. In the limit when we go to a continuous system this becomes the two-dimensional displacement field $\phi_{ij}(x,y,t)$, of a membrane subjected to small vibrations in the (x,y) plane.

Problem 4.1 : A vibrating membrane
Consider a membrane (for instance of a drum) and let the field $\phi(x,y,t)$ measure the displacement of the membrane in the direction orthogonal to the membrane. Argue that for small oscillations the relevant Lagrangian density takes the form

$$\mathcal{L} = -\tfrac{1}{2}Y(\partial_x\phi)^2 - \tfrac{1}{2}Y(\partial_y\phi)^2 + \tfrac{1}{2}\mu(\partial_t\phi)^2\,, \tag{4.15}$$

in rescaled units. Give possible reasons for suppressing a term proportional to $\partial_x\partial_y\phi$ and for choosing equal coefficient for the first two terms. Derive the corresponding Euler-Lagrange equations. Write down the normal modes (characterized by a well-defined frequency) for a square membrane where $0 \leq x, y \leq L$. Thes normal modes can be written as $\sin k_x x\,\sin k_y y\,\cos(\omega t + \alpha)$, where the k_x, k_y are the wave numbers and ω denotes the frequency. Express these in terms of Y and μ and find the propagation velocity of these (transverse) waves.

5 Field theory

As we have seen above, the action S in field theory is no longer a function of a finite number of coordinates, but of fields. These fields are functions defined in a d-dimensional space-time, parametrized by the time t and by $d-1$ spatial coordinates. Henceforth we use a d-vector notation, $x^\mu = (\vec{x}, t)$. Usually we will consider Lorentz invariant field theories. There are many such theories, but the simplest ones are based on scalar fields $\phi(\vec{x}, t)$. For instance, a standard action for a single scalar field $\phi(x) = \phi(\vec{x}, t)$ is given by

$$\begin{aligned} S[\phi(x)] &= \int d^d x \left\{ -\tfrac{1}{2}(\partial_\mu \phi(x))^2 - \tfrac{1}{2} m^2 \phi^2(x) \right\} \\ &= \int dt \int d^{d-1}x \left\{ \tfrac{1}{2}(\partial_t \phi)^2 - \tfrac{1}{2}(\vec{\nabla}\phi)^2 - \tfrac{1}{2} m^2 \phi^2 \right\}, \end{aligned} \tag{5.1}$$

which is indeed Lorentz invariant, owing to the fact that we adopted a metric with signature $(-1, 1, \ldots, 1)$, corresponding to the Lorentz-invariant inner product $x^2 = \vec{x}^2 - t^2$. Observe that here, and throughout these notes, we choose units where $c = 1$. The field equation (or equation of motion) corresponding to (5.1) is the Klein-Gordon equation,

$$(\partial_\mu^2 - m^2)\phi = 0. \tag{5.2}$$

The action (5.1) describes a free scalar field; interactions will be described by terms of higher order in ϕ.

The expression in parentheses in (5.1) is called the Lagrangian *density*, denoted by $\mathcal{L}$, because its integral over space defines the Lagrangian,

$$S[\phi] = \int dt \int d^{d-1}x \; \mathcal{L}(\phi(x), \partial_\mu \phi(x)) = \int dt \, L. \tag{5.3}$$

In order to see that the action (5.1) describes an infinite number of degrees of freedom, we may decompose the field $\phi(\vec{x}, t)$ in terms of a complete set of functions $Y(\vec{x})$,

$$\phi(\vec{x}, t) = \sum_A \phi_A(t) \, Y^A(\vec{x}). \tag{5.4}$$

When $\{A\}$ is a continuous set, the sum is replaced by an integral. For instance, we may have

$$\phi(\vec{x}, t) = (2\pi)^{-\frac{d-1}{2}} \int d^{d-1}k \; \phi_{\vec{k}}(t) \, e^{i\vec{k}\cdot\vec{x}}. \tag{5.5}$$

Substituting this expansion into (5.1) we get

$$S[\phi] = \int dt \left\{ \int d^{d-1}k \, \tfrac{1}{2} \left[|\dot{\phi}_{\vec{k}}(t)|^2 - (\vec{k}^2 + m^2)|\phi_{\vec{k}}(t)|^2 \right] \right\}, \tag{5.6}$$

where we used that for a real scalar field $[\phi_{\vec{k}}(t)]^* = \phi_{-\vec{k}}(t)$, as can be seen from (5.5). We recognize (5.6) as the action for an infinite set of independent harmonic oscillators with frequencies $\sqrt{\vec{k}^2 + m^2}$. (See problem 1.1.)

Let us therefore momentarily return to the case of a single harmonic oscillator. The Lagrangian is equal to

$$L = \tfrac{1}{2}m\dot{q}^2 - \tfrac{1}{2}m\omega^2 q^2. \tag{5.7}$$

Defining the canonical momentum in the standard way,

$$p \equiv \frac{\partial L}{\partial \dot{q}} = m\dot{q}, \tag{5.8}$$

the Hamiltonian reads (from now on it should be clear from the context when p and q are operators, and we will no longer indicate this by using P and Q)

$$H \equiv p\dot{q} - L = \frac{p^2}{2m} + \tfrac{1}{2}m\omega^2 q^2. \tag{5.9}$$

We introduce the raising and lowering operators, $a^\dagger$ and a,

$$\begin{aligned} a &= \frac{1}{\sqrt{2m\hbar\omega}}\Big(m\omega\, q + ip\Big), \\ a^\dagger &= \frac{1}{\sqrt{2m\hbar\omega}}\Big(m\omega\, q - ip\Big). \end{aligned} \tag{5.10}$$

The canonical commutation relations (3.23) imply that

$$[a, a^\dagger] = 1. \tag{5.11}$$

Using the inverse of (5.10),

$$\begin{aligned} q &= \sqrt{\frac{\hbar}{2m\omega}}\Big(a + a^\dagger\Big), \\ p &= -im\omega\sqrt{\frac{\hbar}{2m\omega}}\Big(a - a^\dagger\Big), \end{aligned} \tag{5.12}$$

we rewrite the Hamiltonian as

$$H = \tfrac{1}{2}\hbar\omega(a\, a^\dagger + a^\dagger\, a) = \hbar\omega(a^\dagger\, a + \tfrac{1}{2}). \tag{5.13}$$

In the Heisenberg picture we have time-dependent operators $a(t)$ and $a^\dagger(t)$,

$$a(t) = e^{\frac{i}{\hbar}Ht} a\, e^{-\frac{i}{\hbar}Ht}, \qquad a^\dagger(t) = e^{\frac{i}{\hbar}Ht} a^\dagger\, e^{-\frac{i}{\hbar}Ht}, \tag{5.14}$$

which satisfy

$$\frac{da}{dt} = \frac{i}{\hbar}[H, a], \qquad \frac{da^\dagger}{dt} = \frac{i}{\hbar}[H, a^\dagger]. \tag{5.15}$$

Note that, since $[H, a] = -\hbar\omega\, a$ and $[H, a^\dagger] = \hbar\omega\, a^\dagger$, we can easily derive that

$$a(t) = a\, e^{-i\omega t}, \qquad a^\dagger(t) = a^\dagger\, e^{i\omega t}. \tag{5.16}$$

Obviously in this picture we have the same decomposition as in (5.12),

$$\begin{aligned} q(t) &= \sqrt{\frac{\hbar}{2m\omega}}\Big(a(t) + a^\dagger(t)\Big), \\ p(t) &= -im\omega\sqrt{\frac{\hbar}{2m\omega}}\Big(a(t) - a^\dagger(t)\Big). \end{aligned} \tag{5.17}$$

Note that the operators $q(t)$ and $p(t)$ satisfy the classical equations of motion, $m\dot{q} = p$ and $\dot{p} = -m\omega^2\, q$. It is straightforward to calculate the commutators of the Heisenberg operators. First note that $[a(t), a(t')] = [a^\dagger(t), a^\dagger(t')] = 0$ and $[a(t), a^\dagger(t')] = \exp i\omega(t' - t)$, so that we derive

$$\begin{aligned} [q(t), q(t')] &= \frac{\hbar}{2m\omega}\Big([a(t), a^\dagger(t')] + [a^\dagger(t), a(t')]\Big) \\ &= -\frac{\hbar i}{m\omega}\sin\omega(t - t'). \end{aligned} \tag{5.18}$$

Analogously,

$$[q(t), p(t')] = i\hbar\cos\omega(t - t'). \tag{5.19}$$

For $t = t'$, (5.18) vanishes and (5.19) yields $i\hbar$, which are the usual equal-time results.

We now return to the field theory defined by (5.1). The canonical momentum is defined by the functional derivative,

$$\pi(\vec{x}, t) \equiv \frac{\partial S[\phi]}{\partial\dot{\phi}(\vec{x}, t)}. \tag{5.20}$$

For the case at hand, this yields

$$\pi(\vec{x}, t) = \dot{\phi}(\vec{x}, t). \tag{5.21}$$

The Hamiltonian equals

$$\begin{aligned} H &= \int d^{d-1}x\,\Big\{\pi\dot{\phi} - \mathcal{L}\Big\} \\ &= \int d^{d-1}x\,\Big\{\tfrac{1}{2}\pi^2 + \tfrac{1}{2}(\vec{\nabla}\phi)^2 + \tfrac{1}{2}m^2\phi^2\Big\}, \end{aligned} \tag{5.22}$$

Since this field theory describes just an infinite set of harmonic oscillators, its quantization is obvious. In analogy with (5.17) the field, which now represents an operator acting on a quantum-mechanical Hilbert space, can be decomposed in creation and absorption operators.

In the Heisenberg picture we thus find (see also problem 5.1)

$$
\begin{aligned}
\phi(\vec{x},t) &= \sqrt{\frac{\hbar}{(2\pi)^{d-1}}}\int \frac{d^{d-1}k}{\sqrt{2k_0}}\left\{a(\vec{k})\,e^{i\vec{k}\cdot\vec{x}-ik_0t}+a^\dagger(\vec{k})\,e^{-i\vec{k}\cdot\vec{x}+ik_0t}\right\},\\
\pi(\vec{x},t) &= \sqrt{\frac{\hbar}{(2\pi)^{d-1}}}\int \frac{d^{d-1}k}{\sqrt{2k_0}}(-ik_0)\left\{a(\vec{k})\,e^{i\vec{k}\cdot\vec{x}-ik_0t}-a^\dagger(\vec{k})\,e^{-i\vec{k}\cdot\vec{x}+ik_0t}\right\},
\end{aligned}
\tag{5.23}
$$

where the frequencies are given by $k_0=\sqrt{\vec{k}^2+m^2}$. The reason for the factor $(2k_0)^{-1/2}$ in the integrands is follows from substituting $m=1$ and $\omega=k_0$ in the expressions for a single harmonic oscillator. Note that $\phi(\vec{x},t)$ is a solution of the field equation (5.2), so that the field satisfies the classical equation of motion. Canonical commution relations are now effected by

$$
[\phi(\vec{x},t),\ \pi(\vec{x}\,',t')]_{t=t'}=i\hbar\,\delta^{d-1}(\vec{x}-\vec{x}\,'),
\tag{5.24}
$$

which is equivalent to

$$
[a(\vec{k}),a^\dagger(\vec{k}\,')]=\delta^{d-1}(\vec{k}-\vec{k}\,').
\tag{5.25}
$$

We may also consider the analogue of (5.18) and compute the commutator for the field operators at different space-time points. When these two points, say $(\vec{x},t)$ and $(\vec{x}\,',t')$, are separated by a space-like distance, so that $(\vec{x}-\vec{x}')^2>(t-t')^2$, this commutator should vanish, because we can always transform to another Lorentz frame such that the two points are at equal time. Let us verify that this is indeed the case. Using (5.23) we evaluate (cf. (5.18))

$$
\begin{aligned}
[\phi(\vec{x},t),\phi(\vec{x}\,',t')] &= \frac{\hbar}{(2\pi)^{d-1}}\int\frac{d^{d-1}k\,d^{d-1}k'}{\sqrt{4k_0k_0'}}\Big\{\mathrm{e}^{\mathrm{i}\vec{\mathrm{k}}\cdot\vec{\mathrm{x}}-\mathrm{i}\mathrm{k}_0\mathrm{t}-\mathrm{i}\vec{\mathrm{k}}\,'\cdot\vec{\mathrm{x}}\,'+\mathrm{i}\mathrm{k}_0'\mathrm{t}'}\,[\mathrm{a}(\vec{\mathrm{k}}),\mathrm{a}^\dagger(\vec{\mathrm{k}}\,')]\\
&\qquad +e^{-i\vec{k}\cdot\vec{x}+ik_0t+i\vec{k}\,'\cdot\vec{x}\,'-ik_0't'}\,[a^\dagger(\vec{k}),a(\vec{k}\,')]\Big\},\\
&= \frac{2i\hbar}{(2\pi)^{d-1}}\int\frac{d^{d-1}k}{2k_0}\sin k\cdot(x-x').
\end{aligned}
\tag{5.26}
$$

In this integral, the scalar product $k\cdot(x-x')$ is Lorentz invariant. Furthermore, it can be shown that the integral $\int\frac{d^{d-1}k}{2k_0}$ is also Lorentz invariant, so that (5.26) is a Lorentz invariant function. If $x-x'$ is a space-like vector, we can exploit the Lorentz invariance of (5.26) by performing a Lorentz transformation such that t becomes equal to t'. Then it is obvious that (5.26) vanishes because the integrand is odd in $\vec{k}$.

So we conclude that $[\phi(x),\ \phi(x')]=0$ whenever x and x' are separated by a space-like distance. This phenomenon is known as *local commutativity*, a fundamental property that any relativistic field theory should satisfy. Local quantum operators taken at points that are not causally connected, commute.

We started by introducing field theories as a system of infinitly many degrees of freedom. However, there is a dual interpretation which is known under the term 'second quantization'. By first quantization one means the usual quantum mechanics, used to describe a system with a finite number of degrees of freedom. For instance, take a free particle, whose states are described in terms of a wave number or a momentum vector, say $\vec{p}$. Both classically and quantum-mechanically the energy of this state is determined in terms of the momentum and denoted by $E_{\vec{p}}$. The precise dependence of $E_{\vec{p}}$ on $\vec{p}$ is not important. For instance, for a free relativistic particle of mass μ we would have $E_{\vec{p}} = \sqrt{\vec{p}^2 + \mu^2}$, while in the nonrelativistic case we have $E_{\vec{p}} = \frac{1}{2}\vec{p}^2/\mu$. Now one introduces a Hilbert space, called *Fock space*, consisting of states that describe an arbitrary number of free particles. Assuming that the particles are bosons, the multiparticle states should be symmetric under interchange. Therefore it is sufficient to specify the *occupation numbers* $n_{\vec{p}}$ which give the number of particles with the same momentum $\vec{p}$. The vacuum (or groundstate) of the Fock space is denoted by $|0\rangle$, and is the state that contains no particles. Then we have the one-particle states $|\vec{p}\,\rangle$, the two-particle states $|\vec{p}, \vec{p}\,'\rangle$, and so on. Using the occupation numbers, we can generally denote these states by

$$|n_{\vec{p}_1}, n_{\vec{p}_2}, n_{\vec{p}_3}, \ldots\rangle, \quad \text{with} \quad n_{\vec{p}_i} = 0, 1, 2, \ldots, \tag{5.27}$$

where $\vec{p}_i$ are the possible momenta. The energy of these states is given by

$$E(n_{\vec{p}_i}) = \sum_i n_{\vec{p}_i} \, E_{\vec{p}_i} \, . \tag{5.28}$$

In the Fock space we can define creation and annihilation operators, which increase or decrease the occupation numbers by 1. They are defined by

$$\begin{aligned} a(\vec{p}_i)\, |n_{\vec{p}_1}, n_{\vec{p}_2}, \ldots, n_{\vec{p}_i}, \ldots\rangle &= \sqrt{n_{\vec{p}_i}}\; |n_{\vec{p}_1}, n_{\vec{p}_2}, \ldots, n_{\vec{p}_i} - 1, \ldots\rangle, \\ a^\dagger(\vec{p}_i)\, |n_{\vec{p}_1}, n_{\vec{p}_2}, \ldots, n_{\vec{p}_i}, \ldots\rangle &= \sqrt{n_{\vec{p}_i} + 1}\; |n_{\vec{p}_1}, n_{\vec{p}_2}, \ldots, n_{\vec{p}_i} + 1, \ldots\rangle. \end{aligned} \tag{5.29}$$

With this definition, one can show that

$$[a(\vec{p}_i), a^\dagger(\vec{p}_j)] = \delta_{ij}. \tag{5.30}$$

The energy of the multiparticle states (cf. 3.27) are given by the eigenvalues of the Hamiltonian

$$H_0 = \sum_i a^\dagger(\vec{p}_i)\, a(\vec{p}_i)\, E_{\vec{p}_i}. \tag{5.31}$$

It is easy to introduce interactions into this theory by including terms of higher order in the operators a and $a^\dagger$. For instance, the term

$$H_{\text{int}} = \sum_{i,j,k,l} \delta(\vec{p}_i + \vec{p}_j - \vec{p}_k - \vec{p}_l)\, V_{ijkl}\, a^\dagger(\vec{p}_i)\, a^\dagger(\vec{p}_j)\, a(\vec{p}_k)\, a(\vec{p}_l), \tag{5.32}$$

describes a four-particle interaction in which two particles are annihilated and two other particles are created. The delta function in (5.32) ensures momentum conservation.

The key observation is that the energy spectrum for the multiparticle states coincides with the spectrum of a system of infinitely many harmonic oscillators with frequencies $\hbar^{-1}\, E_{\vec{p}_i}$. Using the operators a and $a^\dagger$ we can now write down fields $\phi(\vec{x}, t)$ by using the expression (5.23) with $\vec{k} = \hbar^{-1}\vec{p}$ and $k_0 = \hbar^{-1}\, E_{\vec{p}}$. The above results can then be cast in the form of a field theory, which, upon quantization, leads to the same Fock space operators as above. For a system of relativistic particles, where $E_{\vec{p}} = \sqrt{\vec{p}^2 + \mu^2}$, this system of harmonic oscillators is precisely described by the field theory defined by (5.1), with $m = \mu/\hbar$. In particular, the Hamiltonian H_0 is equal to (5.22), up to an infinite "zero-point" energy

$$\langle 0|H|0\rangle = \tfrac{1}{2}\sum_i \sqrt{\vec{p}_i^2 + \mu^2}. \tag{5.33}$$

This is one of the characteristic infinities that emerge in quantum field theory, caused by the presence of an infinite number of degrees of freedom. We will return to these infinities in due course.

Problem 5.1 : The complex harmonic oscillator
To exhibit the derivation of (5.23) from the Schrödinger picture, consider the theory (5.1) in one space dimension. For simplicity, assume that the space dimension is compactified to a circle of length L. Show that the field ϕ can be expanded in a Fourier series

$$\phi(x,t) = \frac{1}{\sqrt{L}} \sum_k \phi(k,t)\, \exp(ikx)\,,$$

with k equal to $2\pi/L$ times a (positive or negative) integer. Subsequently, write down the Lagrangian.

Now restrict yourself to two Fourier modes with a fixed value of $|k|$, so that the infinite Fourier sum is replaced by a sum over two terms with $\pm k$, where we choose k positive. Define $\phi_k = \phi$ and $\phi_{-k} = \phi^\dagger$, so that the Lagrangian reads

$$L = \dot{\phi}\dot{\phi}^\dagger - \omega^2 \phi\phi^\dagger\,. \qquad (\omega^2 = k^2 + m^2)$$

For this system of a finite number of degrees of freedom, find the expression for the canonical momenta π and $\pi^\dagger$, associated with ϕ and $\phi^\dagger$, respectively. Then write the canonical commutation relations and give the Hamiltonian. Express ϕ, $\phi^\dagger$, π and $\pi^\dagger$ in terms of the operators

$$a = \frac{1}{\sqrt{2\hbar\omega}}\Big(\omega\phi + i\pi^\dagger\Big), \quad b = \frac{1}{\sqrt{2\hbar\omega}}\Big(\omega\phi^\dagger + i\pi\Big),$$

and their hermitean conjugates. Derive the commutation relations for a, $a^\dagger$, b and $b^\dagger$ and write down the Hamiltonian in terms of these operators. What does this system correspond to?

Derive the operators a, $a^\dagger$, b and $b^\dagger$ in the Heisenberg picture. Reconstruct the field $\phi(x,t)$ by writing the full Fourier sum. Take the limit $L\to\infty$ and compare to the first line in (5.23). Do the same for the canonical momenta. Here we note the Fourier transform in d space-time dimensions (note the sign in the exponential)

$$\pi(\vec{x},t) = (2\pi)^{-\frac{d-1}{2}} \int d^{d-1}k\; \pi(\vec{k},t)\, e^{-i\vec{k}\cdot\vec{x}}.$$

Problem 5.2 : Taking the continuum limit

Express the Hamiltonian (5.22) in terms of the operators $a(\vec{k})$ and $a^\dagger(\vec{k})$. In view of the above presentation it is convenient to consider the field theory (5.1) in a large but finite ($(d-1)$-dimensional) box of volume V and impose periodic boundary conditions. Then we decompose (cf. 3.23),

$$\begin{aligned}\phi(\vec{x},t) &= \frac{1}{\sqrt{V}}\sum_{\vec{k}}\phi(\vec{k},t)e^{i\vec{k}\cdot\vec{x}} = \sum_{\vec{k}}\sqrt{\frac{\hbar}{2Vk_0}}\left\{a(\vec{k})\,e^{i\vec{k}\cdot\vec{x}-ik_0t} + a^\dagger(\vec{k})\,e^{-i\vec{k}\cdot\vec{x}+ik_0t}\right\}, \qquad (5.34)\\ \pi(\vec{x},t) &= \frac{1}{\sqrt{V}}\sum_{\vec{k}}\pi(\vec{k},t)e^{-i\vec{k}\cdot\vec{x}} = \sum_{\vec{k}}\sqrt{\frac{\hbar}{2Vk_0}}(-ik_0)\left\{a(\vec{k})\,e^{i\vec{k}\cdot\vec{x}-ik_0t} - a^\dagger(\vec{k})\,e^{-i\vec{k}\cdot\vec{x}+ik_0t}\right\},\end{aligned}$$

where $\pi(\vec{k},t)\equiv \partial S/\partial\dot\phi(\vec{k},t)$. Determine the commutator $[\phi(\vec{k},t),\pi(\vec{k}',t')]_{t=t'}$ from (5.24) and check the expression for $[a(\vec{k}),a^\dagger(\vec{k}')]$. Give again the Hamiltonian and compare the result with (5.31) and (5.33). Consider the continuum results by making use of the correspondence

$$\sum_{\vec{k}} \longrightarrow \frac{V}{(2\pi)^{d-1}}\int d^{d-1}k\,, \qquad \delta_{\vec{k},\vec{k}'} \longrightarrow \frac{(2\pi)^{d-1}}{V}\,\delta^{d-1}(\vec{k}-\vec{k}')\,. \qquad (5.35)$$

Problem 5.3 : Prove that the integral measure $\int \mathrm{d}^3k\,[2(\vec{k}^2+m^2)^{1/2}]^{-1}$ is Lorentz invariant. This can be done in two ways. First perform a Lorentz transformation (see e.g. De Wit & Smith, appendix A) and express $\mathrm{d}^3k'\,[2(\vec{k}'^2+m^2)^{1/2}]^{-1}$ in terms of the original momenta. Secondly, rewrite the integral as an integral over four momenta $\vec{k}$ and k_0 by including $\delta(k^2+m^2)\,\theta(k_0)$ in the integrand.

Problem 5.4 : Show that $\langle 0|\phi(\vec{x},t)\,\phi(\vec{x},t)|0\rangle$ is divergent.

Problem 5.5 : Wave functions versus fields

Give arguments why a field and a wave function are two different concepts, so that (5.2) should not be regarded as a relativistic generalization of the Schrödinger equation. (This point is even more pressing for fermions where the relativistic wave equation – the Dirac equation – is also a first-order differential equation, just as the Schrödinger equation.) For comparison, consider the single harmonic oscillator and confront the second-order differential equation for the operator $q(t)$ in the Heisenberg picture with the first-order Schrödinger equation. Derive the Schrödinger equation in the "coordinate" representation where we have wave functions $\Psi(\phi(\vec{k}),t)$ depending on the "coordinates" $\phi(\vec{k})$ and the time t. For convenience, consider again the theory (5.1) in a box with periodic boundary conditions. Write down the correct expression for the momenta $\pi(\vec{k})$ in this representation and give the Hamiltonian. Show that the ground state wave function $\Psi_0(\phi(\vec{k}),t)$, which corresponds to the vacuum (i.e. the state with zero occupation numbers) of the Fock space, takes the form (make use of problem 3.1)

$$\Psi_0(\phi(\vec{k}),t) = \exp\Big\{\sum_{\vec{k}}\Big(-\frac{\sqrt{\vec{k}^2+m^2}}{2\hbar}\phi(\vec{k})\phi(-\vec{k}) - \tfrac{1}{2}it\sqrt{\vec{k}^2+m^2} + \tfrac{1}{4}\ln\Big[\frac{\vec{k}^2+m^2}{\pi\hbar}\Big]\Big)\Big\}\,.$$

Note the presence of the zero-point energy.

Problem 5.6 : A particle on a circle

Consider a particle of mass m, moving on a circle C of radius R in the (x,y)-plane. The circle is parametrised by $(x,y)=(R\cos\phi, R\sin\phi)$ and $0\leq\phi<2\pi$. The particle experiences a force described by a periodic potential $V(\phi)=V(\phi+2\pi)$, so that the classical action reads

$$S[\phi] = \int dt\Big\{\tfrac{1}{2}mR^2\Big(\frac{d\phi}{dt}\Big)^2 - V(\phi)\Big\}\ .$$

i) Show that the Hamiltonian of the particle equals

$$H(p_\phi,\phi) = \frac{p_\phi^2}{2mR^2} + V(\phi)\,,$$

with p_ϕ the momentum conjugate to ϕ. After quantization p_ϕ and ϕ are operators satisfying the commutation relation $[\phi,p_\phi]=i\hbar$. How does p_ϕ therefore act on the wave function $\Psi(\phi,t)$? Specify the boundary conditions for $\Psi(\phi,t)$ and determine the eigenvalues of the momentum operator p_ϕ. Finally give the time-dependent Schrödinger equation for the wave function.

By means of the above Hamiltonian we would like to derive a path integral expression for the transition function $W_C(\phi_N,t_N;\phi_0,t_0)\equiv\langle\phi_N|e^{-iH(t_N-t_0)/\hbar}|\phi_0\rangle$. We follow the standard procedure and divide the time interval t_N-t_0 into N pieces of 'length' $\epsilon=(t_N-t_0)/N$, applying the completeness relation $\int_0^{2\pi} d\phi_i \; |\phi_i\rangle\langle\phi_i| = 1$ at any time instant t_i ($i = 1, 2, \ldots, N-1$). In this way we obtain as a first result

$$W_C(\phi_N, t_N; \phi_0, t_0) = \prod_{i=1}^{N-1} \int_0^{2\pi} d\phi_i \; \prod_{j=1}^{N} \langle\phi_j|e^{-iH\epsilon/\hbar}|\phi_{j-1}\rangle \; . \tag{5.36}$$

Subsequently we must determine the matrix element $\langle\phi_j|e^{-iH\epsilon/\hbar}|\phi_{j-1}\rangle$. For this purpose we use the Poisson resummation formula

$$\sum_{n=-\infty}^{\infty} \delta(x-n) = \sum_{\ell=-\infty}^{\infty} e^{2\pi i \ell x} \; . \tag{5.37}$$

Note that the resummation formula expresses the fact that the phase factors on the right-hand side only interfere constructively when the phases are equal to a multiple of 2π.

ii) Show with help of (5.37) that, after neglecting $O(\epsilon^2)$ corrections,

$$\langle\phi_j|e^{-iH\epsilon/\hbar}|\phi_{j-1}\rangle = \sum_{\ell_j=-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{dk_{j-1}}{2\pi} \; e^{i(\phi_j - \phi_{j-1} + 2\pi\ell_j)k_{j-1}} \; e^{-i\epsilon H(\hbar k_{j-1}, \phi_{j-1})/\hbar} \; .$$

Now we also introduce the transition function $W(\phi_N, t_N; \phi_0, t_0)$ for a particle of 'mass' mR^2 that moves subject to the same periodic potential $V(\phi)$ along the full ϕ-axis. (This means that now $-\infty < \phi < \infty$.)

iii) Prove, by substitution of the previous result in (5.36) and by using the path integral expression for $W(\phi_N, t_N; \phi_0, t_0)$,

$$W_C(\phi_N, t_N; \phi_0, t_0) = \sum_{\ell_N=-\infty}^{\infty} W(\phi_N + 2\pi\ell_N, t_N; \phi_0, t_0) \; .$$

Can you physically explain this formula? (Note: ℓ_N is known as the winding number.)

Finally consider the special case of a free particle ($V(\phi) = 0$). Then

$$W(\phi_N, t_N; \phi_0, t_0) = \sqrt{\frac{mR^2}{2\pi i\hbar(t_N - t_0)}} \; \exp\left\{ \frac{imR^2}{2\hbar} \; \frac{(\phi_N - \phi_0)^2}{t_N - t_0} \right\} \; .$$

Because the transition function W_C is periodic in $\phi_N - \phi_0$, we can expand W_C in the Fourier series

$$W_C(\phi_N, t_N; \phi_0, t_0) = \sum_{n=-\infty}^{\infty} C_n(t_N - t_0) \; \frac{e^{in(\phi_N - \phi_0)}}{2\pi} \; .$$

iv) Determine the coefficients $C_n(t_N - t_0)$ by means of a Fourier transform of the result of part iii) and determine with the help of this the eigenvalues of the Hamiltonian. Here, make use of (2.20).

Problem 5.7 : Electromagnetic fields

Consider the Lagrange density for the free photon field $A_\mu(\vec{x}, t)$,

$$\mathcal{L} = -\tfrac{1}{4}(F_{\mu\nu})^2 = -\tfrac{1}{4}(\partial_\mu A_\nu - \partial_\nu A_\mu)^2 \ . \tag{5.38}$$

i) Determine, by considering the variation of the action under $A_\mu \rightarrow A_\mu + \delta A_\mu$, the classical equations of motion for A_μ in their Lorentz covariant form, $\partial^\mu(\partial_\mu A_\nu - \partial_\nu A_\mu) = 0$. Write them in terms of the electric field $\vec{E} = \nabla A_0 - \partial \vec{A}/\partial t$ and the magnetic field $\vec{B} = \nabla \times \vec{A}$.
Suggestion: you may want to use the vector identity $\vec{A} \times (\vec{B} \times \vec{C}) = (\vec{A} \cdot \vec{C})\vec{B} - (\vec{A} \cdot \vec{B})\vec{C}$. What kind of (space- and time-dependent) gauge symmetry do the Lagrange density and the equations of motion for A_μ possess?

We want to quantize the above theory. This requires that we first choose a (so-called) gauge condition (as we will discuss later in these lectures). In what follows we choose the so-called temporal gauge, defined by the condition $A_0 = 0$.

ii) Give the Lagrange density in this gauge and determine again the classical equations of motion. Note that, in comparison with part i), one equation is missing. We return to this shortly.

iii) The Lagrange density in the temporal gauge still contains a residual gauge symmetry. Give this symmetry or derive it from the original symmetry of the original Lagrange density. In addition, write the transformations for $\vec{A}(\vec{k}, t)$, the Fourier transform of $\vec{A}(\vec{x}, t)$.

iv) Determine the canonically conjugate momentum $\vec{\pi}$ corresponding to $\vec{A}$ and express it in terms of $\vec{E}$. Give the Hamiltonian in terms of $\vec{E}$ and $\vec{B}$.
Suggestion: the following identity may be convenient, $(\vec{\nabla} \times \vec{A}) \cdot (\vec{\nabla} \times \vec{A}) = \partial_i A_j \, \partial_i A_j - \partial_i A_j \, \partial_j A_i$.

v) What are the commutation relations of the 'momenta' $\vec{\pi}(\vec{k})$ and the 'coordinates' $\vec{A}(\vec{k})$? What are, in the coordinate representation, the momentum operators and the Hamiltonian. Formulate the time-dependent Schrödinger equation for the wave functional $\Psi[\vec{A}(\vec{k}), t]$. Assumer that the quantization is performed in a finite box of volume V, so that the $\vec{k}$ assume discrete values.

In question ii), we had found that, at the classical level in the temporal gauge, the equation $\nabla \cdot \vec{E} = 0$ is missing. In order to perform the quantization of the Maxwell theory in a correct way, we must therefore explicitly include this equation. We do this by imposing it as a 'constraint' on the wave functional.

vi) Give the above 'constraint' on the wave functional in the coordinate representation. In iii) we determined how $\vec{A}(\vec{k})$ transforms under gauge transformations corresponding to the temporal gauge. Use this to show that the 'constraint' guarantees that $\Psi[\vec{A}(\vec{k}), t]$ is invariant under an infinitesimal gauge transformation.

We will now try to determine the wave functional for the ground state by solving the time-independent Schrödinger equation.

vii) Derive in the usual manner, i.e. from the time-dependent Schrödinger equation, the time-independent Schrödinger equation for a wave functional $\Psi[\vec{A}(\vec{k})]$.

