Path Integrals in Quantum Mechanics

Dirk H. Rischke

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Contents

1 Summary

Lecture 1

Dick Feynman told me:"The electron does anything it likes . . . It just goes in any direction at any speed . . . however it likes, and then you add up the amplitude and it gives you the wave-function." I said to him: "You're crazy." But he wasn't.
Freeman Dyson

The method of **path integrals** presents an alternative way to describe quantum-mechanical and quantum field-theoretical systems. The underlying idea is that a quantum-mechanical particle may not only take the classical trajectory (which extremizes the action) from point $\vec{q}_a$ to point $\vec{q}_b$, but also all other possible trajectories, properly weighted with a complex phase. The quantum-mechanical transition amplitude is then given as "path integral", i.e., the coherent superposition of all these phase factors.

After a short reminder on the dynamics of classical and quantum-mechanical particles given in Chap. 2, in Chap. 3 we will derive the path-integral representation of the quantum-mechanical transition amplitude. We will then explain the connection between the transition amplitude and the Green's function, or propagator, of the Schrödinger equation. A discussion of external gauge fields, which couple to the quantum-mechanical particle, will reveal some peculiar aspects of the path integral. In particular, it will become clear that the latter consists mostly of trajectories which resemble Brownian motion and require a careful treatment when evaluating certain quantities on these trajectories.

In Chap. 4 a few applications will be discussed. We will explicitly compute the propagator of the free Schrödinger equation, and with this in hand, discuss the famous double-slit experiment and the resulting interference pattern, which is a result of the wave nature of the quantum-mechanical particle. In general, the propagator cannot be computed exactly, but in many cases the semiclassical approximation for the propagator has proven useful, for which an analytic expression can be derived. This expression is exact for potential energies which are quadratic in the particle coordinate, e.g., the harmonic oscillator, which is discussed subsequently. The chapter closes with a discussion of the anharmonic oscillator.

Chapter 5 gives an introduction to perturbation theory. First, the Born series for the propagator is presented, followed by a discussion of the scattering matrix and the Feynman-diagram technique. Finally, the generating functional for n–point correlation functions is derived, which is the central object in Quantum Field Theory.

In order to proceed to Quantum Field Theory, Chap. 6 gives a brief discussion on how to make the transition from a classical system of N particles to classical field theory, i.e., a system where $N \to \infty$. The central object is the Lagrange density or Lagrangian, which

defines any given theory. A variational principle allows to derive the classical equation of motion for fields.

The Lagrangian is also the central object for Quantum Field Theory in the functional-integral formulation, as will be explained in Chap. 7. After a brief discussion of non-interacting Klein–Gordon theory as the simplest conceivable field theory, the generating functional for n–point correlation function of this theory is derived in the form of a functional integral, and then explicitly computed. Finally, $\lambda\phi^4$ as an example of an interacting field theory is presented and it is explained how to apply perturbation theory to compute the generating functional. The final Chapter 8 gives a brief discussion how the partition function of Statistical Field Theory can be formulated in terms of a functional integral.

2 Dynamics of Particles

2.1 Dynamics of classical particles

2.1.1 Hamilton's principle

From Classical Mechanics we know that, in classical physics, the dynamics of a particle can be described using **Hamilton's action principle**,

$$\delta S[\vec{q}(t)] = 0 \ , \tag{2.1}$$

where

$$S[\vec{q}(t)] = \int_{t_a}^{t_b} \mathrm{d}t \, L(\vec{q}, \dot{\vec{q}}, t) \tag{2.2}$$

is the **action** along the trajectory of a particle, which is traversed during the time interval $[t_a, t_b]$, and $L(\vec{q}, \dot{\vec{q}}, t)$ represents the **Lagrange function** of the system. Here $\vec{q}$ denotes the vector of the (generalized) coordinates of the particle and $\dot{\vec{q}}$ is the corresponding velocity vector.

Hamilton's principle (2.1) tells us that the actually traversed trajectory corresponds to an **extremum** of the action (2.2). In order to determine the latter, one compares the action for a **competing set** of trajectories in coordinate space, cf. Fig. 2.1. The competing set consists of all trajectories with **fixed initial and final coordinates** $\vec{q}(t_a) \equiv \vec{q}_a$, $\vec{q}(t_b) \equiv \vec{q}_b$. The **classical trajectory** is the one which makes the action stationary (extremizes the action).

According to the laws of variational calculus, Eq. (2.1) leads to the **Euler–Lagrange equations**

$$0 = \frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial L(\vec{q}, \dot{\vec{q}}, t)}{\partial \dot{q}_i} - \frac{\partial L(\vec{q}, \dot{\vec{q}}, t)}{\partial q_i} \ , \quad i = x, y, z \ , \tag{2.3}$$

which are completely equivalent to Newton's equations of motion. If the initial conditions

$$\vec{q}_a \equiv \vec{q}(t_a) \ , \quad \dot{\vec{q}}_a \equiv \dot{\vec{q}}(t_a) \ ,$$

are known, one can determine the position $\vec{q}(t_b)$ and the velocity $\dot{\vec{q}}(t_b)$ of the particle at any later time t_b by solving the Euler–Lagrange equations. This **uniqely** determines the **trajectory** $\vec{q}(t)$ which the particle takes and for which one computes the action (2.2).

2.1.2 Modified Hamilton's principle

The **modified Hamilton's principle** is a formulation which constitutes an alternative to Hamilton's principle,

$$0 = \delta S[\vec{q}(t), \vec{p}(t)] = \delta \int_{t_a}^{t_b} \mathrm{d}t \, \left[\vec{p} \cdot \dot{\vec{q}} - H(\vec{q}, \vec{p}, t) \right] \ , \tag{2.4}$$

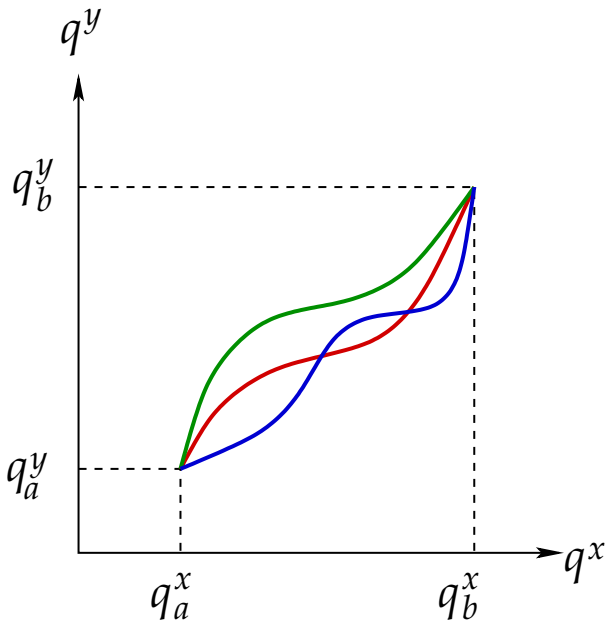


Figure 2.1: Competing set of trajectories in the projection of coordinate space onto the (q^x, q^y) plane.

Here one replaces the Lagrange function in Eq. (2.2) by its Legendre transform,

$$L(\vec{q}, \dot{\vec{q}}, t) = \vec{p} \cdot \dot{\vec{q}} - H(\vec{q}, \vec{p}, t) \ , \tag{2.5}$$

with the **Hamilton function** $H(\vec{q}, \vec{p}, t)$. In contrast to Hamilton's principle one now considers a competing set of trajectories in **phase space**, cf. Fig. 2.2. Note that the coordinates of the initial and final point are fixed, $\vec{q}(t_a) \equiv \vec{q}_a$, $\vec{q}(t_b) \equiv \vec{q}_b$, but the values $\vec{p}(t_a)$, $\vec{p}(t_b)$ of the momentum can vary freely.

The classical trajectory is that which fulfills the **canonical equations**

$$\dot{q}_i = \frac{\partial H(\vec{q}, \vec{p}, t)}{\partial p_i} \ , \quad \dot{p}_i = -\frac{\partial H(\vec{q}, \vec{p}, t)}{\partial q_i} \ , \quad i = x, y, z \ , \tag{2.6}$$

which are completely equivalent to the Euler–Lagrange equations (2.3).

2.2 Dynamics of quantum-mechanical particles

According to Heisenberg's uncertainty principle, in quantum mechanics one cannot simultaneously determine position and velocity (or momentum) of a particle. The central quantity is now the **quantum-mechanical overlap**

$$\langle \vec{q}_b, t_b | \vec{q}_a, t_a \rangle \ , \tag{2.7}$$

which corresponds to the **amplitude** for a **transition** from state $|\vec{q}_a, t_a\rangle$ at time t_a to a state $|\vec{q}_b, t_b\rangle$ at time t_b. The modulus square of the transition amplitude,

$$|\langle \vec{q}_b, t_b | \vec{q}_a, t_a \rangle|^2 \tag{2.8}$$

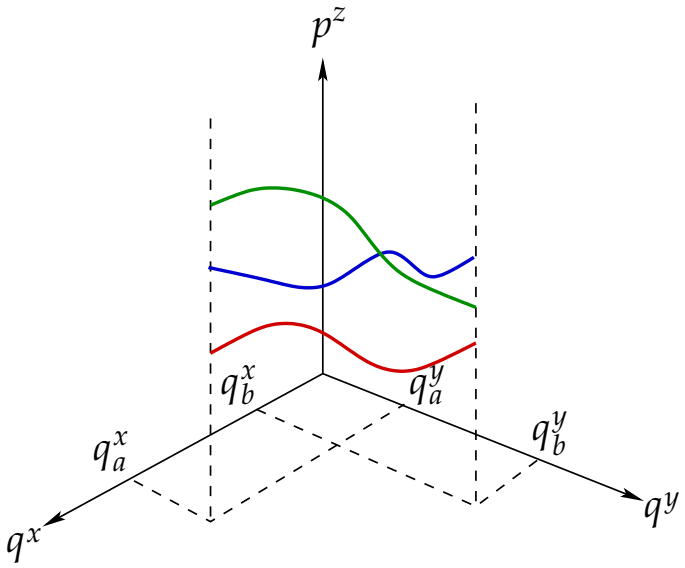


Figure 2.2: Competing set of trajectories in the projection of phase space onto the three-dimensional (q^x, q^y, p^z) subspace.

determines the **probability** for such a transition. In other words, it is the probability to find the particle at time t_b at position $\vec{q}_b$, if it was located at position $\vec{q}_a$ at time t_a.