In view of our experience with harmonic oscillators we expect that the wave functional $\Psi_0[\vec{A}(\vec{k})]$ belonging to the ground state will be a Gaussian functional. Therefore we write

$$\Psi_0[\vec{A}(\vec{k})] = C_0 \exp\left\{\sum_{\vec{k}} A_i(-\vec{k})\, G_{ij}(\vec{k})\, A_j(\vec{k})\right\} \ . \tag{5.39}$$

viii) Determine first from the 'constraint' of vii) the form of $G_{ij}(\vec{k})$.
Suggestion: indicate first which tensorial structure you expect for G_{ij}.

ix) Subsequently, solve the time-independent Schrödinger equation. In other words, determine the ground-state wave functional (you may ignore its normalization) and the (infinite) ground-state energy. Could you have written down the answer for the latter directly? If so, explain your answer.

Problem 5.8 : Winding and momentum states

Consider a field theory in a one-dimensional space corresponding to a circle with circumference L, described by a real scalar field $\phi(x,t)$ with action

$$S[\phi] = \int dt \int_0^L dx \ \left[\tfrac{1}{2}(\partial_t\phi)^2 - \tfrac{1}{2}(\partial_x\phi)^2\right] \ . \tag{5.40}$$

i) Argue that the field ϕ can be expanded as

$$\phi(x,t) = \frac{1}{\sqrt{L}} \sum_k \phi_k(t)\, \mathrm{e}^{2\pi i k x/L} \,, \tag{5.41}$$

where k is an integer. Is ϕ_k real?

ii) Write the action in terms of the ϕ_k. As expected we are then dealing with an (infinite) sum of known quantum-mechanical systems. In this sum we distinguish two contributions, i.e. i.e., $S = S_0 + S_{\rm osc}$, where $S_0 = \int {\rm d}t\ \frac{1}{2}(\partial_t\phi_0)^2$ and $S_{\rm osc}$ comprises the contribution of the oscillations described by the ϕ_k with $k \neq 0$. Determine the conjugate momentum π_k of ϕ_k and give the canonical commutation relations.

iii) Determine the spectrum of the conjugate momenta π_k (in other words, their possible eigenvalues). Clarify your answer on the basis of your knowledge of the quantum-mechanical system described by ϕ_k. In particular, note the conjugate momentum belonging to ϕ_0.

iv) Give the Hamiltonian. Give also the corresponding expression in the 'coordinate' representation.

v) Consider now the case that the field ϕ itself characterizes the position on a circle with radius R, so that we identify ϕ with $\phi + 2\pi R$. Argue that the decomposition of ϕ should be changed now into

$$\phi(x,t) = \frac{2\pi m R}{L}x + \frac{1}{\sqrt{L}}\sum_k \phi_k(t)e^{2\pi i k x/L}\,. \tag{5.42}$$

What are the possible values for the number m? What is their significance? Try to clarify your answer with a figure.

vi) Give the action again and distinguish as before between the two terms S_0 and $S_{\rm osc}$. Give the expressions of the conjugate momenta π_k of ϕ_k and write down the canonical commutation relations.

vii) From the periodicity of ϕ, derive a condition for ϕ_0. What is now the spectrum of the momenta? Pay again attention to the conjugate momentum π_0.

viii) Give the Hamiltonian and the ground-state energy. Let us concentrate on the contributions of the Hamiltonian that are *not* caused by the oscillations described by ϕ_k with $k \neq 0$. Determine the eigenvalues of this (nontrivial) part of the Hamiltonian,

$$E_0(m,n) = \frac{1}{2L}\left[\frac{\hbar^2 n^2}{R^2} + (2\pi R)^2 m^2\right]. \tag{5.43}$$

Describe what happens to these eigenvalues when we change R into $\hbar/2\pi R$. in the context of string theory this phenomenon is known as T-duality.

6 Correlation functions

In principle, one would like to calculate the same kind of quantities for any quantum field theory that one considers in the context of more conventional quantum mechanics. Hence one is interested in the determination of energy levels, scattering amplitudes and the like. In general, however, these caclulations are cumbersome and one usually has to rely on perturbation theory. The way one calculates physically relevant quantities depends often on the context. The reason is that the direct physical significance of the quantum field is not necessarily obvious, as one can always apply field redefinitions. Therefore the intermediate results of the theory often take the form of correlation functions, which can carry different names depending again on the context. These, somewhat abstractly defined functions are the topic of this chapter.

As a first attempt to define correlation functions, let us consider

$$ {}_{t_2}\langle q_2|\, q(t)\, q(t') \cdots |q_1\rangle_{t_1} \quad \text{for} \quad t_2 > t > t' > \cdots > t_1, \tag{6.1} $$

where $|q_i\rangle_{t_i}$ is the eigenstate of the position operator at $t = t_i$. Both states and operators are taken in the Heisenberg picture. To facilitate the notation, let us introduce a so-called time-ordered product,

$$ T(q(t)\, q(t') \cdots) \equiv q(t)\, q(t') \cdots, \qquad \text{if} \quad t > t' > \cdots, \qquad \text{etc.} \tag{6.2} $$

The correlation function $G(t, t', \ldots)$ may then be defined by

$$ G(t, t', \ldots) \equiv \frac{{}_{t_2}\langle q_2|T(q(t)\, q(t') \ldots)|q_1\rangle_{t_1}}{{}_{t_2}\langle q_2|q_1\rangle_{t_1}} + \cdots . \tag{6.3} $$

When the time-ordered product contains n operators q at independent times, $G(t, t', \ldots)$ is called the n-point correlation function. Of course, there is always the possibility of modifiying a correlation function by products of lower-n correlation functions. Such modifications are indicated by the dots in (6.3). Later on we intend to make a specific choice for these modifications, but for the moment we leave them unspecified.

Using the completeness of the states $|q\rangle_t$ for fixed value of t, we can rewrite (6.3) as

$$ \begin{aligned} G(t, t', \ldots) &= \frac{\int dq \int dq' \cdots \; {}_{t_2}\langle q_2|q\rangle_t \; q \; {}_t\langle q|q'\rangle_{t'} \; q' \; {}_{t'}\langle q'| \cdots |q_1\rangle_{t_1}}{{}_{t_2}\langle q_2|q_1\rangle_{t_1}} \\ &= \frac{\int \mathcal{D}q \; q(t)\, q(t') \cdots e^{\frac{i}{\hbar} S[q(t)]}}{\int \mathcal{D}q \; e^{\frac{i}{\hbar} S[q(t)]}}, \end{aligned} \tag{6.4} $$

where both path integrals are defined with boundary conditions

$$ q(t_1) = q_1, \qquad q(t_2) = q_2. \tag{6.5} $$

Correlation functions are not restricted to products of the $q(t)$, but can also contain so-called composite operators, "functions" of the operators $q(t)$ taken at the same instant of time. However, in field theory the definition of such operators requires special care, because products of fields become singular when taken at the same space-time point. We return to this aspect in due course.

As an example let us consider the correlation functions for the harmonic oscillator, first in the operator formalism and then by means of path integral techniques.

6.1 Harmonic oscillator correlation functions; operators

We consider the two-point correlation function defined above in the context of the operator formalism. Here it is customary to adopt different boundary conditions. Rather than the states $|q_1\rangle_{t_1}$ and $|q_2\rangle_{t_2}$, we will choose the groundstates $|0\rangle_{t_1}$ and $|0\rangle_{t_2}$. Because the groundstate energy of the harmonic oscillator is equal to $\frac{1}{2}\hbar\omega$, we have

$$|0\rangle_t = e^{\frac{i\omega t}{2}}|0\rangle, \tag{6.6}$$

and therefore

$${}_{t_2}\langle 0|0\rangle_{t_1} = e^{-\frac{i\omega}{2}(t_2-t_1)}. \tag{6.7}$$

Let us now determine the matrix element ${}_{t_2}\langle 0|q(t)\,q(t')|0\rangle_{t_1}$ for $t_2 > t > t' > t_1$. Using the completeness of the energy eigenstates $|n\rangle_{t_0}$ with $t > t_0 > t'$, we can write

$${}_{t_2}\langle 0|q(t)\,q(t')|0\rangle_{t_1} = \sum_n \;{}_{t_2}\langle 0|q(t)|n\rangle_{t_0}\;{}_{t_0}\langle n|q(t')|0\rangle_{t_1}. \tag{6.8}$$

Using (5.17) we compute

$${}_{t_0}\langle n|q(t')|0\rangle_{t_1} = \sqrt{\frac{\hbar}{2m\omega}}\, e^{\frac{1}{2}i\omega(t_1-3t_0+2t')}\,\delta_{n-1,0}. \tag{6.9}$$

In this way we find

$$\begin{aligned} {}_{t_2}\langle 0|q(t)\,q(t')|0\rangle_{t_1} &= \frac{\hbar}{2m\omega}\exp\left[\tfrac{1}{2}i\omega(t_1-3t_0+2t'-t_2+3t_0-2t)\right] \\ &= \frac{\hbar}{2m\omega}\exp\left[-\tfrac{1}{2}i\omega(t_2-t_1)\right]\exp\left[-i\omega(t-t')\right]. \end{aligned} \tag{6.10}$$

Therefore the two-point correlation function equals

$$\begin{aligned} G(t,t') &= \frac{\hbar}{2m\omega}\left\{\theta(t-t')\,e^{-i\omega(t-t')} + \theta(t'-t)\,e^{i\omega(t-t')}\right\} \\ &= \frac{\hbar}{2m\omega}\left\{\cos\omega(t-t') - i\sin\omega(t-t')[\theta(t-t')-\theta(t'-t)]\right\} \end{aligned} \tag{6.11}$$

where $\theta(t)$ is the step function defined by

$$\theta(t) = \begin{cases} 1 & \text{for } t > 0 \\ 0 & \text{for } t < 0 \end{cases} \tag{6.12}$$

Observe that we could have modified the correlation function by adding a term proportional to the product of two "one-point" correlation functions, containing a single operator $q(t)$ or $q(t')$. However, these terms vanish because of (6.9), so that this aspect may be ignored here. Furthermore we should point out that we have implicitly assumed that t_1 and t_2 are moved to $-\infty$ and $+\infty$, because we have not introduced additional step functions to restrict t and t' to the interval (t_1, t_2).

Now we use the following representation for the θ function,

$$\theta(t) = \lim_{\epsilon \downarrow 0} \frac{-1}{2\pi i} \int_{-\infty}^{\infty} dq \, \frac{e^{-iqt}}{q + i\epsilon}, \tag{6.13}$$

which can be proven by contour integration.[2] Substituting (6.13) into (6.11), we find[3]

$$\begin{aligned} G(t,t') &= \frac{-\hbar}{2m\omega} \frac{1}{2\pi i} \int_{-\infty}^{\infty} dq \, \frac{1}{q + i\epsilon} \left\{ e^{-i(\omega+q)(t-t')} + e^{+i(\omega+q)(t-t')} \right\} \\ &= \frac{-\hbar}{2m\omega} \frac{1}{2\pi i} \int_{-\infty}^{\infty} dq \, e^{-iq(t-t')} \left(\frac{1}{q - \omega + i\epsilon} + \frac{1}{-q - \omega + i\epsilon} \right) \\ &= \frac{\hbar}{m} \frac{1}{2\pi i} \int_{-\infty}^{\infty} dq \, \frac{e^{-iq(t-t')}}{-q^2 + \omega^2 - i\epsilon}. \end{aligned} \tag{6.14}$$

Obviously $G(t,t')$ depends only on $t - t'$ and satisfies the equation

$$(-\partial_t^2 - \omega^2) G(t,t') = \frac{i\hbar}{m} \delta(t - t'). \tag{6.15}$$

To show the latter one uses the Dirac delta function $\delta(t) = \frac{1}{2\pi} \int dq \, e^{iqt}$. Of course, the above equation can also be verified directly for the expression (6.11).

To calculate the real and imaginary part of G, we can use the identity

$$\lim_{\epsilon \downarrow 0} \int dq \, \frac{f(q)}{q - \omega \pm i\epsilon} = \mathrm{P} \int dq \, \frac{f(q)}{q - \omega} \mp i\pi f(\omega), \tag{6.16}$$

[2]The integrand has a pole in the lower half plane. If $t > 0$ then it is possible to close the contour in the lower half plane. The pole is then inside the contour, so the Cauchy integral formula, $f(z) = \frac{1}{2\pi i} \oint dw \, f(w)(w - z)^{-1}$ yields $\theta(t) = 1$. For $t < 0$ the contour can be closed in the upper half plane. Now the pole is outside the contour, so we find $\theta(t) = 0$.

[3]Note that we shift the integration variable of an integral which is not manifestly convergent. The discussion of such subtleties is postponed until later. In the present case there is no difficulty.

where $\mathrm{P}\!\int dq \equiv \lim_{\delta\downarrow 0}\left(\int_{-\infty}^{\omega-\delta} + \int_{\omega+\delta}^{\infty}\right) dq$ is the principal value integral. Substituting (6.16) in (6.14) we easily find

$$\mathrm{Re}\, G(t,t') = \frac{\hbar}{2m\omega}\cos\omega(t-t'), \tag{6.17}$$

and

$$\mathrm{Im}\, G(t,t') = \frac{\hbar}{2m\pi}\,\mathrm{P}\!\int dq\,\frac{e^{-iq(t-t')}}{q^2-\omega^2}\,. \tag{6.18}$$

6.2 Harmonic oscillator correlation functions; path integrals

Next we will consider the correlation functions in the context of the path integral. Although this will turn out to be quite a laborious exercise, we will do this explicitly to demonstrate a number of techniques which are standard in the evaluation of functional integrals. We start by introducing

$$W_J(q_2,t_2;q_1,t_1) = \int \mathcal{D}q\, e^{\frac{i}{\hbar}S[q(t)] + \int_{t_1}^{t_2} dt\, J(t)q(t)}, \tag{6.19}$$

where $J(t)$ is some external source. Just as above we are interested in different boundary conditions, so we define

$$W_J^{(0)}(t_2,t_1) = \int dq_1\, dq_2\; \varphi_0^*(q_2)\, W_J(q_2,t_2;q_1,t_1)\, \varphi_0(q_1)\,, \tag{6.20}$$

with $\varphi_0(q) = {}_t\langle q|0\rangle_t$ the groundstate wave function (which is time-independent). Now we consider

$$\begin{aligned} G(t,t') &\equiv \frac{\delta}{\delta J(t)}\frac{\delta}{\delta J(t')}\ln W_J^{(0)}\Big|_{J=0} \\ &= \frac{\int \mathcal{D}q\, q(t)\, q(t')\, e^{\frac{i}{\hbar}S}}{\int \mathcal{D}q\, e^{\frac{i}{\hbar}S}} - \left(\frac{\int \mathcal{D}q\, q(t)\, e^{\frac{i}{\hbar}S}}{\int \mathcal{D}q\, e^{\frac{i}{\hbar}S}}\right)\left(\frac{\int \mathcal{D}q\, q(t')\, e^{\frac{i}{\hbar}S}}{\int \mathcal{D}q\, e^{\frac{i}{\hbar}S}}\right), \end{aligned} \tag{6.21}$$

where the integration over $q_{1,2}$ according to (6.20) has been implied in every path integral. Observe that the overall normalization of the path integral cancels in this definition. This is one of the reason why in practice one does not worry so much about these (ill-defined) factors. The definition of two-point correlation function shows the modification by products of lower correlation functions that we alluded to in the text below (6.3) and (6.12). In the two-point function these terms vanish, at least for the harmonic oscillator, but in the general case there are important reasons for including these terms. The above definition can easily be generalized to n-point correlation functions,[4]

$$G(t,t',t'',\ldots) = \frac{\delta}{\delta J(t)}\frac{\delta}{\delta J(t')}\frac{\delta}{\delta J(t'')}\cdots \ln W_J^{(0)}\Big|_{J=0}. \tag{6.22}$$

[4]These correlation functions are called the *connected* correlation functions for reasons that we do not yet explain. In later chapters we often denote these correlation functions by $\langle q(t)\, q(t')\, q(t'')\cdots\rangle$.

Again this definition leads to modifications by products of lower-n correlation functions. With this particular definition one can show from the results that we are about to present, that all $n > 2$ correlation functions for the harmonic oscillator (or, more generally, for any action quadratic in q) vanish (cf. problem 6.1).

We now apply the above formulae to the harmonic oscillator. Subsequently we will compare the result with (6.14). First we evaluate the path integral (6.19) in the semiclassical approximation (which is exact for an action quadratic in q). We therefore expand $q(t)$ about a classical solution $q_0(t)$ with $q_0(t_1) = q_1$ and $q_0(t_2) = q_2$ as an infinite sum,

$$q(t) = q_0(t) + \sum_{n=1}^{\infty} q_n \sin \frac{n\pi(t-t_1)}{t_2 - t_1}, \tag{6.23}$$

which gives rise to the following expression for the action,

$$S[q(t)] = S[q_0] + \sum_{n=1}^{\infty} \tfrac{1}{4} m\, q_n^2 \left\{ \frac{n^2\pi^2}{(t_2-t_1)^2} - \omega^2 \right\} (t_2 - t_1). \tag{6.24}$$

Note that terms linear in q_0 do not appear since those vanish due to the equations of motion (i.e., $q_0(t)$ is a stationary "point" for the action $S[q(t)]$). Then

$$\begin{aligned} W_J &= \exp\left\{ \frac{i}{\hbar} S[q_0] + \int dt\, J(t) q_0(t) \right\} \qquad (6.25)\\ &\times \int \mathcal{D}q \exp\left\{ \frac{i}{\hbar}\frac{m}{4}(t_2-t_1) \sum_{n=1}^{\infty} q_n^2 \left[\frac{n^2\pi^2}{(t_2-t_1)^2} - \omega^2 \right] + \sum_{n=1}^{\infty} q_n \int dt\, J(t) \sin \frac{n\pi(t-t_1)}{t_2-t_1} \right\} \end{aligned}$$

Observe that only the first factor depends on the boundary values $q_{1,2}$. Now we redefine the integration variables q_n in the path integral by a shift proportional to J such as to eliminate the term linear in q_n. This leads to

$$\begin{aligned} W_J &= \exp\left\{ \frac{i}{\hbar} S[q_0] + \int dt\, J(t)\, q_0(t) + \tfrac{1}{2} \int dt\, dt'\, J(t)\, G_0(t,t')\, J(t') \right\} \\ &\qquad \times \int \mathcal{D}q \exp\left\{ \frac{i}{\hbar}\frac{m}{4}(t_2-t_1) \sum_{n=1}^{\infty} q_n^2 \left[\frac{n^2\pi^2}{(t_2-t_1)^2} - \omega^2 \right] \right\}, \end{aligned} \tag{6.26}$$

where

$$G_0(t,t') = -\frac{\hbar}{i} \frac{2}{m(t_2-t_1)} \sum_{n=1}^{\infty} \frac{\sin \frac{n\pi(t-t_1)}{t_2-t_1} \sin \frac{n\pi(t'-t_1)}{t_2-t_1}}{\frac{n^2\pi^2}{(t_2-t_1)^2} - \omega^2}, \tag{6.27}$$

which is periodic in t and t' separately with periodicity $2(t_2 - t_1)$. Note that

$$\left(-\frac{\partial^2}{\partial t^2} - \omega^2 \right) G_0(t,t') = \frac{i\hbar}{m} \delta(t-t'), \tag{6.28}$$

where $\delta(t-t')$ is the δ-function for functions on the (t_1, t_2) interval that vanish at the boundary. Outside this interval, the result follows from periodicity.

There are now three expressions that we have to evaluate. First of all we should simplify the expression for (6.27), then we should calculate the Gaussian integral over the q_n, and finally we should determine the integrals over q_1 and q_2 to convert to the same states as in the operator formalism (cf.

6.2.1 Evaluating G_0

It is possible to further evaluate G_0. First we write

$$G_0(t,t') = \frac{i\hbar}{mT}\sum_{n=1}^{\infty}\Big[\cos\frac{n\pi(t-t')}{T} - \cos\frac{n\pi(t+t'-2t_1)}{T}\Big]\Big[\frac{n^2\pi^2}{T^2}-\omega^2\Big]^{-1}, \tag{6.29}$$

where $T = t_2 - t_1$. Now we make use of the following formula,

$$\frac{1}{T}\sum_{n=1}^{\infty}\frac{\cos\frac{n\pi(\tau+T)}{T}}{\frac{n^2\pi^2}{T^2}-\omega^2} = \frac{1}{2\omega^2 T} - \frac{\cos\omega\tau}{2\omega\sin\omega T}\,. \tag{6.30}$$

This result follows from Fourier decomposing $\cos\omega\tau$ in the interval $-T<\tau<T$ in terms of functions $\cos(n\pi\tau/T)$. Note that, while the left-hand side is periodic under $\tau\to\tau+2T$, the right-hand side is not. By exploiting the periodicity of the left-hand side, τ must first be selected such that it is contained in the interval $(-T,T)$.

Now apply the above formula to (6.29), with in the first term $\tau = t-t'-T$ when $t_1<t'<t<t_2$, or $\tau = t-t'+T$ when $t_1<t<t'<t_2$, and in the second term $\tau = t+t'-t_1-t_2$ where $t_1<t,t'<t_2$. This leads to

$$\begin{aligned} G_0(t,t') \;=\; \frac{i\hbar}{2m\omega}\Big\{ &-\theta(t-t')\sin\omega(t-t') - \theta(t'-t)\sin\omega(t'-t) \qquad (6.31)\\ &-\cos\omega(t-t')\,\cot\omega T + \frac{\cos\omega(t+t'-t_1-t_2)}{\sin\omega T}\Big\}, \qquad (t_1<t,t'<t_2) \end{aligned}$$

where the first term in (6.29) corresponds to the first three terms in the formula above. As one easily verifies, this result satisfies again the differential equation (6.15), just as the result (6.11) obtained by means of the operator formalism. We expect to derive the same result (6.11) by means of path integrals. It therefore follows that the remaining terms that we are about to evaluate, must be a solution of the homogeneous equation corresponding to (6.15). As we shall see, this is indeed the case.

6.2.2 The integral over q_n

Let us now discuss the second line in (6.26), which is a path integral independent of the boundary values $q_{1,2}$. There are two ways to evaluate this integral. The easiest one is to observe that this integral is precisely the path integral for the harmonic oscillator, evaluated in chapter 2, with boundary condition $q_1 = q_2 = 0$. Using (3.28) it thus follows that

$$\int \mathcal{D}q \exp\left\{\frac{i}{\hbar}\frac{m}{4}(t_2-t_1)\sum_{n=1}^{\infty} q_n^2 \left[\frac{n^2\pi^2}{(t_2-t_1)^2} - \omega^2\right]\right\} = \sqrt{\frac{m\omega}{2\pi i\hbar \sin\omega(t_2-t_1)}}. \tag{6.32}$$

In a more explicit evaluation one computes the Gaussian integrals. First we write the path integral measure as

$$\int \mathcal{D}q \longrightarrow \prod_{n=1}^{\infty}\int_{-\infty}^{\infty} dq_n. \tag{6.33}$$

Integration over the q_n yields

$$\begin{aligned}
&\int \mathcal{D}q \exp\left\{\frac{i}{\hbar}\frac{m}{4}(t_2-t_1)\sum_{n=1}^{\infty} q_n^2 \left[\frac{n^2\pi^2}{(t_2-t_1)^2} - \omega^2\right]\right\} \\
&\quad = \left\{\prod_{n=1}^{\infty}\left(\frac{4i\hbar(t_2-t_1)}{m\pi\, n^2}\right)\right\}^{\frac{1}{2}} \left\{\prod_{n=1}^{\infty}\left(1-\frac{\omega^2(t_2-t_1)^2}{\pi^2\, n^2}\right)\right\}^{-\frac{1}{2}}.
\end{aligned} \tag{6.34}$$

This yields a result proportional to (6.32).[5] The ill-defined proportionality factor is independent of ω and should be absorbed into the definition of the path integral; this is in accord with the prescription based on the Wiener measure discussed in chapter 2. Combining (6.26) and (6.32), we find

$$\begin{aligned}
W_J(q_2,t_2;q_1,t_1) &= \sqrt{\frac{m\omega}{2\pi i\hbar \sin\omega(t_2-t_1)}} \\
&\quad \times \exp\left\{\frac{i}{\hbar}S[q_0] + \int dt\, J(t)q_0(t) + \tfrac{1}{2}\int dt\, dt'\, J(t)\, G_0(t,t')\, J(t')\right\}.
\end{aligned} \tag{6.36}$$

6.2.3 The integrals over q_1 and q_2

Now we are ready to calculate the two-point correlation function of the groundstate in the path integral formalism. We recall that the classical solution for the harmonic oscillator reads

$$q_0(t) = \frac{1}{\sin\omega(t_2-t_1)}\Big\{q_2\sin\omega(t-t_1) - q_1\sin\omega(t-t_2)\Big\}, \tag{6.37}$$

which leads to the action

$$S_{cl} = \frac{m\omega}{2\sin\omega(t_2-t_1)}\left\{\left(q_1^2+q_2^2\right)\cos\omega(t_2-t_1) - 2q_1q_2\right\}. \tag{6.38}$$

[5] Note the formula

$$\frac{\sin x}{x} = \prod_{n=1}^{\infty}\left(1-\frac{x^2}{\pi^2\, n^2}\right), \tag{6.35}$$

which can be derived from (6.30) by first putting $\tau = -T$ and multiplying by ω; subsequently one integrates over ω and fixes the integration constant by comparing for $x = 0$.

Furthermore, the groundstate wave function takes the form

$$\varphi_0(q) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left\{-\frac{m\omega}{2\hbar}q^2\right\}. \tag{6.39}$$

Hence $W_J^{(0)}(t_2,t_1)$ is given by

$$\begin{aligned} W_J^{(0)} &= \sqrt{\frac{m\omega}{2\pi i\hbar\sin\omega(t_2-t_1)}}\sqrt{\frac{m\omega}{\pi\hbar}}\;\exp\left\{\tfrac{1}{2}\int dt\,dt'\,J(t)\,G_0(t,t')\,J(t')\right\} \\ &\times\;\int dq_1\,dq_2\exp\left\{\frac{m\omega}{2\hbar}\left[-q_1^2-q_2^2+\frac{i}{\sin\omega(t_2-t_1)}\left[(q_1^2+q_2^2)\cos\omega(t_2-t_1)-2q_1q_2\right]\right.\right. \\ &\qquad\qquad\left.\left.+\frac{2\hbar}{m\omega\sin\omega(t_2-t_1)}(J_1q_1+J_2q_2)\right]\right\}, \end{aligned} \tag{6.40}$$

where

$$\begin{aligned} J_1 &= -\int_{t_1}^{t_2} dt\,J(t)\,\sin\omega(t-t_2), \\ J_2 &= \int_{t_1}^{t_2} dt\,J(t)\,\sin\omega(t-t_1). \end{aligned} \tag{6.41}$$

The integral can be written as

$$\int dq_1\,dq_2\exp\left\{\frac{m\omega}{\hbar}\left[-\tfrac{1}{2}\sum_{i,j=1,2}q_i\,A_{ij}\,q_j+\frac{\hbar}{m\omega\sin\omega(t_2-t_1)}\sum_{i=1,2}J_i\,q_i\right]\right\}, \tag{6.42}$$

where the matrix A equals

$$A=\frac{-i}{\sin\omega(t_2-t_1)}\begin{pmatrix} e^{i\omega(t_2-t_1)} & -1 \\ -1 & e^{i\omega(t_2-t_1)}\end{pmatrix}. \tag{6.43}$$

This integral can be evaluated explicitly and we find

$$\left(\frac{m\omega}{2\hbar}\right)^{-1}\sqrt{\frac{\pi^2}{\det A}}\exp\left\{\frac{\hbar}{2m\omega\sin^2\omega(t_2-t_1)}\sum_{i,j=1,2}J_i\,\left(A^{-1}\right)_{ij}\,J_j\right\}. \tag{6.44}$$

Combining this with (6.40) and using

$$\det A=-2i\frac{\exp i\omega(t_2-t_1)}{\sin\omega(t_2-t_1)}\,,\qquad A^{-1}=\tfrac{1}{2}\begin{pmatrix} 1 & e^{-i\omega(t_2-t_1)} \\ e^{-i\omega(t_2-t_1)} & 1\end{pmatrix}$$

yields

$$\begin{aligned} W_J^{(0)}(t_2,t_1) &= e^{-\frac{i\omega}{2}(t_2-t_1)}\exp\left\{\frac{\hbar}{2m\omega\sin^2\omega(t_2-t_1)}\int dt\,dt'\,J(t)\,f(t,t')\,J(t')\right\} \\ &\times\exp\left\{\tfrac{1}{2}\int dt\,dt'\,J(t)\,G_0(t,t')\,J(t')\right\}, \end{aligned} \tag{6.45}$$

where

$$\begin{aligned}
f(t,t') &= \tfrac{1}{2}\Big\{ \sin\omega(t-t_1)\sin\omega(t'-t_1) + \sin\omega(t-t_2)\sin\omega(t'-t_2)\Big\} \\
&\quad -\tfrac{1}{2}e^{-i\omega(t_2-t_1)}\Big\{ \sin\omega(t-t_2)\sin\omega(t'-t_1) + \sin\omega(t-t_1)\sin\omega(t'-t_2)\Big\} \\
&= \tfrac{1}{2} i \sin\omega(t_2-t_1)\Big\{ e^{-i\omega(t_2-t_1)}\cos\omega(t-t') - \cos\omega(t+t'-t_1-t_2)\Big\} . \qquad (6.46)
\end{aligned}$$

This function satisfies the homogeneous version of the differential equation (6.15), as was claimed earlier.

6.3 Conclusion

Observe that the logarithm of (6.45) depends quadratically on J, so that only the two-point correlation function is nonvanishing, a result that we have alluded to below (6.22). The two-point correlation function is now given by

$$G(t,t') = G_0(t,t') + \frac{\hbar}{m\omega \sin^2 \omega(t_2-t_1)}\, f(t,t'). \qquad (6.47)$$

Substituting (6.31) and (6.46) one reproduces the original result (6.11) obtained in the operator method. This is the desired result. To obtain the correct result we had to pay attention to the correct boundary conditions, which are linked to the choice of the matrix elements used in the definition of the correlation functions. The crucial contribution to the correlation function is represented by G_0, which is itself independent of the choice of the matrix element and satifies the inhomogenous differential equation (6.15). In practical calculations the question of boundary conditions is often not explicitly addressed.

Problem 6.1 :
Evaluate the discretized path integral

$$W_J = \int \prod_i \mathrm{d}q_i \, \exp\Big\{ -\tfrac{1}{2}\sum_{i,j} q_i\, A_{ij}\, q_j + \sum_i J_i\, q_i \Big\} .$$

Define the (connected) correlation functions according to (6.22) and show that only the two-point function is nonvanishing and proportional to the inverse of the matrix A_{ij}. Argue from this that the two-point function for the harmonic oscillator must satisfy the differential equation (6.15).

Problem 6.2 : Time ordering and commutation relations
Evaluate, using the procedure described in the first part of this chapter, the correlation functions $\langle q(t)\, p(t')\rangle$ and $\langle p(t)\, p(t')\rangle$ for the harmonic oscillator. Using $p = m\,\dot q$, which is valid

in the Heisenberg picture, we may write the result as $m\langle q(t)\,\dot q(t')\rangle$ and $m\langle \dot q(t)\,p(t')\rangle$, respectively. Assume that the time derivative can be written outside the correlation functions and compare the results. Argue why they coincide for the first and not for the second correlation function. Now consider the correlation functions involving q and $\dot q$ by including a second source in the path integral that couples to $\dot q$. Argue that in this case time derivatives can be taken outside the correlation functions. How would you evaluate correlation functions of q and p operators using path integrals. Can you see how the discrepancy between correlation functions of q and/or p and correlation functions of q and/or $m\,\dot q$ arises in this context? (In the path-integral derivation, ignore possible subtleties with the boundeary conditions.)

Problem 6.3 : In equation (6.21) we have shown explicitly that the two-point correlation function equals

$$\begin{aligned}\langle q(t)q(t')\rangle &= \frac{\delta}{\delta J(t)}\frac{\delta}{\delta J(t')}\ln W_J^{(0)}\Big|_{J=0} \\ &= \langle 0|T(q(t)\,q(t'))|0\rangle - \langle 0|q(t)|0\rangle\,\langle 0|q(t')|0\rangle,\end{aligned} \tag{6.48}$$

where $|0\rangle$ denotes the normalized groundstate of the system. Show in a similar manner, thus by functional differentiation, that the four-point correlation function obeys

$$\begin{aligned}\langle q(t)\,q(t')\,q(t'')\,q(t''')\rangle &= \frac{\delta}{\delta J(t)}\frac{\delta}{\delta J(t')}\frac{\delta}{\delta J(t'')}\frac{\delta}{\delta J(t''')}\ln W_J^{(0)}\Big|_{J=0} \\ &= \langle 0|T(q(t)\,q(t')\,q(t'')\,q(t'''))|0\rangle \\ &\quad -\langle 0|T(q(t)\,q(t'))|0\rangle\,\langle 0|T(q(t'')\,q(t'''))|0\rangle \\ &\quad -\langle 0|T(q(t)\,q(t''))|0\rangle\,\langle 0|T(q(t')\,q(t'''))|0\rangle \\ &\quad -\langle 0|T(q(t)\,q(t'''))|0\rangle\,\langle 0|T(q(t')\,q(t''))|0\rangle,\end{aligned}$$

if we assume that the potential $V(q)$ is an even function in q, so that expectation values of an odd number of q operators, such as $\langle 0|q(t)|0\rangle$ and $\langle 0|T(q(t)\,q(t')\,q(t''))|0\rangle$, vanish.

Problem 6.4 : For the harmonic oscillator we have found that

$$W_J^{(0)} = \exp\left\{\tfrac{1}{2}\int dt\int dt'\,J(t)\,G(t,t')\,J(t')\right\}, \tag{6.49}$$

with the two-point correlation function $\langle q(t)\,q(t')\rangle \equiv G(t,t')$ given by equation (6.11). Using the results of problems 4.1 and 4.3, show that in this case $\langle 0|T(q(t)\,q(t'))|0\rangle = G(t,t')$ and that

$$\langle 0|T(q(t)\,q(t')\,q(t'')\,q(t'''))|0\rangle = G(t,t')\,G(t'',t''')+G(t,t'')\,G(t',t''')+G(t,t''')\,G(t',t''). \tag{6.50}$$

Argue generally why there is no ambiguity in the value of $G(t,t')$ at equal times $t = t'$. Is the same true for $\langle 0|T(q(t)\, p(t'))|0\rangle$? (cf. problem 6.2).

Problem 5.5 : Anharmonic socillator
Consider now an anharmonic oscillator with Hamiltonian

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2 + \frac{1}{2\ell^2} m\omega^2 q^4, \tag{6.51}$$

where the last term is a small perturbation. Prove that in lowest-order perturbation theory the groundstate energy of the anharmonic oscillator equals

$$E_0 \simeq \frac{\hbar\omega}{2} + \frac{m\omega^2}{2\ell^2} \langle 0|T(q(t)\, q(t)\, q(t)\, q(t))|0\rangle = \frac{\hbar\omega}{2}\left(1 + \frac{3}{4}\frac{\hbar}{m\omega\ell^2}\right). \tag{6.52}$$

7 Euclidean Theory

In the previous chapters we have discussed path integrals in quantum mechanics and quantum field theory and we encountered Gaussian integrals such as,

$$\int \mathcal{D}q\ \exp\left\{\frac{i}{\hbar}\int dt\ \left[\tfrac{1}{2} m\dot{q}^2 - \tfrac{1}{2} m\omega^2 q^2\right]\right\}, \tag{7.1}$$

$$\int \mathcal{D}\phi\ \exp\left\{\frac{i}{\hbar}\int d^d x\ \left[-\tfrac{1}{2}(\partial_\mu\phi)^2 - \tfrac{1}{2} m^2\phi^2\right]\right\}. \tag{7.2}$$

The exponential functions in the integrand have purely imaginary exponents, so that the integrals are ill-defined. One way to deal with this problem is to add a small *negative* imaginary term to ω^2 or m^2, so that the integrals converge[6]. At the end one puts the imaginary part to zero. This is in line with the $i\varepsilon$ modification in the correlation functions (cf. 4.14). Another way (which is not unrelated) is to perform an analytic continuation of the time variable t to imaginary time. Therefore we define the so-called Euclidean time variable τ by

$$\tau \equiv i\, t. \tag{7.3}$$

The term Euclidean is derived from the fact that the Lorentz-invariant length $\vec{x}^2 - t^2$ is replaced by the Euclidean length $\vec{x}^2 + \tau^2$. The correlation functions in Minkowski space are then *defined* by analytic continuation from the corresponding functions evaluated in Euclidean space. To see how such an analytic continuation must be performed, consider the two-point correlation function

$$\langle q(t)\, q(0)\rangle = \frac{i\hbar}{2\pi m}\int_{-\infty}^{\infty} dk_0 \frac{e^{-ik_0 t}}{k_0^2 - \omega^2 + i\varepsilon}. \tag{7.4}$$

[6]We recall that Gaussian integrals $\int_{-\infty}^{\infty} dx\ \exp(-a\, x^2)$ can also be defined for complex a provided that $\mathrm{Re}\, a > 0$.

Now the $i\varepsilon$ term prescribes how one should deal with the poles on the integration countour. This is related to the time direction (and thus to causality), because the $i\varepsilon$ modification was induced by the time ordering of the operators in the correlation functions (see the discussion in the previous chapter). Often one has to deal with (momentum) integrals that contain the correlation functions and one can then avoid the poles by rotating the integration contour away from the real axis. Such a rotation is called a Wick rotation. It rotates the integration contour along the real axis to an integration along the imaginary k_0-axis by closing these contours in the upper-right and lower-left quadrants and using Cauchy's theorem. Obviously one can only rotate such that one avoids the poles at $k_0 = \pm(\omega - i\varepsilon)$, as these would give rise to extra contributions. Therefore the $i\varepsilon$-modification prescribes how the analytic continuation should be done.

Let us consider the Wick rotation in some detail and establish some of the rules. (The reader may also consult De Wit & Smith section 8.2.) The integration contour integrals such as (7.4) is thus rotated counter-clockwise over $\pi/2$, so that k_0 is purely imaginary and related to the real "Euclidean" variable by $k_0 = ik_E$. The Wick rotation then leads to[7]

$$\int_{-\infty}^{\infty} dk_0 \longrightarrow \int_{-i\infty}^{i\infty} dk_0 = i\int_{-\infty}^{\infty} dk_E. \tag{7.5}$$

Consistency requires that delta functions change according to

$$\delta(k_0) \longrightarrow -i\,\delta(k_E). \tag{7.6}$$

Hence the analytic continuation of (7.4) leads to

$$\langle q(-i\tau)\,q(0)\rangle = \frac{\hbar}{2\pi m}\int_{-\infty}^{\infty} dk_E \frac{e^{-ik_E\tau}}{k_E^2+\omega^2}. \tag{7.7}$$

From the Dirac representation of the delta function, one deduces from (7.6) that the Wick rotation for the time variable should be taken in the *opposite* direction (so that $tk_0 = \tau k_E$). A clockwise rotation leads to (7.3), so that

$$\begin{aligned} \int_{t_1}^{t_2} dt &\longrightarrow -i\int_{\tau_1}^{\tau_2} d\tau, \\ \delta(t) &\longrightarrow i\,\delta(\tau). \end{aligned} \tag{7.8}$$

With these rules the exponents in (7.1) and (7.2) change according to

$$\frac{i}{\hbar}S[q] \longrightarrow \frac{1}{\hbar}\int d\tau\,\left\{-\tfrac{1}{2}m(dq/d\tau)^2 - \tfrac{1}{2}m\omega^2 q^2\right\} \equiv -\frac{1}{\hbar}S^E[q], \tag{7.9}$$

[7]For indefinite integrals the integration variable k_E can always be changed into $-k_E$, so that the sign in the relation between k_0 and k_E is not very important. However, for a finite integration range the sign is important as it will define the boundary values of the integration contour after the Wick rotation.

$$\frac{i}{\hbar}S[\phi] \longrightarrow \frac{1}{\hbar}\int d^dx_E \left\{-\tfrac{1}{2}(\partial_\tau\phi)^2 - \tfrac{1}{2}(\nabla\phi)^2 - \tfrac{1}{2}m^2\phi^2\right\} \equiv -\frac{1}{\hbar}S^E[\phi]. \tag{7.10}$$

The Euclidean action S^E is thus real and positive, so that the Gaussian integration is well defined. It is customary to define also a Euclidean Lagrangian (density) from the action by means of the relation

$$S^E[q(\tau)] \equiv \int d\tau L^E(q(\tau), \dot{q}(\tau)) \quad \text{with} \quad \dot{q} = \frac{dq}{d\tau}. \tag{7.11}$$

Just as in chapter 2 we can derive a path-integral representation for the transition function,

$$W^E(q_2, \tau_2; q_1, \tau_1) = \langle q_2|e^{-\frac{1}{\hbar}H(\tau_2-\tau_1)}|q_1\rangle = \int_{\substack{q(\tau_1)=q_1\\ q(\tau_2)=q_2}} \mathcal{D}q(\tau)\; e^{-\frac{1}{\hbar}S^E[q(\tau)]}. \tag{7.12}$$

The usefulness of this expression, which is a path integral over a real exponential factor and not over a phase factor, will become clear in due course.

Let us now briefly consider the expressions for the Euclidean path integral for the free particle and the harmonic oscillator. For the free particle (cf. problem 3.1) we have $L^E = \frac{1}{2}m\dot{q}^2$. One easily finds

$$S^E_{cl} = \frac{m}{2(\tau_2-\tau_1)}\left(q_2-q_1\right)^2, \tag{7.13}$$

and

$$W^E(q_2, \tau_2; q_1, \tau_1) = \sqrt{\frac{m}{2\pi\hbar(\tau_2-\tau_1)}}\,\exp\left\{\frac{-m(q_2-q_1)^2}{2\hbar(\tau_2-\tau_1)}\right\}, \tag{7.14}$$

which is clearly the analytic continuation of the result found in problem 3.1.

For the harmonic oscillator (cf. problem 3.3) we have $L^E = \frac{1}{2}m\dot{q}^2 + \frac{1}{2}m\omega^2q^2$. The solution to the Euler-Lagrange equation is $q_0(\tau) = A\sinh\omega(\tau-\tau_0)$, which contains two arbitrary constants A and τ_0. With the usual boundary conditions this becomes

$$q_0(\tau) = \frac{q_2\sinh\omega(\tau-\tau_1) - q_1\sinh\omega(\tau-\tau_2)}{\sinh\omega(\tau_2-\tau_1)}. \tag{7.15}$$

From this classical solution we calculate the classical action S^E_{cl}, which determines the q-dependence of the transition matrix

$$W^E = f(\tau_1-\tau_2)e^{-S^E_{cl}[q]/\hbar}. \tag{7.16}$$

As explained in chapter 3, the function f can be determined in various ways, and one finds

$$W^E = \sqrt{\frac{m\omega}{2\pi\hbar\sinh\omega(\tau_2-\tau_1)}}\,\exp\left\{\frac{-m\omega\left[(q_1^2+q_2^2)\cosh\omega(\tau_2-\tau_1) - 2q_1q_2\right]}{2\hbar\sinh\omega(\tau_2-\tau_1)}\right\}. \tag{7.17}$$

By analytic continuation this is related to the results derived in problem 3.3.

The Euclidean theory is also interesting in its own right and Euclidean path integrals have many interesting applications in physics. One of them is in equilibrium statistical mechanics. To see this, consider the Euclidean version of (2.24),

$$\begin{aligned} W^E(q_2,\tau_2;q_1,\tau_1) &= \sum_n \langle q_2|n\rangle\, e^{-E_n(\tau_2-\tau_1)/\hbar}\,\langle n|q_1\rangle \\ &= \sum_n \varphi_n(q_2)\,\varphi_n^*(q_1)\,e^{-\beta E_n}\,, \end{aligned} \tag{7.18}$$

with

$$\beta \equiv \frac{\tau_2-\tau_1}{\hbar}\,. \tag{7.19}$$

This expression is proportional to a matrix element of the density operator ρ_β for a statistical ensemble with temperature $T=(k\beta)^{-1}$,

$$\rho_\beta \equiv \frac{\mathrm{e}^{-\beta H}}{Z_\beta} = \frac{\sum_n |n\rangle\,\mathrm{e}^{-\beta E_n}\,\langle n|}{Z_\beta}, \tag{7.20}$$

which satisfies $\rho_\beta=\rho_\beta^\dagger$ and $\langle q|\rho_\beta|q\rangle \geq 0$ for all $|q\rangle$. The normalization factor Z_β is just the partition function, defined by

$$Z_\beta = \sum_n e^{-\beta E_n}. \tag{7.21}$$

(which gives $Z_\beta = \sum_n N_n e^{-\beta E_n}$ in case of a degeneracy N_n of the energy level E_n). This expression can also be written as

$$Z_\beta = \sum_n \int dq\;\varphi_n(q)\,\varphi_n^*(q)\,e^{-\beta E_n} = \int_{-\infty}^{\infty} dq_1\,dq_2\;W^E(q_1,q_2)\,\delta(q_1-q_2), \tag{7.22}$$

where in the second equation we used (7.18). In this way we find a path-integral representation for the partition function, [8]

$$Z_\beta = \int_{q(0)=q(\beta\hbar)} \mathcal{D}q\;\exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau\;L^E(q,\dot q)\right\}, \tag{7.23}$$

where we now integrate over all *periodic* paths, i.e. functions $q(\tau)$ that satisfy $q(0)=q(\hbar\beta)$. The original real-time coordinate is thus replaced by a a compactified imaginary-time coordinate, whose range extends over $\hbar\beta$.

To illustrate the above result, take, for instance, $L^E=\frac{1}{2}m\dot q^2+V(q)$ and consider the path integral for high temperature. (More precisely, for temperatures such that $\hbar\beta$ is small as compared to the typical scale set by the variations of the potential.) In that case the paths cannot deviate too much from their boundary values, since this will induce large values for

[8] In the limit of zero temperature ($\beta\to\infty$) the groundstate dominates the partition sum (7.21) and we are dealing with the Euclidean theory whose analytic continuation leads to the Minkowski theory.

the kinetic energy which suppresses the integrand in (7.23). Hence we may approximate $\int_0^{\hbar\beta} d\tau\, V(q(\tau))$ by $\hbar\beta V(\frac{1}{2}[q_1+q_2])$, so that

$$W^E(q_2,\hbar\beta;q_1,0) \approx \exp\left\{-\beta V(\tfrac{1}{2}[q_1+q_2])\right\} \int \mathcal{D}q \exp\left\{-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau \tfrac{1}{2}m\dot{q}^2\right\}. \tag{7.24}$$

The calculation of the path integral is now simple. From (7.14) we find

$$W^E(q_2,\hbar\beta;q_1,0) \approx \exp\left\{-\beta V(\tfrac{1}{2}[q_1+q_2])\right\} \sqrt{\frac{m}{2\pi\hbar^2\beta}} \exp\left\{\frac{-m(q_2-q_1)^2}{2\hbar^2\beta}\right\}. \tag{7.25}$$

Using (7.22) then gives

$$Z_\beta = \sqrt{\frac{m}{2\pi\hbar^2\beta}} \int dq\; e^{-\beta V(q)}, \tag{7.26}$$

which is just the partition function based on the Boltzmann distribution.

We will now calculate the partition function of the harmonic oscillator from (7.17). However, we will allow ourselves a small extension and evaluate (7.23) for both periodic and antiperiodic paths. The partition function will be denoted by $Z_\beta^{(\pm)}$ corresponding to the boundary condition $q(\hbar\beta) = \pm q(0)$. (We will motivate that extension later in these lectures). The result is

$$\begin{aligned} Z_\beta^{(\pm)} &= \int dq \sqrt{\frac{m\omega}{2\pi\hbar\sinh\beta\hbar\omega}} \exp\left\{\frac{-m\omega(\cosh\beta\hbar\omega \mp 1)\, q^2}{\hbar\sinh\beta\hbar\omega}\right\} \\ &= \sqrt{\frac{m\omega}{2\pi\hbar\sinh\beta\hbar\omega}} \sqrt{\frac{\pi\hbar\sinh\beta\hbar\omega}{m\omega(\cosh\beta\hbar\omega\mp 1)}} \\ &= \left(e^{\beta\hbar\omega/2} \mp e^{-\beta\hbar\omega/2}\right)^{-1}. \end{aligned} \tag{7.27}$$

Therefore

$$Z_\beta^{(+)} = \frac{e^{-\beta\hbar\omega/2}}{1-e^{-\beta\hbar\omega}} = \sum_{n=0}^{\infty} e^{-\beta\hbar\omega(n+\frac{1}{2})}, \tag{7.28}$$

and

$$Z_\beta^{(-)} = \left(\sum_{n=0}^{1} e^{-\beta\hbar\omega(n-\frac{1}{2})}\right)^{-1}. \tag{7.29}$$

We see that the partition function for periodic boundary conditions is that of a quantum harmonic oscillator, as expected. It turns out that the *inverse* partition function for antiperiodic boundary conditions equals the partition function of a "fermionic" harmonic oscillator (which has a groundstate with energy $-\frac{1}{2}\hbar\omega$ and an excited state with energy $\frac{1}{2}\hbar\omega$). It is not easy to explain why we get the inverse partition function. This has to do with the fact that fermionic path integrals require the use of so-called anticommuting c-numbers. The significance of this statement will be explained in due course.

We end this chapter by computing the euclidean correlation function for the harmonic oscillator in the operator formulation. The canonical momentum was defined in terms of the real-time (Minkowski) theory,

$$p(t) = \frac{\partial L(q,\dot{q})}{\partial \dot{q}}, \quad \text{where} \quad \dot{q} = \frac{dq}{dt}. \tag{7.30}$$

In the imaginary-time formulation, the relation between p and q reads

$$p = i\,\frac{\partial L^E(q,\dot{q})}{\partial \dot{q}}, \quad \text{where} \quad \dot{q} = \frac{dq}{d\tau}. \tag{7.31}$$

Quantum-mechanically, p and q are still represented by the same (Schrödinger) operators satisfying the standard commutation relation $[q,p] = i\,\hbar$. In the Heisenberg picture we have to deal with the operators

$$q(\tau) = e^{\frac{1}{\hbar}H\tau} q\, e^{-\frac{1}{\hbar}H\tau}, \qquad p(\tau) = e^{\frac{1}{\hbar}H\tau} p\, e^{-\frac{1}{\hbar}H\tau}, \tag{7.32}$$

which can be decomposed in terms of creation and annihilation operators $a(\tau) = a\exp(-\omega\tau)$ and $a^\dagger(\tau) = a^\dagger\exp(\omega\tau)$ in the usual manner (cf. (5.17)),

$$\begin{aligned} q(\tau) &= \sqrt{\frac{\hbar}{2m\omega}}\Big(a(\tau) + a^\dagger(\tau)\Big), \\ p(\tau) &= -im\omega\sqrt{\frac{\hbar}{2m\omega}}\Big(a(\tau) - a^\dagger(\tau)\Big). \end{aligned} \tag{7.33}$$

Observe that $p(\tau)$ satifies $p = im\,\dot{q}$. The reality conditions in the Minkowski case ($q^\dagger(t) = q(t)$, etc.) have to be replaced by the so-called reflection positivity conditions,

$$q(\tau)^\dagger = q(-\tau)\,, \quad p(\tau)^\dagger = p(-\tau). \tag{7.34}$$

Note that the factor i in (7.31) is crucial for the reality of $p(\tau)$.

Now we are ready to compute correlation functions in the Euclidean formalism. For the harmonic oscillator the two-point function is computed as in chapter 6,

$$\begin{aligned} G(\tau,\tau') &= \frac{{}_{\tau_2}\langle 0|T(q(\tau)\,q(\tau'))|0\rangle_{\tau_1}}{{}_{\tau_2}\langle 0|0\rangle_{\tau_1}} \\ &= \frac{\hbar}{2m\omega}\Big\{\theta(\tau-\tau')e^{-\omega(\tau-\tau')} + \theta(\tau'-\tau)e^{\omega(\tau-\tau')}\Big\}. \end{aligned} \tag{7.35}$$

We use again the integral representation (6.13) of the θ-function to find

$$G(\tau,\tau') = \frac{\hbar}{2m\omega}\frac{-1}{2\pi i}\int_{-\infty}^{\infty} dq \frac{1}{q+i\epsilon}\left(e^{-i(q-i\omega)(\tau-\tau')} + e^{+i(q-i\omega)(\tau-\tau')}\right). \tag{7.36}$$

We shift the integration contour a distance ω into the upper half of the complex q-plane. As we don't encounter poles in the integrand, which falls off at infinity, we thus obtain

$$G(\tau,\tau') = \frac{\hbar}{2\pi m}\int_{-\infty}^{\infty} dq\,\frac{e^{-iq(\tau-\tau')}}{q^2+\omega^2}\,. \tag{7.37}$$

This is precisely (7.7), which was derived by analytic continuation of the real-time correlation function.

The above Euclidean correlation functions pertain to the case of zero temperature. At finite temperature the correlation functions take the form of ensemble averages. For instance, the two-point function reads ($0 \leq \tau, \tau' < \hbar\,\beta$)

$$G_\beta(\tau,\tau') = \mathrm{Tr}\left[\rho_\beta\, T_\tau(q(\tau)\,q(\tau'))\right] - \mathrm{Tr}\left[\rho_\beta\, q(\tau)\right]\mathrm{Tr}\left[\rho_\beta\, q(\tau')\right], \tag{7.38}$$

where T_τ denotes the ordering with respect to the Euclidean time variable τ. One can show that this correlation functions corresponds to the derivative of the logarithm of the partition function (which equals the free energy times $-\beta$) with respect to an external source (see problem 5.5).

Problem 7.1 :
Following the derivation in chapter 2, present the corresponding derivation of the Euclidean path integral (7.12).

Problem 7.2 :
Consider the limit of (7.17) for $T = \tau_2 - \tau_1 \to \infty$ and derive the groundstate energy and wave function of the harmonic oscillator. Try to do the same for (7.14) and explain why matters are more subtle in this case.

Problem 7.3 :
Prove that $G(\tau,\tau')$ as given in (7.37) is a solution of $(\partial_\tau^2 - \omega^2)G(\tau,\tau') = -\frac{\hbar}{m}\,\delta(\tau-\tau')$.

Problem 7.4 :
The correlation function G_β is defined in (7.38) with τ and τ' belonging to the interval $(0,\hbar\beta)$. Show that it actually depends on the difference $\tau-\tau'$, which is thus restricted to the interval $-\hbar\beta < \tau-\tau' \leq \hbar\beta$. Prove that G_β takes the same value for $\tau-\tau' = -\hbar\beta$, 0, $\hbar\beta$. Restrict $\tau-\tau'$ to the left-half of the interval (so $-\hbar\beta < \tau-\tau' \leq 0$) and prove the periodicity property $G_\beta(\tau-\tau') = G_\beta(\tau-\tau'+\hbar\,\beta)$.

Problem 7.5 :

Write down the path-integral representation for Z_β in the presence of a source term $\int d\tau\; J(\tau)\, q(\tau)$. Argue that J must be periodic and show that the correlation function (7.38) corresponds to the second derivative of $\ln Z_\beta$ with respect to the external source. Subsequently, argue that the correlation function can be expanded in terms of functions periodic in $\tau - \tau'$ with frequencies equal to $\omega_n = \pi n/(\hbar\,\beta)$ where n are *even* integers. These frequencies are known as the Matsubara frequencies.

Problem 7.6 :
Using the τ-periodicity property, derive, for the harmonic oscillator, an expansion of $G_\beta(\tau - \tau')$ in terms of the even Matsubara frequencies along the lines of what we did in chapter 6 (i.e., expand the variables $q(\tau)$ in terms of periodic functions). Show that it satisfies

$$(\partial_\tau^2 - \omega^2)\, G_\beta(\tau - \tau') = -\frac{\hbar}{m}\,\delta(\tau - \tau')\,,$$

for $0 \leq \tau, \tau' < \hbar\,\beta$. Moreover, prove that in the zero-temperature limit, by converting the sum into an integral, one obtains (7.37).

Problem 7.7 : Flux periodicity
Consider an electrically charged particle with mass m and charge q moving on a circle C of radius R in the (x, y)-plane. Inside the circle is a magnetic field such that the flux encircled by C is equal to Φ. The circle is parametrized by $(x, y) = (R\cos\theta, R\sin\theta)$ and $0 \leq \theta < 2\pi$. The classical action then reads

$$S_\Phi[\theta] = \int dt \Big\{ \tfrac{1}{2} m R^2\, \dot\theta^2 + qR\,\dot\theta A \Big\}\,,$$

with $A = \Phi/2\pi R$ the magnitude of the vector potential along the circle due to the enclosed flux. (Observe that the second term in the right-hand side equals (in cartesian coordinates) precisely the well-known interaction term $\int dt\; q\,\dot{\vec{x}} \cdot \vec{A}(\vec{x})$, which is responsible for the Lorentz force.)

i) Give the expression for the momentum p_θ and show that the Hamiltonian takes the form

$$H(p_\theta, \theta) = \frac{(p_\theta - \hbar\Phi/\Phi_0)^2}{2mR^2}\,,$$

with $\Phi_0 = h/q$ the flux quantum for this problem. After quantisation p_θ and θ are two operators satisfying the commutation relation $[\theta, p_\theta] = i\hbar$. How does p_θ act therefore on the wavefunction $\Psi(\theta, t)$? Specify the boundary conditions on $\Psi(\theta, t)$ and determine the eigenfunctions and eigenvalues of the operator p_θ.

ii) Determine the eigenvalues of the Hamiltonian. What is your conclusion concerning the energy spectrum $\{E_\nu(\Phi)\}$ and $\{E_\nu(\Phi+\Phi_0)\}$?

With this Hamiltonian we can now derive a path-integral expression for the transition function $W_{C,\Phi}(\theta_1,t_1;\theta_0,t_0) \equiv \langle\theta_1|e^{-iH(t_1-t_0)/\hbar}|\theta_0\rangle$ in the usual way. Following the same steps as in problem 3.6, the result takes the form

$$W_{C,\Phi}(\theta_1,t_1;\theta_0,t_0) = \sum_{\ell=-\infty}^{\infty} W_\Phi(\theta_1+2\pi\ell,t_1;\theta_0,t_0) \ ,$$

where $W_\Phi(\theta_1,t_1;\theta_0,t_0)$ is the transition function for a particle with 'mass' mR^2 and charge q that freely moves along the entire θ-axis. This means that $-\infty<\theta<\infty$, while the path-integral expression for $W_\Phi(\theta_1,t_1;\theta_0,t_0)$ takes the form

$$W_\Phi(\theta_1,t_1;\theta_0,t_0) = \int \mathcal{D}\theta \; e^{iS_\Phi[\theta]/\hbar} \ ,$$

with $S_\Phi[\theta]$ the classical action defined above.

iii) Using the explicit form of the action, show that

$$W_\Phi(\theta_1,t_1;\theta_0,t_0) = e^{i(\theta_1-\theta_0)\Phi/\Phi_0} W_{\Phi=0}(\theta_1,t_1;\theta_0,t_0) \ . \tag{7.39}$$

Use the expression for the path integral for a free particle (cf. problem 3.1) to determine the corresponding partition function $Z_\beta(\Phi)$. To do this, first present the expression for the partition function as a sum over ℓ and determine the periodicity of $Z_\beta(\Phi)$.

iv) Subsequently, use the Poisson resummation rule (5.37) (integrated over a suitably chosen function) and rewrite the previous result. Argue now that the resulting expression is in agreement with your conclusions in i) and ii).

8 Tunneling and instantons

Tunneling is one of the most interesting phenomena in quantum mechanics, which cannot be described in perturbation theory in $\hbar$. It turns out that the Euclidean path integrals introduced in the previous chapter offer a convenient framework for obtaining quantitative results, at least in the semiclassical approximation. In certain cases this involves dealing with so-called *instanton* solutions, as we will demonstrate shortly. Our starting point is the path-integral representation of the Euclidean transition function,

$$W^E(q_2,\tau_2;q_1,\tau_1) = \langle q_2|e^{-\frac{1}{\hbar}H(\tau_2-\tau_1)}|q_1\rangle = \int_{\substack{q(\tau_1)=q_1\\ q(\tau_2)=q_2}} \mathcal{D}q(\tau)\; e^{-\frac{1}{\hbar}S^E[q(\tau)]} \, . \tag{8.1}$$

From this expression we intend to extract information about the energies and certain matrix elements by considering the limit of large T. We will restrict ourselves to the Euclidean Lagrangian $L^E = \frac{1}{2}\dot{q}^2 + V(q)$. In the semiclassical approximation we need the classical trajectory. Hence we must consider solutions of the equations of motion, which read

$$\ddot{q} = \frac{\partial V}{\partial q} \,. \tag{8.2}$$

We assume that $V(q)$ is bounded from below and by adding a suitable constant we ensure that its minimum value is precisely equal to zero. Hence $V(q) \geq 0$. One easily verifies (e.g. by multiplying the above equation with $\dot{q}$) that $\frac{1}{2}\dot{q}^2 - V(q)$ is a constant of the motion. Hence we write

$$\tfrac{1}{2}\dot{q}^2 - V(q) = E \,, \tag{8.3}$$

with E a constant. Note that E is the energy for a particle moving in the (negative) potential $-V(q)$. Obviously

$$\dot{q} = \pm\sqrt{2(E + V(q))} \,, \tag{8.4}$$

which can be integrated and yields the solution

$$\tau_2 - \tau_1 = \pm \int_{q_1}^{q_2} \frac{\mathrm{d}q}{\sqrt{2(E + V(q))}} \,. \tag{8.5}$$

The Euclidean action $S^E_{cl}[q_0]$ corresponding to the classical path $q_0(\tau)$,

$$S^E_{cl}[q] = \int_{\tau_1}^{\tau_2} \mathrm{d}\tau \Big(\tfrac{1}{2}\dot{q}^2 + V(q)\Big) \,, \tag{8.6}$$

is obviously nonnegative for any trajectory, provided that $\tau_2 > \tau_1$. When the initial and final times, τ_1 and τ_2, tend to $\pm\infty$, then the action will diverge, unless the endpoints $q(\tau_{1,2})$ correspond to absolute minima of the potential (where $V = 0$), *and* the velocity will tend to zero. This implies that finite action solutions for infinite time intervals must have $E = 0$, at least for solutions of the equation of motion (8.2). The action for solutions can be written in a variety of ways,

$$\begin{aligned} S^E_{cl}[q_0] &= \int_{\tau_1}^{\tau_2} \mathrm{d}\tau \Big(\dot{q}^2 - E\Big) = -E(\tau_2 - \tau_1) + \int_{\tau_1}^{\tau_2} \mathrm{d}\tau \, \dot{q}^2 \\ &= \int_{\tau_1}^{\tau_2} \mathrm{d}\tau \Big(|\dot{q}|\sqrt{2(E + V(q))} - E\Big) = -E(\tau_2 - \tau_1) + \operatorname{sgn}\dot{q} \int_{q_1}^{q_2} \mathrm{d}q \, \sqrt{2(E + V(q))} \,. \end{aligned} \tag{8.7}$$

In the last expression we assumed that $\dot{q}$ is of the same sign throughout the trajectory.

In the semiclassical approximation, discussed in chapter 3, we expand about a classical trajectory with boundary values $q(\tau_{1,2}) = q_{1,2}$, keeping terms quadratic in the deviations from this trajectory over which we subsequently integrate (cf. (3.5),(3.10)). Formally this integral leads to a determinant of a differential operator. Up to certain normalizations we thus find

$$W^E(q_2,\tau_2;q_1,\tau_1) \propto \Big[\det\Big(-\partial_\tau^2+V''(q_0(\tau))\Big)\Big]^{-1/2}\, e^{-S^E_{cl}[q_0(\tau)]/\hbar}\,\Big\{1+\mathrm{O}(\hbar)\Big\}\,, \tag{8.8}$$

where $V''=\partial^2V/\partial q^2$ and the differential operator in the determinant acts on functions that vanish at the boundaries $\tau_{1,2}$. It is now clear why we are interested in classical paths with finite action, because otherwise, the above expression will simply vanish. It is sometimes convenient to consider ratios of determinants to avoid some of the subtleties with normalization factors. Therefore one often divides the above determinant by the determinant of a similar operator, but now with V'' replaced by a suitably chosen constant (such as the value of V'' taken at a minimum of the potential). The latter determinant is known from the explicit expression for the transition function of the harmonic oscillator (7.17). Setting $\tau_2=-\tau_1=T/2$ we rewrite (8.8) as

$$W^E(q_2,\tau_2;q_1,\tau_1) = \sqrt{\frac{\omega}{2\pi\hbar\sinh\omega T}}\;K\,e^{-S^E_{cl}[q_0(\tau)]/\hbar}\,\Big\{1+\mathrm{O}(\hbar)\Big\}\,, \tag{8.9}$$

where

$$K=\left|\frac{\det\big(-\partial_\tau^2+\omega^2\big)}{\det\big(-\partial_\tau^2+V''(q_0(\tau))\big)}\right|^{\frac{1}{2}}\,. \tag{8.10}$$

The factor K depends on T and on ω. In principle ω is chosen such that K remains finite in the limit for large T. Later we will see that subtleties may arise when T tends to infinity, but for the moment we ignore possible complications and continue.

To elucidate our strategy let us first consider a simple example of a potential with a single minimum, say at $q=a$, so that $V(a)=0$. We consider the Euclidean path integral for boundary values $q_1=q_2=a$. There is only a single solution connecting these endpoints, namely $q(\tau)=a$, which has vanishing action. Any other classical trajectory starting at $q_1=a$ will have a certain velocity and thus a finite energy at $q=a$; however, once the particle moves away from $q=a$ it will never return and acquire more and more kinetic energy and thus increase its action until it reaches the endpoint q_2, which cannot be equal to a.

Choosing $\omega^2=V''(a)$, the factor K equals unity and we find

$$W^E(a,T/2;a,-T/2)=\sqrt{\frac{\omega}{2\pi\hbar\sinh\omega T}}\;\stackrel{T\to\infty}{\longrightarrow}\;\sqrt{\frac{\omega}{\pi\hbar}}e^{-\omega T/2}\,. \tag{8.11}$$

This shows that the groundstate energy is equal to $\frac{1}{2}\hbar\omega$, up to higher orders in $\hbar$, while the overlap of $|a\rangle$ with the groundstate $|0\rangle$ satisfies $|\langle a|0\rangle| = [\omega/\pi\hbar]^{1/4}$. This result is obtained in the semiclassical approximation and is exact for the harmonic oscillator (cf. problem 7.2).

Figure 1: A double-well potential $V(q)$ and the instanton solution, which gives the classical trajectory for a particle moving between the maxima of $-V(q)$ in a time interval T.