We now want to write the amplitude (2.7) in a somewhat different form. The **time-evolution operator** is

$$\hat{U}(t, t_0) = \hat{T} \exp\left[-\frac{i}{\hbar}\int_{t_0}^{t} \mathrm{d}t'\, \hat{H}(t')\right] . \tag{2.9}$$

Let the Schrödinger state $|\psi(t)\rangle_S$ at time t_0 be identical with the corresponding Heisenberg state $|\psi\rangle_H$,

$$|\psi(t_0)\rangle_S = |\psi\rangle_H .$$

Using the time-evolution operator (2.9) the time evolution of this state reads

$$|\psi(t)\rangle_S = \hat{U}(t, t_0)\,|\psi(t_0)\rangle_S \equiv \hat{U}(t, t_0)\,|\psi\rangle_H .$$

The corresponding **wave function** follows by projection onto a coordinate-space state,

$$\psi(\vec{q}, t) \equiv \langle\vec{q}|\psi(t)\rangle_S = \langle\vec{q}|\,\hat{U}(t, t_0)\,|\psi\rangle_H \equiv \langle\vec{q}, t|\psi\rangle_H ,$$

where we introduced the **time-dependent coordinate-space state**

$$|\vec{q}, t\rangle \equiv \hat{U}(t_0, t)\,|\vec{q}\rangle , \tag{2.10}$$

noting that $\hat{U}^\dagger(t, t_0) = \hat{U}(t_0, t)$. With this we can now write the amplitude (2.7) as follows:

$$\begin{aligned} \langle\vec{q}_b, t_b|\vec{q}_a, t_a\rangle &= \langle\vec{q}_b|\,\hat{U}^\dagger(t_0, t_b)\,\hat{U}(t_0, t_a)\,|\vec{q}_a\rangle = \langle\vec{q}_b|\,\hat{U}(t_b, t_0)\,\hat{U}(t_0, t_a)\,|\vec{q}_a\rangle \\ &\equiv \langle\vec{q}_b|\,\hat{U}(t_b, t_a)\,|\vec{q}_a\rangle , \end{aligned} \tag{2.11}$$

where we used the convolution property

$$\hat{U}(t_b, t_0)\,\hat{U}(t_0, t_a) \equiv \hat{U}(t_b, t_a) \tag{2.12}$$

of the time-evolution operator. Equation (2.11) is the starting point for deriving the so-called **path-integral formula** of the quantum-mechanical transition amplitude (2.7), as will be explained in the next chapter.

3 Path Integrals

3.1 Path integrals in phase space

We decompose the time interval $[t_a, t_b]$ into N pieces of equal length τ, $t_b - t_a = N\,\tau$, so that

$$t_n = t_a + n\tau \;, \quad n = 0, \ldots, N \;, \quad t_0 = t_a \;, \;\; t_N = t_b \;.$$

Using the convolution property (2.12) we write

$$\hat{U}(t_b, t_a) = \hat{U}(t_b, t_{N-1})\,\hat{U}(t_{N-1}, t_{N-2}) \cdots \hat{U}(t_2, t_1)\,\hat{U}(t_1, t_a) \equiv \prod_{n=1}^{N} \hat{U}(t_n, t_{n-1}) \;, \tag{3.1}$$

so that Eq. (2.11) assumes the form

$$\langle \vec{q}_b, t_b | \vec{q}_a, t_a \rangle = \langle \vec{q}_b | \prod_{n=1}^{N} \hat{U}(t_n, t_{n-1})\,|\vec{q}_a\rangle \;. \tag{3.2}$$

We now insert to the left of each time-evolution operator a complete set of coordinate-space eigenstates and to the right a complete set of momentum eigenstates. In order to distinguish the individual sets, we label them with an index corresponding to the respective time step t_n,

$$\mathbb{1} = \int \mathrm{d}^3\vec{q}_n\,|\vec{q}_n\rangle\langle\vec{q}_n| \;, \quad \mathbb{1} = \int \mathrm{d}^3\vec{p}_n\,|\vec{p}_n\rangle\langle\vec{p}_n| \;, \quad n = 1, \ldots, N \;. \tag{3.3}$$

Then it follows from Eq. (3.2) that

$$\begin{aligned} \langle \vec{q}_b, t_b | \vec{q}_a, t_a \rangle \;\; &= \;\; \int \left[\prod_{n=1}^{N} \mathrm{d}^3\vec{q}_n\,\mathrm{d}^3\vec{p}_n \right] \langle \vec{q}_b | \vec{q}_N \rangle \langle \vec{q}_N |\, \hat{U}(t_N, t_{N-1})\,|\vec{p}_N\rangle \langle \vec{p}_N | \vec{q}_{N-1}\rangle \\ &\times \;\; \langle \vec{q}_{N-1} |\, \hat{U}(t_{N-1}, t_{N-2})\,|\vec{p}_{N-1}\rangle \langle \vec{p}_{N-1} | \vec{q}_{N-2}\rangle \;\cdots\; \langle \vec{q}_1 |\, \hat{U}(t_1, t_a)\,|\vec{p}_1\rangle \langle \vec{p}_1 | \vec{q}_a\rangle \;. \end{aligned} \tag{3.4}$$

For $N \to \infty$ the time intervals τ become infinitesimally small, $\tau \to 0$, so that one can approximate the integral in the exponent of the time-evolution operator according to the mean-value theorem of integral calculus,

$$\int_{t_{n-1}}^{t_n} \mathrm{d}t'\,\hat{H}(t') = \tau\,\hat{H}\,(t_{n-1} + \lambda\,\tau) + O(\tau^2) \;, \quad \lambda \in [0, 1] \;.$$

In this limit, one can also expand the exponential to leading order in τ

$$\hat{U}(t_n, t_{n-1}) = \hat{T}\,\exp\left[-\frac{i}{\hbar} \int_{t_{n-1}}^{t_n} \mathrm{d}t'\,\hat{H}(t') \right] = \mathbb{1} - \frac{i\,\tau}{\hbar}\,\hat{H}\,(t_{n-1} + \lambda\,\tau) + O(\tau^2) \;. \tag{3.5}$$

The time-ordering operator plays no role if we terminate the expansion of the exponential function after the linear term in τ. The matrix elements of the time-evolution operator appearing in Eq. (3.4) then assume the following form:

$$\langle \vec{q}_n | \, \hat{U}(t_n, t_{n-1}) \, | \vec{p}_n \rangle = \langle \vec{q}_n | \vec{p}_n \rangle - \frac{i\,\tau}{\hbar} \, \langle \vec{q}_n | \, \hat{H} \, (t_{n-1} + \lambda\,\tau) \, | \vec{p}_n \rangle + O(\tau^2) \; . \tag{3.6}$$

Usually the Hamilton operator is a function of the momentum and the position operator,

$$\hat{H}(t) \equiv H(\hat{\vec{q}}, \hat{\vec{p}}, t) \; .$$

The matrix element of the Hamilton operator between momentum and coordinate-space eigenstates is then simply the **expectation value** of the Hamilton operator,

$$\langle \vec{q}_n | \, \hat{H} \, (t_{n-1} + \lambda\,\tau) \, | \vec{p}_n \rangle \equiv H(\vec{q}_n, \vec{p}_n, t_{n-1} + \lambda\,\tau) \, \langle \vec{q}_n | \vec{p}_n \rangle \; . \tag{3.7}$$

Putting all this together we obtain for Eq. (3.6)

$$\begin{aligned} \langle \vec{q}_n | \, \hat{U}(t_n, t_{n-1}) \, | \vec{p}_n \rangle &= \left[1 - \frac{i\,\tau}{\hbar} \, H(\vec{q}_n, \vec{p}_n, t_{n-1} + \lambda\,\tau) + O(\tau^2) \right] \, \langle \vec{q}_n | \vec{p}_n \rangle \\ &= \exp\left(-\frac{i\,\tau}{\hbar} \, H_n \right) \, \langle \vec{q}_n | \vec{p}_n \rangle \; , \end{aligned} \tag{3.8}$$

where we reversed the expansion of the exponential function in the last step and abbreviated

$$H_n \equiv H(\vec{q}_n, \vec{p}_n, t_{n-1} + \lambda\,\tau) \; .$$

Note that the exponent in Eq. (3.8) is just a **function** and no longer operator-valued.

As is known from the lectures on Quantum Mechanics, the quantum-mechanical overlap of momentum and coordinate-space eigenstates are plane waves,

$$\langle \vec{q}_n | \vec{p}_m \rangle = \frac{1}{\sqrt{2\pi\hbar}^3} \, \exp\left(\frac{i}{\hbar} \, \vec{q}_n \cdot \vec{p}_m \right) \; . \tag{3.9}$$

If we insert Eqs. (3.8) and (3.9) into Eq. (3.4), we obtain with

$$\langle \vec{q}_b | \vec{q}_N \rangle = \delta^{(3)}(\vec{q}_b - \vec{q}_N)$$

the expression

$$\begin{aligned} \langle \vec{q}_b, t_b | \vec{q}_a, t_a \rangle &= \int \prod_{n=1}^{N} \frac{\mathrm{d}^3\vec{q}_n \, \mathrm{d}^3\vec{p}_n}{(2\pi\hbar)^3} \, \delta^{(3)}(\vec{q}_b - \vec{q}_N) \, \exp\left\{ \frac{i}{\hbar} \left[(\vec{q}_N - \vec{q}_{N-1}) \cdot \vec{p}_N - \tau\, H_N \right.\right. \\ &\quad \left.\left. + (\vec{q}_{N-1} - \vec{q}_{N-2}) \cdot \vec{p}_{N-1} - \tau\, H_{N-1} + \; \cdots \; + (\vec{q}_1 - \vec{q}_a) \cdot \vec{p}_1 - \tau\, H_1 \right] \right\} \\ &= \int \prod_{n=1}^{N-1} \mathrm{d}^3\vec{q}_n \prod_{n=1}^{N} \frac{\mathrm{d}^3\vec{p}_n}{(2\pi\hbar)^3} \, \exp\left[\frac{i}{\hbar} \sum_{n=1}^{N} \tau \left(\frac{\vec{q}_n - \vec{q}_{n-1}}{\tau} \cdot \vec{p}_n - H_n \right) \right] \; , \end{aligned} \tag{3.10}$$

where we have set $\vec{q}_0 \equiv \vec{q}_a$ and $\vec{q}_N \equiv \vec{q}_b$. In the limit $N \to \infty$, $\tau \to 0$ we have

$$\sum_{n=1}^{N} \tau \;\longrightarrow\; \int_{t_a}^{t_b} \mathrm{d}t \;, \quad \frac{\vec{q}_n - \vec{q}_{n-1}}{\tau} \;\longrightarrow\; \frac{\mathrm{d}\vec{q}}{\mathrm{d}t} \equiv \dot{\vec{q}} \;, \tag{3.11}$$

so that

$$\langle \vec{q}_b, t_b | \vec{q}_a, t_a \rangle \;\longrightarrow\; \int_{\vec{q}(t_a)=\vec{q}_a}^{\vec{q}(t_b)=\vec{q}_b} \mathcal{D}\vec{q}\mathcal{D}\vec{p}\, \exp\left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} \mathrm{d}t \, \left[\vec{p}\cdot\dot{\vec{q}} - H(\vec{q},\vec{p},t) \right] \right\} \;. \tag{3.12}$$

Here we introduced the symbolic notation

$$\mathcal{D}\vec{q} \equiv \lim_{N\to\infty} \prod_{n=1}^{N-1} \mathrm{d}^3\vec{q} \;, \quad \mathcal{D}\vec{p} \equiv \lim_{N\to\infty} \prod_{n=1}^{N} \frac{\mathrm{d}^3\vec{p}}{(2\pi\hbar)^3} \;. \tag{3.13}$$

Equation (3.12) is the so-called **path-integral** or **functional-integral representation** of the quantum-mechanical transition amplitude. It states that **every possible** trajectory $(\vec{q}(t), \vec{p}(t))$ in **phase space**, which leads from position $\vec{q}_a = \vec{q}(t_a)$ to position $\vec{q}_b = \vec{q}(t_b)$ for arbitrary values of the momenta $\vec{p}_a = \vec{p}(t_a)$ and $\vec{p}_b = \vec{p}(t_b)$, is weighted with a phase factor

$$\exp\left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} \mathrm{d}t \, \left[\vec{p}\cdot\dot{\vec{q}} - H(\vec{q},\vec{p},t) \right] \right\} \;, \tag{3.14}$$

and then one sums (integrates) over all trajectories. This situation corresponds to that which we already encountered in the discussion of the **modified Hamilton's principle** in Sec. 2.1.2. According to Eq. (2.4), the **classical trajectory** corresponds to that for which the argument of the phase factor (3.14) becomes **stationary** (or is extremized). However, in **quantum mechanics** also all other possible trajectories are allowed.