8.1 The double-well potential

Let us now consider the more complicated case of a double-well symmetric potential, $V(q) = V(-q)$, with minima at $q = \pm a$. Just as above we will choose the boundary values $q_{1,2}$ equal to the positions of the classical minima. Hence two different transition functions are of interest, namely

$$\begin{aligned} W(\pm a, T/2; \pm a, -T/2) &= \langle \pm a | e^{-HT/\hbar} | \pm a \rangle \,, \\ W(\pm a, T/2; \mp a, -T/2) &= \langle \pm a | e^{-HT/\hbar} | \mp a \rangle \,, \end{aligned} \tag{8.12}$$

where we identified certain matrix elements by virtue of the reflection symmetry $q \leftrightarrow -q$. Because this is a symmetry of the Hamiltonian, energy eigenfunctions $\psi(q)$ must be either symmetric or antisymmetric in q. Classically there are two independent groundstates $q = \pm a$. Without tunneling, these states would acquire the same semiclassical energy equal to $\frac{1}{2}\hbar\omega$, where $\omega^2 = V''(a) = V''(-a)$. However, due to quantum tunneling the two states will mix and this causes a shift in the energy levels, such that the symmetric state acquires the lowest energy. Our goal is to calculate these shifts in the energy levels in the semiclassical approximation.

Let us first keep T finite. In that case there is again a unique classical solution with $q_1 = q_2 = \pm a$, which is equal to $q(\tau) = a$. This solution has zero energy and zero action. Also there is always a solution with $q_1 = -q_2 = \pm a$, which is shown in Fig. 1. This solution is known as the instanton[9]. The corresponding solution $-q(\tau)$ is called anti-instanton. Let us first discuss some of its properties. For finite T the classical trajectory connecting the two maxima in $-V(q)$ must carry a finite energy, simply because the particle should move away

[9] In the limit $T \to \infty$ the instanton solution may be regarded as a finite-energy static soliton in $1+1$ dimensions. To see this, let q also depend on a real time variable t and interprete τ as a spatial coordinate.

from the maximum with a nonzero velocity. For the instanton this velocity equals $\sqrt{2E}$, so that the endpoints of the solution are approached linearly, i.e.

$$q(\tau) \approx \pm a + \sqrt{2E}(\tau \mp \tfrac{1}{2}T)\,, \qquad \text{for} \qquad \tau \to \pm\tfrac{1}{2}T\,. \tag{8.13}$$

A number of features changes when T becomes infinite. In that case the velocity at $q = \pm a$ must vanish, because otherwise the particle will reach the other maximum in a finite time (after which it continues to move beyond the second maximum and will never return). So E must be zero. This implies that the particle reaches the endpoints at $q = \pm a$ in an exponentially slow manner. We can determine this from (8.5). Assuming that we choose τ_1 and $\tau_2 > \tau_1$ to be large enough so that the particle moves closely to one of the two maxima. Then we may approximate the potential around $q = \pm a$ by $V = \frac{1}{2}\omega^2(q \mp a)^2$, so that

$$\tau_2 - \tau_1 \approx \pm\frac{1}{\omega}\int_{q(\tau_1)}^{q(\tau_2)} \frac{\mathrm{d}q}{a \mp q} = -\frac{1}{\omega}\ln\frac{a \mp q(\tau_2)}{a \mp q(\tau_1)}\,. \tag{8.14}$$

This leads to ($|\tau| \gg 1$)

$$q(\tau) \approx \pm a\Big[1 - c\, e^{-\omega|\tau|}\Big]\,, \tag{8.15}$$

with c some positive constant. The action (8.7) remains finite in the $T \to \infty$ limit and receives its contribution mainly from the center of the instanton solution, where the velocity differs substantially from zero. An explicit solution is discussed in problem 8.1.

There is a subtlety in the $T \to \infty$ limit, because if T is really infinite, then there is no reason to insist that the instanton solution goes through the origin. Stated differently, the fact that the boundaries in τ have been shifted to infinity implies that we regain translational symmetry in τ. If $q_0(\tau)$ is a solution, then also $q_0(\tau+\kappa)$, with κ some arbitrary finite constant must be a solution of (8.2). Hence we are dealing with a continuous set of solutions and we

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Consider then the action

$$S[q(t,\tau)] = \int \mathrm{d}t\,\mathrm{d}\tau\,\Big(\tfrac{1}{2}(\partial_t q)^2 - \tfrac{1}{2}(\partial_\tau q)^2 - V(q)\Big)\,.$$

For static solutions q satisfies the equation of motion $\partial_\tau^2 q = V'(q)$, which is just (8.2), and defines some extended object in one dimension. Its energy equals $\int \mathrm{d}\tau\,(\partial_\tau q)^2$, with the integral extended to the whole τ-interval. (Previously this quantity was identified with the action, (cf. (8.7)), where the integration constant E (which is *not* the energy of the extended object) must vanish in order that the energy be finite.) The energy of the extended object receives its relevant contributions from the region around $\tau = 0$, where the derivative differs appreciably from zero, so that the energy density is concentrated here. Hence we describe a extended object localized at $\tau = 0$. However, τ is just the Euclidean time variable, so that in some sense we are describing a (somewhat smeared out) "event" at $\tau = 0$. This motivated the name "instanton", or "pseudoparticle", for this solution.
In a field theory in 1 time dimension and $d-1$ space dimensions we can thus define instantons as finite-action solutions of the d-dimensional Euclidean version of the theory. These solutions can be regarded as static finite-energy solutions of a theory in 1 time and d space dimensions.

can thus consider two solutions that are arbitrarily close, i.e., $q' = q_0 + \delta q$. Subsituting both sides into the differential equation (8.2), assuming that both q' and q_0 satisfy the equation, and retaining terms linear in δq, we find that δq must satisfy the differential equation

$$\Big[-\partial_\tau^2 + V''(q_0(\tau)) \Big] \delta q(\tau) = 0 \,. \tag{8.16}$$

The function $\delta q(\tau)$ is called a *zero-mode*, because it represents an eigenfunction of the differential operator with zero eigenvalue. So whenever we have a continuous set of solutions there is an associated set of zero modes that satisfy the above equation. Continuous degeneracies always appear whenever a system has a continuous symmetry. In the case at hand, the symmetry is provided by the translations in τ and the zero-mode solution takes the form $\delta q = \dot q_0$, simply because $q_0(\tau+\kappa) \approx q_0(\tau) + \kappa \dot q(\tau) + \mathrm{O}(\kappa^2)$. Indeed, one easily verifies that $\dot q_0$ is a solution of the differential equation (8.16). As long as T is finite, the zero-mode solution poses no difficulty; the shifted solutions do not satisfy the appropriate boundary condition and $\dot q_0$ does not vanish at $\tau = \pm T/2$.[10] Obviously the presence of the boundary conditions suppresses the degeneracy, but when T is infinite this suppression does not take place.

Hence if the time interval is really infinite then there are many solutions that move between maxima of $-V(q)$ in an infinite time interval. First of all, the (anti-)instanton solution itself can we shifted arbitrarily, but furthermore we can glue together a set of instanton and anti-instanton solutions, separated by infinite (or at least large compared to $1/\omega$) time intervals. While there is precisely one exact classical solution when the time interval is finite, there is an infinite number of *approximate* solutions that become closer and closer to an exact solution in the $T \to \infty$ limit. Furthermore, the ratio of determinants K defined in (6.9) will diverge, because the differential operator in the numerator has zero-modes whose eigenvalues vanish as shown in (8.16).

We should stress that these two features, the degeneracy of the solutions and the presence of the zero-modes, are intimately connected. Both seem to lead to divergences, but as it turns out their combined effect will remain finite. With this in mind let us proceed and evaluate first the one-instanton contributions. We thus want to determine the semiclassical contribution of one-instanton solutions to the functional integral with boundary values $q(-\infty) = -a$ and $q(\infty) = a$. For an infinite time interval, we are confronted by an infinite variety of instanton solutions, which we can characterize by the time τ_0 at which the solution is zero. We will call τ_0 the "position" of the instanton. Previously, with a finite symmetric time interval $(-T/2, T/2)$, the instanton's position was necessarily equal to $\tau = 0$, because of symmetry reasons. However, for an infinite time interval we can shift τ to $\tau - \tau_0$ and

[10]Remember that we are taking the determinant of a differential operator acting on functions that vanish on the boundary.

obtain an instanton at τ_0.

Now we want to extract the integration over the instanton position outside the functional integral. We do this by means of the following trivial identity,

$$\int_{-\infty}^{\infty} \mathrm{d}\tau_0 \; |\dot{q}(\tau_0)| \, \delta(q(\tau_0)) = 1 \,, \tag{8.17}$$

which holds for any function $q(\tau_0)$ that vanishes precisely once along the infinite τ-axis. As we will be considering a path integral with boundary values $q = \pm a$ at $\tau = \pm\infty$, we know that any function must have an odd number of zeroes. By restricting the semiclassical corrections to the one-instanton sector, we assume precisely one zero. Later we shall include other solutions.

Inserting this identity under the functional integral, interchanging the order of τ_0 integration with the path-inegral and identifying q in (8.17) with the function $q(\tau)$ in the path integral, we obtain the following result,

$$W(a,\infty;-a,-\infty) = \int_{-\infty}^{\infty} \mathrm{d}\tau_0 \int_{\substack{q(-\infty)=-a\\ q(\infty)=a}} \mathcal{D}q(\tau) \; \delta(q(\tau_0)) \, |\dot{q}(\tau_0)| \; e^{-\frac{1}{\hbar}S^E[q(\tau)]} \,. \tag{8.18}$$

The path integral thus extends over all possible trajectories between $q = \mp a$ at $\tau = \mp\infty$ which vanish (once) at a given time τ_0. According to (8.18) the path integral factorizes into two parts, one associated with paths running from $q(-\infty) = -a$ to $q(\tau_0) = 0$, and the other one corresponding to paths running from $q(\tau_0) = 0$ to $q(\infty) = a$. These two path integrals can subsequently be evaluated in the semiclassical approximation. Because of the boundary value at τ_0, there are no problems with degenerate solutions and corresponding zero-modes.

In principle, the semiclassical approximation is rather straightforward. Because of the symmetry of the potential the classical action associated with the positive or the negative branch of the instanton solution is equal to one-half of the action of a full instanton. In what follows, we denote the action of a full instanton by S_0, so that the semiclassical results equals $\exp(-\frac{1}{2}S_0/\hbar)$, times a determinant factor corresponding to the integral over the small deviations about the classical instanton solution. We write this determinant in a form that is familiar from the Gel'fand-Yaglom representation (see problem 3.5), but now in the context of Euclidean time τ. For instance, for the time interval $(\tau_0, \tau_0 + T/2)$ we write

$$\det \Big[-\partial_\tau^2 + V''(q_0(\tau)) \Big]\Big|_{q_0(\tau_0)=0;\; q_0(T/2)=a} = 2\pi\hbar \, \Psi(\tau_0 + T/2, \tau_0) \,, \tag{8.19}$$

and there are similar expressions for different boundary values. We return to the definition and the subsequent evaluation of Ψ shortly. For the moment we note that we need a similar expression for the time-interval $(\tau_0 - T/2, \tau_0)$. Furthermore, we also have to incorporate the factor $|\dot{q}(\tau)|$ that appears in (8.18), but as deviations of the classical trajectories induce corrections of order $\sqrt{\hbar}$, we can approximate it by its classical value. According to (8.4), this value is equal to $\sqrt{2V(0)}$. Hence we write

$$\int_{\substack{q(-\infty)=-a\\ q(\infty)=a}} \mathcal{D}q(\tau)\;\delta(q(\tau_0))\,|\dot q(\tau_0)|\;\mathrm{e}^{-\frac{1}{\hbar}S^E[q(\tau)]} = \frac{1}{2\pi\hbar}\sqrt{\frac{2V(0)}{\Psi(\tau_0+T/2,\tau_0)\,\Psi(\tau_0,\tau_0-T/2)}}\;\mathrm{e}^{-S_0/\hbar}\,. \tag{8.20}$$

At this point we should first discuss the definition and evaluation of the function $\Psi(\tau,\tau')$, which is a function of the (Euclidean) time difference $\tau-\tau'$. It is defined by the following conditions,

$$\Big[-\partial_\tau^2 + V''(q_0(\tau))\Big]\Psi(\tau,\tau') = 0\,,\qquad \Psi\Big|_{\tau=\tau'} = 0\,,\quad \frac{\mathrm{d}\Psi}{\mathrm{d}\tau}\Big|_{\tau=\tau'} = 1\,. \tag{8.21}$$

Hence Ψ satisfies a time-independent Schrödinger equation with τ playing the role of the coordinate and the τ-dependent potential given by $V''(q_0(\tau))$. Note that this potential is a function of τ through a given instanton path $q_0(\tau)$. For reference purposes, let us assume that $q_0(\tau)$ is the (anti)instanton solution centered at $\tau=\tau_0$ in the middle of a τ-interval of size T, where T is supposed to tend to infinity. Therefore the potential $V''(q_0(\tau))$ behaves as follows. It is symmetric in $(\tau-\tau_0)$ and for $|\tau-\tau_0|\gg 1$ it tends to a positive constant $\omega^2 = V''(a)$. Around $\tau=\tau_0$ it exhibits a dip. It becomes negative and its minimum at $\tau=\tau_0$ is equal to $V''(0)$.

The second-order differential equation (8.21) has two independent solutions. We will define these two independent solutions and use them extensively to decompose the various solutions of the differential equations with various boundary and/or normalization conditions. One solution that we have already encountered, is proportional to the zero-mode solution. It is symmetric in $\tau-\tau_0$ and we define it by $\varphi(\tau)=\dot q_0(\tau)/\dot q_0(\tau_0)$, so that its value at $\tau=\tau_0$ is normalized to unity. The second independent solution can therefore be chosen antisymmetric in $\tau-\tau_0$. We denote it by $\psi(\tau)$ and we normalize it by requiring $\dot\psi(\tau_0)=1$. Obviously ψ itself vanishes at $\tau=\tau_0$. The so-called Wronskian associated with these solutions, defined by $\varphi\dot\psi-\psi\dot\varphi$, is constant and its value is equal to unity, as one can verify at $\tau=\tau_0$. Asymptotically, solutions to the differential equation behave as $\exp[\pm\omega(\tau-\tau_0)]$. However, we know that the zero-mode solution φ vanishes asymptotically (this is qualitatively clear, but follows explicitly from (8.15)), so that we expect the second solution ψ to contain an exponentially increasing factor. Therefore, the two solutions satisfy the following properties

$$\begin{aligned} &\varphi(\tau_0)=1\,, && \dot\varphi(\tau_0)=0\,, && \varphi(\tau)\approx C_+\,\mathrm{e}^{-\omega|\tau-\tau_0|} \quad \text{for }\ |\tau-\tau_0|\to\infty\,, \\ &\psi(\tau_0)=0\,, && \dot\psi(\tau_0)=1\,, && \psi(\tau)\approx \mathrm{sgn}(\tau-\tau_0)\,C_-\,\mathrm{e}^{\omega|\tau-\tau_0|} \quad \text{for }\ |\tau-\tau_0|\to\infty\,. \end{aligned} \tag{8.22}$$

From the value of the Wronskian we derive that C_+ and C_- are not independent and satisfy the condition $2\omega\, C_+\, C_- = 1$.

Armed with this information we determine straigthforwardly, in the limit $T \to \infty$, the two functions Ψ in (8.20).

$$\Psi(\tau_0 + T/2, \tau_0) \approx C_-\, \mathrm{e}^{\omega T/2}\,, \qquad \Psi(\tau_0, \tau_0 - T/2) \approx \frac{1}{2\omega\, C_+}\, \mathrm{e}^{\omega T/2}\,. \tag{8.23}$$

The first result is rather obvious. To determine second one one first writes the solution for $\Psi(\tau, \tau_0 - T/2)$ near $\tau \approx \tau_0 - T/2$, which is equal to $\omega^{-1} \sinh[\omega(\tau - \tau_0 + T/2)]$. This solution decomposes into φ and ψ and by matching the exponential factors far away from the instanton locations, one can determine the explicit decomposition,

$$\Psi(\tau, \tau_0 - T/2) = \frac{\mathrm{e}^{\omega \mathrm{T}/2}}{2\omega C_+}\, \varphi(\tau) + \frac{\mathrm{e}^{-\omega \mathrm{T}/2}}{2\omega C_-}\, \psi(\tau)\,. \tag{8.24}$$

When choosing $\tau = \tau_0$, the second term proportional to ψ vanishes so that one obtains the required result (8.23). Of course, for a specific example the above results can be worked out explicitly, as we will see in problem 8.2. Later on in this chapter, we will have to consider a similar matching for the multi-instanton solutions.

After this digression we continue the determination of (8.20). First we rewrite the corresponding expression as

$$\sqrt{\frac{\omega}{\pi\hbar}}\, \mathrm{e}^{-\omega T/2} \sqrt{\frac{S_0}{2\pi\hbar}}\, K'\, \mathrm{e}^{-S_0/\hbar}\,. \tag{8.25}$$

Subsequently we establish that $\Psi(\tau_0 + T/2, \tau_0)\, \Psi(\tau_0, \tau_0 - T/2) \approx C_-^2 \exp(\omega T)$, and we use this result to rewrite the (positive) factor K' as

$$K' = \lim_{T\to\infty} \sqrt{\frac{V(0)}{\omega\, S_0}} \sqrt{\frac{e^{\omega T}}{\Psi(\tau_0 + T/2, \tau_0)\, \Psi(\tau_0, \tau_0 - T/2)}} = \sqrt{\frac{V(0)}{S_0\, \omega\, C_-^2}}\,. \tag{8.26}$$

Integrating (8.25) over the instanton position τ_0 leads to an extra factor T,

$$W(a, \infty; -a, -\infty) = \lim_{T\to\infty} \sqrt{\frac{\omega}{\pi\hbar}}\, e^{-\omega T/2} \sqrt{\frac{S_0}{2\pi\hbar}}\, K'\, T\, e^{-S_0/\hbar}\,. \tag{8.27}$$

Clearly this answer does not depend exponentially on T, due to the degeneracy of the one-instanton solutions, so that we cannot extract a value for the energy.

Before continuing let us explain the reasons for extracting the prefactor $\sqrt{S_0/(2\pi\hbar)}$ in (8.25). The factor $\sqrt{S_0}$ in the numerator is precisely the norm of the zero-mode $\dot{q}_0$, as can be seen from (8.7) upon subtituting $E = 0$. The factor $\sqrt{2\pi\hbar}$ in the denominator arises because of the fact that we were dealing with a path integral in which the paths are fixed at some intermediate value (namely at τ_0). Each integration over a point of the path at a given time carries a factor $1/\sqrt{2\pi\hbar}$, as is shown in (2.21). These factors are almost completely cancelled by the appropriate measure of the path integral. The very same factor in (8.19) is a remnant of this. Compared to a path integral over unrestricted paths, a path integral over paths fixed at some intermediary time, carries a relative factor $1/\sqrt{2\pi\hbar}$. When integrating over the intermediary position, the correponding Gaussian integral yields a factor $\sqrt{2\pi\hbar}$, so that the relative factor disappears.

The multi-instanton solutions can now be treated in the same way. Hence we consider the contribution in the path integral of paths $q(\tau)$ that cross the τ-axis $2n+1$ times and approximate them by an alternating sequence of $n+1$ instanton and n anti-instanton solutions. Here we assume that the instantons remain localized and separated by infinite time intervals, the so-called *dilute-instanton approximation*. Again we use the trick based on (8.17) to write the path integral as an integral over instanton positions $\tau_0 \ll \tau_2 \ll \cdots \ll \tau_{2n-2} \ll \tau_{2n}$ and anti-instanton positions $\tau_1 \ll \tau_3 \ll \cdots \ll \tau_{2n-1}$. Keeping the (anti-)instanton positions fixed for the moment, we are interested in the functional integral

$$\int_{\substack{q(-\infty)=-a\\ q(\infty)=a}} \mathcal{D}q(\tau) \left(\sum_{i=0}^{2n} \delta(q(\tau_i))\, |\dot{q}(\tau_i)| \right) \mathrm{e}^{-\frac{1}{\hbar} S^E[q(\tau)]} \,. \tag{8.28}$$

This integral can be evaluated and gives rise to the following result

$$\left(\frac{1}{2\pi\hbar}\right)^{\frac{2n+2}{2}} \sqrt{\frac{(2V(0))^{2n+1}}{\Psi(T/2,\tau_{2n})\,\Psi(\tau_{2n},\tau_{2n-1})\cdots\Psi(\tau_1,\tau_0)\,\Psi(\tau_0,-T/2)}}\; \mathrm{e}^{-(2n+1)S_0/\hbar} \,. \tag{8.29}$$

To further determine this expression we need an expression for $\Psi(\tau_{i+1},\tau_i)$, where τ_i and τ_{i+1} denote two consecutive, widely separated (anti-)instanton postitions. It can be obtained by considering $\Psi(\tau,\tau_i)$ at an intermediate value between de instanton and anti-instanton and comparing its form by extrapolating from both sides. Obviously $\Psi(\tau,\tau_i) = \psi_i(\tau) \approx C_-\, \exp[\omega(\tau-\tau_i)]$, where the subscript i indicates that the functionφ_i is defined with respect to the i-th (anti)instanton, and one must be able to write this as a linear combination for the functions φ_{i+1} and ψ_{i+1}, but now defined with respect to the (anti)instanton at τ_{i+1}. Matching the exponentials $\mathrm{e}^{\omega\tau}$ leads to

$$\Psi(\tau,\tau_i) = \frac{C_-\,\mathrm{e}^{-\omega\tau_i}}{C_+\,\mathrm{e}^{-\omega\tau_{i+1}}}\; \varphi_{i+1}(\tau) + \alpha\,\psi_{i+1}(\tau) \,, \tag{8.30}$$

where α is some unknown coefficient. From this expression one derives

$$\Psi(\tau_{i+1},\tau_i) \approx 2\,\omega\, C_-^2\, \mathrm{e}^{\omega(\tau_{i+1}-\tau_i)} \,. \tag{8.31}$$

Substituting this result we obtain the following result for (8.28),

$$\sqrt{\frac{\omega}{\pi\hbar}}\;\mathrm{e}^{-\omega T/2}\left[\sqrt{\frac{S_0}{2\pi\hbar}}\,K'\mathrm{e}^{-S_0/\hbar}\right]^{2n+1}, \tag{8.32}$$

where K' was defined earlier in (8.26).

Subequently we integrate over the $2n+1$ (anti-)instanton positions. However, we have to take into account that every instanton must be followed by an anti-instanton, and vice versa, until one reaches the end. Hence the integral takes the form

$$\int_{-T/2}^{T/2}\mathrm{d}\tau_{2n}\int_{-T/2}^{\tau_{2n}}\mathrm{d}\tau_{2n-1}\cdots\int_{-T/2}^{\tau_2}\mathrm{d}\tau_1\int_{-T/2}^{\tau_1}\mathrm{d}\tau_0=\frac{1}{(2n+1)!}\,T^{2n+1}\,. \tag{8.33}$$

Substituting this expression into the path integral and summing over all multi-instanton configurations gives rise to

$$W(a,\infty;-a,-\infty)=\lim_{T\to\infty}\sqrt{\frac{\omega}{\pi\hbar}}\;e^{-\omega T/2}\sum_{n=0}^{\infty}\frac{1}{(2n+1)!}\left[\sqrt{\frac{S_0}{2\pi\hbar}}\,K'\,T\,\mathrm{e}^{-S_0/\hbar}\right]^{2n+1}. \tag{8.34}$$

Of course, the same result is obtained when interchanging the endpoints and considering paths running from $q=a$ to $q=-a$. But multi-instanton solutions contribute also when the endpoints are identical, except that the numbers of instantons and anti-instantons must then be equal, so that the sum runs over even powers of T,

$$W(a,\infty;a,-\infty)=\lim_{T\to\infty}\sqrt{\frac{\omega}{\pi\hbar}}\;e^{-\omega T/2}\sum_{n=0}^{\infty}\frac{1}{(2n)!}\left[\sqrt{\frac{S_0}{2\pi\hbar}}\,K'\,T\,\mathrm{e}^{-S_0/\hbar}\right]^{2n}. \tag{8.35}$$

Note that we included the zero-instanton contribution.

Both results (8.34) and (8.35) can be summed and we obtain

$$\begin{aligned}W(a,\infty;\pm a,-\infty)=&\lim_{T\to\infty}\tfrac{1}{2}\sqrt{\frac{\omega}{\pi\hbar}}\;\mathrm{e}^{-\omega T/2}\\&\times\left\{\exp\left[\sqrt{\frac{S_0}{2\pi\hbar}}\,K'\,T\,\mathrm{e}^{-S_0/\hbar}\right]\pm\exp\left[-\sqrt{\frac{S_0}{2\pi\hbar}}\,K'\,T\,\mathrm{e}^{-S_0/\hbar}\right]\right\}.\end{aligned} \tag{8.36}$$

After this summation the result depends exponentially on T and we can extract the results for the energy and the wave functions. We clearly distinguish two exponential factors corresponding to two different intermediate states in the evolution operator. One corresponds to the ground state, which we expect to be symmetric. The other one, corresponding to an exited state, is antisymmetric in $q\to -q$. We denotes these states by $|S\rangle$ and $|A\rangle$ and we use that $\langle -a|S\rangle=\langle a|S\rangle$ and $\langle -a|A\rangle=-\langle a|A\rangle$. In this way we extract the correponding energy levels denoted by E_S and E_A,

$$E_{\substack{S\\A}}=\tfrac{1}{2}\hbar\omega\mp\hbar\sqrt{\frac{S_0}{2\pi\hbar}}\,K'\,\mathrm{e}^{-S_0/\hbar}\,. \tag{8.37}$$

As expected, the ground state (with energy E_S) is symmetric under the reflection symmetry $q \to -q$ (cf. problem 8.3). Observes that these answers cannot be obtained form standard perturbation theory, which would yield a power series in $\hbar$.

8.2 The periodic potential

As a third application we consider the periodic potential with minima at $q = na$, with n an integer, where periodicity interval of the potential is equal to a. Then the eigenstates of the Hamiltonian can be chosen such that they are simultaneously eigenstates of the translation operator $\mathcal{T}$, which shifts the coordinate q to $q + a$. This translation operator commutes with the Himoltonian and must be a unitary operator, so that its eigenvalues can be written as a phase factor. Hence we expect that eigenfunctions $\psi(q)$ will be quasi-periodic, i.e., they will satisfy $\psi(q + Na) = \exp(i\theta N)\,\psi(q)$ for some angle θ. This property will be confirmed below.

Let us now repeat the semiclassical instanton approximation. Using the same steps as above, we can sum over the solutions consisting of instanton and anti-instantons. However, in this case there is no correlation in the ordering of instantons and anti-instantons as an instanton does not have to be followed by an anti-instanton. The integration over n_+ instanton and n_- anti-instanton positions yields therefore a factor

$$\frac{T^{n_+}}{n_+!}\,\frac{T^{n_-}}{n_-!}\,.$$

The transition function between two states $|\ell a\rangle$ and $|(\ell + N)a\rangle$ therefore takes the form

$$W((\ell+N)a,\infty;\ell a,-\infty) = \lim_{T\to\infty}\sqrt{\frac{\omega}{\pi\hbar}}\,\mathrm{e}^{-\omega T/2}\sum_{n_+-n_-=N}^{\infty}\frac{1}{n_+!\,n_-!}\left[\sqrt{\frac{S_0}{2\pi\hbar}}\,K'\,T\,\mathrm{e}^{-S_0/\hbar}\right]^{n_++n_-}. \tag{8.38}$$

Using the following representation of the Kronecker-delta for integers n,

$$\delta_{n,0} = \frac{1}{2\pi}\int_{-\pi}^{\pi}\mathrm{d}\theta\;\mathrm{e}^{i\theta n}\,, \tag{8.39}$$

and inserting it into the above expression with n replaced by $N - n_+ + n_-$, we can perform the sums in (8.38) under the θ-integral by summing over unrestricted integers $n_\pm$. The instantons and anti-instantons thus yield a factor

$$\exp\left[\sqrt{\frac{S_0}{2\pi\hbar}}\,K'\,T\,\mathrm{e}^{-S_0/\hbar\mp i\theta}\right], \tag{8.40}$$

respectively. The final result takes the form

$$\begin{aligned} W((\ell+N)a,\infty;\ell a,-\infty) &= \lim_{T\to\infty}\sqrt{\frac{\omega}{\pi\hbar}}\,\mathrm{e}^{-\omega T/2} \\ &\quad\times\frac{1}{2\pi}\int_{-\pi}^{\pi}\mathrm{d}\theta\;\mathrm{e}^{i\theta N}\exp\left[2\cos\theta\sqrt{\frac{S_0}{2\pi\hbar}}\,K'\,T\,\mathrm{e}^{-S_0/\hbar}\right]. \end{aligned} \tag{8.41}$$

In (8.41) we distinguish a variety of exponential factors associated with continuous band of energies

$$E_\theta = \tfrac{1}{2}\hbar\omega - 2\hbar\cos\theta\sqrt{\frac{S_0}{2\pi\hbar}}\,K'\,\mathrm{e}^{-S_0/\hbar}\,. \tag{8.42}$$

Denote the corresponding eigenstates by $|\theta\rangle$ and insert a complete set of eigenstates into $\langle(\ell+N)a|\exp(-HT/\hbar)|\ell a\rangle$. In the approximation that we are working with, only the states $|\theta\rangle$ contribute, as is obvious from (8.41), so that we conclude

$$\langle(\ell+N)a|\theta\rangle\,\langle\theta|\ell a\rangle = \sqrt{\frac{\omega}{\pi\hbar}}\,\mathrm{e}^{i\theta N}\,, \tag{8.43}$$

or

$$\langle(\ell+N)a|\theta\rangle = \mathrm{e}^{i\theta N}\,\langle\ell a|\theta\rangle\,, \qquad \text{and} \qquad |\langle\ell a|\theta\rangle| = \left[\frac{\omega}{\pi\hbar}\right]^{\frac{1}{4}}. \tag{8.44}$$

We conclude that we are dealing with a continuous band of eigenstates with energy (8.42), characterized by an angle θ, which has a two-fold degeneracy. This band structure is very characteristic in solid-state physics and is, for instance, extremely relevant when describing the behaviour of electrons in solids.

Problem 8.1 :
Consider the (anti-)instanton solutions for the double-well potential

$$V(q) = \frac{\omega^2}{8a^2}(a^2-q^2)^2\,, \tag{8.45}$$

and show that (for $T=\infty$) it takes the form

$$q(\tau) = a\tanh\Big[\tfrac{1}{2}\omega(\tau-\tau_0)\Big]\,, \tag{8.46}$$

where τ_0 is the instanton "position" (the time where the velocity is maximal and q vanishes). Finally show that the action equals $S^E_{cl}[q(\tau)] = \frac{2}{3}\omega a^2$.

Problem 8.2 :
Reconsider the Gel'fand-Yaglom method for the calculation of determinants for the Euclidean case (cf. problem 3.5). As before the semiclassical result takes the form $F(\tau',\tau)\,\exp(-S/\hbar)$, with S the action corresponding to the classical path. The prefactor is equal to

$$F(\tau,\tau') = \frac{1}{\sqrt{2\pi\hbar\Psi(\tau,\tau')}}\,,$$

where Ψ is proportional to the determinant of the differential operator $[-\partial_\tau^2+V''(q_0(\tau))]$ for functions that vanish at the boundary. Prove that Ψ is a solution of the differential equation

$$\Big[-\partial_\tau^2 + V''(q_0(\tau))\Big]\Psi(\tau,\tau') = 0\,, \tag{8.47}$$

with boundary conditions $\Psi(\tau', \tau') = 0$ and $\partial_\tau \Psi(\tau, \tau')|_{\tau=\tau'} = 1$. Discuss the large-time behaviour.

Problem 8.3 :
Consider (8.36) and the matrix elements of $\exp(-HT/\hbar)$ in the two-dimensional space spanned by the states $|\pm a\rangle$. Insert a complete set of eigenstates and argue that only two of them, denoted by $|S\rangle$ and $|A\rangle$, contribute. Identify their corresponding energies with (8.37). Find the overlap of the eigenfunctions with the states $|\pm a\rangle$ and show that $\langle a|S\rangle = \langle -a|S\rangle$, $\langle a|A\rangle = -\langle -a|A\rangle$ and $|\langle a|S\rangle| = |\langle a|A\rangle| = [\omega/(4\pi\hbar)]^{1/4}$. Interpret this result.

Problem 8.4 :
Show that V'' in the instanton background corresponding to the potential (8.45) takes the form

$$V'' = \frac{\omega^2}{2a^2}(3q^2 - a^2) = \tfrac{1}{2}\omega^2 \left[2 - \frac{3}{\cosh^2 \tfrac{1}{2}\omega(\tau - \tau_0)} \right] . \tag{8.48}$$

We consider the differential equation (8.47). This is just like solving the Schrödinger equation with (8.48) as a potential for which we must determine the zero-energy solution. One such solution is already known, as it correponds to the zero-mode. Show that it equals (with certain normalization)

$$\varphi(\tau) = \frac{1}{\cosh^2(\omega(\tau - \tau_0)/2)} .$$

This is the true groundstate wave function for the potential (8.48). It is nowhere zero and vanishes exponentially at infinity. Show that it satisfies the following properties

$$\varphi(\tau_0) = 1 , \qquad \dot\varphi(\tau_0) = 0 , \qquad \varphi(\tau) \approx 4\mathrm{e}^{-\omega|\tau-\tau_0|} \text{ for } \tau \to \pm\infty .$$

Prove that all zero-energy solutions behave asymptotically as $\exp(\pm\omega\tau)$ and can be chosen symmetric or antisymmetric under $(\tau-\tau_0) \to -(\tau-\tau_0)$. We are interested in the independent solution ψ (but only for large and positive τ) that satisfies the boundary conditions

$$\psi(\tau_0) = 0 , \qquad \dot\psi(\tau_0) = 1 .$$

Show that any two solutions with equal eigenvalues, say f and g, have a constant Wronskian $f\,\dot g - \dot f\,g$. For φ and ψ use this observation to prove that

$$\varphi\,\dot\psi - \dot\varphi\,\psi = 1$$

Solve this equation at large τ to obtain an asymptotic prediction for ψ.

With the help of the above results show that the Gel'fand-Yaglom function Ψ behaves as

$$\Psi(\tau_0 + T/2, \tau_0) \approx \frac{1}{8\omega}\,\mathrm{e}^{\omega T/2}.$$

Determine also $\Psi(\tau_0, \tau_0 - T/2)$ by matching the solution at $\tau \approx \tau_0 - T/2$ to a linear combination of φ and/or ψ. Calculate the constant K' and, using the result for the instanton action found in problem 6.1, derive that the energies of the lowest-lying states are equal to

$$E_{\substack{S\\A}} = \tfrac{1}{2}\hbar\omega \mp 2\sqrt{\frac{\hbar\omega^3 a^2}{\pi}}\,\mathrm{e}^{-\frac{2}{3}\omega a^2/\hbar}\,.$$

.

Problem 8.5 :
Consider a particle in a two-dimensional plane and denote its position $\vec{q}$ in polar coordinates by $q(\cos\theta, \sin\theta)$. The particle is constrained to move on the circle $q = R$ and the Euclidean action of the particle is, therefore, simply

$$S^E[\vec{q}] = \int \mathrm{d}\tau\;\tfrac{1}{2}(\dot{\vec{q}})^2 = \int \mathrm{d}\tau\;\tfrac{1}{2}R^2(\dot{\theta})^2\;.$$

We want to calculate the transition function $W(\theta_2, T/2; \theta_1, -T/2)$ in the semiclassical approximation (which is exact here). What are the classical paths that contribute to this transition function? Calculate the classical action for each of them.

Using the (real-time) result of problem 3.6, part iii), write down the exact transition function. Identify the contribution from the the various paths and observe that the prefactor depends on T, and not on θ_1 and θ_2, as expected.

The exponential factors do not obviously yield the expected behaviour for large T. Use the Poisson resummation formula (5.37) such that the expected form is obtained and identify the contribution from the energy eigenvalues and the wave functions. Consider the dependence on $\theta_2 - \theta_1$ for large and small T and explain the result.

Next consider a relativistic field theory for a complex scalar field $\phi(x) \equiv |\phi(x)|e^{i\theta(x)}$, which is also constrained to take values on the circle $|\phi(x)| = R/\sqrt{2}$. The relevant Euclidean action is now

$$S^E[\phi] = \int \mathrm{d}^4x\;\partial_\mu\phi^*\partial^\mu\phi = \int \mathrm{d}^4x\;\tfrac{1}{2}R^2(\partial_\mu\theta)^2\;.$$

We want to calculate again the transition function $W(\theta_2, T/2; \theta_1, -T/2)$, where θ_1 and θ_2 are constant (i.e., they do not depend on the space coordinates), in the semiclassical approximation (which is exact). Determine again the classical paths subject to these boundary conditions and the corresponding value of the action. Assume a finite volume V of space at this point.

Observing that the result obtained is almost entirely the same as that found above for a single particle, try to justify the prefactor in the transition function, and use the Poisson resummation formula exactly as above. Then take the limit $V \to \infty$. What is now your conclusion about the $(\theta_2 - \theta_1)$-dependence of the transition function in general and the groundstate wave function in particular?

9 Perturbation theory

For most actions S we cannot explicitly calculate the path integral. However, we will show that we can describe the path integral in perturbation theory in terms of an infinite series of so-called *Feynman diagrams*. Consider an action S which is not only quadratic in the fields but also includes higher-order terms. We write

$$S[\phi] = S_0[\phi] + S_I[\phi], \tag{9.1}$$

where $S_0[\phi]$ denotes the part of S quadratic in ϕ, while $S_I[\phi]$ contains the higher-order terms. The path integral W can be written as

$$W = \int \mathcal{D}\phi \, \exp\left\{\frac{i}{\hbar} S_0[\phi]\right\} \exp\left\{\frac{i}{\hbar} S_I[\phi]\right\}. \tag{9.2}$$

In chapter 4 the following identity was derived

$$\int \mathcal{D}\phi \exp\left\{\frac{i}{\hbar} S_0[\phi] + J \cdot \phi\right\} = \exp\left\{\tfrac{1}{2}(J, \Delta J)\right\}, \tag{9.3}$$

where Δ is the two-point function of the free theory, determined by S_0. Clearly the two-point function is directly proportional to the inverse of the quadratic term in the action. Note that we use a compact notation, where

$$J \cdot \phi \equiv \int dx \, J(x) \, \phi(x) \quad \text{and} \quad (J, \Delta J) \equiv \int dx \, dy \, J(x) \, \Delta(x,y) \, J(y). \tag{9.4}$$

If the quadratic term in the action is equal to $\frac{1}{2}(\phi, A\phi)$ then $\Delta = i\hbar \, A^{-1}$. The two-point function Δ is often called the *propagator*. The path-integral measure $\mathcal{D}\phi$ is normalized such that $\int \mathcal{D}\phi \, \exp[\frac{i}{\hbar} S_0] = 1$.

Using (9.3) we get

$$\begin{aligned} \int \mathcal{D}\phi \, \phi_1 \cdots \phi_n \exp\left\{\frac{i}{\hbar} S_0[\phi]\right\} &= \int \mathcal{D}\phi \, \frac{\partial}{\partial J_1} \cdots \frac{\partial}{\partial J_n} \, \exp\left\{\frac{i}{\hbar} S_0[\phi] + J \cdot \phi\right\}\Big|_{J=0} \\ &= \frac{\partial}{\partial J_1} \cdots \frac{\partial}{\partial J_n} \, \exp\left\{\tfrac{1}{2}(J, \Delta J)\right\}\Big|_{J=0}. \end{aligned} \tag{9.5}$$

To compute (9.2) we expand $\exp\left\{\frac{i}{\hbar}S_I[\phi]\right\}$ as a power series in terms of the fields; (9.2) can be written as

$$W = \exp\left\{\frac{i}{\hbar}S_I\left[\partial/\partial J\right]\right\} \exp\left\{\tfrac{1}{2}(J,\Delta J)\right\}\Big|_{J=0}. \tag{9.6}$$

To be more specific and to clarify what is meant by $S_I\left[\partial/\partial J\right]$ we discuss an example based on the action

$$S = \int d^d x \left(\mathcal{L}_0 + \lambda\phi^4(x)\right), \tag{9.7}$$

where $\mathcal{L}_0$ is the quadratic part of L. The coupling constant λ must be taken negative in order that the potential be bounded from below. Then (9.2) becomes

$$W = \int \mathcal{D}\phi \exp\left\{\frac{i}{\hbar}\int d^d x\; \lambda\phi^4(x)\right\} \exp\left\{\frac{i}{\hbar}S_0[\phi]\right\}. \tag{9.8}$$

The first term, $\exp\{\frac{i}{\hbar}S_I\}$, can be expanded as a power series

$$\exp\left\{\frac{i}{\hbar}S_I[\phi]\right\} = 1 + \frac{i\lambda}{\hbar}\int d^d x\, \phi^4(x) - \frac{\lambda^2}{2\hbar^2}\left\{\int d^d x\, \phi^4(x)\right\}^2 + \cdots \tag{9.9}$$

We focus on $\int \mathcal{D}\phi \int d^d x\, \phi^4(x) \exp\left\{S_0[\phi]\right\}$, treating higher-order terms as perturbations. With (9.5) this is equal to

$$\int d^d x \left(\frac{\partial}{\partial J(x)}\right)^4 \exp\left\{\tfrac{1}{2}(J,\Delta J)\right\} = \int d^d x \left(\frac{\partial}{\partial J(x)}\right)^4 \exp\left\{\tfrac{1}{2}\int d^d y\, d^d z\; J(y)\,\Delta(y,z)\,J(z)\right\}. \tag{9.10}$$

Using $\frac{\partial J(y)}{\partial J(x)} = \delta^d(x-y)$ one easily finds this to be equal to

$$\begin{aligned}\int d^d x &\left\{3\Delta^2(x,x) + 6\Delta(x,x)\left(\int d^d y\, \Delta(x,y)J(y)\right)^2 + \left(\int d^d y\, \Delta(x,y)J(y)\right)^4\right\} \\ &\times \exp\left\{\tfrac{1}{2}\int d^d z\, d^d z'\; J(z)\,\Delta(z,z')\,J(z')\right\}.\end{aligned} \tag{9.11}$$

The correspondence with Feynman diagrams is given by associating to each propagator $\Delta(x,y)$ a line with end points labelled by x and y, to each source term $J(x)$ a cross labelled by x and to each term originating from $\phi^n(x)$ an n-point vertex labelled by x (an n-point vertex is a point where n lines join. Furthermore, one should integrate over the variables associated with the internal lines. In terms of Feynman diagrams the expression (9.11) is shown in Fig. 2. The coefficients of the three terms in (9.11) are combinatorial factors which are related to the number of ways in which a diagram can be formed by connecting propagators and vertices. Indeed, there are three different ways to connect the four lines of the vertex by two propagators and six different ways to connect only two lines.

Observe that we did not put the source equal to zero in (9.11). Only the first term therefore represents a contribution to the path integral (9.8). The subsequent terms contribute,

Figure 2: Diagrammatic representation of (7.11).

however, to the two- and four-point correlation function, which follow from taking further derivatives with respect to $J(x)$, before putting $J(x)$ to zero.

In principle it is straightforward to work out all these expressions including the combinatorial factors. In practice these manipulations are summarized in a number of simple rules, the so-called Feynman rules, which succinctly specify the correspondence between a diagram and its mathematical expression and prescribe in simple terms how to obtain the combinatorial factors, without necessarily having to refer to long expressions such as the ones above. These rules can be applied to any field theory. We refer to De Wit & Smith (in particular to chapter 2) for further details.

In (9.11) one observes that propagators appear whose space-time arguments coincide. They are caused by the fact that in (9.10) and (9.11) we are considering correlation functions of fields taken at the same point in space-time. We have already observed, at the end of chapter 3 (cf. problem 3.3), that such products become singular. The same phenomenon happens here. To see this consider the propagator for Klein-Gordon theory, which follows directly from (6.14) by integrating over all the different harmonic oscillators described by the field theory. Hence

$$\Delta(x,y) = \frac{\hbar}{i(2\pi)^d} \int d^dk \, \frac{e^{i\vec{k}\cdot(\vec{x}-\vec{y}) - ik_0(x_0-y_0)}}{-k_0^2 + \vec{k}^{\,2} + m^2 - i\epsilon}. \tag{9.12}$$

Obviously Δ satisfies the equation

$$\frac{i}{\hbar}\left(\nabla^2 - \partial_0^2 - m^2\right)\Delta(x,y) = -\delta^d(x-y). \tag{9.13}$$

For $x=y$ we find

$$\Delta(x,x) = \frac{\hbar}{i(2\pi)^d} \int d^dk \, \frac{1}{-k_0^2 + \vec{k}^{\,2} + m^2 - i\epsilon}, \tag{9.14}$$

which diverges unless we are in $d = 1$ dimensions, where we are dealing with just one harmonic oscillator. The singularity is thus caused by the fact that, in field theory, we are dealing with an infinite number of harmonic oscillators (the singularity is called "ultraviolet" because it is associated with large momenta; observe that the degree of divergence grows with the dimension).

Let us first study these singularities in a little more detail. Because of Lorentz invariance, the propagator is not only singular for $x = y$, but everywhere on the light cone (thus for $(x-y)^2 = 0$). Therefore we switch to the Euclidean case, where the singularity occurs only at $x = y$. In d dimensions we thus consider the following differential equation,

$$\left(\partial_i^2 - m^2\right) \Delta(x-y) = -\hbar\, \delta^d(x-y). \tag{9.15}$$

Writing $r = \mid \vec{x} - \vec{y} \mid$, we use the ansatz

$$\Delta(x-y) = -\frac{\hbar}{\Omega_d} \frac{f(mr)}{r^{d-2}}\,, \tag{9.16}$$

where

$$\Omega_d = \frac{2\pi^{d/2}}{\Gamma(d/2)}\,, \tag{9.17}$$

is the surface area of a unit sphere S^{d-1} embedded in d dimensions. This ansatz implies that the dimensionless function f must satisfy the equation

$$f''(mr) - \frac{d-3}{mr} f'(mr) - f(mr) = 0\,. \qquad (r > 0) \tag{9.18}$$

Equation (9.18) is a modified Bessel equation (cf. problem 7.4). Integrating (9.15) over a ball of radius R centered at the origin, we obtain

$$\int_{B_R} d^d x\ \left(\partial_i^2 - m^2\right) \Delta(x) = -\hbar\,. \tag{9.19}$$

Using Gauss' law we rewrite the first term as a surface integral. In this way we find

$$1 + (d-2)\, f(mR) - mR\, f'(mR) + m^2 \int_0^R dr\, r\, f(mr) = 0. \tag{9.20}$$

Upon differentiation with respect to R one finds again (9.18). Assuming that f is regular at the origin and that $d \neq 2$, one readily concludes that $f(0) = -(d-2)^{-1}$.

For $m = 0$ we thus recover the Coulomb potential in d dimensions,

$$\Delta(x-y) = \frac{\hbar}{\Omega_d} \frac{1}{d-2} \frac{1}{r^{d-2}}\,, \qquad (d \neq 2) \tag{9.21}$$

Problem 9.1 :
For $d = 1$ prove that the solution of (9.15) equals

$$\Delta(x) = \frac{\hbar}{2m} e^{-m|x|} + C_1\, e^{mx} + C_2\, e^{-mx}\,, \tag{9.22}$$

where C_1 and C_2 are arbitrary constants. Give physical arguments why one should choose $C_1 = C_2 = 0$. Consider also the case $m = 0$.

Problem 9.2 :
For $d = 2$ we assume that $rf(mr)$ is regular near the origin. Show that (9.20) then leads to

$$\Delta(x - y) = \frac{\hbar}{2\pi} \ln m|x - y| \,, \tag{9.23}$$

for $x - y \approx 0$, while for large values of $|x - y|$ we have an exponential damping factor proportional to $\exp(-m|x - y|)$. Convert to complex coordinates $z = x + iy$ and write the massless equation in terms of these coordinates. Show that the general solution away from $x - y = 0$ can be written as the sum of two arbitrary functions $f(z)$ and $g(\bar{z})$, i.e. a holomorphic and an antiholomorphic function. Argue that the special solution of the inhomogenous equation

$$\Delta(x - y) = \frac{\hbar}{2\pi} \ln \mu|x - y| \,, \tag{9.24}$$

with μ an arbitrary constant, is indeed of that form. This is the Coulomb potential in two dimensions. Demonstrate that the above result is consistent with the limit $d \to 2$ of (9.21).

Problem 9.3 :
Solve (9.18) and (9.19) at $R = 0$ for $d = 3$ and prove that the most general solution for $\Delta(x)$ follows from

$$f(mr) = e^{-mr} + A \sinh mr,$$

where A is an arbitrary constant. For $A = 0$ one obtains the Yukawa potential

$$\Delta_{d=3} = -\hbar \, \frac{e^{-mr}}{4\pi r}. \tag{9.25}$$

Give a systematic comparison of the short and long distance behaviour of the propagators in various dimensions, both for $m \neq 0$ and $m = 0$.

Problem 9.4 : Green's functions with non-zero mass
Consider the expression for Δ in d Euclidean dimensions,

$$\Delta(\vec{x}) = \frac{\hbar}{(2\pi)^d} \int \mathrm{d}^d k \, \frac{e^{i\vec{k}\cdot\vec{x}}}{\vec{k}^2 + m^2}.$$

Show that it can be written as

$$\Delta(\vec{x}) = \frac{\hbar}{(2\pi)^d} \int_0^\infty \mathrm{d}s \int \mathrm{d}^d k \; e^{-s(k^2+m^2)+i\vec{k}\cdot\vec{x}} \,.$$

Perform the integral over the component of $\vec{k}$ parallel to $\vec{x}$ and over the transverse components of $\vec{k}$. Prove the following result $(r = |\vec{x}|)$,

$$\Delta(r) = \frac{\hbar\, m^{d-2}}{(4\pi)^{d/2}} \int_0^\infty \frac{\mathrm{d}s}{s^{d/2}}\; \exp\Big[-s - \frac{(mr)^2}{4s}\Big] .$$

The modified Bessel functions are defined by

$$K_\nu(x) = \frac{x^\nu}{2^{\nu+1}} \int_0^\infty \frac{\mathrm{d}s}{s^{\nu+1}}\; \exp\Big[-s - \frac{x^2}{4s}\Big] .$$

Show that $x^{-\nu}\, K_\nu(x)$ satisfies the differential equation (9.18) for appropriately chosen ν. The asymptotic behaviour of K_ν is given by

$$\begin{aligned} K_\nu(x) &\overset{x\to\infty}{\sim} \sqrt{\frac{\pi}{2x}}\, e^{-x}\Big(1 + \frac{4\nu^2-1}{8x} + \mathrm{O}(x^{-2})\Big) , \\ K_\nu(x) &\overset{x\to 0}{\sim} \frac{2^{\nu-1}\,\Gamma(\nu)}{x^\nu}\Big(1 + \mathrm{O}(x)\Big) . \end{aligned}$$

Verify the asymptotic statements made in the text.

Problem 9.5 : Loops in connected graphs

Consider the path integral $W = \exp\left\{\frac{i}{\hbar} S_I[\partial/\partial J]\right\} \exp\left\{\frac{1}{2}(J, \Delta J)\right\}|_{J=0}$. The expansion of $\exp\left\{\frac{i}{\hbar} S_I\right\}$ into a power series leads to an expansion of W, which can be represented by Feynman graphs. Similar expansions are obtained for the n-point Green's functions (correlation functions) by differentiating n more times with respect to the source $J(x_i)$, before putting J to zero. Here x_i are the space-time coordinates $(i = 1, \ldots, n)$ associated with the Green's function. The corresponding diagrams then have n external lines, i.e. propagators that emanate from a vertex at space-time point x_i, with no other propagators attached. The other side of this propagator is then connected to the main body of the diagram. Obviously, we call a diagram *connected* when it can *not* be divided into two parts without cutting one of the lines.

For a field theory with translational symmetry it is convenient to perform a Fourier transformation and to consider the Feynman graphs in momentum space. The Green's functions then depend on n momenta (subject to energy-momentum conservation). Connected diagrams can be classified by the number of loops L, the number of independent momentum integrations once energy-momentum conservation has been imposed at every vertex.

Show that a connected graph with V vertices and I internal and E external lines has $I - V + 1$ loops. The Feynman graphs are proportional to some power of $\hbar$, which is related to the number of loops. To determine this power, argue that propagators are of order $\hbar$ and vertices of order $1/\hbar$. Show that as a result connected Feynman graphs are proportional to

$\hbar^{I+E-V} = \hbar^{L+E-1}$ and conclude that a loop expansion of a diagram with E external lines corresponds to an expansion in orders of $\hbar$.

Problem 9.6 : Functional of connected graphs

In the case of a free field theory coupled to an external source we have seen that (apart from a normalization factor) $W = \exp\left\{\frac{1}{2}(J, \Delta J)\right\}$ and that $\ln W = \frac{1}{2}(J, \Delta J)$ therefore consists of only a connected diagram $\times\!\!-\!\!\!-\!\!\!-\!\!\times$. The fact that $\ln W$ can be written as a sum of only connected diagrams turns out to be a general property for any field theory.

To see this consider some generic theory with an interaction Lagrangian $g\,\mathcal{L}_I$. Possible interactions with external sources may be included in it. A general graph can always be written as the product of powers of the expressions for *connected* graphs. Let us denote the contribution of a given connected graph $[i]$ by $g^{s_i}\,\Gamma[i]$, where s_i defines the number of vertices of the graph (which equals the power of the coupling constant g). For simplicity, assume that there is only one kind of vertex. Note that $g^{s_i}\,\Gamma[i]$ contains all combinatorial factors, i.e. the ones that are encountered when the full diagram is precisely equal to the single connected graph $[i]$. Prove now that a general (dis)connected contribution to W that contains n_i diagrams of type $[i]$ is equal to

$$\Gamma(\{n_i\}) = \prod_i \frac{(g^{s_i}\,\Gamma[i])^{n_i}}{n_i!},$$

Since W is the sum of all the above contributions for all possible graphs, it follows that

$$W = \sum_{\{n_i\}} \Gamma(\{n_i\}) = \prod_i \left(\sum_{n_i=0}^{\infty} \frac{(g^{s_i}\,\Gamma[i])^{n_i}}{n_i!} \right) = \exp\left\{ \sum_i g^{s_i}\,\Gamma[i] \right\}.$$

Hence, $\ln W$ is just the sum of the connected diagrams. How do connected diagrams depend on the total volume of the system? (Suppress external sources here). Argue that $\ln W$ rather than W itself is the quantity that is of physcial interest.

Problem 9.7 :

To show explicitly in a nontrivial example that $\ln W$ consists of the sum of only connected diagrams, we consider the path integral

$$W_{\tilde{J}} = \int \mathcal{D}\phi \;\exp\left\{-\tfrac{1}{2}(\phi, \Delta^{-1}\phi) + \tfrac{1}{2}(\phi, \tilde{J}\phi)\right\}, \tag{9.26}$$

where $(\phi, \tilde{J}\phi) = \int \mathrm{d}^d x\; \tilde{J}(x)\phi^2(x)$. Show that $W_{\tilde{J}}$ is proportional to $(\det(\Delta^{-1} - \tilde{J}))^{-1/2}$ by performing the Gaussian integral. Making use of equation (3.7), prove subsequently that

$$W_{\tilde{J}} = W_{\tilde{J}=0}\;\exp\left\{-\tfrac{1}{2}\mathrm{Tr}\;\ln(1 - \Delta\tilde{J})\right\}.$$

Now consider the Feynman diagrams corresponding to (9.26), with propagators Δ and vertices describing the coupling to $\tilde{J}$. How many loops do these diagrams have? Write down the connected Feynman diagram with n sources $\tilde{J}$, including its combinatorial factor. Show that its result coincides with the above equation when extracting the n-th order term of the logarithm. Is this consistent with the result proven in problem 7.6?

Problem 9.8 : Consider a field theory with two real fields, ϕ en A, described by the Lagrangian

$$\mathcal{L} = -\tfrac{1}{2}(\partial_\mu \phi)^2 - \tfrac{1}{2} m^2\, \phi^2 - \lambda\, \phi^4 - \tfrac{1}{2} A^2 + A(\mu^2 + g\, \phi^2)\,.$$

1. Give the propagators and vertices. Determine the dimension of the fields and the coupling-constant and mass parameters λ, g, μ^2 and m^2.
2. Calculate the self-energy diagrams in the tree approximation and give the masses for the *physical* particles described in this approximation. Subsequently give the full propagators in the tree approximation and use these in the next three questions.
3. Calculate the (three) self-energy diagrams for the field ϕ in the one-loop approximation. Give the mass-shift of ϕ in that approximation. (Note: do *not* try to evaluate the integrals.) For which value of g does the mass shift vanish?
4. Calculate the mass shift for the field A in the one-loop approximation. What do you conclude?
5. Solve the equations of motion for A en substitute the result into the Lagrangian, which will then depend only on ϕ. Show that this corresponds to integrating out the field A in the path integral.
6. Evaluate now again the mass of the field ϕ in tree approximation and compare the result with that of question 2 above.
7. Calculate again the self-energy diagrams in the one-loop approximation? Compare the result with that obtained in question 3.

Problem 9.9 : The large-N limit

Consider the action for N real scalar fields ϕ_i ($i = 1 \ldots N$) and one real scalar field σ, given by

$$S[\phi_i, \sigma] = \int d^4x \left\{ -\tfrac{1}{2} \sum_i (\partial_\mu \phi_i)^2 - \tfrac{1}{2} m^2 \sum_i \phi_i^2 + \sigma \sum_i \phi_i^2 + \tfrac{1}{2} c\, \sigma^2 \right\}. \qquad (9.27)$$

i) Give the expressions for the propagators and the vertices of the action.

ii) Calculate the selfenergy diagrams for the fields ϕ_i and σ with one closed loop (do not evaluate the corresponding momentum integrals). Argue by considering the inverse (connected) 2-point correlation function (use the Dyson equation) in the one-loop approximation that these results are valid for *large* values of c.

iii) Calculate the one-loop diagram with a single external σ-line. Express the result into the (divergent) momentum integral

$$T(m^2) = \int \frac{\mathrm{d}^4 p}{i(2\pi)^4} \, \frac{1}{p^2 + m^2} \,. \tag{9.28}$$

How does the result depend on N?

iv) We are interested in the (connected) correlation functions of the fields ϕ_i. To that order introduce a source term J_i for every field ϕ_i. The relevante correlation functions are then given by

$$\langle \phi_{i_1}(x_1) \ldots \phi_{i_n}(x_n) \rangle = \frac{\delta}{\delta J_{i_1}(x_1)} \cdots \frac{\delta}{\delta J_{i_n}(x_n)} \ln Z[J_i] \bigg|_{J_i=0} \,. \tag{9.29}$$

Determine the value of c such that this theory is equivalent with the one given by an action without the field σ, but with a four-point coupling between the ϕ_i fields with coupling strength $-g/N$.

Subsequently we assume that c is equal to this special value that you found in iv). Now we consider the limit of large N with g constant for all correlation functions (9.29).

v) Consider diagrams with only external ϕ-lines, coupled via internal σ-line, but *without* loops formed *exclusively* by ϕ-propagators. Show that only the disconnected tree diagrams contribute in the limit $N \to \infty$.

vi) Add a loop of exclusively internal ϕ-propagators. This loop couples through σ-lines to the rest of the diagram. Show which diagrams contribute in the limit $N \to \infty$. Generalize this argument to several ϕ-loops and prove that, in the limit $N \to \infty$, only the two-point *connected* correlation functions (9.29) are nonzero. The theory therefore behaves as a free field theory in this limit.

vii Prove, in the $N \to \infty$ limit, that the quantum corrections only give rise to changes in the ϕ-mass. Denote this modified mass by M. Show that M satisfies the following equation,

$$M^2 = m^2 + 4g\, T(M^2) \,. \tag{9.30}$$

Do this by first expanding the right-hand side to g with the aid of the one-loop result. Subsequently, show that both sides of the equation describe the same diagrams.

viii) Give, for large N, the leading expression for the full propagator belonging to the field σ. This expression contains again a divergent integral, which depends on M^2. In this approximation, can you say something about whether σ can correspond to a possible physical particle?

10 More on Feynman diagrams

Here we follow sections 2.4, 2.5 and 2.6 of De Wit & Smith. We also consider part of the problems at the end of chapter 2.

Problem 10.1 : Auxiliary fields

Consider the following Lagrangian of real fields A and F in four spacetime dimensions,

$$\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_m + \mathcal{L}_g \,, \tag{10.1}$$

where

$$\mathcal{L}_0 = -\tfrac{1}{2}\partial_\mu A\, \partial^\mu A + \tfrac{1}{2}F^2 \,, \quad \mathcal{L}_m = mFA \,, \quad \mathcal{L}_g = gFA^2 \,. \tag{10.2}$$

i) Show that, classically, this theory is equivalent to a self-interacting theory of one real scalar.

ii) Due to the A-F mixing introduced in $\mathcal{L}_m$ the quadratic part of the Lagrangian $\mathcal{L}$ is not diagonal in field space. Therefore, the propagators form a 2×2-matrix with off-diagonal entries. Show that the propagators for this model read

$$\Delta(p^2) = \begin{pmatrix} \Delta_{AA}(p^2) & \Delta_{AF}(p^2) \\ \Delta_{FA}(p^2) & \Delta_{FF}(p^2) \end{pmatrix} = \frac{1}{i(2\pi)^4}\frac{1}{p^2+m^2}\begin{pmatrix} 1 & -m \\ -m & -p^2 \end{pmatrix} . \tag{10.3}$$

iii) Write down the Feynman rules corresponding to $\mathcal{L}$. Represent the AA-propagator by a straight line, the FF-propagator by a wiggly line. The propagators Δ_{AF} and Δ_{FA} are represented by lines which are straight at the end associated with the A-field and turn wiggly at the end associated with the F-field.

We note that the Lagrangian has special properties, as is reflected for example in the fact that

$$\frac{\partial}{\partial m}\mathcal{L}_m = \frac{1}{2g}\frac{\partial}{\partial A}\mathcal{L}_g \,. \tag{10.4}$$

Such properties lead to intricate relations among the diagrams generated by $\mathcal{L}$. We will derive such a relation in the following. We introduce sources for the fields A and F and the path-integral representation for the generating functional

$$Z[J] = \int \mathcal{D}A\,\mathcal{D}F \exp\left[i\int \mathrm{d}^4y\, \mathcal{L} + \int \mathrm{d}^4y(J_A A + J_F F)\right] . \tag{10.5}$$

iv) Derive the relation

$$\frac{\partial}{\partial m} Z[J] + \frac{im}{2g} \int \mathrm{d}^4 y \frac{\delta Z[J]}{\delta J_F(y)} + \frac{1}{2g} Z[J] \int \mathrm{d}^4 y J_A(y) = 0 \,. \tag{10.6}$$

(Hint: use that the path integral over a (functional) derivative with respect to a field vanishes,

$$\int \mathcal{D}\phi \, \frac{\delta}{\delta \phi(x)} G[\phi] = 0 \,, \tag{10.7}$$

as well as

$$\int \mathcal{D}\phi \, H[\phi] \int \mathrm{d}x \, \frac{\partial^2}{\partial x^2} \phi(x) = 0 \,, \tag{10.8}$$

for functionals $G[\phi]$ and $H[\phi]$.)

v) Rewrite the identity (10.6) in terms of the generating functional of *connected* correlation functions $W[J] = \ln Z[J]$.

From above identities one can now deduce many non-trivial relations between different graphs. To pick out the specific graphs contributing to a correlation function one functionally differentiates with respect to the sources and then sets the sources to zero. Let us define

$$\begin{aligned} D_{AA}(x_1, x_2) &= \frac{\delta}{\delta J_A(x_1)} \frac{\delta}{\delta J_A(x_2)} W[J_A, J_F] \Big|_{J_A = 0 = J_F} \,, \\ \Gamma_{FAA}(x_1, x_2, x_3) &= \frac{\delta}{\delta J_F(x_1)} \frac{\delta}{\delta J_A(x_2)} \frac{\delta}{\delta J_A(x_3)} W[J_A, J_F] \Big|_{J_A = 0 = J_F} \,. \end{aligned} \tag{10.9}$$

vi) What do $D_{AA}(x_1, x_2)$ and $\Gamma_{FAA}(x_1, x_2, x_3)$ represent? Draw the tree diagrams that contribute to these two functions. (Hint: Don't forget that there is a off-diagonal piece in the propagator which induces a mixing between the fields.)

We now turn to a specific example of the sort of relations that hold between different connected correlation functions,

$$\frac{\partial}{\partial m} D_{AA}(x_1, x_2) = -\frac{im}{2g} \int \mathrm{d}^4 y \; \Gamma_{FAA}(y, x_1, x_2) \,. \tag{10.10}$$

vii) Prove the relation (10.10) by making use of the result found in v). Why does the relation (10.10) hold to all orders in perturbation theory?

We note that upon Fourier transformation the quantities defined in (10.9) read

$$\begin{aligned} &\int \mathrm{d}^4 x_1 \, \mathrm{d}^4 x_2 \, \mathrm{e}^{ip_1 \cdot x_1 + ip_2 \cdot x_2} \, D_{AA}(x_1, x_2) = \\ &\qquad (2\pi)^4 \, \delta^{(4)}(p_1 + p_2) \, D_{AA}(p_1, p_2) \,. \\ &\int \mathrm{d}^4 x_1 \, \mathrm{d}^4 x_2 \, \mathrm{d}^4 x_3 \, \mathrm{e}^{ip_1 \cdot x_1 + ip_2 \cdot x_2 + ip_3 \cdot x_3} \, \Gamma_{FAA}(x_1, x_2, x_3) = \\ &\qquad (2\pi)^4 \, \delta^{(4)}(p_1 + p_2 + p_3) \, \Gamma_{FAA}(p_1, p_2, p_3) \,. \end{aligned} \tag{10.11}$$

The δ-functions arise due to translational invariance.

viii) Prove that the relation (10.10) in momentum space is given by

$$\frac{\partial}{\partial m} D_{AA}(p,-p) = -\frac{im}{2g}\ \Gamma_{FAA}(0,p,-p)\,. \tag{10.12}$$

ix) Verify the relation (10.12) explicitely at tree-level approximation using the set of Feynman rules deduced in iii). You may ignore factors of $i(2\pi)^4$.

Problem 10.2 : Field rederinitions

Consider a real scalar field ϕ coupled to an external field H in four spacetime dimensions. The Lagrangian is given by

$$\mathcal{L}_1 = -\tfrac{1}{2}\,(\partial\phi)^2 - \tfrac{1}{2}\,m^2\phi^2 - g\,\phi[2(\partial\phi)^2 + m^2\phi^2] - g^2\phi^2[2(\partial\phi)^2 + \tfrac{1}{2}m^2\phi^2] + H\phi\,. \tag{10.13}$$

In this exercise we will restrict ourselves to tree diagrams.

i) Write down the Feynman rules for this theory.

ii) Calculate the connected tree diagram(s) that involve two H-fields (without external ϕ lines). Call the resulting expression $D(p_1,p_2)$, where p_1 and p_2 denote the incoming momenta associated with the H-fields.

iii) Calculate the connected tree diagram(s) involving three H-fields (without external ϕ lines). Call the resulting expression $T(p_1,p_2,p_3)$, where p_1, p_2 and p_3 are the incoming momenta associated with the H-fields.