3.2 Path integrals in coordinate space

If the Hamilton operator is a quadratic function of the momentum operator,

$$\hat{H}(t) = \frac{\hat{\vec{p}}^{\,2}}{2m} + V(\hat{\vec{q}}, t) \;, \tag{3.15}$$

the (infinitely many) momentum integrations in Eq. (3.12) can be performed exactly, since they are just (shifted) Gaussian integrals. In order to see this, we consider Eq. (3.10) and insert Eq. (3.15)

$$H_n = H(\vec{q}_n, \vec{p}_n, t_{n-1} + \lambda\,\tau) = \frac{\vec{p}_n^{\,2}}{2m} + V(\vec{q}_n, t_{n-1} + \lambda\,\tau) \;.$$

Completing the square leads to

$$\frac{\vec{p}_n^{\,2}}{2m} - \frac{\vec{q}_n - \vec{q}_{n-1}}{\tau}\cdot\vec{p}_n = \frac{1}{2m}\left(\vec{p}_n - m\,\frac{\vec{q}_n - \vec{q}_{n-1}}{\tau} \right)^2 - \frac{m}{2}\left(\frac{\vec{q}_n - \vec{q}_{n-1}}{\tau} \right)^2 \;. \tag{3.16}$$

If we substitute the integration variable

$$\vec{p}_n \longrightarrow \vec{p}_n' = \vec{p}_n - m\,\frac{\vec{q}_n - \vec{q}_{n-1}}{\tau}\ ,$$

we realize that all momentum integrals decouple and, since they are Gaussian integrals, can be immediately computed with the help of the well-known formula

$$\int_{-\infty}^{\infty} \mathrm{d}x\, e^{-ax^2} = \sqrt{\frac{\pi}{a}}\ , \quad a > 0\ , \tag{3.17}$$

resulting in

$$\int \frac{\mathrm{d}^3\vec{p}_n'}{(2\pi\hbar)^3}\, \exp\left(-\frac{i\,\tau}{\hbar}\,\frac{\vec{p}_n'^{\,2}}{2m}\right) = \left[\int_{-\infty}^{\infty} \frac{\mathrm{d}p}{2\pi\hbar}\, \exp\left(-\frac{i\,\tau}{2m\hbar}\,p^2\right)\right]^3 = \sqrt{\frac{m}{2\pi i\tau\hbar}}^{\,3}\ . \tag{3.18}$$

Here a remark is in order. Because of the factor i in the exponent this is actually not a true Gaussian integral in the sense of Eq. (3.17). However, with the help of Euler's formula, some results from integral tables [5], as well as $\cos\frac{\pi}{4} = \sin\frac{\pi}{4} = 1/\sqrt{2}$ we obtain the same result as in Eq. (3.17):

$$\begin{aligned}\int_{-\infty}^{\infty} \mathrm{d}x\, e^{-iax^2} &= \int_{-\infty}^{\infty} \mathrm{d}x\, \cos(ax^2) - i\int_{-\infty}^{\infty} \mathrm{d}x\, \sin(ax^2) \\ &= \sqrt{\frac{\pi}{2a}}\,(1-i) = \sqrt{\frac{\pi}{a}}\left(\cos\frac{\pi}{4} - i\sin\frac{\pi}{4}\right) = \sqrt{\frac{\pi}{a}}\,e^{-i\pi/4} = \sqrt{\frac{\pi}{ia}}\ .\end{aligned} \tag{3.19}$$

With the remaining term from completing the square, cf. Eq. (3.16), we obtain for Eq. (3.10)

$$\begin{aligned}\langle \vec{q}_b, t_b | \vec{q}_a, t_a\rangle &= \sqrt{\frac{m}{2\pi i\tau\hbar}}^{\,3N} \int \prod_{n=1}^{N-1} \mathrm{d}^3\vec{q}_n \\ &\times\ \exp\left\{\frac{i}{\hbar}\sum_{n=1}^{N}\tau\left[\frac{m}{2}\left(\frac{\vec{q}_n - \vec{q}_{n-1}}{\tau}\right)^2 - V(\vec{q}_n, t_{n-1} + \lambda\,\tau)\right]\right\}\ .\end{aligned} \tag{3.20}$$

In the limit $N \to \infty$, $\tau \to 0$ this becomes with the help of Eq. (3.11)

$$\begin{aligned}\langle \vec{q}_b, t_b | \vec{q}_a, t_a\rangle &\longrightarrow \mathcal{N}\int_{\vec{q}(t_a)=\vec{q}_a}^{\vec{q}(t_b)=\vec{q}_b} \mathcal{D}\vec{q}\, \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b} \mathrm{d}t\, \left[\frac{m}{2}\,\dot{\vec{q}}^{\,2} - V(\vec{q},t)\right]\right\} \\ &\equiv \mathcal{N}\int_{\vec{q}(t_a)=\vec{q}_a}^{\vec{q}(t_b)=\vec{q}_b} \mathcal{D}\vec{q}\, \exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b} \mathrm{d}t\, L(\vec{q},\dot{\vec{q}},t)\right] \\ &\equiv \mathcal{N}\int_{\vec{q}(t_a)=\vec{q}_a}^{\vec{q}(t_b)=\vec{q}_b} \mathcal{D}\vec{q}\, \exp\left\{\frac{i}{\hbar}\,S[\vec{q}(t)]\right\}\ ,\end{aligned} \tag{3.21}$$

where we used the Lagrange function

$$L(\vec{q},\dot{\vec{q}},t) = \frac{m}{2}\,\dot{\vec{q}}^{\,2} - V(\vec{q},t) \tag{3.22}$$

and the definition (2.2) of the action. The normalization constant

$$\mathcal{N} = \lim_{\substack{N \to \infty \\ \tau \to 0}} \sqrt{\frac{m}{2\pi i \tau \hbar}}^{3N}$$

is in principle not well defined, but this does matter since we can always renormalize the transition amplitude by multiplying with a constant phase factor. Equation (3.21) is the **path-integral representation** of the quantum-mechanical transition amplitude in **coordinate space**. It tells us that we must weigh **every** trajectory $\vec{q}(t)$ with the phase factor $e^{iS[\vec{q}(t)]/\hbar}$ and then sum (integrate) over **all possible** trajectories in coordinate space. The situation is illustrated in Fig. 3.1. All possible trajectories connecting the fixed initial point $\vec{q}_a$ at time t_a with the fixed final point $\vec{q}_b$ at time t_b are allowed. According to Hamilton's principle (2.1), the **classical trajectory** corresponds to that which makes the action **stationary** (or extremizes it). However, **quantum mechanically** also all other possible trajectories are allowed.

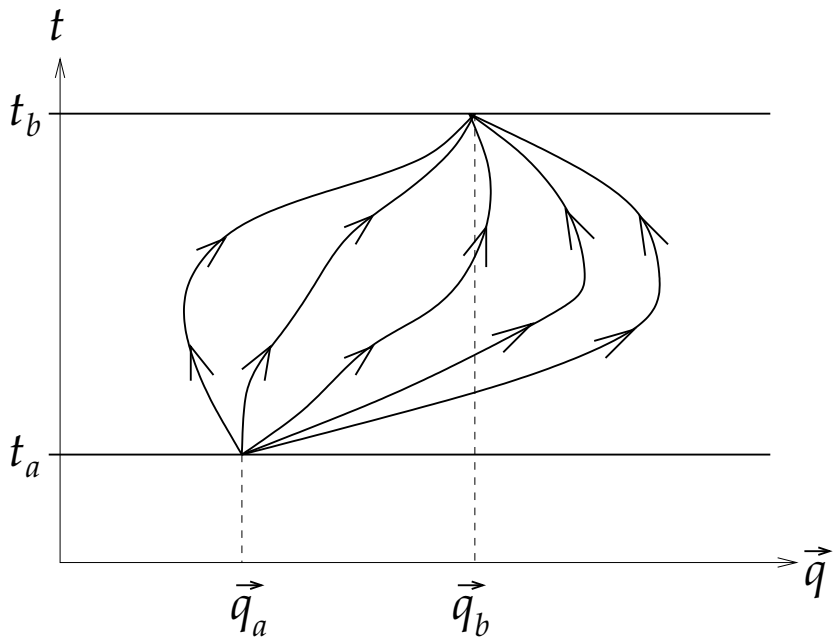


Figure 3.1: Visualization of the path integral in the space-time diagram.

Of central importance in weighing the individual trajectories is the question how large the action on a given trajectory is compared to Planck's quantum of action $\hbar$. In the limit $\hbar \to 0$ the ratio $S[\vec{q}(t)]/\hbar$ becomes arbitrarily large. The phase factors on trajectories away from the classical trajectory, where $S[\vec{q}(t)]$ becomes stationary (and usually assumes a minimum), can thus assume arbitrary (complex) values (of modulus one). The contributions of these trajectories in the path integral (3.21) mutually cancel. In contrast, in the vicinity of the classical trajectory the phase factors all assume similar values due to the stationarity of the action. Thus, only contributions from trajectories near the classical one "survive". Therefore, the limit $\hbar \to 0$ corresponds to the **classical limit**.

3.3 Transition amplitude and Green's function

Let us consider the **free** time-dependent Schrödinger equation,

$$0 = \left(i\hbar \frac{\partial}{\partial t} - \hat{H}_0 \right) \psi(\vec{q}, t) \; , \tag{3.23}$$

where

$$\hat{H}_0 \equiv -\frac{\hbar^2}{2m} \Delta_q \tag{3.24}$$

is the **free** Hamilton operator. This is a **homogeneous** wave equation, which can be solved by Fourier decomposition,

$$\psi(\vec{q}, t) = \frac{1}{(2\pi)^4} \int \mathrm{d}\omega \, \mathrm{d}^3\vec{k} \, \tilde{\psi}(\omega, \vec{k}) \, e^{-i(\omega t - \vec{k}\cdot\vec{q})} \; . \tag{3.25}$$

If we insert this into the Schrödinger equation (3.23), we obtain

$$0 = \frac{1}{(2\pi)^4} \int \mathrm{d}\omega \, \mathrm{d}^3\vec{k} \left(\hbar\,\omega - \frac{\hbar^2 \vec{k}^{\,2}}{2m} \right) \tilde{\psi}(\omega, \vec{k}) \, e^{-i(\omega t - \vec{k}\cdot\vec{q})} \; .$$

Since plane waves constitute a complete and orthogonal function system, this can only vanish if the term in parentheses vanishes, i.e., if the **dispersion relation**

$$\hbar\,\omega(\vec{k}) = \frac{\hbar^2 \vec{k}^{\,2}}{2m} \tag{3.26}$$

holds. We take this into account in the Fourier decomposition (3.25) by making the Ansatz

$$\tilde{\psi}(\omega, \vec{k}) = \tilde{\psi}(\vec{k}) \, \delta(\omega - \omega(\vec{k})) \tag{3.27}$$

for the Fourier coefficients. We obtain

$$\psi(\vec{q}, t) = \frac{1}{(2\pi)^4} \int \mathrm{d}\omega \, \mathrm{d}^3\vec{k} \, \tilde{\psi}(\vec{k}) \, \delta(\omega - \omega(\vec{k})) \, e^{-i(\omega t - \vec{k}\cdot\vec{q})} = \frac{1}{(2\pi)^4} \int \mathrm{d}^3\vec{k} \, \tilde{\psi}(\vec{k}) \, e^{-i(\omega(\vec{k})t - \vec{k}\cdot\vec{q})} \; . \tag{3.28}$$

The coefficients $\tilde{\psi}(\vec{k})$ can be determined from the initial conditions,

$$\psi(\vec{q}, 0) = \frac{1}{(2\pi)^4} \int \mathrm{d}^3\vec{k} \, \tilde{\psi}(\vec{k}) \, e^{i\vec{k}\cdot\vec{q}} \; , \tag{3.29}$$

i.e., after Fourier transformation

$$\begin{aligned} \int \mathrm{d}^3\vec{q} \, e^{-i\vec{p}\cdot\vec{q}} \, \psi(\vec{q}, 0) &= \frac{1}{(2\pi)^4} \int \mathrm{d}^3\vec{k} \, \tilde{\psi}(\vec{k}) \int \mathrm{d}^3\vec{q} \, e^{i(\vec{k}-\vec{p})\cdot\vec{q}} \\ &= \frac{1}{(2\pi)^4} \int \mathrm{d}^3\vec{k} \, \tilde{\psi}(\vec{k}) \, (2\pi)^3 \delta^{(3)}(\vec{k} - \vec{p}) \\ &= \frac{1}{2\pi} \, \tilde{\psi}(\vec{p}) \; , \end{aligned}$$

or

$$\tilde{\psi}(\vec{k}) = 2\pi \int \mathrm{d}^3\vec{q}\, e^{-i\vec{k}\cdot\vec{q}}\, \psi(\vec{q},0)\ . \tag{3.30}$$

If we insert this into Eq. (3.28), we obtain

$$\psi(\vec{q},t) = \frac{1}{(2\pi)^3} \int \mathrm{d}^3\vec{k} \int \mathrm{d}^3\vec{r}\ e^{-i\omega(\vec{k})t + i\vec{k}\cdot(\vec{q}-\vec{r})}\, \psi(\vec{r},0)\ . \tag{3.31}$$

We define the function

$$G(\vec{q},t;\vec{r},0) \equiv \frac{1}{(2\pi)^3} \int \mathrm{d}^3\vec{k}\, e^{-i\omega(\vec{k})t + i\vec{k}\cdot(\vec{q}-\vec{r})}\ . \tag{3.32}$$

Then, Eq. (3.31) can be written as

$$\psi(\vec{q},t) = \int \mathrm{d}^3\vec{r}\, G(\vec{q},t;\vec{r},0)\, \psi(\vec{r},0)\ . \tag{3.33}$$

The physical interpretation of this equation is that the initial condition $\psi(\vec{r},0)$ is "propagated" to the time t and position $\vec{q}$ via the function $G(\vec{q},t;\vec{r},0)$. One should note that one has to integrate over all $\vec{r}$ at initial time $t = 0$. A graphical visualization is shown in Fig. 3.2.

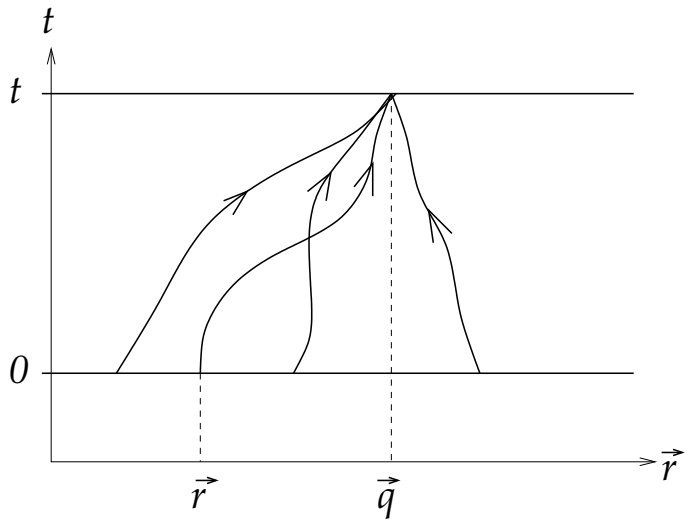


Figure 3.2: Propagation of the initial condition $\psi(\vec{r},0)$ at time $t = 0$ and all positions $\vec{r}$ with the help of the propagator $G(\vec{q},t;\vec{r},0)$.

This is very similar to the discussion of wave propagation in Classical Electrodynamics. For this reason, $G(\vec{q},t;\vec{r},0)$ is also called **propagator**. This function is actually a **Green's function**, because if we act with the free Schrödinger operator

$$i\hbar\frac{\partial}{\partial t} - \hat{H}_0$$

onto the result (3.33), we obtain

$$\left(i\hbar\,\frac{\partial}{\partial t}-\hat{H}_0\right)\psi(\vec{q},t)=\int \mathrm{d}^3\vec{r}\,\left(i\hbar\,\frac{\partial}{\partial t}-\hat{H}_0\right)G(\vec{q},t;\vec{r},0)\,\psi(\vec{r},0)\;.$$

Since $\psi(\vec{q},t)$ is supposed to be a solution of the free Schrödinger equation (3.23) for all times $t>0$, the right-hand side has to vanish. This is fulfilled if

$$\left(i\hbar\,\frac{\partial}{\partial t}-\hat{H}_0\right)G(\vec{q},t;\vec{r},0)=\delta(t)\,\delta^{(3)}(\vec{q}-\vec{r})\;, \tag{3.34}$$

since then

$$\left(i\hbar\,\frac{\partial}{\partial t}-\hat{H}_0\right)\psi(\vec{q},t)=\delta(t)\,\psi(\vec{q},0)=0\quad\forall\,t>0\;.$$

Equation (3.34) is just the defining equation for the Green's function of the Schrödinger equation.

In Eq. (3.33) we can relabel coordinates and times,

$$\psi(\vec{q}_b,t_b)=\int \mathrm{d}^3\vec{q}_a\,G(\vec{q}_b,t_b;\vec{q}_a,t_a)\,\psi(\vec{q}_a,t_a)\;. \tag{3.35}$$

We now show that the transition amplitude (2.7) is identical to the **Green's function** (3.32) of the Schrödinger equation. To this end, we relate the wave function at position $\vec{q}_b$ and time t_b to the wave function at position Ort $\vec{q}_a$ and time t_a by inserting a complete set of states,

$$\mathbb{1}=\int \mathrm{d}^3\vec{q}_a\,|\vec{q}_a,t_a\rangle\,\langle\vec{q}_a,t_a|\;, \tag{3.36}$$

to obtain

$$\psi(\vec{q}_b,t_b)=\langle\vec{q}_b,t_b|\psi\rangle_H=\int \mathrm{d}^3\vec{q}_a\,\langle\vec{q}_b,t_b|\vec{q}_a,t_a\rangle\,\langle\vec{q}_a,t_a|\psi\rangle_H=\int \mathrm{d}^3\vec{q}_a\,\langle\vec{q}_b,t_b|\vec{q}_a,t_a\rangle\,\psi(\vec{q}_a,t_a)\;. \tag{3.37}$$

The comparison with Eq. (3.35) yields

$$G(\vec{q}_b,t_b;\vec{q}_a,t_a)\equiv\langle\vec{q}_b,t_b|\vec{q}_a,t_a\rangle\;,\quad\text{q.e.d.} \tag{3.38}$$

The transition amplitude is thus nothing but the **propagator** or the **Green's function** of the Schrödinger equation. In Sec. 4.1, we will also prove this by an explicit calculation for the free case, $V(\vec{q},t)=0$.

Lecture 2

3.4 Gauge fields

Let us consider a particle in an electromagnetic field. As is well-known from the lectures on Classical Electrodynamics, the electric and magnetic fields can be written as

$$\vec{E}(\vec{q},t)=-\vec{\nabla}\varphi(\vec{q},t)-\partial_t\vec{A}(\vec{q},t)\;, \tag{3.39}$$

$$\vec{B}(\vec{q},t)=\vec{\nabla}\times\vec{A}(\vec{q},t)\;, \tag{3.40}$$

where $\varphi(\vec{q},t)$ is the so-called "scalar" potential and $\vec{A}(\vec{q},t)$ is the vector potential. A non-vanishing scalar potential is in principle already included in our previous discussion, as in this case the potential energy is simply

$$V(\vec{q},t) \equiv \mathfrak{q}\varphi(\vec{q},t) \;, \tag{3.41}$$

where $\mathfrak{q}$ is the electric charge of the particle. However, a non-vanishing vector potential $\vec{A}$ requires changes to the previous discussion. As is well-known from the lectures on Classical Mechanics, in this case the Hamilton function reads

$$H(\vec{q},\vec{p},t) = \frac{1}{2m}\,\left[\vec{p} - \mathfrak{q}\,\vec{A}(\vec{q},t)\right]^2 + V(\vec{q},t) \;. \tag{3.42}$$