We want to compare this result to the result one obtains in a theory where the H-field has an extra coupling to ϕ^2,

$$\mathcal{L}_2 = \mathcal{L}_1 + g\,\phi^2 H\,. \tag{10.14}$$

Due to the additional interaction term in $\mathcal{L}_2$ there is a new vertex.

iv) Argue that there are no contributions from the new vertex to the connected diagrams $D(p_1,p_2)$ calculated in ii).

v) There are now new connected tree diagrams involving three H-fields due to the new $\phi^2 H$ vertex. Show that these new diagram(s) cancel against $T(p_1,p_2,p_3)$ evaluated in iii).

vi) Explain the results obtained under iv) and v) by arguing that $\mathcal{L}_2$ is related to a free field theory by a field-redefinition in the latter of the form $\phi \to a\,\phi + b\,\phi^2$. Determine the values of a and b.
Hint: consider the path integral representation

$$W[H] = \int \mathcal{D}\phi \; \mathrm{e}^{\frac{i}{\hbar}\int[\mathcal{L}_0 + H\phi]}, \tag{10.15}$$

where

$$\mathcal{L}_0 = -\tfrac{1}{2}\,(\partial\phi)^2 - \tfrac{1}{2}\,m^2\phi^2\,. \tag{10.16}$$

You may ignore any subtleties involving a Jacobian that might arise when performing a field-redefinition in this expression.

vii) For the theory defined by $\mathcal{L}_1$, draw the connected tree-diagrams that involve four H-fields.

viii) Argue now (without performing a calculation) that these diagrams will exactly cancel against contributions coming from the extra tree-diagrams that involve the $\phi^2 H$ vertices in $\mathcal{L}_2$. Draw these diagrams.

We now consider two interacting field theories, $\mathcal{L}_3(\phi)$ and $\mathcal{L}_4(\phi)$, that are related by a local field redefinition of the form $\phi \to a\,\phi + b\,\phi^2 + c\,\phi^3 + \cdots$. To calculate the correlation functions of the fields ϕ we can add an external source J, coupled to ϕ, to both $\mathcal{L}_3$ and $\mathcal{L}_4$,

$$\mathcal{L}_3 \;\to\; \mathcal{L}_3 + J\phi\,, \tag{10.17}$$

$$\mathcal{L}_4 \;\to\; \mathcal{L}_4 + J\phi\,, \tag{10.18}$$

and differentiate with respect to J in the usual fashion (setting J to zero afterwards).

ix) Argue that the 4-point functions corresponding to $\mathcal{L}_3$ and $\mathcal{L}_4$ differ by terms that correspond to diagrams that involve extra source interactions $\phi^n J$ with $n > 1$, where J is the source used to generate the correlation functions. Indicate the three kinds of diagrams that involve these vertices and that contribute to the 4-point function. (recall that we only consider tree diagrams).

x) Suppose now that we put the diagrams of the 4-point function "on the mass shell". By this we mean that we multiply each external line with $p_i^2 + m^2$, where p_i is the momentum associated with that line. After thus having removed the propagator poles associated with the external lines, we take $p_i^2 \to -m^2$. Show that the 4-point functions corresponding to $\mathcal{L}_3$ and $\mathcal{L}_4$ are now equal, *i.e.* the extra diagrams based on the $\phi^n J$ vertices do not contribute here.

xi) Can you describe in words what you think is the significance of the result proven in x). Furthermore, argue that the Jacobian that we suppressed in vi) when performing a field redefinition in (10.15) may be regarded as a closed-loop effect.

11 Fermionic harmonic oscillator states

Consider a simple extension of the harmonic oscillator, described by the following Hamiltonian

$$H = \begin{pmatrix} \dfrac{p^2}{2m} + \frac{1}{2}m\omega^2\, q^2 - \frac{1}{2}\hbar\omega & 0 \\ 0 & \dfrac{p^2}{2m} + \frac{1}{2}m\omega^2\, q^2 + \frac{1}{2}\hbar\omega \end{pmatrix} . \tag{11.1}$$

Note that this Hamiltonian does not describe two harmonic oscillators, nor a harmonic oscillator in two dimensions. From the harmonic oscillator spectrum it is clear that we have a groundstate of vanishing energy, while each of the excited states is doubly degenerate and has energy equal to $\hbar\omega$, $2\hbar\omega$, $3\hbar\omega, \ldots$. The corresponding wave functions have therefore two components. The degeneracy is indicative of a symmetry (called *supersymmetry*), which we shall discuss elsewhere. Now we concentrate on the Hamiltonian itself.

First we introduce the usual creation and annihilation operators a and $a^\dagger$ in terms of p and q. To describe the extension to the two-component system we introduce two further operators,

$$b = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} , \qquad b^\dagger = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} . \tag{11.2}$$

It is our intention to interpret these operators again as creation and annihilation operators. Before doing so, we note the following properties,

$$b^2 = b^{\dagger 2} = 0 \,, \qquad \{b, b^\dagger\} \equiv b\, b^\dagger + b^\dagger\, b = \mathbf{1} \,. \tag{11.3}$$

In terms of these operators the Hamiltonian takes a rather symmetric form,

$$H = \hbar\,\omega(a^\dagger\, a + b^\dagger\, b) \,, \tag{11.4}$$

(the operators a and $a^\dagger$ act uniformly on both components of the wave function, so that they are proportional to the two-by-two identity matrix). The interpretation of creation/annihilation operators is based on

$$[H, a] = -\hbar\omega\, a \,, \qquad [H, b] = -\hbar\omega\, b \,, \tag{11.5}$$

so that, when acting on an eigenstate of the Hamiltonian, a and b lower the energy by $\hbar\,\omega$, while their hermitean conjugates raise the energy by this amount. The Hamiltonian can also be written as

$$H = \frac{p^2}{2m} + \tfrac{1}{2} m\omega^2\, q^2 + \tfrac{1}{2} m\omega\, [\psi^\dagger, \psi]\,, \tag{11.6}$$

where $\psi \equiv \sqrt{\frac{\hbar}{m}}\, b$.

Eventually we want to extend this system to a field theory. As we discussed earlier, a (free) field theory can be regarded as a theory describing an infinite number of harmonic oscillators. With this in mind, we generalize the above system to an arbitrary number N of harmonic oscillators, each extended to a 2×2 matrix. In that case we have creation and annihilation operators a_i, b_i, $a_i^\dagger$ and $b_i^\dagger$, where $i = 1, 2, \ldots, N$, satisfying the (anti)commutation relations

$$[a_i, a_j] = [a_i^\dagger, a_j^\dagger] = 0\,, \qquad [a_i, a_j^\dagger] = \delta_{ij}\,, \tag{11.7}$$

$$\{b_i, b_j\} = \{b_i^\dagger, b_j^\dagger\} = 0\,, \qquad \{b_i, b_j^\dagger\} = \delta_{ij}\,. \tag{11.8}$$

The Hamiltonian

$$H = \sum_{i=1}^{N} \Big\{ \frac{p_i^2}{2m} + \tfrac{1}{2} m\omega^2\, q_i^2 + \tfrac{1}{2} m\omega\, [\psi_i^\dagger, \psi_i] \Big\} \tag{11.9}$$

describes N harmonic oscillators with a $2^N \times 2^N$ matrix extension. The latter because N operators ψ_i with the required anticommutation relations can only be realized in a 2^N-dimensional space. The excited states in this theory exhibit again a degeneracy. However, this degeneracy is due to our choice of parameters and the resulting supersymmetry can be broken rather easily, for instance by changing the factor in front of the $\psi^\dagger\psi$ term. For the purpose of this chapter supersymmetry is not important, but it makes the discussion somewhat more elegant.

In view of the anticommutation relations, the states produced by applying the creation operators $b_i^\dagger$ are antisymmetric under exchange: defining states $|i,j\rangle \equiv b_i^\dagger\, b_j^\dagger|0\rangle$, where $|0\rangle$ is some state that is not annihilated be the creation operators, we have $|i,j\rangle = -|j,i\rangle$. This implies that the states associated with the operators $b_i^\dagger$ are to be interpreted as *fermions*. When extending the above models to a field theory, they should be viewed in the context of second quantization, as explained in chapter 3. The conclusion is that such a field-theoretic extension will describe particles with Fermi-Dirac statistics.

For the moment we postpone the extension to a relativistic field theory and first discuss how to deal with systems with anticommuting coordinates and momenta, with the aim of eventually setting up a path integral formulation for fermions. We will therefore first develop the classical Lagrangian and Hamiltonian formulations in terms of coordinates that are anticommuting. Naively, it is clear that the following Lagrangian would lead to the Hamiltonian (9.6),

$$\mathcal{L} = \tfrac{1}{2} m\, \dot{q}^2 - \tfrac{1}{2} m\omega^2\, q^2 + im\, \psi^\dagger\, \dot{\psi} - m\omega\, \psi^\dagger\, \psi\,. \tag{11.10}$$

In the Lagrangian the quantities ψ and $\psi^\dagger$ are taken as anticommuting and we ignored a possible constant term. When passing to the Hamiltonian the coordinate $\psi^\dagger$ will play the role of the canonical momentum and the time derivative of ψ cancels. There exists an appropriate canonical bracket, which after quantization, leads to operators ψ and $\psi^\dagger$ whose anticommutator is proportional to the identity. Before exhibiting this in detail we introduce so-called *anticommuting* c-numbers.

Problem 11.1 :
Write down the two-component wave functions (in the coordinate representation) for the three lowest-energy states corresponding to the Hamiltonian (11.1).

Problem 11.2 :
Consider the case $N = 2$, where we have four-component wave functions. Construct the four-component space by choosing $|0,0\rangle$ as the state that is annihilated by both b_1 and b_2. Argue that such a state can always be found. By acting on it with $b_1^\dagger$ and $b_2^\dagger$ construct the four remaining states $|1,0\rangle$, $|0,1\rangle$ and $|1,1\rangle$. Write the operators b_i and $b_i^\dagger$ as four-by-four matrices and write down the Hamiltonian (11.6) in matrix form. Write down the wave function for the groundstate and the first excited states.

Problem 11.3 :
It is possible to construct operators that give transitions between the degenerate states. Show that the so-called supercharges,

$$\begin{aligned} Q_1 &= \sqrt{\hbar\omega}(a^\dagger\, b + a\, b^\dagger)\,, \\ Q_2 &= i\sqrt{\hbar\omega}(a^\dagger\, b - a\, b^\dagger)\,, \end{aligned}$$

commute with the Hamiltonian and must therefore be such operators. Somewhat unexpectedly, it thus turns out that we are dealing with two independent supersymmetries. Show that both supercharges annihilate the groundstate. Write the bosonic and fermionic states in terms of products of creation operators acting on the groundstate, and show that Q_i changes a bosonic state into a fermionic one, and vice versa. Finally show that

$$\{Q_i, Q_j\} = 2H\,\delta_{ij}\,. \tag{11.11}$$

Prove from this result that zero-energy states must be annihilated by Q_i. Can you construct a conserved bosonic operator other than the Hamiltonian? Can you give an interpretation of this operator?

Problem 11.4 :
Generalize the various results of chapter 1 to argue that the path integral for the Hamiltonian (11.1), which now takes the form of a two-by-two matrix, takes the form

$$
\begin{aligned}
W(q_2,t_2;q_1,t_1) &= \sqrt{\frac{m\omega}{2\pi i\hbar\sin\omega(t_2-t_1)}} \\
&\quad\times\exp\left\{\frac{im\omega}{2\hbar\sin\omega(t_2-t_1)}\Big[(q_1^2+q_2^2)\cos\omega(t_2-t_1)-2q_1q_2\Big]\right\} \\
&\quad\times\begin{pmatrix} e^{\frac{1}{2}i\omega(t_2-t_1)} & \\ 0 & e^{-\frac{1}{2}i\omega(t_2-t_1)}\end{pmatrix} . \qquad (11.12)
\end{aligned}
$$

Evaluate now the partition function for this model at finite temperature and show that it is given by $Z_\beta^{(+)}/Z_\beta^{(-)}$, where $Z_\beta^{(\pm)}$ was defined in chapter 5. Reread the text following (5.28). What is your conclusion?

12 Anticommuting c-numbers

In this chapter we briefly introduce the mathematical concepts that form the basis for the so-called anticommuting c-numbers and exhibit how to perform practical calculations with them.

The Grassmann Algebra :
Anticommuting c-numbers can be discussed within the context of *Grassman algebras*. We start by considering anticommuting c-numbers θ_i satisfying

$$\theta_i\,\theta_j = -\theta_j\,\theta_i\,. \qquad (12.1)$$

The numbers θ_i are taken to be real, i.e. $\theta_i^\dagger = \theta_i$. Under conjugation the order of anticommuting c-numbers is reversed. For instance, we have $(\theta_i\theta_j)^\dagger = \theta_j\theta_i = -\theta_i\theta_j$.

On the basis of n such anticommuting objects one defines an n-dimensional Grassmann algebra with n *generators* $\theta_1,\ldots,\theta_n$. Each element $P(\theta)$ of the algebra can be decomposed in the following way

$$P(\theta) = p^{(0)} + \theta_i\,p_i^{(1)} + \sum_{i>j}\theta_i\theta_j\,p_{ij}^{(2)} + \cdots + \theta_n\theta_{n-1}\cdots\theta_1\,p^{(n)}\,, \qquad (12.2)$$

where summation over repeated indices is implied. The total number of independent terms in (12.2) is at most 2^n. A monomial $\theta_{i_1}\ldots\theta_{i_p}$ is called a monomial of degree p. Monomials of odd (even) degree are anticommuting (commuting) objects. The square of a monomial vanishes unless its degree is zero, in which case we have an ordinary c-number. Monomials of degree higher than the dimension of the Grassmann algebra vanish identically. It is not difficult to define differentiation and integration on the Grassmann algebra. As we shall see below, the application of functional methods to fermions does not require major modification.

Differentiation on the Grassmann algebra ;
We distinguish two different derivatives on the Grassmann algebra, called *right* and *left* derivatives. The derivative of a general element of the algebra is obtained by differentiating its monomials and resumming the result. To calculate the right (left) derivative with respect to θ_i we must, in every monomial, permute θ_i to the right (left) and then drop it. If $\epsilon[i]$ is the sign of the permutation needed to bring θ_i to the right (left), and $\epsilon[i] = 0$ when θ_i does not occur in the monomial, then the right (left) derivative of a monomial can be written in the following way,

$$\frac{\partial}{\partial \theta_{i_k}} \Big(\theta_{i_1} \cdots \theta_{i_{k-1}} \theta_{i_k} \theta_{i_{k-1}} \cdots \theta_{i_m} \Big) = \epsilon[i_k] \Big(\theta_{i_1} \ldots \theta_{i_{k-1}} \theta_{i_{k+1}} \ldots \theta_{i_m} \Big) . \tag{12.3}$$

Unless specified otherwise, we shall always use left derivatives.

Although the expression $P(\theta)$ for an element of the Grassmann algebra is not a function of θ in the strict mathematical sense, most of the properties of left and right derivatives of $P(\theta)$ are similar to the properties of derivatives of ordinary functions. For example if $\delta\theta_i$ denotes an additional "infinitesimal" anticommuting c-number we can symbolically write for (12.3)

$$\frac{\partial}{\partial \theta} P(\theta) = \lim_{\delta\theta_i \to 0} \frac{1}{\delta\theta_i} \Big\{ P(\theta_1, \ldots, \theta_i + \delta\theta_i, \ldots \theta_n) - P(\theta_1, \ldots, \theta_i. \ldots \theta_n) \Big\} . \tag{12.4}$$

The chain rule holds in the same form as for commuting numbers

$$\frac{\partial}{\partial \theta_i} P(\alpha(\theta)) = \frac{\partial}{\partial \theta_i} \alpha_j(\theta) \, \frac{\partial}{\partial \alpha_j} P(\alpha), \tag{12.5}$$

where P is an element of a Grassmann algebra on the basis of the α's, and α is an element of a Grassmann algebra with the θ's as its generators. However, the order in which one writes the terms in (12.5) is important for anticommuting parameters; for right derivatives, the order of the two terms is interchanged! Also Leibniz' rule has a direct analogue. For instance, for left derivatives we have

$$\frac{\partial}{\partial \theta} \Big(f(\theta) \, g(\theta) \Big) = \left(\frac{\partial}{\partial \theta} f(\theta) \right) g(\theta) \pm f(\theta) \left(\frac{\partial}{\partial \theta} g(\theta) \right) , \tag{12.6}$$

where the plus (minus) sign is valid for an even (odd) "function" $f(\theta)$.

Integration over the Grassmann algebra :
We construct the analogue of the indefinite one-dimensional integral (for a suitable class of functions)

$$\int_{-\infty}^{\infty} \mathrm{d}x \; f(x)$$

for the case of anticommuting c-numbers, which we denote by

$$\int \mathrm{d}\theta \; P(\theta).$$

As a starting point for its construction we require that the following property of the integral over commuting parameters,

$$\int_{-\infty}^{\infty} \mathrm{d}x \, f(x) = \int_{-\infty}^{\infty} \mathrm{d}x \, f(x+a) \,, \tag{12.7}$$

which is valid for any finite a, holds also for an integral over anticommuting parameters. Also we assume that the standard rules for taking linear combinations of integrals remain valid. We now consider a one-dimensional integral. A general element of the one-dimensional Grassmann algebra is decomposed as

$$P(\theta) = a + \theta \, b \,, \tag{12.8}$$

with a and b arbitrary, and θ anticommuting. The expression analogous to (12.7) for anticommuting numbers is

$$\int \mathrm{d}\theta \, P(\theta) = \int d\theta \, P(\theta + \alpha), \tag{12.9}$$

for any anticommuting α. Substituting (12.8) into (12.9), we find that the latter requires

$$\int d\theta \; \alpha \, b = 0 \,, \tag{12.10}$$

for any α and b. Hence we must define

$$\int \mathrm{d}\theta \; [\text{any element not depending on } \theta] = 0. \tag{12.11}$$

Consequently we are left with the integral over θ, which we simply normalize to unity,

$$\int \mathrm{d}\theta \, \theta \equiv 1 \,. \tag{12.12}$$

Multiple integrals can be understood as iterated integrals, leading to the anticommuting symbols[11] $\mathrm{d}\theta_i$. Integration over anticommuting numbers turns out to be equivalent to taking the left derivative

$$\int \mathrm{d}\theta \, P(\theta) = \frac{\partial}{\partial\theta} P(\theta) \,. \tag{12.13}$$

[11] It is possible to set up differential forms with both commuting and anticommuting coordinates. In that case the forms $\mathrm{d}x$ are anticommuting and the forms $\mathrm{d}\theta$ are commuting.

Also the rules of partial integration apply for integrals over anticommuting parameters. In analogy with

$$\int_{-\infty}^{\infty} \mathrm{d}x\, \frac{\partial}{\partial x} f(x) = 0\,,$$

one can easily show that

$$\int \mathrm{d}\theta\, \frac{\partial}{\partial \theta} P(\theta) = 0\,. \tag{12.14}$$

Gaussian integrals and the superdeterminant :
In the previous discussions on path integrals, generalized Gaussian integrals played an important role. We now discuss their evaluation for anticommuting variables. The generalization of a Gaussian integral over complex commuting variables,

$$\int \left(\prod_i \frac{\mathrm{d}\bar{z}_i\, \mathrm{d}z_i}{2\pi\, i}\right)\, \exp(-(\bar{z}, Az)) = (\det A)^{-1}\,, \tag{12.15}$$

is easy to find.[12] Using the integration rule for anticommuting quantities one derives straightforwardly

$$\int \left(\prod_i \mathrm{d}\theta_i\, \mathrm{d}\bar{\theta}_i\right)\, \exp(\bar{\theta}, A\theta) = \det A\,. \tag{12.16}$$

Note that A is required to be a positive-definite hermitean matrix in order that the integral (12.15) converges, whereas (12.16) is valid for arbitrary A.

It is also possible to define Gaussian integrals over real variables. We give the result without further derivation

$$\int \left(\prod_i \frac{\mathrm{d}x_i}{\sqrt{2\pi}}\right)\, \exp\left(-\tfrac{1}{2}(x, Ax)\right) \;=\; \frac{1}{\sqrt{\det A}}\,, \tag{12.17}$$

$$\int \left(\prod_i \mathrm{d}\theta_i\right)\, \exp\left(\tfrac{1}{2}(\theta, A\theta)\right) \;=\; \pm\sqrt{\det A}\,. \tag{12.18}$$

In this case the matrix A should be symmetric and positive definite in (12.17) and antisymmetric in (12.18). The quantity $(\det A)^{1/2}$, with A antisymmetric, is sometimes called a Pfaffian in the mathematical literature. One can show that the Pfaffian is a monomial in each of the eigenvalues of the matrix, a property which is obvious from (12.18).

Gaussian integrals can be used to define the determinant of a matrix acting in superspace, the space of commuting and anticommuting coordinates. Vectors in this space are decomposed in terms of commuting and anticommuting variables, x and θ, respectively. Linear transformations in superspace can be written as matrices acting on these coordinates,

$$\begin{pmatrix} x \\ \theta \end{pmatrix} \longrightarrow \begin{pmatrix} x' \\ \theta' \end{pmatrix} = \begin{pmatrix} A & D \\ C & B \end{pmatrix} \begin{pmatrix} x \\ \theta \end{pmatrix}\,, \tag{12.19}$$

[12] Use $z = x + iy$ and $\mathrm{d}\bar{z}\, \mathrm{d}z/2i = \mathrm{d}x\, \mathrm{d}y$.

where the submatrices A and B have commuting, and C and D have anticommuting elements. One can now construct the so-called superdeterminant of a superspace matrix M

$$M = \begin{pmatrix} A & D \\ C & B \end{pmatrix} \tag{12.20}$$

by calculating a generalized Gaussian integral over commuting and anticommuting variables,

$$\frac{1}{\det M} = \int \frac{\mathrm{d}\bar{z}\,\mathrm{d}z}{2\pi i}\,\mathrm{d}\bar{\theta}\,\mathrm{d}\theta\ \exp(-(\bar{z},Az) - (\bar{z},D\theta) - (\bar{\theta},Cz) - (\bar{\theta},B\theta))\,. \tag{12.21}$$

This integral can be evaluated formally by making a shift in integration variables,

$$\begin{aligned} \theta &\longrightarrow \theta - B^{-1}Cz\,, \\ \bar{\theta} &\longrightarrow \bar{\theta} - \bar{z}DB^{-1}\,. \end{aligned}$$

Subsequently, using (12.15) and (12.16) leads to the following result for the superdeterminant

$$\det M = \frac{\det(A - DB^{-1}C)}{\det B} = \frac{\det A}{\det(B - CA^{-1}D)}\,. \tag{12.22}$$

The second form can be obtained by performing a similar shift, but now in the integration variables z and $\bar{z}$. Both results for the superdeterminant become plausible when we write M as a product of two matrices,

$$M = \begin{pmatrix} A & 0 \\ C & 1 \end{pmatrix} \begin{pmatrix} 1 & A^{-1}D \\ 0 & B - CA^{-1}D \end{pmatrix}, \tag{12.23}$$

or, alternatively,

$$M = \begin{pmatrix} 1 & D \\ 0 & B \end{pmatrix} \begin{pmatrix} A - DB^{-1}C & 0 \\ B^{-1}C & 1 \end{pmatrix}. \tag{12.24}$$

Precisely as for the conventional determinant one has a product rule for the superdeterminant

$$\det(M_1M_2) = \det M_1\ \det M_2\,. \tag{12.25}$$

To show this we first introduce the notion of the *supertrace*,

$$\mathrm{Tr}\,M \equiv \mathrm{Tr}\,A - \mathrm{Tr}\,B\,, \tag{12.26}$$

where the trace operation on the right-hand side is the conventional one applied to the submatrices A and B. Owing to the minus sign in front of the submatrix B, which acts exclusively in the anticommuting sector, the supertrace satisfies the characteristic cyclicity property of a trace,

$$\mathrm{Tr}(M_1M_2) = \mathrm{Tr}(M_2M_1)\,. \tag{12.27}$$

This allows one to straightforwardly derive (see problem 10.2)

$$\operatorname{Tr}\ln(M_1 M_2) = \operatorname{Tr}\ln M_1 + \operatorname{Tr}\ln M_2\,. \tag{12.28}$$

We now write M as the product of two triangular matrices according to (12.23) or (12.24), and use (12.28) to construct $\operatorname{Tr}\ln M$. This then shows that

$$\operatorname{Tr}\ln M = \ln\det M\,, \tag{12.29}$$

with $\det M$ as defined by (12.22). This then suffices to establish the product rule (12.25) by means of (12.28). Here we note that the exponent and the logarithm of a matrix in superspace are defined by series expansions, precisely as for ordinary matrices.

An important aspect of determinants is that they occur in the definition of the Jacobian of a transformation. A similar situation exists for superdeterminants. Indeed for a transformation in superspace

$$(x,\theta) \rightarrow (x(\hat{x},\hat{\theta}), \theta(\hat{x},\hat{\theta}))\,, \tag{12.30}$$

we may write

$$\int \mathrm{d}x\,\mathrm{d}\theta\; P(x,\theta) = \int \mathrm{d}\hat{x}\,\mathrm{d}\hat{\theta}\; J(x(\hat{x},\hat{\theta}))\, P(x(\hat{x},\hat{\theta}), \theta(\hat{x},\hat{\theta}))\,, \tag{12.31}$$

where

$$J(x(\hat{x},\theta), \theta(\hat{x},\hat{\theta})) = \pm\det\begin{pmatrix} \frac{\partial x}{\partial \hat{x}} & \frac{\partial x}{\partial \hat{\theta}} \\ \frac{\partial \theta}{\partial \hat{x}} & \frac{\partial \theta}{\partial \hat{\theta}} \end{pmatrix}\,. \tag{12.32}$$

In (12.31) the fermionic derivatives are right derivatives. The correctness of (12.31) is entirely obvious for linear transformations. For instance, we may redefine the integration variables (x,θ) of the Gaussian integral (12.21) according to a linear transformation (12.19) and recover (12.32) by using the product rule. But (12.32) holds for general nonsingular transformation as well.

Problem 12.1 :
Prove that the determinant of an $n\times n$ antisymmetric matrix vanishes when n is odd. Derive the same result on the basis of (12.18).

Problem 12.2 :
Prove the cyclicity property (12.27). Use the Campbell-Baker-Hausdorff formula for ordinary matrices

$$(\exp A)(\exp B) = \exp(A + B + \text{repeated commutators of } A \text{ and } B),$$

to show the validity of (12.28).

Problem 12.3 :
An intermediate step in the proof of (12.32) is to show that it holds for an integral over a two-dimensional Grassmann algebra. Parametrize the transformation $\theta_i(\hat\theta_1,\hat\theta_2)$ according to (12.2), and demonstrate the validity of (12.32) by explicit calculation. Show also the validity of (12.32) for an integral over one commuting and one anticommuting parameter.

13 Phase space with commuting and anticommuting coordinates and quantization

Consider a system with Lagrangian L depending on a commuting coordinate q and two anticommuting coordinates, c and d,

$$L(q,\dot q,c,\dot c,d) = \tfrac{1}{2}m\dot q^2 + i d\dot c - V(d,c,q)\,. \tag{13.1}$$

Naively one defines the action for given 'trajectories' $q(t)$, $d(t)$ and $c(t)$ as the time integral of the above Lagrangian and applies Hamilton's principle to obtain the equations of motion. Requiring the action to be stationary under changes of $q(t)$, $c(t)$ and $d(t)$, ignoring the various boundary terms that arise in the variation of the action, leads to the following differential equations,

$$m\ddot q + \frac{\partial V}{\partial q} \;=\; 0\,, \tag{13.2}$$

$$i\dot d + \frac{\partial V}{\partial_R c} \;=\; 0\,, \tag{13.3}$$

$$i\dot c - \frac{\partial V}{\partial_L d} \;=\; 0\,, \tag{13.4}$$

where the suffix R (L) on the fermionic derivatives denotes right(left)-differentiation. Obviously, the Lagrangian and the equations of motion can only be interpreted in the context of a Grassmann algebra, as introduced in the previous chapter. However, there is a subtlety with the boundary conditions and thus with the application of Hamilton's principle for the fermionic trajectories, because the Lagrangian (13.1) contains terms that are at most *linear* in the time derivative of the fermionic coordinates. The corresponding equations of motion (13.3-13.4) are therefore first-order differential equations, whose solution becomes unique once the trajectory is specified at one instant of time. So unlike for the coordinate $q(t)$, where one has a second-order differential equation, whose determination requires to fix the trajectory at two different instants of time, Hamilton's principle can only be consistently applied for the fermionic coordinates provided one fixes only *one* of the endpoints for the trajectories specified by $c(t)$ and $d(t)$. More explicitly, suppose we consider trajectories at times t satisfying $t_1 \leq t \leq t_2$ and we fix $q(t_1) = q_1$, $q(t_2) = q_2$, $d(t_2) = d_2$ and $c(t_1) = c_1$. The solutions of (13.2-13.4) are then uniquely determined. The endpoint values $d(t_1)$ and $c(t_2)$ are left unrestricted and will follow from the classical equations of motion. The action, whose variation subject to these boundary conditions leads to the equations of motion, is equal to

$$S[q(t), d(t), c(t)] = -id(t_2)\, c(t_2) + \int_{t_1}^{t_2} \mathrm{d}t\; L(q, \dot{q}, c, \dot{c}, d)\,. \tag{13.5}$$

We now proceed with the canonical formulation of the theory. Canonical momenta are defined in the usual manner,

$$p = \frac{\partial L}{\partial \dot{q}}\,, \qquad p_c = -i\frac{\partial L}{\partial_R \dot{c}}\,. \tag{13.6}$$

Hence $p_c = d$, whereas the canonical momentum associated with d vanishes.[13]

The Hamiltonian is defined by

$$H = p\,\dot{q} + ip_c\,\dot{c} - L\,. \tag{13.7}$$

Because the Lagrangian is at most linear in the time derivatives of the fermionic coordinates, the Hamiltonian takes the simple form,

$$H(q, p, c, p_c) = \frac{p^2}{2m} + V(p_c, c, q)\,. \tag{13.8}$$

Hamilton's equations can be derived straightforwardly[14] from the Euler-Lagrange equations,

$$\frac{\mathrm{d}p}{\mathrm{d}t} = \frac{\partial L}{\partial q}\,, \qquad \frac{\mathrm{d}p_c}{\mathrm{d}t} = -i\frac{\partial L}{\partial_R c}\,, \qquad 0 = i\frac{\partial L}{\partial_L p_c}\,, \tag{13.9}$$

by considering the change of H under a variation of $p, q, \dot{q}, p_c, c$ and $\dot{c}$. When collecting all the terms, the variations proportional to $\delta\dot{q}$ and $\delta\dot{c}$ cancel by virtue of (13.6). Using (13.9), the result then takes the form,

$$\delta H = -\dot{p}\,\delta q + \delta p\,\dot{q} + i\delta p_c\,\dot{c} - i\dot{p}_c\,\delta c\,, \tag{13.10}$$

[13] The conditions $p_c = d$ and $p_d = 0$ impose constraints on the phase space. We solve these constraints by simply restricting the phase space coordinates to q, p, c and d, but note that there exists a general and more elaborate theory of phase-space constraints, originally introduced by Dirac.

[14] Remember that the Lagrangian is a function of coordinates and velocities, while the Hamiltonian is a function of coordinates and momenta. Consequently, partial derivatives of the Lagrangian and the Hamiltonian are not the same, although one conventionally uses the same notation.

which yields Hamilton's equations,

$$
\begin{aligned}
\dot p &= -\frac{\partial H}{\partial q}\,, \qquad \dot q = \frac{\partial H}{\partial p}\,,\\
\dot p_c &= i\frac{\partial H}{\partial_R c}\,, \qquad \dot c = -i\frac{\partial H}{\partial_L p_c}\,.
\end{aligned} \tag{13.11}
$$

Assuming that the variation in (13.9) are determined by their time evolution, we can substitute (13.11) and show that the Hamiltonian is a constant of the motion, as expected.

As usual Hamilton's equations describe the time evolution in phase space, but here in a phase space consisting of both commuting and anticommuting coordinates. Consider now a function $u(q(t),p(t),c(t),p_c(t);t)$ of coordinates and momenta, with possibly an explicit dependence on t. The time derivative of such a function can be written in the usual form,

$$
\frac{\mathrm{d}u}{\mathrm{d}t} = (u,H) + \frac{\partial u}{\partial t}\,, \tag{13.12}
$$

where the bracket (A,B) is a generalization of the usual Poisson bracket and can be defined as

$$
(A,B) \equiv \frac{\partial A}{\partial q}\,\frac{\partial B}{\partial p} - \frac{\partial A}{\partial p}\,\frac{\partial B}{\partial q} - i\,\frac{\partial A}{\partial_R c}\,\frac{\partial B}{\partial_L p_c} - i\,\frac{\partial A}{\partial_R p_c}\,\frac{\partial B}{\partial_L c}\,. \tag{13.13}
$$

This bracket applies to 'functions' A and B that can be commuting or anticommuting, but obvious care is required in the order of writing the various terms. It obviously takes its values in the Grassmann algebra. We note the following relations,

$$
(A,B)^\dagger = -(B^\dagger,A^\dagger)\,, \qquad (B,A) = -(-)^{AB}\,(A,B)\,, \tag{13.14}
$$

where in the exponent AB is the product of the degrees of A and B, so that $(-)^{AB}$ equals -1 when both A and B are anticommuting (i.e. of odd degree), while in all other cases it is equal to $+1$. We return to the precise definition of hermitean conjugation shortly. To derive the relation above, one may for instance assume that c and p_c are real. Note, however, that right and left derivatives must be conjugate to each other.