How does this change the path-integral representation (3.20) of the transition amplitude? As one can readily convince oneself, the discussion is unaffected until Eq. (3.10). The modifications occur when integrating out the momenta. Completing the square, cf. Eq. (3.16), now reads

$$\begin{aligned}
&\frac{1}{2m}\left[\vec{p}_n - \mathfrak{q}\,\vec{A}(\vec{q}_n,\bar{t}_n)\right]^2 - \frac{\vec{q}_n-\vec{q}_{n-1}}{\tau}\cdot\vec{p}_n \\
&= \frac{1}{2m}\left[\vec{p}_n - \mathfrak{q}\,\vec{A}(\vec{q}_n,\bar{t}_n)\right]^2 - \frac{\vec{q}_n-\vec{q}_{n-1}}{\tau}\cdot\left[\vec{p}_n - \mathfrak{q}\,\vec{A}(\vec{q}_n,\bar{t}_n)\right] - \mathfrak{q}\,\vec{A}(\vec{q}_n,\bar{t}_n)\cdot\frac{\vec{q}_n-\vec{q}_{n-1}}{\tau} \\
&= \frac{1}{2m}\,\left[\vec{p}_n - \mathfrak{q}\,\vec{A}(\vec{q}_n,\bar{t}_n) - m\,\frac{\vec{q}_n-\vec{q}_{n-1}}{\tau}\right]^2 - \frac{m}{2}\,\left(\frac{\vec{q}_n-\vec{q}_{n-1}}{\tau}\right)^2 \\
&\quad - \mathfrak{q}\,\vec{A}(\vec{q}_n,\bar{t}_n)\cdot\frac{\vec{q}_n-\vec{q}_{n-1}}{\tau} \;,
\end{aligned} \tag{3.43}$$

where, for the sake of brevity, we have denoted $\bar{t}_n \equiv t_{n-1}+\lambda\tau$. The momentum integration can now be performed as before, but the substitution of the integration variable reads

$$\vec{p}_n \longrightarrow \vec{p}_n' = \vec{p}_n - \mathfrak{q}\,\vec{A}(\vec{q}_n,\bar{t}_n) - m\,\frac{\vec{q}_n-\vec{q}_{n-1}}{\tau} \;.$$

Finally, instead of Eq. (3.20) we arrive at

$$\begin{aligned}
\langle\vec{q}_b,t_b|\vec{q}_a,t_a\rangle &= \sqrt{\frac{m}{2\pi i\tau\hbar}}^{3N}\int\prod_{n=1}^{N-1}\mathrm{d}^3\vec{q}_n \\
&\times\exp\left\{\frac{i}{\hbar}\sum_{n=1}^{N}\tau\left[\frac{m}{2}\left(\frac{\vec{q}_n-\vec{q}_{n-1}}{\tau}\right)^2 - V(\vec{q}_n,\bar{t}_n) + \mathfrak{q}\,\vec{A}(\vec{q}_n,\bar{t}_n)\cdot\frac{\vec{q}_n-\vec{q}_{n-1}}{\tau}\right]\right\} \;.
\end{aligned} \tag{3.44}$$

In the limit $N\to\infty$, $\tau\to 0$, the continuous version of this equation reads

$$\langle\vec{q}_b,t_b|\vec{q}_a,t_a\rangle \longrightarrow \mathcal{N}\int_{\vec{q}(t_a)=\vec{q}_a}^{\vec{q}(t_b)=\vec{q}_b}\mathcal{D}\vec{q}\,\exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b}\mathrm{d}t\,\left[\frac{m}{2}\,\dot{\vec{q}}^{\,2} - V(\vec{q},t) + \mathfrak{q}\,\vec{A}(\vec{q},t)\cdot\dot{\vec{q}}\right]\right\} \;. \tag{3.45}$$

Indeed, the argument under the integral in the exponent is the Lagrange function of a charged particle in the presence of electromagnetic fields, well-known from the lectures on Classical Mechanics,

$$L(\dot{\vec{q}}, \vec{q}, t) = \frac{m}{2}\,\dot{\vec{q}}^{\,2} - V(\vec{q}, t) + \mathfrak{q}\,\vec{A}(\vec{q}, t) \cdot \dot{\vec{q}}\,. \tag{3.46}$$

Everything seems to be as expected, however, there is a mistake hiding in the discretized version (3.44) of the path integral. This goes back to an ambiguity in evaluating the expectation value (3.6). The attentive reader will have noticed that this expectation value arose from inserting complete sets of position and momentum states (3.3) between the various factors of $U(t_n, t_{n-1})$ in Eq. (3.2), leading to Eq. (3.4). However, before inserting the momentum states, we could have evaluated the expectation value

$$\langle \vec{q}_n |\, \hat{U}(t_n, t_{n-1})\, | \vec{q}_{n-1} \rangle$$

This would have lead to an ambiguity as to whether replace the position operator $\hat{\vec{q}}$ contained in $H(\hat{\vec{p}}, \hat{\vec{q}}, t)$ with the eigenvalue $\vec{q}_n$ or $\vec{q}_{n-1}$. Instead of Eq. (3.6) we could have taken the "democratic" version

$$\begin{aligned}
&\langle \vec{q}_n |\, \hat{U}(t_n, t_{n-1})\, | \vec{q}_{n-1} \rangle = \langle \vec{q}_n | \vec{q}_{n-1} \rangle - \frac{i\,\tau}{\hbar}\, \langle \vec{q}_n |\, H\left(\hat{\vec{p}}, \hat{\vec{q}}, \bar{t}_n\right)\, | \vec{q}_{n-1} \rangle + O(\tau^2) \\
&= \langle \vec{q}_n | \vec{q}_{n-1} \rangle - \frac{i\,\tau}{2\hbar}\, \langle \vec{q}_n |\, \left[H\left(\hat{\vec{p}}, \vec{q}_n, \bar{t}_n\right) + H\left(\hat{\vec{p}}, \vec{q}_{n-1}, \bar{t}_n\right) \right]\, | \vec{q}_{n-1} \rangle + O(\tau^2)\,,
\end{aligned} \tag{3.47}$$

i.e., where the arithmetic mean of $\hat{H}$ evaluated at $\vec{q}_n$ and at $\vec{q}_{n-1}$ is used. We could have re-exponentiated this "average" version of $\hat{H}$ and only then inserted the complete set of momentum states. In Eq. (3.10) we would then have to make the replacement

$$H_n = H(\vec{p}_n, \vec{q}_n, \bar{t}_n) \longrightarrow \frac{1}{2}\left[H(\vec{p}_n, \vec{q}_n, \bar{t}_n) + H(\vec{p}_n, \vec{q}_{n-1}, \bar{t}_n) \right]\,. \tag{3.48}$$

As we will see in the following, this does not affect the previous discussion with only a scalar potential $V(\vec{q}, t)$, but it does make a difference when a vector potential $\vec{A}(\vec{q}, t)$ is included.

The question is, which one of the prescriptions of including a vector potential is correct, the discretized version (3.44), or the one where $\vec{A}(\vec{q}_n, \bar{t}_n)$ is replaced by the arithmetic mean $\frac{1}{2}\left[\vec{A}(\vec{q}_n, \bar{t}_n) + \vec{A}(\vec{q}_{n-1}, \bar{t}_n)\right]$ (and possibly $V(\vec{q}_n, \bar{t}_n)$ by $\frac{1}{2}\left[V(\vec{q}_n, \bar{t}_n) + V(\vec{q}_{n-1}, \bar{t}_n)\right]$)? This can be decided by checking whether the transition amplitude, which is identical to the propagator, leads to the correct Schrödinger equation of a charged particle in an electromagnetic field. Our starting point is Eq. (3.37), where we only take an infinitesimal step τ in time, i.e.,

$$\psi(\vec{x}, t+\tau) = \langle \vec{x}, t+\tau | \psi \rangle_H = \int \mathrm{d}^3\vec{y}\, \langle \vec{x}, t+\tau | \vec{y}, t \rangle\, \langle \vec{y}, t | \psi \rangle_H = \int \mathrm{d}^3\vec{y}\, \langle \vec{x}, t+\tau | \vec{y}, t \rangle\, \psi(\vec{y}, t)\,, \tag{3.49}$$

where we have denoted $\vec{q}_b \equiv \vec{x}$, $t_b \equiv t+\tau$, $\vec{q}_a \equiv \vec{y}$, $t_a \equiv t$ for the sake of convenience. The propagator (3.44) for an infinitesimal time step reads

$$\langle \vec{x}, t+\tau | \vec{y}, t \rangle = \sqrt{\frac{m}{2\pi i \tau \hbar}}^3 \times \exp\left(\frac{i}{\hbar} \tau \left\{ \frac{m}{2} \left(\frac{\vec{x}-\vec{y}}{\tau} \right)^2 - \frac{1}{2} \left[V(\vec{x}, \bar{t}) + V(\vec{y}, \bar{t}) \right] + \frac{\mathfrak{q}}{2} \left[\vec{A}(\vec{x}, \bar{t}) + \vec{A}(\vec{y}, \bar{t}) \right] \cdot \frac{\vec{x}-\vec{y}}{\tau} \right\} \right) , \tag{3.50}$$

where $\bar{t} \equiv t + \lambda\tau$, $\lambda \in [0,1]$. There is no longer an integration over any intermediate positions, since $N = 1$ and the product over integrations $\mathrm{d}^3\vec{q}_n$ in Eq. (3.44) is empty. Moreover, there is just a single term in the sum over n in the exponent. For the moment, we have considered the "democratic" version (3.48) of the Hamilton function, which leads to the arithmetic means $\frac{1}{2}\left[V(\vec{x}, \bar{t}) + V(\vec{y}, \bar{t})\right]$ and $\frac{1}{2}\left[\vec{A}(\vec{x}, \bar{t}) + \vec{A}(\vec{y}, \bar{t})\right]$. Afterwards we will investigate what happens when using the original version (3.44), i.e., when only $V(\vec{x}, \bar{t})$ and $\vec{A}(\vec{x}, \bar{t})$ appear in Eq. (3.50) instead of the arithmetic means. We now insert Eq. (3.50) into Eq. (3.49), substitute the integration variable $\vec{\xi} \equiv \vec{y} - \vec{x}$, and Taylor-expand all quantities which depend on $\vec{y} = \vec{x} + \vec{\xi}$ to second order in $\vec{\xi}$ around the position $\vec{x}$ (why up to second order is sufficient will be explained below). The result is

$$\begin{aligned} \psi(\vec{x}, t+\tau) = {} & \sqrt{\frac{m}{2\pi i \tau \hbar}}^3 \int \mathrm{d}^3\vec{\xi} \, \exp\left(\frac{im}{2\hbar\tau} \vec{\xi}^2 \right) \\ & \times \exp\left\{ -\frac{i}{\hbar}\tau \left[V(\vec{x}, \bar{t}) + \frac{1}{2} \vec{\xi} \cdot \vec{\nabla} V(\vec{x}, \bar{t}) + \frac{1}{4} \sum_{i,j=1}^{3} \xi_i \xi_j \partial_i \partial_j V(\vec{x}, \bar{t}) + \mathcal{O}(\xi^3) \right] \right\} \\ & \times \exp\left\{ -\frac{i\mathfrak{q}}{\hbar} \vec{\xi} \cdot \left[\vec{A}(\vec{x}, \bar{t}) + \frac{1}{2} \vec{\xi} \cdot \vec{\nabla} \vec{A}(\vec{x}, \bar{t}) \right] + \mathcal{O}(\xi^3) \right\} \\ & \times \left[\psi(\vec{x}, t) + \vec{\xi} \cdot \vec{\nabla} \psi(\vec{x}, t) + \frac{1}{2} \sum_{n,m=1}^{3} \xi_n \xi_m \partial_n \partial_m \psi(\vec{x}, t) + \mathcal{O}(\xi^3) \right] . \end{aligned} \tag{3.51}$$

In the next step, we also expand all exponential functions involving V and $\vec{A}$ to second order in $\vec{\xi}$. We then encounter (complex) Gaussian integrals of the type

$$\int \mathrm{d}^3\vec{\xi} \, \exp\left(\frac{im}{2\hbar\tau} \vec{\xi}^2 \right) = \sqrt{\frac{2\pi i \hbar \tau}{m}}^3 , \tag{3.52}$$

$$\int \mathrm{d}^3\vec{\xi} \, \xi_i \xi_j \exp\left(\frac{im}{2\hbar\tau} \vec{\xi}^2 \right) = \delta_{ij} \sqrt{\frac{2\pi i \hbar \tau}{m}}^3 \frac{i\hbar\tau}{m} , \quad i,j = 1,2,3 . \tag{3.53}$$

Integrals over odd powers of ξ_i vanish by symmetry. We now see why an expansion up to second order in $\vec{\xi}$ was sufficient: each power of ξ_i under the $\mathrm{d}^3\vec{\xi}$ integral results in a factor of $\sqrt{\tau}$ after integration. In the limit $\tau \to 0$, only terms which are $\sim \tau^{3/2}$, and thus cancel the $\tau^{-3/2}$ in the prefactor, lead to a non-vanishing result. Higher powers of ξ_i produce additional factors of $\sqrt{\tau}$, which then vanish when $\tau \to 0$.

Since there is a prefactor τ in the terms involving the potential V, we actually do not need to keep any but the leading term in the Taylor expansion of V: all (non-vanishing) higher-order terms lead to factors which are at least $\sim \tau^2$, and thus vanish in the limit $\tau \to 0$. This also explains why it does not matter whether we take $V(\vec{q}_n, \bar{t}_n)$ in Eq. (3.44) or the arithmetic mean $\frac{1}{2}\left[V(\vec{q}_n, \bar{t}_n) + V(\vec{q}_{n-1}, \bar{t}_n)\right]$. Collecting all relevant terms, we obtain

$$\begin{aligned}
\psi(\vec{x}, t+\tau) &= \left[1 - \frac{i}{\hbar}\tau V(\vec{x}, \bar{t})\right] \sqrt{\frac{m}{2\pi i\tau\hbar}}^3 \int \mathrm{d}^3\vec{\xi}\, \exp\left(\frac{im}{2\hbar\tau}\vec{\xi}^2\right) \\
&\times \left\{1 - \frac{i\mathfrak{q}}{\hbar}\sum_{i=1}^{3}\xi_i A_i(\vec{x}, \bar{t}) - \frac{i\mathfrak{q}}{2\hbar}\sum_{i,j=1}^{3}\xi_i\xi_j\left[\partial_j A_i(\vec{x}, \bar{t})\right] - \frac{\mathfrak{q}^2}{2\hbar^2}\sum_{i,j=1}^{3}\xi_i\xi_j A_i(\vec{x}, \bar{t}) A_j(\vec{x}, \bar{t})\right\} \\
&\times \left[\psi(\vec{x}, t) + \sum_{n=1}^{3}\xi_n\partial_n\psi(\vec{x}, t) + \frac{1}{2}\sum_{n,m=1}^{3}\xi_n\xi_m\partial_n\partial_m\psi(\vec{x}, t)\right] \\
&= \left[1 - \frac{i}{\hbar}\tau V(\vec{x}, \bar{t})\right] \sqrt{\frac{m}{2\pi i\tau\hbar}}^3 \int \mathrm{d}^3\vec{\xi}\, \exp\left(\frac{im}{2\hbar\tau}\vec{\xi}^2\right) \\
&\times \left\{\psi(\vec{x}, t) - \frac{i\mathfrak{q}}{\hbar}\sum_{i,n=1}^{3}\xi_i\xi_n A_i(\vec{x}, \bar{t})\partial_n\psi(\vec{x}, t) - \frac{i\mathfrak{q}}{2\hbar}\sum_{i,j=1}^{3}\xi_i\xi_j\left[\partial_j A_i(\vec{x}, \bar{t})\right]\psi(\vec{x}, t)\right. \\
&\quad \left. - \frac{\mathfrak{q}^2}{2\hbar^2}\sum_{i,j=1}^{3}\xi_i\xi_j A_i(\vec{x}, \bar{t}) A_j(\vec{x}, \bar{t})\psi(\vec{x}, t) + \frac{1}{2}\sum_{n,m=1}^{3}\xi_n\xi_m\partial_n\partial_m\psi(\vec{x}, t)\right\} . \qquad (3.54)
\end{aligned}$$

Applying the Gaussian integrals (3.52), (3.53), we then obtain

$$\begin{aligned}
\psi(\vec{x}, t+\tau) &= \left[1 - \frac{i}{\hbar}\tau V(\vec{x}, \bar{t})\right]\left\{\psi(\vec{x}, t) + \frac{\mathfrak{q}\tau}{m}\vec{A}(\vec{x}, \bar{t})\cdot\vec{\nabla}\psi(\vec{x}, t) + \frac{\mathfrak{q}\tau}{2m}\left[\vec{\nabla}\cdot\vec{A}(\vec{x}, \bar{t})\right]\psi(\vec{x}, t)\right. \\
&\qquad \left. - \frac{i\mathfrak{q}^2\tau}{2m\hbar}\vec{A}^2(\vec{x}, \bar{t})\psi(\vec{x}, t) + \frac{i\hbar\tau}{2m}\Delta\psi(\vec{x}, t)\right\} \\
&= \psi(\vec{x}, t) - \frac{i}{\hbar}\tau V(\vec{x}, \bar{t})\psi(\vec{x}, t) + \frac{\mathfrak{q}\tau}{m}\vec{A}(\vec{x}, \bar{t})\cdot\vec{\nabla}\psi(\vec{x}, t) + \frac{\mathfrak{q}\tau}{2m}\left[\vec{\nabla}\cdot\vec{A}(\vec{x}, \bar{t})\right]\psi(\vec{x}, t) \\
&\quad - \frac{i\mathfrak{q}^2\tau}{2m\hbar}\vec{A}^2(\vec{x}, \bar{t})\psi(\vec{x}, t) + \frac{i\hbar\tau}{2m}\Delta\psi(\vec{x}, t) + \mathcal{O}(\tau^2) , \qquad (3.55)
\end{aligned}$$

where we kept all terms linear in τ. We can now reorder the terms and employ

$$\lim_{\tau\to 0}\frac{\psi(\vec{x}, t+\tau) - \psi(\vec{x}, t)}{\tau} = \frac{\partial}{\partial t}\psi(\vec{x}, t)$$

to obtain in the limit $\tau \to 0$

$$\begin{aligned}
i\hbar\frac{\partial}{\partial t}\psi(\vec{x}, t) &= -\frac{\hbar^2}{2m}\Delta\psi(\vec{x}, t) + V(\vec{x}, t)\psi(\vec{x}, t) + \frac{i\hbar\mathfrak{q}}{m}\vec{A}(\vec{x}, t)\cdot\vec{\nabla}\psi(\vec{x}, t) \\
&\quad + \frac{i\hbar\mathfrak{q}}{2m}\left[\vec{\nabla}\cdot\vec{A}(\vec{x}, t)\right]\psi(\vec{x}, t) + \frac{\mathfrak{q}^2}{2m}\vec{A}^2(\vec{x}, t)\psi(\vec{x}, t) \\
&= \left\{\frac{1}{2m}\left[\hat{\vec{p}} - \mathfrak{q}\,\vec{A}(\vec{x}, t)\right]^2 + V(\vec{x}, t)\right\}\psi(\vec{x}, t) . \qquad (3.56)
\end{aligned}$$

This is the correct result for the Schrödinger equation of a particle in an electromagnetic field, since the Hamilton operator is

$$\hat{H} \equiv \frac{1}{2m}\left[\hat{\vec{p}} - \mathfrak{q}\,\vec{A}(\vec{x},t)\right]^2 + V(\vec{x},t)\;, \tag{3.57}$$

which is the quantum-mechanical analogue of the classical Hamilton function (3.42).

Finally, we can answer the question what would have happened if had not used the arithmetic mean $\frac{1}{2}\left[\vec{A}(\vec{x},\bar{t}) + \vec{A}(\vec{y},\bar{t})\right]$, but simply $\vec{A}(\vec{x},\bar{t})$. Then there would be no need to Taylor-expand $\frac{1}{2}\vec{A}(\vec{y},\bar{t})$ and the term $\frac{1}{2}\vec{\xi}\cdot\vec{\nabla}A(\vec{x},\bar{t})$ in Eq. (3.51) would be absent. Tracing this all the way to the final result (3.56), the term $\sim \vec{\nabla}\cdot\vec{A}(\vec{x},t)$ would be absent. This would have prevented us from combining the terms to the correct Hamilton operator (3.57), i.e., we would not have obtained the correct Schrödinger equation. Therefore, taking the arithmetic mean of the vector potential in Eq. (3.50) is not a matter of choice: it is the **only** choice that reproduces the **correct** Schrödinger equation. In consequence, the "democratic" version (3.48) of the Hamilton function is in general the safe, and therefore better, choice. It is just a coincidence that this choice does not matter if $\vec{A}(\vec{q},t) = 0$ and only the scalar potential $V(\vec{q},t) \neq 0$.

3.5 Midpoint rule, Ito integral, Brownian motion, and gauge transformations

In the last section, instead of the arithmetic mean $\frac{1}{2}\left[\vec{A}(\vec{q}_n,\bar{t}_n) + \vec{A}(\vec{q}_{n-1},\bar{t}_n)\right]$ we could have also taken the vector potential at the midpoint $(\vec{q}_n + \vec{q}_{n-1})/2$, since its Taylor expansion around $\vec{q}_n$ reads

$$\begin{aligned}\vec{A}\left(\frac{\vec{q}_n+\vec{q}_{n-1}}{2},\bar{t}_n\right) &= \vec{A}(\vec{q}_n,\bar{t}_n) + \left(\frac{\vec{q}_n+\vec{q}_{n-1}}{2} - \vec{q}_n\right)\cdot\vec{\nabla}_q\vec{A}(\vec{q}_n,\bar{t}_n) + \mathcal{O}\left((\vec{q}_n-\vec{q}_{n-1})^2\right)\\ &= \vec{A}(\vec{q}_n,\bar{t}_n) - \frac{\vec{q}_n-\vec{q}_{n-1}}{2}\cdot\vec{\nabla}_q\vec{A}(\vec{q}_n,\bar{t}_n) + \mathcal{O}\left((\vec{q}_n-\vec{q}_{n-1})^2\right)\end{aligned} \tag{3.58}$$

and is thus to first order in $\vec{q}_n - \vec{q}_{n-1}$ identical with the Taylor expansion of the arithmetic mean around $\vec{q}_n$,

$$\frac{1}{2}\left[\vec{A}(\vec{q}_n,\bar{t}_n) + \vec{A}(\vec{q}_{n-1},\bar{t}_n)\right] = \vec{A}(\vec{q}_n,\bar{t}_n) + \frac{1}{2}\,(\vec{q}_{n-1}-\vec{q}_n)\cdot\vec{\nabla}_q\vec{A}(\vec{q}_n,\bar{t}_n) + \mathcal{O}\left((\vec{q}_n-\vec{q}_{n-1})^2\right)\;. \tag{3.59}$$

Since we only needed the first-order term in the calculation of the previous section, the **"midpoint rule"**, i.e., replacing $\vec{A}(\vec{q}_n,\bar{t}_n)$ by $\vec{A}\left(\frac{\vec{q}_n+\vec{q}_{n-1}}{2},\bar{t}_n\right)$ in Eq. (3.44), would have also given the correct Schrödinger equation.