When applied to the phase space coordinates the only nonvanishing brackets are,

$$
(q,p) = 1\,, \qquad (c,p_c) = -i\,. \tag{13.15}
$$

Quantization is now implemented by replacing the phase-space coordinates by operators and the bracket by $(i\hbar)^{-1}$ times the corresponding (anti)commutators,

$$
(A,B) \longrightarrow \frac{1}{i\hbar}\Big\{A\,B - (-)^{AB}\,B\,A\Big\}\,. \tag{13.16}
$$

In particular this yields the canonical (anti)commutation relations,

$$
[q,p] = i\hbar\,, \qquad \{c,p_c\} = \hbar\,, \tag{13.17}
$$

while all other (anti)commutators vanish.

So in this way we naturally arive at the same kind of theory described in chapter 9. We should point out that at this point it may seem natural to associate hermitean operators to c and p_c, because both the 'kinetic term' $ip_c\dot{c}$ in the Lagrangian (13.1) and the boundary term $-ip_c(t_2)\,c(t_2)$ in the action (13.5), are real under

$$c^\dagger = c\,, \qquad p_c^\dagger = p_c\,. \tag{13.18}$$

This conjugation is compatible with the anticommutation relation $\{c,p_c\} = \hbar$. However, there is a second type of conjugation, namely

$$c^\dagger = p_c\,, \qquad p_c^\dagger = c\,, \tag{13.19}$$

which is also compatible with the anticommutator, while the contribution in the action from the kinetic term changes only by boundary terms. As it turns out, this is the conjugation that is physically relevant. For the matrix representation of the anticommutator introduced in chapter 9, this was indeed the case as c and p_c correspond to b and $b^\dagger$ defined in (11.2). This is imposed on us because c and p_c are nilpotent operators.

Hence we have now reobtained the matrix model of chapter 9 starting with an extended dynamical system based on both commuting and anticommuting coordinates and momenta. Whether or not one chooses to make use of the matrix formulation is now a matter of convenience. We should stress that in this way we cannot formulate arbitrary matrix Hamiltonians, but only the ones that eventually admit an interpretation in terms of bosons and fermions. In the next chapter we derive the path integral formulation for the anticommuting fields.

Problem 13.1 :
Reconsider the path integral (1.16), which involves an integral over the trajectories $q(t)$ and $p(t)$. Specify the boundary conditions and consider the expression in the continuum limit. Show that Hamilton's principle leads to the Hamilton equations for p and q, with these boundary conditions.

Problem 13.2 :
Consider a theory based on five real fields, denoted by a five-component vector

$$\Phi = \begin{pmatrix} \Phi_0 \\ \Phi_1 \\ \Phi_2 \\ \Phi_3 \\ \Phi_4 \end{pmatrix}\,. \tag{13.20}$$

The action has a form reminiscent of the Dirac action for fermions,

$$S = -\tfrac{1}{2}\int \mathrm{d}^4x\ \bar{\Phi}(\beta^\mu\partial_\mu + M\ )\Phi\,, \tag{13.21}$$

and is thus at most linear in spacetime derivatives. Here, however the fields are *commuting* and therefore describe bosons. The conjugate vector is defined by $\bar{\Phi} = \Phi^T\eta$, with η a symmetric 5×5 matrix ($\eta^T = \eta$) satisfying $\eta^2 = \mathbf{1}$, and Φ^T denotes the transposed of the vector Φ.
The four matrices β^μ and the matrix η are given by

$$\beta^0 = \begin{pmatrix} 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad \beta^1 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{pmatrix}, \quad \beta^2 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix},$$

$$\beta^3 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \quad \eta = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & -1 \end{pmatrix}.$$

i) Give the mass dimension of the parameter M and the field Φ. Verify that the matrices $(\eta\,\beta^\mu)$ are antisymmetric. Show that $\bar{\chi}\beta^\mu\rho = -\bar{\rho}\beta^\mu\chi$ for two arbitrary five-component vectors χ and ρ.

ii) Derive the equations of motion for Φ. Use them to express Φ_0, Φ_1, Φ_2, and Φ_3 in terms of Φ_4 and give the equation satisfied by Φ_4. What are the degrees of freedom that this Langrangian describes?

The phase space, described in terms of the coordinates Φ_i and their canonically conjugate momenta, is reduced by a number of constraints. We now consider these constraints.

iii) Determine the canonically conjugate momentum for each of the fields Φ_i. Note that, because the Langrangian does not contain any time derivatives of Φ_1, Φ_2 and Φ_3, their canonically conjugate momenta are zero. For this reason, we can solve for these three fields using their equations of motion.

iv) The relevant phase space quantities are hence Φ_0 and Φ_4, and their conjugate momenta. Show that these quantities are subject to a constraint as well. As a result, the effective phase space is smaller. Give the dimension of the effective phase space and argue that this result is in agreement with the result obtained in ii).

v) There exist many relations among products of matrices β^μ. Show that $\beta^\mu\beta^\mu\beta^\mu$ is proportional to β^μ for arbitrary values of μ. A more general relation (which you are not asked to prove) is

$$\beta^\mu\beta^\nu\beta^\lambda + \beta^\lambda\beta^\nu\beta^\mu = \beta^\mu\eta^{\nu\lambda} + \beta^\lambda\eta^{\nu\mu}\,, \tag{13.22}$$

where $\eta^{\mu\nu}$ is the Minkowski metric. Derive from this relation an identity for $\not{p}^3$, where $\not{p} \equiv \beta^\mu p_\mu$. Using this identity and the equations of motion (in matrix form, i.e. not the component form), show that each of the components of Φ satisfies the Klein-Gordon equation.

vi) Show that the propagator of the field Φ (which can be defined as the vacuum expectation value of the time-ordered product of $\bar{\Phi}(x)$ and $\Phi(y)$ in momentum space), is given by

$$\Delta(p) = \frac{1}{i(2\pi)^4}\,\frac{1}{p^2+M^2-i\epsilon}\,\frac{i\not{p}(i\not{p}-M)+p^2+M^2}{M}\,, \tag{13.23}$$

vii) The propagator has a singularity for $p^2 = -M^2$. What can you say about the residue of the 5×5 matrix ? Analyse the residue by choosing $p^\mu = (\vec{0}, p^0)$ and studying the propagator in the limit $p^0 \to \pm M$. Explain the result.

We now add a complex scalar field scalar σ to the model, accompanied by an interaction with the field Φ, which has a form similar to the interaction of a gauge field with σ, i.e.

$$S' = -\int \mathrm{d}^4x\,\Big[|\partial_\mu\sigma|^2 + m^2|\sigma|^2 + ieV^\mu\left[\sigma^*(\partial_\mu\sigma) - (\partial_\mu\sigma^*)\sigma\right]\Big]\,. \tag{13.24}$$

Here V^μ is given by $V^\mu = \bar{\Phi}\beta^\mu u$ with u a constant 5-component vector.

viii) Draw the two 1-loop self energy diagrams of the σ field. Argue that one of them does not contribute.

Problem 13.3 :

We consider a field theory for a complex anti-commuting field $\psi(x)$. We have already seen in chapter 9 that a natural term in the Lagrangian will be $\int \mathrm{d}^3x\ \psi^\dagger(x) i\partial_t\psi(x)$, but we still need to find a term depending on the gradients of $\psi(x)$.

In the non-relativistic limit we know that the energy of a (spinless) fermion with momentum $\vec{p}$ and mass m is equal to $E(\vec{p}) = \vec{p}^2/2m$. Argue that this requirement leads to the Lagrangian

$$L(\psi^\dagger,\psi) = \int \mathrm{d}^3x\ \psi^\dagger(\vec{x},t)\left\{i\partial_t + \frac{\nabla^2}{2m}\right\}\psi(\vec{x},t)\ , \tag{13.25}$$

by showing that the field-equation for $\psi(\vec{x},t)$ has the plane-wave solutions $\psi(\vec{p})\exp[i\vec{p}\cdot\vec{x} - iE(\vec{p})\,t]$.

For a relativistic fermion we must also include the spin of the particle and $\psi(x)$ becomes a spinor (i.e. a vector in spin-space, whose dimension will be specified later on). We still expect the term $\int \mathrm{d}^3x\ \psi^\dagger(x) i\partial_t \psi(x)$, where the components of the spinor fields are contracted as in a complex inner product, but the gradient term must be modified because the energy of a particle with momentum $\vec{p}$ and mass m is now equal to $\sqrt{\vec{p}^2+m^2}$. To see how this can be achieved consider the Lagrangian

$$L(\psi^\dagger,\psi) = \int d^3x\ \psi^\dagger(x)\left\{i\partial_t + i\alpha^i\partial_i - \beta m\right\}\psi(x)\ , \tag{13.26}$$

with α^i and β matrices in spin-space. What is the field-equation for $\psi(x)$ and $\psi(\vec{p})$, respectively? Derive from the latter that the correct relativistic energy is obtained if $\{\alpha^i,\alpha^j\} = 2\delta^{ij}$, $\{\alpha^i,\beta\} = 0$ and $\{\beta,\beta\} = 2$. Finally, show that by introducing the Dirac matrices $\gamma^0 = -i\beta$ and $\gamma^i = -i\beta\alpha^i$, the Lagrangian can be rewritten as

$$L(\bar{\psi},\psi) = -\int \mathrm{d}^3x\ \bar{\psi}(x)\left\{\gamma^\mu\partial_\mu + m\right\}\psi(x)\ , \tag{13.27}$$

where $\bar{\psi}(x) = \psi^\dagger(x)\beta = i\psi^\dagger(x)\gamma^0 = \psi^\dagger\gamma_4$. Calculate also $\{\gamma^\mu,\gamma^\nu\}$. Finally write down a plane-wave expansion, analogous to (3.23), for solutions of the field equation that follows from (13.27). This equation is the celebrated Dirac equation. (For more details, consult sections 5.1-3 of *Field Theory in Particle Physics*, where also the Lorentz invariance of the action corresponding to the Lagrangian (13.27) is shown.)

Problem 13.4 :
Consider the following fermionic field theory in one space and one time dimension with the Lagrangian

$$L_0 = \int \mathrm{d}x\ i\psi^\dagger(x,t)(\partial_t + \partial_x)\psi(x,t)\ . \tag{13.28}$$

i) Write down the field equation and give its (plane-wave) solutions.

ii) Derive how the fermion fields should transform in order that this Lagrangian density (or the action) be invariant under Lorentz transformations. Use here that under a Lorentz transformation with $\beta = v/c$, we have

$$x' \pm t' = \sqrt{\frac{1\mp\beta}{1\pm\beta}}\,(x\pm t)\ ,$$

In addition we introduce an interaction with an electromagnetic field A_μ, via

$$\partial_t + \partial_x \rightarrow \partial_t + \partial_x - iA_t - iA_x\ .$$

This leads to a Lagrangian that we will denote by L_1. The electric charge is defined by the coupling of the fermions to the field A_t, and is thus given by

$$Q = \int \mathrm{d}x \; \psi^\dagger(x,t)\psi(x,t) \; . \tag{13.29}$$

We now assume that the spatial coordinate x parametrizes a circle with circumference L; the x-integrations then extend from 0 tot L.[15] Furthermore we assume $A_t = 0$ and restrict A_x to a constant value, so that $\Phi = LA_x$ equals the magnetic flux through the circle. At this stage it is possible to prove that a time-independent A_x can always be chosen equal to a constant in a certain interval by using a suitable gauge transformation. We will not derive this, but consequences of this fact will become apparent in the results below.

iii) Argue that the field ψ can be expanded in the following Fourier series

$$\psi(x,t) = \frac{1}{\sqrt{L}} \sum_k \psi(k,t) \; \exp(ikx) \, ,$$

where k is equal to $2\pi/L$ times an integer n (which can be of either sign).

iv) Write down the Lagrangian L_1, the Hamiltonian and the charge Q in terms of the Fourier modes. Prove that the charge does not depend on the time by using the field equations.

v) Determine the conjugate momenta and the anticommutation relations for $\psi(k)$ and $\psi^\dagger(k)$ in the Schrödinger representation. Consider the commutation relations of the Hamiltonian with $\psi(k)$ and $\psi^\dagger(k)$. Identify creation and annihilation operators (such that creation operators increase the energy of a state).

vi) Argue that the wave function in the 'coordinate representation' is a 'function' of the anticommuting coordinates $\psi(k)$. Define the momentum and write down the Schrödinger equation in the coordinate representation (cf. Problem 3.5). Give the ground-state wave function.

vii) Give the decomposition of the Heisenberg field $\psi(x,t)$ as a Fourier series in terms of the creation and annihilation operators found above. For $A_x = 0$, justify the following decomposition for the Heisenberg field (in the $L \to \infty$ limit)

$$\psi(x,t) = \sqrt{\frac{\hbar}{2\pi}} \int_0^\infty \mathrm{d}k \; \Big[a(k)\, e^{ikx - i\omega t} + b^\dagger(k)\, e^{-ikx + i\omega t} \Big] \; ,$$

with $\omega = k \geq 0$, and identify the operators $a(k)$ and $b(k)$ in terms of the $\psi(k)$.

[15] In the limit $L \to \infty$ we can use $\sum_k \to (L/2\pi) \int_{-\infty}^{\infty} dk$. We also remind you of the relation $\sum_n \exp(2\pi i n x) = \sum_l \delta(x - l)$, where on both sides of the equation the sum extends over all integers.

viii) Calculate the anticommutator of the Heisenberg fields $\psi^\dagger(x_1, t_1)$ and $\psi(x_2, t_2)$ in the special case that $A_x = 0$. Consider this result in the limit $L \to \infty$ and prove that it is in agreement with Lorentz invariance.

ix) Consider again (for $A_x \neq 0$) the Hamiltonian in terms of the creation and annihilation operators and show that the energy spectrum does not change under $\Phi \to \Phi + 2\pi$. Give an expression for the (infinite) energy of the groundstate, i.e., the state of lowest energy, which depends on the flux Φ. Sketch the energy of the one-particle states (with respect to the energy of the groundstate) as a function of k, first for $\Phi = 0$ and then for a value of Φ between 0 and 2π. Stress the qualitative differences.

x) Consider the charge operator and give the expression for the (infinite) charge of the groundstate. Give also the charge of the one-particle states (with respect to the charge of the groundstate).

xi) The infinite energy and charge of the groundstate is characteristic for a system with infinitely many degrees of freedom. Of course, these expressions are not really well defined. In practice one ignores these infinite contributions and there are good arguments that justify this. However, in this case the expressions depend on the value of the flux Φ. Show that the charge of the groundstate is insensitive to small changes in the value of Φ, but changes with an amount ΔQ when we let the flux increase from 0 to 2π. Determine the value for ΔQ.

xii) Add a second fermion field, but now with Lagrangian

$$L_2 = \int \mathrm{d}x \; i\psi_2^\dagger(x, t)(\partial_t - \partial_x - iA_t + iA_x)\psi_2(x, t) \; .$$

Determine the value of ΔQ for the combined system described by $L_1 + L_2$.[16]

Problem 13.5 :

In this exercise we will derive the plane-wave expansion for a Dirac field $\psi(t, \vec{x})$ in three spacetime dimensions and canonically quantize it. Consider the Lagrangian density describing a free massive fermion in three spacetime dimensions (we take c, the velocity of light, equal to $c = 1$),

$$\mathcal{L} = i\,\psi^\dagger\,\partial_t\psi + \psi^\dagger\,\sigma_3\,\vec{\sigma}\cdot\vec{\nabla}\,\psi - m\,\psi^\dagger\sigma_3\psi\,, \qquad (13.30)$$

[16]We should add that systems with $\Delta Q \neq 0$ are called *anomalous* and give rise to a violation of charge conservation.

where σ_i are the Pauli matrices satisfying $\sigma_i\sigma_j = \delta_{ij}\,\mathbf{1} + i\,\varepsilon_{ijk}\sigma_k$, and conventially represented by

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\,, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\,, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\,. \tag{13.31}$$

The vector arrow denotes vectors in the two spatial dimensions, *i.e.*,

$$\vec{x} = (x_1, x_2)\,, \quad \vec{p} = (p_1, p_2)\,, \quad \vec{\nabla} = (\partial_1, \partial_2)\,, \quad \vec{\sigma} = (\sigma_1, \sigma_2)\,. \tag{13.32}$$

and the inner product is the usual one, $\vec{x}\cdot\vec{y} = x_1\,y_1 + x_2\,y_2$. Note that ψ is a spinor with two components.

i) Derive the field equations for $\psi(t, \vec{x}\,)$ and $\psi^\dagger(t, \vec{x}\,)$.

ii) Consider plane wave solutions $\psi(t, \vec{x}\,) \sim \psi(\vec{p}\,)\,\mathrm{e}^{i\vec{p}\cdot\vec{x} - ip_0 t}$ and show that they must satisfy the equation

$$\begin{pmatrix} p_0 & ip_1 + p_2 \\ ip_1 - p_2 & -p_0 \end{pmatrix} \psi(\vec{p}) = m\,\psi(\vec{p})\,. \tag{13.33}$$

Show that, to have non-trivial solutions $\psi(\vec{p})$ to the above equation, p_0 must satisfy

$$p_0 = \pm\omega(\vec{p}\,)\,, \quad \text{where} \quad \omega(\vec{p}\,) = \sqrt{\vec{p}^{\;2} + m^2}\,. \tag{13.34}$$

Argue that this indicates that the theory based on (13.30) is relativistically invariant.

iii) Assume that the field is placed in a box with volume V and that periodic boundary conditions are imposed. Argue that $\psi(t, \vec{x})$ can be expanded as

$$\psi(t, \vec{x}\,) = \frac{1}{\sqrt{V}} \sum_{\vec{p}} \psi(t, \vec{p}\,)\,\mathrm{e}^{i\vec{p}\cdot\vec{x}}\,. \tag{13.35}$$

Give the possible values of the momenta $\vec{p}$ and write down the Lagrangian in terms of $\psi(t, \vec{p})$ and $\psi^\dagger(t, \vec{p})$.

iv) Determine the conjugate momentum $\pi(t, \vec{p}\,)$ of $\psi(t, \vec{p}\,)$ and prove that the Hamiltonian is given by

$$H = \sum_{\vec{p}} \psi^\dagger(t, \vec{p}\,)\,\sigma_3(-i\,\vec{\sigma}\cdot\vec{p} + m)\,\psi(t, \vec{p}\,)\,. \tag{13.36}$$

Show that $\sigma_3(-i\,\vec{\sigma}\cdot\vec{p} + m)$ is hermitean (so that the Hamiltonian is hermitean) and argue that its eigenvalues are equal to $\pm\omega(\vec{p})$, where $\omega(\vec{p})$ was defined in (13.34).

v) We now choose a basis for $\psi(t,\vec{p}\,)$ in such a way that the Hamiltonian becomes diagonal. The eigenvectors of $\sigma_3(-i\,\vec{\sigma}\cdot\vec{p}+m)$ with eigenvalue $\omega(\vec{p}\,)$ and $-\omega(\vec{p}\,)$ are denoted by $u_\alpha(\vec{p}\,)$ and $v_\alpha(\vec{p}\,)$, respectively. They take the form

$$u_\alpha(\vec{p}\,) = \sqrt{m+\omega}\begin{pmatrix} 1 \\ \dfrac{ip_1 - p_2}{m+\omega} \end{pmatrix}, \qquad v_\alpha(\vec{p}\,) = \sqrt{m+\omega}\begin{pmatrix} \dfrac{ip_1 + p_2}{m+\omega} \\ 1 \end{pmatrix}. \tag{13.37}$$

Show that these eigenvectors are orthogonal and normalized according to

$$v^\dagger u = u^\dagger v = 0\,, \qquad u^\dagger u = v^\dagger v = 2\omega\,. \tag{13.38}$$

(We note in passing that $u^\dagger\sigma_3 u = 2m$ and $v^\dagger\sigma_3 v = -2m$.)

Using $u(\vec{p}\,)$ and $v(\vec{p}\,)$ we decompose the two-component field $\psi_\alpha(t,\vec{p}\,)$ according to

$$\psi_\alpha(t,\vec{p}\,) = \sqrt{\frac{\hbar}{2\omega}}\Big[\,c_+(t,\vec{p})\,u_\alpha(\vec{p}\,) + c_-(t,\vec{p})\,v_\alpha(\vec{p}\,)\Big]\,. \tag{13.39}$$

Subsequently we proceed to quantize the system in the Schrödinger picture, promoting the modes of ψ to time-independent operators $\psi_\alpha(\vec{p}\,)$, and the modes of the conjugate momentum to momentum operators $\pi(\vec{p}\,)$. The conjugate momentum was already considered in iv).

vi) Impose the canonical quantization conditions and give the value of the anti-commutators,

$$\Big\{\psi_\alpha(\vec{p}\,),\psi_\beta(\vec{p}\,')\Big\}\,, \qquad \Big\{\psi^\dagger_\alpha(\vec{p}\,),\psi_\beta(\vec{p}\,')\Big\} \quad \text{and} \quad \Big\{\psi^\dagger_\alpha(\vec{p}\,),\psi^\dagger_\beta(\vec{p}\,')\Big\}\,. \tag{13.40}$$

Here $\alpha,\beta = 1,2$ denote spinor components. Subsequently derive the anti-commutation relations for the Schrödinger picture operators $c_\pm(\vec{p}\,)$ and $c^\dagger_\pm(\vec{p}\,)$, making use of (13.38).

vii) Express the Hamilton operator H in terms of $c^\dagger_\pm(\vec{p}\,)$ and $c_\pm(\vec{p}\,)$. Evaluate the commutator between the Hamiltonian H and the operators $c^\dagger_\pm(\vec{p}\,)$ and $c_\pm(\vec{p}\,)$; identify which of these operators play the role of annihilation operators ($a(\vec{p}\,)$, $b(\vec{p}\,)$) and of creation operators ($a^\dagger(\vec{p}\,)$, $b^\dagger(\vec{p}\,)$). Convert now to the Heisenberg picture with operators $a(t,\vec{p}\,)$, $b(t,\vec{p}\,)$, $a^\dagger(t,\vec{p}\,)$ and $b^\dagger(t,\vec{p}\,)$ and determine the time dependence of these operators.

viii) Express the quantum field $\psi(t,\vec{x}\,)$ in terms of the Schrödinger picture creation and annihilation operators. Give the corresponding expression in the large volume limit. Does this result satisfy the field equation and why (not)?

ix) Give the energy of the ground state $\langle 0|H|0\rangle$. Discuss the size and the sign for given $\vec{p}$. Did you expect this result?

14 Path integrals for fermions

Let us return to the model of chapter 8 and consider the path integral. There are several ways in which one can proceed. First we may stay within the matrix formulation with two-component wave functions. We can follow the same steps as in chapter 1, taking into account that we have a matrix Hamiltonian and that the states carry an extra quantum number. Obviously the transition function then takes the form of a two-by-two matrix and we have

$$W(q_2,t_2;q_1,t_1)=\int_{\substack{q(t_1)=q_1\\ q(t_2)=q_2}}\mathcal{D}q(t)\,\mathcal{D}\frac{p(t)}{2\pi\hbar}\;\exp\Big\{\frac{i}{\hbar}\int_{t_1}^{t_2}\mathrm{d}t\,\Big[p(t)\,\dot q(t)-H(p(t),q(t))\Big]\Big\}\,. \qquad (14.1)$$

We remind the reader (cf. 1.16) that the boundary conditions on $p(t)$ are such that we integrate over $p(t_1)$, while $p(t_2)$ is left unrestricted (so that the result satifies the product rule(1.12); cf. exercise 2.8).

Formally this is the same result as found before except that we are dealing with two-by-two matrices. We already evaluated the corresponding expressions for the model of chapter 9 in problem 9.4. However, we prefer to avoid a matrix formulation here. Ultimately we are interested in a field theory consisting of an infinite number of oscillators, so that the matrices will become infinite-dimensional and impossible to deal with. Our goal is therefore to find a description in terms of anticommuting variables, such that the anticommuting degrees of freedom can be treated in parallel with the commuting ones and no matrices are necessary. The material presented in the previous chapters makes it rather straightforward to set up such a formulation.

First we introduce a way of dealing with matrices where matrix multiplication is implemented by means of integrals over anticommuting c-numbers. Consider two-by-two matrices A_{ij}, where $i,j=0,1$. To each matrix we associate an element of the Grassmann algebra,

$$A(\bar\alpha,\alpha)\equiv A_{00}+\bar\alpha\,A_{10}+A_{01}\,\alpha+\bar\alpha\,A_{11}\,\alpha\,, \qquad (14.2)$$

where α and $\bar\alpha$ are two anticommuting c-numbers. Multiplication of two matrices A and B is now implemented by performing the following integral over anticommuting c-numbers,

$$\int\mathrm{d}\bar\beta\,\mathrm{d}\alpha\;e^{\alpha\bar\beta}\,A(\bar\alpha,\alpha)\,B(\bar\beta,\beta)=(AB)(\bar\alpha,\beta)\,. \qquad (14.3)$$

In other words, the above integral over the product of two Grassmann algebra elements associated with matrices A and B yields the element of the Grassmann algebra corresponding to the matrix product AB. This result is easy to verify by writing out the expression for the integral and using the results for integrals over anticommuting c-numbers.

Note that the Grassmann-algebra valued form corresponding to the unit matrix is equal to

$$\mathbf{1} \longrightarrow \mathbf{1}(\bar\alpha,\alpha) = 1 + \bar\alpha\,\alpha = e^{\bar\alpha\,\alpha}\,. \tag{14.4}$$

We also need the following expression in the limit where ϵ is small,

$$\exp\left[\epsilon\begin{pmatrix} A_{00} & A_{01} \\ A_{10} & A_{00}+A_{11}\end{pmatrix}\right] \longrightarrow \exp\Big[\bar\alpha\,\alpha + \epsilon A(\bar\alpha,\alpha)\Big] + \mathrm{O}(\epsilon^2)\,. \tag{14.5}$$

This result follows straightforwardly from a power series expansion of the exponential.

Also the ordinary trace over the matrix can be evaluated as an integral, as well as the graded trace, introduced in chapter 9, where certain entries of the matrix contribute with opposite sign. The reader can easily verify the following results

$$\mathrm{Tr}\,(A) \equiv A_{00} + A_{11} = -\int \mathrm{d}\bar\alpha\,\mathrm{d}\alpha\; e^{-\alpha\bar\alpha}\,A(\bar\alpha,\alpha)\,, \tag{14.6}$$

$$\mathrm{Tr}\,((-)^F A) \equiv A_{00} - A_{11} = \int \mathrm{d}\bar\alpha\,\mathrm{d}\alpha\; e^{\alpha\bar\alpha}\,A(\bar\alpha,\alpha)\,. \tag{14.7}$$

Finally we note that hermitean conjugation of the matrix is consistent with hermitean conjugation of the corresponding element of the Grassmann algebra (according to the prescription given in chapter 9), where $\alpha^\dagger = \bar\alpha$ and $\bar\alpha^\dagger = \alpha$. This leads to

$$(A^\dagger)(\bar\alpha,\alpha) = (A(\bar\alpha,\alpha))^\dagger\,. \tag{14.8}$$

For a unitary matrix we thus have

$$\int \mathrm{d}\bar\beta\,\mathrm{d}\alpha\; e^{\alpha\bar\beta}\,A(\bar\alpha,\alpha)\,(A(\bar\beta,\beta))^\dagger = e^{\bar\alpha\beta}\,. \tag{14.9}$$

Rather than setting up a path integral expression for the matrix valued Hamiltonian, we start from the corresponding Grassmann-algebra valued expression, which we denote by $W(q_2,t_2,\bar\alpha_2;q_1,t_1,\alpha_1)$. The approach is the same as in chapter 1. We divide a time interval (t_0,t_N) into N intervals (t_i,t_{i+1}) with $t_{i+1}-t_i=\Delta$, so that $t_N - t_0 = N\Delta$. Then we approximate the path integral by a product of path integrals with small time increments Δ, so that $W(q_N,t_N,\bar\alpha_N;q_0,t_0,\alpha_0)$ can be written as

$$\begin{aligned} W(q_N,t_N,\bar\alpha_N;q_0,t_0,\alpha_0) &= \int dq_{N-1}\cdots\int dq_1\int \mathrm{d}\bar\alpha_{N-1}\,\mathrm{d}\alpha_{N-1}\cdots\int \mathrm{d}\bar\alpha_1\,\mathrm{d}\alpha_1 \\ &\times\left(\prod_{i=1}^{N-1} e^{\alpha_i\,\bar\alpha_i}\right) W(q_N,t_N,\bar\alpha_N;q_{N-1},t_{N-1},\alpha_{N-1})\cdots W(q_1,t_1,\bar\alpha_1;q_0,t_0,\alpha_0). \end{aligned} \tag{14.10}$$

The matrix product is correctly implemented by virtue of (12.3). The Hamiltonian is now a two-by-two matrix, which depends on the operators P and Q, which we decompose according to (12.2). For small values of Δ we may write

$$W(q_{i+1},t_{i+1},\bar\alpha_{i+1};q_i,t_i,\alpha_i) = \langle q_{i+1}|e^{\bar\alpha_{i+1}\,\alpha_i-\frac{i}{\hbar}H(P,Q,\bar\alpha_{i+1},\alpha_i)\Delta}|q_i\rangle \tag{14.11}$$
$$\approx \langle q_{i+1}|q_i\rangle\,\mathbf{1} - \frac{i\Delta}{\hbar}\begin{pmatrix} \langle q_{i+1}|H_{00}(P,Q)|q_i\rangle & \langle q_{i+1}|H_{01}(P,Q)|q_i\rangle \\ \langle q_{i+1}|H_{10}(P,Q)|q_i\rangle & \langle q_{i+1}|H_{00}(P,Q)+H_{11}(P,Q)|q_i\rangle \end{pmatrix},$$

so that for vanishing H we obtain the unit matrix. As a consequence of this parametrization H_{00} represents the part of the Hamiltonian that acts uniformly on the two-dimensional vector space (cf. 12.5).[17] Inserting a complete set of eigenstates of the momentum operator then leads to

$$\begin{aligned} W &= \int \mathrm{d}p_i\,\langle q_{i+1}|p_i\rangle\langle p_i|e^{\bar\alpha_{i+1}\,\alpha_i-\frac{i}{\hbar}H(P,Q,\bar\alpha_{i+1},\alpha_i)\Delta}|q_i\rangle \\ &\approx \int\frac{\mathrm{d}p_i}{2\pi\hbar}\,\exp\left(\bar\alpha_{i+1}\,\alpha_i+\frac{i}{\hbar}\left[p_i(q_{i+1}-q_i)-H(p_i,q_i,\bar\alpha_{i+1},\alpha_i)\Delta\right]\right), \end{aligned}\tag{14.12}$$

where the two-component character resides in the Grassmann-valued character of the Hamiltonian, so that there is no need for indicating the two-component nature of the states. As before we made use of (1.7) and of the fact that Δ is small.

Putting the previous expressions together we thus obtain (observe that there is no dependence on $\bar\alpha_0$ and α_N)

$$\begin{aligned} W(q_N,t_N,\bar\alpha_N;q_0,t_0,\alpha_0) &= \prod_{i=1}^{N-1}\int dq_i\,\mathrm{d}\bar\alpha_i\,\mathrm{d}\alpha_i\,\prod_{i=0}^{N-1}\int\frac{dp_i}{2\pi\hbar} \\ &\times\exp\left(\bar\alpha_N\,\alpha_N-\sum_{i=1}^{N}\bar\alpha_i(\alpha_i-\alpha_{i-1})\right) \\ &\times\exp\left(\frac{i}{\hbar}\Delta\sum_{i=0}^{N-1}\left[\frac{p_i(q_{i+1}-q_i)}{\Delta}-H(p_i,q_i,\bar\alpha_{i+1},\alpha_i)\right]\right) \\ &= \prod_{i=1}^{N-1}\int dq_i\,\mathrm{d}\bar\alpha_i\,\mathrm{d}\alpha_i\,\prod_{i=0}^{N-1}\int\frac{dp_i}{2\pi\hbar} \\ &\times\exp\left(\bar\alpha_N\,\alpha_N+\frac{i}{\hbar}\Delta\sum_{i=0}^{N-1}\left[\frac{i\hbar\bar\alpha_{i+1}(\alpha_{i+1}-\alpha_i)}{\Delta}+\frac{p_i(q_{i+1}-q_i)}{\Delta}-H(p_i,q_i,\bar\alpha_{i+1},\alpha_i)\right]\right). \end{aligned}\tag{14.13}$$

The boundary conditions on the fermionic path are in accord with the description given in the previous chapter and the boundary term $\bar\alpha_N\alpha_N$ coincides with the corresponding term

[17] Observe that the matrix Hamiltonian, such as given in (11.1), does not correspond directly to the Grassmann-parameter representation $H(P,Q,\bar\alpha_{i+1},\alpha_i)$ according to (12.2); instead the relationship proceeds through (14.11).

in the action (13.5). Observe that this term, which actually vanishes against a similar term, is important for establishing the decomposition rule,

$$\int \mathrm{d}q_2\, \mathrm{d}\bar{\beta}\, \mathrm{d}\alpha\; e^{\alpha\bar{\beta}}\, W(q_3, t_3, \bar{\alpha}; q_2, t_2, \alpha)\; W(q_2, t_2, \bar{\beta}; q_1, t_1, \beta) = W(q_3, t_3, \bar{\alpha}; q_1, t_1, \beta)\,. \tag{14.14}$$

The continuum limit is now straightforward and after rescaling of $\bar{\alpha}$ and α with a factor $\hbar^{-1/2}$, we have

$$\begin{aligned} W(q_2, t_2, \bar{\alpha}_2; q_1, t_1, \alpha_1) = \int \mathcal{D}q(t) \int \mathcal{D}\frac{p(t)}{2\pi\hbar} \int \mathcal{D}\frac{\bar{\alpha}(t)}{\sqrt{\hbar}} \int \mathcal{D}\frac{\alpha(t)}{\sqrt{\hbar}} \\ \times \exp\left(\frac{i}{\hbar}\left[-i\bar{\alpha}(t_2)\,\alpha(t_2) + \int_{t_1}^{t_2} \mathrm{d}t\, \Big[i\bar{\alpha}(t)\,\dot{\alpha}(t) + p(t)\,\dot{q}(t) - H(p(t), q(t), \bar{\alpha}(t), \alpha(t))\Big]\right]\right)\,, \end{aligned} \tag{14.15}$$

where the various trajectories have the following characteristic properties:

$$q(t_1) = q_1\,, \quad q(t_2) = q_2\,, \quad \alpha(t_1) = \alpha_1\,, \quad \bar{\alpha}(t_2) = \bar{\alpha}_2\,, \tag{14.16}$$

and there is no integration over $p(t_2)$, $\alpha(t_2)$ and $\bar{\alpha}(t_1)$ (which are not contained in the integrand), while we do integrate over $p(t_1)$. Obviously, the term in the exponent, including the boundary term, is precisely the action defined earlier in (13.5). This garantuees that the $\hbar \to 0$ limit leads to the correct classical results. In the Hamiltonian, we have absorbed the $\sqrt{\hbar}$ from the rescaling of the fermionic coordinates into the definition of the matrix elements of H.

Let us momentarily return to the discrete version. It is possible to obtain the expression for the trace (with respect to the original matrix indices) of the path integral by using (12.6). Hence we integrate (14.13) over $\bar{\alpha}_N$ and α_0 with an exponential factor $-\exp(-\alpha_0\bar{\alpha}_N)$. Therefore the exponent in (14.13) will explicitly contain the following combination of terms

$$-\bar{\alpha}_N(-\alpha_0 - \alpha_{N-1}) - \sum_{i=1}^{N-1} \bar{\alpha}_i(\alpha_i - \alpha_{i-1})\,.$$

The trace over the bosonic states is implemented by taking the integral over $q_N = q_0$, as was shown in (5.21). Close inspection now shows that the combined trace coincides with

$$\begin{aligned} \mathrm{Tr}\, W \;=\; & -\prod_{i=0}^{N-1} \int dq_i\, \mathrm{d}\bar{\alpha}_i\, \mathrm{d}\alpha_i \prod_{i=0}^{N-1} \int \frac{dp_i}{2\pi\hbar} \\ & \times \exp\left(\frac{i}{\hbar}\Delta \sum_{i=0}^{N-1}\left[\frac{i\hbar\bar{\alpha}_{i+1}(\alpha_{i+1} - \alpha_i)}{\Delta} + \frac{p_i(q_{i+1} - q_i)}{\Delta} - H(p_i, q_i, \bar{\alpha}_{i+1}, \alpha_i)\right]\right)\,. \end{aligned}$$

for *antiperiodic* fermionic paths, i.e. paths satisfying $\bar{\alpha}_N = -\bar{\alpha}_0$ and $\alpha_N = -\alpha_0$, and *periodic* bosonic paths with $q_N = q_0$. After converting to the Euclidean case, we can thus obtain a closed expression for the partition function for a theory where the original Hamiltonian is a matrix, in which the matrix degrees of freedom are incorporated by anticommuting coordinates and momenta, whose treatment is very analogous to the treatment of commuting coordinates and momenta.

With these results, we can evaluate the fermionic path integral and set up a perturbation expansion in terms of Feynman diagrams, precisely as for the bosonic theories. Of course, one must be aware of various minus signs that show up in actual calculations, due to the anticommuting nature of the fermionic coordinates or fields. We mention two of them.

First consider the definition of fermionic correlation functions. On the basis of the path integral representation the correlation function should exhibit the fact that the fermion operators are anticommuting. More explicitly, it is clear that one should have

$$\langle \alpha(t)\,\bar\alpha(t')\rangle = -\langle \bar\alpha(t')\,\alpha(t)\rangle\,, \tag{14.17}$$

for a correlation function defined by

$$\langle \alpha(t)\,\bar\alpha(t')\rangle = \frac{\int \mathcal{D}\phi\,\alpha(t)\,\bar\alpha(t')\,e^{\frac{i}{\hbar}S[\phi]}}{\int \mathcal{D}\phi\,e^{\frac{i}{\hbar}S[\phi]}}\,, \tag{14.18}$$

where ϕ generically denotes all the variables in the path integral. For the operator definition the minus sign in (14.18) implies that one must take a modified time-ordered product,

$$T(a(t)\,\bar\alpha(t')) = \theta(t-t')\,\alpha(t)\,\bar\alpha(t') - \theta(t'-t)\,\bar\alpha(t')\,\alpha(t)\,. \tag{14.19}$$

Secondly, in the evaluation of Feynman diagrams it turns out that a closed loop associated with a fermion line acquires an overall minus sign. We will discuss an example of this in problem 12.4.

Problem 14.1 :
Consider the Hamiltonian $H(\bar\alpha,\alpha) = \hbar\omega\,\bar\alpha\alpha$, which corresponds in matrix notation to

$$H = \begin{pmatrix} 0 & 0 \\ 0 & \hbar\omega \end{pmatrix}\,,$$

and calculate the transition function $W(\bar\alpha_N, t_N; \alpha_0, t_0)$ by first explicitly performing the integrations $\int d\bar\alpha_{N-1}d\alpha_{N-1}\ldots\int d\bar\alpha_1 d\alpha_1$ in the path integral (14.13) and then taking the limit $N\to\infty$ and $\Delta\to 0$ such that $N\Delta = t_N - t_0$ remains fixed. (It is convenient to perform the integrals starting from the left, i.e. from α and $\bar\alpha$ with the highest index values.) Compare the result with equation (11.12) and explain the differences. Calculate the transition function also by immediately making use of the continuum limit of the path integral, i.e. find the classical trajectories $\alpha(t)$ and $\bar\alpha(t)$, write the transition function as $f(t_N - t_0)\, e^{iS_{cl}/\hbar}$ and determine $f(t_N - t_0)$, for instance by requiring that the evolution operator for one of the states takes the expected form (semiclassical approximation). Note once more the relevance of the boundary term at $t = t_2$. (Comment: in the continuum limit the Hamiltonian reads $H(\bar\alpha, \alpha) = \omega\, \bar\alpha\alpha$, because of the rescaling of the fermionic coordinates by $\sqrt{\hbar}$.)

Problem 14.2 :
We have seen in chapter 8 that the Hamiltonian of the fermionic harmonic oscillator is $H = \hbar\omega b^\dagger b$, which has the eigenstates $|0\rangle$ and $|1\rangle = b^\dagger|0\rangle$. In matrix notation the transition function is therefore

$$W_{ij}(t_N; t_0) = \langle i|e^{-iH(t_N - t_0)/\hbar}|j\rangle \ .$$

We now introduce the so-called coherent states $|\alpha\rangle \equiv \exp(-\alpha b^\dagger)|0\rangle = |0\rangle + |1\rangle\alpha$, where α is again an anti-commuting number that also anticommutes with the operators b and $b^\dagger$. Prove that these coherent states obey $b|\alpha\rangle = \alpha|\alpha\rangle$, $\langle\alpha'|\alpha\rangle = e^{\bar\alpha'\alpha}$ and $\int d\bar\alpha\, \mathrm{d}\alpha\ e^{-\bar\alpha\alpha}|\alpha\rangle\langle\alpha| = 1$. Furthermore, show now that

$$W(\bar\alpha_N, t_N; \alpha_0, t_0) = \langle\alpha_N|e^{-iH(t_N - t_0)/\hbar}|\alpha_0\rangle.$$

Can you understand on the basis of these results that the action,

$$S[\bar\alpha, \alpha] = -i\hbar\bar\alpha(t_2)\alpha(t_2) + \int_{t_1}^{t_2} dt\ \{i\hbar\bar\alpha\dot\alpha - H(\bar\alpha, \alpha)\}\ ,$$

appearing in the path integral for $W(\bar\alpha_N, t_N; \alpha_0, t_0)$, is not hermitian if one uses the physically relevant conjugation introduced in equation (13.19)? (Hint: To facilitate matters, consider the path integral in the special case $H = 0$.) Determine also $S^\dagger[\bar\alpha, \alpha]$ and explain why this is the desired result by writing a path integral representation for complex conjugate matrix element of the evolution operator.

Problem 14.3 :
Calculate, using the fermionic harmonic oscillator Hamiltonian $H = \hbar\omega\, b^\dagger b$ and the modified time-ordered product of (14.19), the two-point correlation function $G(t, t') = \langle b(t)\, b^\dagger(t')\rangle$. Here $b(t)$ and $b^\dagger(t)$ are the usual annihilation and creation operators in the Heisenberg picture and the average is with respect to the groundstate $|0\rangle$. Show that it can be written as

$$G(t, t') = \frac{-1}{2\pi i}\int_{-\infty}^{\infty} dq\ \frac{e^{-iq(t-t')}}{q - \omega + i\epsilon}\ .$$

Therefore, $G(t, t')$ now obeys the first-order differential equation $(i\partial_t - \omega)\, G(t, t') = i\delta(t - t')$. Obtain the same result by path-integral methods, i.e. by functional differentiation of the logarithm of

$$W_J^{(0)} = \int \mathcal{D}\bar\alpha\, \mathcal{D}\alpha\ \exp\left(\frac{i}{\hbar} S[\bar\alpha,\alpha] + \int \mathrm{d}t\ \{\bar J(t)\alpha(t) + \bar\alpha(t) J(t)\}\right)\ .$$

Problem 14.4 :
Consider a theory based on the Lagrangian

$$S[q,\bar\alpha,\alpha] = -\tfrac{1}{2} m\,\dot q^2 + \tfrac{1}{2} m\omega^2\, q^2 + i\bar\alpha\dot\alpha - (\omega' + g\,q)\bar\alpha\alpha\,,$$

and calculate the contribution from a closed fermion loop to the two-point correlation function $\langle q(t)\, q(t')\rangle$. (Ignore that the actual integral vanishes). Pay particular attention to the overall sign and analyze how a closed-fermion loop is always accompanied by an extra minus sign. For this purpose one may use the representation (6.7).

Problem 14.5 :
Write the partition function for the (Euclidean) harmonic oscillator with antiperiodic boundary conditions as

$$Z_\beta^{(-)} = \int_{\mathrm{AP}} \mathcal{D}q(\tau) \exp\left(-\frac{m}{\hbar}\int_0^{\hbar\beta} d\tau\ q(\tau)\Big[-\frac{\mathrm{d}^2}{\mathrm{d}\tau^2} + \omega^2\Big] q(\tau)\right) \propto \left(\det{}_{\mathrm{AP}}\Big[-\frac{\mathrm{d}^2}{\mathrm{d}\tau^2} + \omega^2\Big]\right)^{-1/2}$$

Also consider the corresponding expression of the fermionic partition function

$$Z_\beta^{\mathrm{fermion}} = \int_{\mathrm{AP}} \mathcal{D}\bar\alpha(\tau)\ \mathcal{D}\alpha(\tau) \exp\left(-\frac{1}{\hbar}\int_0^{\hbar\beta} d\tau\ \bar\alpha(\tau)\Big[\frac{\mathrm{d}}{\mathrm{d}\tau} + \omega\Big]\alpha(\tau)\right) \propto \det{}_{\mathrm{AP}}\Big[\frac{\mathrm{d}}{\mathrm{d}\tau} + \omega\Big]$$

15 Regularization and renormalization

The momentum integrals we have to perform in the calculation of Feynman diagrams are often divergent. We distinguish two kinds of divergences: ultraviolet divergences (UV), where the divergence comes from the behaviour at large integration momenta and infrared divergences (IR) caused by singular behaviour of the integrands at small momenta. The latter usually arise when the fields are massless. The UV divergences can be characterized by their so-called *superficial degree of divergence.* An integral of the type

$$\int \mathrm{d}^d p\ \frac{p^\beta}{(p^2+m^2)^\alpha}\ , \tag{15.1}$$

is called finite when $2\alpha-\beta > d$, logarithmically divergent when $2\alpha-\beta = d$, linearly divergent when $2\alpha - \beta = d - 1$, and so on.

In the presence of divergences we need a mathematical prescription to deal with the integrands and to perform algebraic manipulations on the Feynman diagrams. Such a prescription is called a regularization method. The method can usually be implemented by making certain modifications to the Lagrangian. We mention four methods.

1. *Higher-derivative regularization*:
   We can introduce higher-derivative terms into the Lagrangian, for instance by introducing the term

   $$\mathcal{L} = -\xi^{-1}(\Box\phi)^2 \qquad \text{in additon to} \qquad \mathcal{L} = -(\partial_\mu\phi)^2$$

   Then the propagators are modified according to

   $$\frac{1}{q^2} \longrightarrow \frac{\xi}{q^2(q^2+\xi)}\,,$$

   which makes most of the integrals finite. In the limit $\xi \to \infty$ these divergences reappear. In theories where an invariance principle relates the kinetic term to the interactions, such as a gauge theory or a so-called non-linear sigma model, this method usually renders the theory finite beyond but not at the one-loop level.

2. *Pauli-Villars regularization*:
   In this regularization method we add massive regulator fields to the Lagrangian, some with the "wrong" metric and/or statistics. A field ϕ will usually be replaced in the interaction Lagrangian by a linear combination involving regulator fields ϕ_i,

   $$\phi \longrightarrow \phi + \sum_i \phi_i$$

   The masses, metric and statistics of the regulator fields ϕ_i are chosen such that the sum of the diagrams containing both the original and the regulator fields become finite. The divergences reappear in the limit that the regulator masses are taken to infinity. To use this method we must choose the same momentum parametrization for corresponding diagrams that involve the original field and the regulator fields. Otherwise the result of this regularization may become ambiguous, due to the fact that one is not allowed to shift the integration variables in certain divergent integrals. In this method special care is required to preserve symmetries of the original theory.

3. *Analytic regularization*:
   Here the propagators are changed by replacing $(p^2+m^2)^{-1}$ by $(p^2+m^2)^{-\lambda}$ with λ complex. The integrals are then defined by making an analytic continuation in λ. To preserve symmetries in this approach is often problematic.

4. *Dimensional regularization*
   In most theories nothing refers specifically to the number d of space-time dimensions. The integrals are defined by an analytic continuation from a region in the parameter d where the integrals do exist. Divergences then emerge as poles at $d = 4$. The method is applicable to a large class of theories. It has problems in the presence of symmetries that explicitly depend on the dimension, e.g. chiral symmetry, supersymmetry, conformal symmetry. We refer to De Wit & Smith for an introduction to this method.

After having introduced a regulator scheme we can rigorously deal with the amplitudes. However, at the end of the calculation we wish to remove the regulators again, for instance, by letting the mass of the regulator fields go infinity (in Pauli-Villars) or by finally taking the limit $d \longrightarrow 4$ (in dimensional regularization). In this way we still recover the original infinities, and our next task is to remove or absorb them in order to get finite physical quantities. The method for this is called *renormalization*: one absorbs the infinities of the theory in a well-defined manner into the original parameters of the theory. The renormalization procedure is described in chapter 7 of De Wit & Smith. The reader may be worried that different regularization methods yield different answers, but these (finite) differences can be consistently removed by finite renormalizations, so that at the end the results will coincide (at least in perturbation theory).

Here we give a more formal treatment of renormalization theory. We start with some definitions.

1. A *one-particle irreducible* graph (1PI) is a graph which cannot be divided into two disconnected pieces by cutting only one internal line.

2. *Superficial degree of divergence* (D_Γ) of a 1PI diagram Γ is the overall divergence that one naively extracts by counting powers of integration momenta. This is the leading power in λ if we make the replacement $p \longrightarrow \lambda p$ (external momenta are kept fixed). For one-loop diagrams it is the highest possible degree of divergence. Therefore for a one-loop diagram, being superficially finite implies that it is UV finite, but being superficially divergent does not imply that the actual expression is necessarily divergent. At higher loops a superficially finite integral may still diverge in certain domains of the integration region, for instance those domains that correspond to divergent subdiagrams. We will give an example of this in due course.

A 1PI diagram generally leads to an expression that involves a number of momentum integrals (one for each propagator), momentum-conserving delta functions (one for each vertex) and an integrand that consists of a product of propagators and vertices, i.e.,

$$\int \mathrm{d}^d p \cdots \delta^d(p) \ldots \left(\frac{1}{p^2 + m^2} \cdots \right) , \tag{15.2}$$

so that the number of integration variables equals the number of propagators I, the number of δ-functions equals the number of vertices V, and the last part between the curly brackets denotes the product of all propagators and vertices. Because we are dealing with a connected graph, all but one of the the δ-functions can be integrated out. The remaining one is a δ-function that only contains the external momenta, expressing energy-momentum conservation. Therefore the number of independent integration momenta is reduced by $V-1$. This number is equal to the number of loops L. so that we have

$$L = I - V + 1 . \tag{15.3}$$

Let us now distinguish different types of internal lines, corresponding to different types of fields ϕ_i. The number of internal lines (propagators) of type i in a given graph is denoted by I_i. The propagators are given by the diagonal terms in the Lagrangian quadratic in the fields. (For simplicity we assume that we either diagonalize the kinetic terms or treat off-diagonal terms as interactions). Because the term in the Lagrangian quadratic in the fields that contains the highest number of derivatives is conventionally not multiplied by a dimensional constant, it determines the dimension d_i of the field ϕ_i. Let us assume that the highest number of derivatives in the part of the Lagrangian quadratic in ϕ_i equals α_i, so that (schematically) we have a term $\mathcal{L}_0 \sim \phi_i\, \partial^{\alpha_i}\, \phi_i$ in the Lagrangian. As the action is dimensionless (in units where $\hbar = 1$) the Lagrangian has dimension $[\text{mass}]^d$. Therefore the dimension of ϕ_i is equal to

$$d_i = \frac{d - \alpha_i}{2}. \tag{15.4}$$

By defining the field dimension in this way the behaviour of the propagator for asymptotically large (Euclidean) momenta is gouverned by the dimension. The propagator associated with ϕ_i behaves as

$$\Delta_i(p) \sim \frac{1}{p^{\alpha_i}} = p^{2d_i - d} , \qquad \text{for } p \to \infty. \tag{15.5}$$

Consider a few examples. For the Klein-Gordon Lagrangian

$$\mathcal{L} = -\tfrac{1}{2}(\partial_\mu \phi)^2 - \tfrac{1}{2} m^2 \phi^2,$$

we have $\alpha = 2$. So $d_\phi = \frac{1}{2}(d-2)$ and the propagator behaves as p^{-2} at large p. For the Dirac Lagrangian

$$\mathcal{L} = -\overline{\psi}(\partial\!\!\!/ + m)\psi,$$

we have $\alpha = 1$. So $d_\psi = \frac{1}{2}(d-1)$ and the propagator behaves as p^{-1} at large p. For the Lagrangian

$$\mathcal{L} = -\tfrac{1}{2}(\Box\phi)^2 - \tfrac{1}{2}m_1^2(\partial_\mu\phi)^2 - \tfrac{1}{2}m_2^2\phi^2\,,$$

we have $\alpha = 4$. So $d_\phi = \frac{1}{2}(d-4)$ and the propagator behaves as p^{-4} at large p.

Let us now consider the vertices. We label different types of vertices by α and denote the number of these vertices by V_α, such that the total number of vertices equals $V = \sum_\alpha V_\alpha$. With each type of vertex we associate a coupling constant g_α. Assuming that the vertex of type α contains n_i^α fields ϕ_i, then the dimension of the vertex is given by

$$\delta_\alpha = \sum_i n_i^\alpha\, d_i + \text{ number of space-time derivatives.} \tag{15.6}$$

With the above definitions it is clear that a propagator gives rise to $2d_i - d$ and a vertex to $\delta_\alpha - \sum_i n_i^\alpha\, d_i$ momentum factors in the integrand. The number of momentum integrations is fixed by the number L of closed loops. Therefore the superficial degree of divergence of the diagram is equal to

$$\begin{aligned} D_\Gamma &= d\,L + \sum_\alpha V_\alpha\Big(\delta_\alpha - \sum_i n_i^\alpha\, d_i\Big) + \sum_i I_i(2d_i - d) \\ &= \Big(\sum_i I_i - \sum_\alpha V_\alpha + 1\Big)d + \sum_\alpha V_\alpha\Big(\delta_\alpha - \sum_i n_i^\alpha d_i\Big) + \sum_i I_i(2d_i - d) \\ &= d + \sum_\alpha V_\alpha(\delta_\alpha - d) + \sum_i d_i\Big(2I_i - \sum_\alpha V_\alpha n_i^\alpha\Big)\;. \end{aligned} \tag{15.7}$$

Subsequently we note that in a 1PI diagram the total number of fields ϕ_i emanating from the vertices must be equal to the sum of the number of endpoints of the internal lines and one of the endpoints of the external lines associated with ϕ_i. Thus we obtain the equality

$$E_i + 2I_i = \sum_\alpha n_i^\alpha\, V_\alpha\,, \tag{15.8}$$

where E_i is the number of external lines associated with the field ϕ_i. Using this relation then leads to the result

$$D_\Gamma = d - \sum_\alpha V_\alpha\,(d - \delta_\alpha) - \sum_i E_i\, d_i. \tag{15.9}$$

This remarkably simple result expresses the superficial degree of divergence in terms of $d - \delta_\alpha$, the dimension of the coupling constant g_α, and the dimensions of the external fields (d_i). If $D_\Gamma \geq 0$ then the diagram Γ is called superficially divergent: $D_\Gamma = 0$ corresponds to a logarithmic divergence, $D_\Gamma = 1$ to a linear one, etc. For $D_\Gamma < 0$ the diagram Γ is called superficially finite.

Suppose now that the dimension of the interaction is not larger than d, i.e. $\delta \leq d$, so that the theory has no coupling constants of negative dimensions. In that case the maximal degree of divergence will not increase in higher orders of perturbation theory and depends only on the number of external lines. Theories that satisfy this condition are called: *renormalizable by power counting*. They are thus characterized by coupling constants with non-negative dimensions. Theories with coupling constants that are positive are called *superrenormalizable*, because in that case the degree of divergence will decrease with the number of interactions. On the other hand, in the presence of coupling constants of negative dimension (15.9) tells us that the superficial degree of divergence will grow with the number of interactions. Then short-distance behaviour becomes worse (i.e. more divergent) in higher orders of perturbation theory. A well-known example is gravity in four space-time dimensions, which is not renormalizable by power counting. The coupling constant is Newton's constant, which has negative dimension. A somewhat more subtle example is the Proca theory (see Problem 15.5).

Now that we can classify the graphs according to their superficial degree of divergence we can discuss the renormalization procedure. First we expand the superficially divergent 1PI graphs in a Taylor series in the external momenta. Such an expansion will be of the form

$$a + b_\mu \, p^\mu + c_{\mu\nu} \, p^\mu p^\nu + \ldots \qquad (15.10)$$

where the expansion coefficients now carry a superficial degree of divergence of $D, D{-}1, D{-}2$, etc. The expansion about zero momenta may be troublesome, in particular in the presence of massless particles, but this is a technical problem that we leave aside.

We are now in a position to state the *subtraction procedure* of Bogoliubov, which is defined in a perturbation theory as an iterative procedure.

1. Calculate in perturbation theory, until one encounters a 1PI diagram Γ, whose superficial degree of divergence, D_Γ, is larger than or equal to zero. We expand those diagrams in a Taylor series in terms of the external momenta as described above.

2. Add to the Lagrangian extra terms (counterterms) chosen to precisely cancel (to this order in perturbation theory) all the superficially divergent terms in the Taylor expansion. These counterterms have the structure of the original diagrams shrunk to a point and may contain a certain number of derivatives. Their dimension is given by

$$\delta_{ct} = \sum_i E_i d_i \, , \; \sum_i E_i d_i + 1 \, , \ldots \, , \; \sum_i E_i d_i + D_\Gamma \, . \qquad (15.11)$$

3. Continue the calculation using the modified Lagrangian.

According to Hepp's theorem this procedure eliminates all divergences, not only the superficial ones.

To illustrate the renormalization procedure, let us once more consider the example of the ϕ^4 theory in four dimensions. We have only two classes of superficially divergent 1PI diagrams For the selfenergy diagrams, which have $D = 2$, the first two terms in the Taylor expansion, $\Pi(p) = A + Bp^2$, are superficially divergent; the constant A is quadratically ($D = 2$), and the constant B logarithmically ($D = 0$) divergent. There is no three-point function. For the four-point function we have only a superficially logarithmically divergent constant C. Hence the counterterms take the form

$$\mathcal{L}_{ct} = -\tfrac{1}{2}A\phi^2 - \tfrac{1}{2}B(\partial_\mu\phi)^2 + \tfrac{1}{24}C\phi^4,$$

where A, B and C are expressed by power series in the coupling constant. However, these terms already occur in the original Lagrangian, so that we can simply absorb these terms into the original quantities, fields and coupling constants, of the theory,

$$\mathcal{L}_{total} = \mathcal{L} + \mathcal{L}_{ct} = -\tfrac{1}{2}(1+B)(\partial_\mu\phi)^2 - \tfrac{1}{2}(m^2 + A)\phi^2 - (\lambda - \tfrac{1}{24})C\phi^4\,.$$

Such theories are called *renormalizable*: the infinities can be absorbed into the original parameters, order by order in perturbation theory.

It is now clear that when a theory is not renormalizable by power counting, we have to introduce more and more different counterterms when going to higher orders in perturbation theory. Therefore such theories have no predictive power. They are called *non-renormalizable*. Also, such theories require additions to the Lagrangian that have more and more derivatives. This will have direct consequences for the unitarity and causality properties of the theory.

We close with some more definitions. A Lagrangian is called *strictly renormalizable* if it is renormalizable by power counting *and* it is the most general Lagrangian with interactions of dimension $\delta \leq d$. A Lagrangian that is not of the most general form can still be renormalizable because fewer counterterms are required than indicated by the general argument. This happens in the presence of a symmetry (or an approximate symmetry if the symmetry breaking is sufficiently "soft").

In the presence of symmetries it must be shown that the regularization and renormalization preserves the symmetry. This is particularly difficult for non-linear symmetries. The transformation properties of the fields introduce new vertices, which are not present in the original Lagrangian. We have to allow counterterms for these vertices also which leads to a renormalization of the transformation properties, and verify that this is consistent with the renormalization of the Lagrangian. Such complications occur for instance in the non-linear

$O(N)$ sigma model, in two-dimensional gravitation, for the BRST transformation in gauge symmetries and for certain supersymmetry models.

Problem 15.1 :
Consider a ϕ^3 interaction in four space-time dimensions. Write down the superficially divergent 1PI graphs. Consider the two-loop self-energy graphs, which are superficially finite. Show that some of these graphs are still infinite and that this divergence is related to certain subdiagrams. Do we need counterterms beyond two loops?

Problem 15.2 :
For the Lagrangian

$$\mathcal{L} = -\tfrac{1}{2}(\partial_\mu \phi)^2 - \tfrac{1}{2}m^2\phi^2 - \lambda\phi^4,$$

verify that

$$d_\phi = \tfrac{1}{2}(d-2).$$

The dimension of the ϕ^2 term is thus equal to $d-2$, and the dimension of the ϕ^4 term equals $\delta = 2d-4$. Because $\mathcal{L}$ must have dimension d, the dimension of the coupling constant is $d - \delta_\alpha$, so that $\dim[m^2] = 2$ (as expected) and $\dim[\lambda] = 4-d$. Show that $D_\Gamma = 4 - E$.

Problem 15.3 :
Consider interacting fermions ψ and scalars ϕ in d dimensions with the interaction Lagrangian $\mathcal{L}_I \sim (\bar\psi\phi\psi)$. We know already that $d_\phi = \frac{1}{2}(d-2)$, $d_\psi = \frac{1}{2}(d-1)$, so that $\delta = \frac{3}{2}d - 2$. Eq. (15.9) then gives

$$D_\Gamma = d + V\Big(\frac{d}{2} - 2\Big) - E_\psi \frac{d-1}{2} - E_\phi \frac{d-2}{2}.$$

Argue that in four dimensions the superficial degree of divergence depends only on the external lines. In four dimensions this theory needs also counterterms other than $(\bar\psi\phi\psi)$, namely proportional to ϕ, ϕ^3 and ϕ^4, so it is not strictly renormalizable. In two dimensions the theory is renormalizable when we allow shifting the ϕ field by an infinite constant.

Problem 15.4 :
Show that for a $(\phi)^N$ theory in two dimensions the field dimension and the dimension of the interaction terms are zero. This gives

$$D_\Gamma = 2 - 2V.$$

Therefore the superficially divergent diagrams are those with only a single interaction vertex. Argue that the theory is not strictly renormalizable because the counterterms are of the form ϕ^{N-2}, ϕ^{N-4}, ... Consequently the theory

$$\mathcal{L} = -\tfrac{1}{2}(\partial_\mu\phi)^2 - \tfrac{1}{2}\mu^2\phi^2 + \lambda_0\phi^N + \lambda_1\phi^{N-2} + \lambda_2\phi^{N-4} + \cdots \,,$$

is strictly renormalizable. Can you say something about the possible renormalizability of the $SO(N)$ nonlinear sigma model in two dimensions, defined by the Lagrangian

$$\mathcal{L} = -\tfrac{1}{2}\frac{(\partial_\mu\vec{\phi})^2}{(1+\lambda\vec{\phi}^2)^2}\,.$$

where $\vec{\phi}$ is an $(N-1)$-dimensional vector of scalar fields $(\phi^1,\ldots,\phi^{N-1})$. The above model is called the $SO(N)$ nonlinear sigma model because it is invariant under $SO(N)$.

Problem 15.5 :
Argue that the following Lagrangian of a massive vector field is *not* renormalizable by power counting in four dimensions.

$$\mathcal{L} = -\tfrac{1}{4}(\partial_\mu V_\nu - \partial_\nu V_\mu)^2 - \tfrac{1}{2}M^2V_\mu^2 + ieV_\mu\,\bar{\psi}\gamma^\mu\psi - \bar{\psi}(\partial\!\!\!/ + m)\psi.$$

Note that the dimension of the vector field is generically equal to 1, but since the longitudinal component carries no derivatives in $\mathcal{L}$, its dimension is equal to 2. Therefore the interaction of this field component to the fermions has $\delta = 5$. The form of the propagator,

$$\frac{\eta_{\mu\nu} + p_\mu p_\nu/M^2}{p^2+M^2}$$

indeed behaves as $(p)^0$ for longitudinal components.

Problem 15.6 :
Consider a vector field A_μ coupled to a real scalar field ϕ and a spinor field ψ in four space-time dimensions, described by the Lagrangian

$$\mathcal{L} = -\tfrac{1}{4}(\partial_\mu A_\nu - \partial_\nu A_\mu)^2 - \tfrac{1}{2}(M/q)^2\left|(\partial_\mu - iqA_\mu)\mathrm{e}^{iq\phi/M}\right|^2 - \bar{\psi}(\partial\!\!\!/ - igA\!\!\!/ + m)\psi\,.$$

Show that the Lagrangain is invariant under gauge transformations, under which A_μ transforms according to $A_\mu \to A_\mu + \partial_\mu\xi$ and $\exp iq\phi/M$ en ψ under suitably chosen phase transformations. Here $\xi(x)$ is an arbitrary function of space and time. Give both phase transformations. Determine also how ϕ transforms.

Give now all terms quadratic in the fields A_μ and ϕ. Argue that the inverse propagator takes the form of a 5×5 matrix and determine this matrix. Does the propagator exist? (Try to motivate the answer in two different ways: both on the basis of the explicit matrix and on the basis of a more general argument.)

Argue that $\phi = 0$ is an admissable gauge condition. Determine now the propagator for A_μ. What are the fysical bosonic states of given momentum described by the resulting Lagrangian? (Note: we do not ask for a detailed derivation.)

Is the theory renormalizable by power counting and why (not)? Give the expression for the fermion self-energy diagram in the one-loop approximation (note that there is just one diagram different from zero) and determine the degree of divergence of the corresponding integral. What kind of counterterms do you expect to need to absorb the infinities of the integral? (Give qualitative arguments; do *not* calculate the integral or the coefficients of these counterterms.)

We now choose another gauge condition. Previously we imposed a gauge condition by adding a term $-\frac{1}{2}(\lambda\partial \cdot A)^2$ to the Lagrangian. Now we choose a modification of this term, namely

$$\mathcal{L}_{g.f.} = -\frac{1}{2}(\lambda\partial_\mu A^\mu + M\lambda^{-1}\phi)^2 \,.$$

Calculate again the propagators for A_μ and ϕ. What are in this case the physical bosonic states for given momentum described by the corresponding Lagrangian. Compare your result with your previous answer and give your comments.

In the last formulation is the theory renormalizable by power counting and why (not)? Give the expression for the fermion self-energy diagram in the one-loop approximation and determine again the degree of divergence of the integral. In this case, what are the counterterms that you need to absorb the infinities?

Determine the difference between the expressions for the fermion self-energy diagram in the two gauges on the mass shell, i.e. sandwiched between spinors that satisfy the Dirac equation $(i\not{p} + m)u = 0$ (this implies that $p^2 + m^2 = 0$). Did you expect this result and why (not)?

16 Further reading

Here we list a number of textbooks on quantum field theory. In the text we have referred a number of times to and occasionally used text from:

- B. de Wit and J. Smith, Field theory in particle physics (Elsevier, 1986).

This book is aimed at particle physics and is intended for experimentalists and beginning theorists. There are other many books on quantum field theory and applications, at various levels. For the convenience of the reader we present a list below:

- A.A. Abrikosov, L.P. Gorkov and I.E. Dzyaloshinskii, Quantum Field Theoretical Methods in Statistical Physics (second edition, Pergamon, Oxford, 1965).
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