This observation can be put into a more general context. Let $\varphi(q)$ be an analytic function (which thus has a Taylor expansion) and let $q(t)$ be a particular trajectory in one-dimensional coordinate space with $t \in [a,b]$. Consider the time interval $[a,b]$ of length $b-a$ and divide this into N pieces of length $\tau = (b-a)/N$. This gives the partition of

the time interval into a set of discrete times $t_n \equiv a + n\tau$, $n = 0, 1, \ldots, N$, with $t_0 = a$, $t_N = b$. The positions of the particle at the times t_n are

$$q_n \equiv q(t_n) \ , \quad q_0 = q(a) = q_a \ , \quad q_N = q(b) = q_b \ . \tag{3.60}$$

Now consider the identity (the "telescope sum")

$$\varphi(q_b) - \varphi(q_a) = \sum_{n=0}^{N-1} \left[\varphi(q_{n+1}) - \varphi(q_n)\right] \ . \tag{3.61}$$

We expand both $\varphi(q_n)$ and $\varphi(q_{n+1})$ into Taylor series around a particular point

$$u_n \equiv q_n + \lambda(q_{n+1} - q_n) \ , \quad \lambda \in [0, 1] \ , \tag{3.62}$$

in the interval $[q_n, q_{n+1}]$. These Taylor expansions read up to second order in $(q_{n+1} - q_n)^2$:

$$\begin{aligned}
\varphi(q_n) &= \varphi(u_n) + (q_n - u_n)\varphi'(u_n) + \frac{1}{2}(q_n - u_n)^2\varphi''(u_n) + \mathcal{O}\left((q_n - u_n)^3\right) \\
&= \varphi(u_n) - \lambda(q_{n+1} - q_n)\varphi'(u_n) + \frac{\lambda^2}{2}(q_{n+1} - q_n)^2\varphi''(u_n) + \mathcal{O}\left((q_{n+1} - q_n)^3\right) \ , \\
\varphi(q_{n+1}) &= \varphi(u_n) + (q_{n+1} - u_n)\varphi'(u_n) + \frac{1}{2}(q_{n+1} - u_n)^2\varphi''(u_n) + \mathcal{O}\left((q_{n+1} - u_n)^3\right) \\
&= \varphi(u_n) + (1 - \lambda)(q_{n+1} - q_n)\varphi'(u_n) + \frac{(1 - \lambda)^2}{2}(q_{n+1} - q_n)^2\varphi''(u_n) \\
&\quad + \mathcal{O}\left((q_{n+1} - q_n)^3\right) \ .
\end{aligned} \tag{3.63}$$

Thus, Eq. (3.61) becomes

$$\begin{aligned}
&\varphi(q_b) - \varphi(q_a) \\
&= \sum_{n=0}^{N-1} \left[(q_{n+1} - q_n)\varphi'(u_n) + \left(\frac{1}{2} - \lambda\right)(q_{n+1} - q_n)^2\varphi''(u_n) + \mathcal{O}\left((q_{n+1} - q_n)^3\right)\right] \\
&= \sum_{n=0}^{N-1} \tau \left[\frac{q_{n+1} - q_n}{\tau}\varphi'(u_n) + \left(\frac{1}{2} - \lambda\right)\frac{(q_{n+1} - q_n)^2}{\tau}\varphi''(u_n) + \mathcal{O}\left(\frac{(q_{n+1} - q_n)^3}{\tau}\right)\right] \ .
\end{aligned} \tag{3.64}$$

In the limit $N \to \infty$, $\tau \to 0$, we can convert the sum into an integral and obtain after some reordering of terms the astonishing result

$$\int_{q_a}^{q_b} \mathrm{d}q \, \frac{\mathrm{d}\varphi(q)}{\mathrm{d}q} = \int_a^b \mathrm{d}t \, \frac{\mathrm{d}q}{\mathrm{d}t} \, \frac{\mathrm{d}\varphi(q)}{\mathrm{d}q} = \varphi(q_b) - \varphi(q_a) - \left(\frac{1}{2} - \lambda\right) \int_a^b \mathrm{d}t \, \frac{\mathrm{d}q^2}{\mathrm{d}t} \, \frac{\mathrm{d}^2\varphi(q)}{\mathrm{d}q^2} + \mathcal{O}(\mathrm{d}q^3) \ . \tag{3.65}$$

Why is this astonishing? From the "normal" rules of integral calculus we would have expected that the value of the integral on the left-hand side is the first term, $\varphi(q_b) - \varphi(q_a)$. The second term is "anomalous" in the sense that it can only appear if $\mathrm{d}q^2$ is of order $\mathrm{d}t$ (or $\mathrm{d}q \sim \sqrt{\mathrm{d}t}$), because then the integrand is finite and not infinitesimally small. Or in

other words, if $\mathrm{d}q$ is of order $\mathrm{d}t$ (such that the velocity $\dot{q} = \mathrm{d}q/\mathrm{d}t$ is finite), the second term is infinitesimally small and can be simply neglected (such as all other higher-order terms).

Are there physical situations, where the change in position $\mathrm{d}q$ is of order $\sqrt{\mathrm{d}t}$ instead of $\mathrm{d}t$? In fact, this is the case in **diffusion processes** such as **Brownian motion**. Here, the velocity of the particles is $\mathrm{d}q/\mathrm{d}t \sim 1/\sqrt{\mathrm{d}t} \to \infty$, because the particle motion is discontinuous when it scatters off other particles. It was precisely in this context that K. Ito encountered an integral of the type (3.65). In his case, $\lambda = 0$ and the "diffusion constant" is the coefficient $1/2$ in front of the second term in Eq. (3.65). That is why we would like to call the integral (3.65) the **generalized Ito integral**.

How is this of relevance for our discussion of gauge fields in the previous section? There we indeed found that the result of the Gaussian integration was that the "displacement" $\mathrm{d}q \equiv \xi \sim \sqrt{\tau} \equiv \sqrt{\mathrm{d}t}$! So the trajectories entering the path integral are actually of the same type that particles take in Brownian motion! But irrespective of whether the trajectories are smooth, such that $\dot{q} < \infty$, or discontinuous like Brownian motion, such that $\mathrm{d}q^2/\mathrm{d}t$ is finite, there is actually **one case** where the anomalous term in Eq. (3.65) does not appear: if we apply the **midpoint rule**, i.e., $\lambda = 1/2$ in the Taylor expansion of $\varphi(q)$. This further elucidates the importance of the midpoint rule in the calculation of path integrals.

Finally, let us discuss the importance of our findings for **gauge transformations** of the vector potential,

$$\vec{A}(\vec{q},t) \longrightarrow \vec{A}'(\vec{q},t) = \vec{A}(\vec{q},t) + \vec{\nabla}_q \Lambda(\vec{q},t) \;, \tag{3.66}$$

where $\Lambda(\vec{q},t)$ is a scalar function. This adds a term

$$\frac{i\mathfrak{q}}{\hbar} \int_{t_a}^{t_b} \mathrm{d}t\, \dot{\vec{q}} \cdot \vec{\nabla}_q \Lambda(\vec{q},t) \equiv \frac{i\mathfrak{q}}{\hbar} \int_{\vec{q}_a}^{\vec{q}_b} \mathrm{d}\vec{q} \cdot \vec{\nabla}_q \Lambda(\vec{q},t) \tag{3.67}$$

to the exponent in the propagator (3.45). This is the three-dimensional generalization of the Ito integral (3.65). Applying the midpoint rule ($\lambda = 1/2$), there is no term $\sim \Delta_q \Lambda(\vec{q},t)$,

$$\frac{i\mathfrak{q}}{\hbar} \int_{\vec{q}_a}^{\vec{q}_b} \mathrm{d}\vec{q} \cdot \vec{\nabla}_q \Lambda(\vec{q},t) \equiv \frac{i\mathfrak{q}}{\hbar} \left[\Lambda(\vec{q}_b,t_b) - \Lambda(\vec{q}_a,t_a)\right] \;, \tag{3.68}$$

and the gauge-transformed propagator reads

$$G'(\vec{q}_b,t_b;\vec{q}_a,t_a) = \exp\left[\frac{i\mathfrak{q}}{\hbar}\,\Lambda(\vec{q}_b,t_b)\right] G(\vec{q}_b,t_b;\vec{q}_a,t_a) \exp\left[-\frac{i\mathfrak{q}}{\hbar}\,\Lambda(\vec{q}_a,t_a)\right] \;. \tag{3.69}$$

This corresponds to an (unobservable) change of the phase of the wave function,

$$\begin{aligned}
\psi'(\vec{q}_b,t_b) &= \int \mathrm{d}^3\vec{q}_a\, G'(\vec{q}_b,t_b;\vec{q}_a,t_a)\, \psi'(\vec{q}_a,t_a) \\
&= \exp\left[\frac{i\mathfrak{q}}{\hbar}\,\Lambda(\vec{q}_b,t_b)\right] \\
&\times \int \mathrm{d}^3\vec{q}_a\, G(\vec{q}_b,t_b;\vec{q}_a,t_a) \exp\left[-\frac{i\mathfrak{q}}{\hbar}\,\Lambda(\vec{q}_a,t_a)\right] \exp\left[\frac{i\mathfrak{q}}{\hbar}\,\Lambda(\vec{q}_a,t_a)\right] \psi(\vec{q}_a,t_a) \\
&= \exp\left[\frac{i\mathfrak{q}}{\hbar}\,\Lambda(\vec{q}_b,t_b)\right] \psi(\vec{q}_b,t_b) \;.
\end{aligned} \tag{3.70}$$

4 Applications

Lecture 3

In this chapter, we study various applications of path integrals. For a particle obeying the non-interaction Schrödinger equation, the propagator can be exactly computed. The simplest application of path integrals is scattering of particles through a double slit. The path integral (in a very simple approximation) provides an easy way to understand the emerging interference pattern. We then discuss the semi-classical approximation, which is based on a Taylor expansion of the potential energy up to second order in derivatives. For the harmonic oscillator, this approximation becomes exact. As a non-trivial example, we finally discuss the anharmonic oscillator.

4.1 Propagator of free Schrödinger equation

In this section, we calculate the transition amplitude for the free Schrödinger equation from the path-integral formulation. Since the kinetic energy is in principle a quadratic function of the coordinates, cf. Eq. (3.20), the path integral is of Gaussian type and can therefore be exactly evaluated. The starting point is Eq. (3.20), where we set $V(\vec{q},t) \equiv 0$,

$$\langle \vec{q}_b, t_b | \vec{q}_a, t_a \rangle = \sqrt{\frac{m}{2\pi i \tau \hbar}}^{3N} \int \left[\prod_{m=1}^{N-1} \mathrm{d}^3 \vec{q}_m \right] \, \exp\left[\frac{i\,m}{2\hbar\tau} \sum_{n=1}^{N} (\vec{q}_n - \vec{q}_{n-1})^2 \right] \, . \tag{4.1}$$

We integrate successively over the coordinates $\vec{q}_n$. The coordinate $\vec{q}_1$ appears in two terms in the sum in the exponent, such that the $\vec{q}_1$ integral is

$$\int \mathrm{d}^3 \vec{q}_1 \, \exp\left\{ \frac{i\,m}{2\hbar\tau} \left[(\vec{q}_2 - \vec{q}_1)^2 + (\vec{q}_1 - \vec{q}_0)^2 \right] \right\} \, . \tag{4.2}$$

We rewrite the exponent in the form

$$\begin{aligned} (\vec{q}_2 - \vec{q}_1)^2 + (\vec{q}_1 - \vec{q}_0)^2 &= \vec{q}_2^{\,2} + \vec{q}_0^{\,2} - 2\,\vec{q}_1 \cdot (\vec{q}_2 + \vec{q}_0) + 2\,\vec{q}_1^{\,2} \\ &= 2 \left(\vec{q}_1 - \frac{\vec{q}_2 + \vec{q}_0}{2} \right)^2 - \frac{1}{2} (\vec{q}_2 + \vec{q}_0)^2 + \vec{q}_2^{\,2} + \vec{q}_0^{\,2} \\ &= 2\,\vec{q}_1^{\,\prime\,2} + \frac{1}{2} (\vec{q}_2 - \vec{q}_0)^2 \, , \end{aligned}$$

where we defined

$$\vec{q}_1^{\,\prime} \equiv \vec{q}_1 - \frac{\vec{q}_2 + \vec{q}_0}{2} \, .$$

If we substitute this variable in the $\vec{q}_1$ integral in Eq. (4.2), we can immediately evaluate this integral (it is again of Gaussian type),

$$\begin{aligned}
&\int \mathrm{d}^3\vec{q}_1 \, \exp\left\{\frac{i\,m}{2\hbar\tau}\,\left[(\vec{q}_2-\vec{q}_1)^2+(\vec{q}_1-\vec{q}_0)^2\right]\right\} \\
&= \exp\left[\frac{i\,m}{2\hbar(2\tau)}\,(\vec{q}_2-\vec{q}_0)^2\right]\int \mathrm{d}^3\vec{q}_1' \, \exp\left(\frac{2i\,m}{2\hbar\tau}\,\vec{q}_1'^{\,2}\right) \\
&= \exp\left[\frac{i\,m}{2\hbar(2\tau)}\,(\vec{q}_2-\vec{q}_0)^2\right]\,\sqrt{\frac{\pi i\tau\hbar}{m}}^{\,3} \,. \qquad (4.3)
\end{aligned}$$

We observe that the result from the Gaussian integration combines with three of the $3N$ roots in the prefactors of the path integral in Eq. (4.1) to give

$$\sqrt{\frac{m}{2\pi i\tau\hbar}\,\frac{\pi i\tau\hbar}{m}}^{\,3} = \frac{1}{\sqrt{2}^3} \,. \qquad (4.4)$$

Simultaneously, the time interval τ in the exponential function was replaced by 2τ.

We now integrate over $\vec{q}_2$, which also occurs in two terms in the exponent,

$$\int \mathrm{d}^3\vec{q}_2 \, \exp\left\{\frac{i\,m}{2\hbar\tau}\,\left[(\vec{q}_3-\vec{q}_2)^2+\frac{1}{2}\,(\vec{q}_2-\vec{q}_0)^2\right]\right\} \,. \qquad (4.5)$$

A similar manipulation of the exponent as in the previous case yields

$$\begin{aligned}
(\vec{q}_3-\vec{q}_2)^2+\frac{1}{2}\,(\vec{q}_2-\vec{q}_0)^2 &= \vec{q}_3^{\,2}+\frac{1}{2}\,\vec{q}_0^{\,2}-2\,\vec{q}_2\cdot\left(\vec{q}_3+\frac{1}{2}\,\vec{q}_0\right)+\frac{3}{2}\,\vec{q}_2^{\,2} \\
&= \frac{3}{2}\left[\vec{q}_2-\frac{2}{3}\left(\vec{q}_3+\frac{1}{2}\,\vec{q}_0\right)\right]^2-\frac{2}{3}\left(\vec{q}_3+\frac{1}{2}\,\vec{q}_0\right)^2+\vec{q}_3^{\,2}+\frac{1}{2}\,\vec{q}_0^{\,2} \\
&= \frac{3}{2}\,\vec{q}_2'^{\,2}+\frac{1}{3}\,(\vec{q}_3-\vec{q}_0)^2 \,,
\end{aligned}$$

where we defined

$$\vec{q}_2' \equiv \vec{q}_2-\frac{2}{3}\left(\vec{q}_3+\frac{1}{2}\,\vec{q}_0\right) \,.$$

Inserting this into Eq. (4.5) we obtain

$$\begin{aligned}
&\int \mathrm{d}^3\vec{q}_2 \, \exp\left\{\frac{i\,m}{2\hbar\tau}\,\left[(\vec{q}_3-\vec{q}_2)^2+\frac{1}{2}\,(\vec{q}_2-\vec{q}_0)^2\right]\right\} \\
&= \exp\left[\frac{i\,m}{2\hbar(3\tau)}\,(\vec{q}_3-\vec{q}_0)^2\right]\int \mathrm{d}^3\vec{q}_2' \, \exp\left(\frac{3i\,m}{4\hbar\tau}\,\vec{q}_2'^{\,2}\right) \\
&= \exp\left[\frac{i\,m}{2\hbar(3\tau)}\,(\vec{q}_3-\vec{q}_0)^2\right]\,\sqrt{\frac{4\pi i\tau\hbar}{3m}}^{\,3} \,. \qquad (4.6)
\end{aligned}$$

The result from the Gaussian integration combines with three of the prefactors from Eq. (4.1) and with the factor $1/\sqrt{2}^3$ from Eq. (4.4) to give

$$\sqrt{\frac{m}{2\pi i\tau\hbar}\,\frac{4\pi i\tau\hbar}{3m}\,\frac{1}{2}}^{\,3} = \frac{1}{\sqrt{3}^3} \,.$$

We now continue to integrate over the variables $\vec{q}_m$. When integrating over the variable $\vec{q}_j$ the time interval $j\tau$ in the denominator of the exponent increases by τ, i.e., it becomes $(j+1)\tau$. Simultaneously, three of the $3N$ prefactors in Eq. (4.1) partially cancel with the result of the $\vec{q}_j$ integration, and we obtain a factor $1/\sqrt{j+1}^3$. If we continue to do this until $j = N-1$, we obtain with $\vec{q}_0 \equiv \vec{q}_a$, $\vec{q}_N \equiv \vec{q}_b$, and $N\tau \equiv t_b - t_a$ the final result

$$\langle \vec{q}_b, t_b | \vec{q}_a, t_a \rangle = \sqrt{\frac{m}{2\pi i\hbar(t_b - t_a)}}^3 \exp\left[\frac{i\,m}{2\hbar(t_b - t_a)}\,(\vec{q}_b - \vec{q}_a)^2\right] . \tag{4.7}$$

We now show that this expression is identical with the propagator (3.32) of the Schrödinger equation. To this end we just need to realize that also the integral in that equation is a (shifted) Gaussian integral (at least after analytic continuation into the complex plane, in order to guarantee convergence). With the dispersion relation (3.26) we obtain

$$\begin{aligned} G(\vec{q}, t; \vec{r}, 0) &= \frac{1}{(2\pi)^3} \int \mathrm{d}^3\vec{k}\, \exp\left[-\frac{i\hbar t}{2m}\,\vec{k}^{\,2} + i\vec{k}\cdot(\vec{q} - \vec{r})\right] \\ &= \frac{1}{(2\pi)^3} \int \mathrm{d}^3\vec{k}\, \exp\left\{-\frac{i\hbar t}{2m}\left[\vec{k} - \frac{m}{\hbar t}\,(\vec{q} - \vec{r})\right]^2 + \frac{i\,m}{2\hbar t}\,(\vec{q} - \vec{r})^2\right\} \\ &= \frac{1}{(2\pi)^3}\sqrt{\frac{2\pi m}{i\hbar t}}^3 \exp\left[\frac{i\,m}{2\hbar t}\,(\vec{q} - \vec{r})^2\right] \\ &= \sqrt{\frac{m}{2\pi i\hbar t}}^3 \exp\left[\frac{i\,m}{2\hbar t}\,(\vec{q} - \vec{r})^2\right] . \end{aligned} \tag{4.8}$$

With the obvious replacements $\vec{q} \to \vec{q}_b$, $\vec{r} \to \vec{q}_a$, and $t \to t_b - t_a$ this is identical with Eq. (4.7), q.e.d.

In order to understand the effect of the propagator (4.8), we consider a particle which is localized at the origin, $\vec{r} = 0$, at $t = 0$. The corresponding wave function is a delta function,

$$\psi(\vec{r}, 0) = \delta^{(3)}(\vec{r}) . \tag{4.9}$$

According to Eq. (3.33) the wave function at a later time $t > 0$ is then

$$\psi(\vec{q}, t) = \int \mathrm{d}^3\vec{r}\, G(\vec{q}, t; \vec{r}, 0)\; \delta^{(3)}(\vec{r}) = G(\vec{q}, t; 0, 0) = \sqrt{\frac{m}{2\pi i\hbar t}}^3 \exp\left(\frac{i\,m}{2\hbar t}\,\vec{q}^{\,2}\right) , \tag{4.10}$$

where we have used Eq. (4.8). Apparently, for this initial condition the wave function only depends on the distance $q = |\vec{q}|$ from the origin (the location of the particle at $t = 0$), $\psi(\vec{q}, t) \equiv \psi(q, t)$, it is a **spherical wave**. In addition, the particular initial condition ensures that wave function and propagator are identical. We decompose the wave function into its real and imaginary part,

$$\psi(q, t) = -\frac{1}{\sqrt{2}}\sqrt{\frac{m}{2\pi\hbar t}}^3 (1 + i)\left[\cos\left(\frac{m\,q^2}{2\hbar t}\right) + i\sin\left(\frac{m\,q^2}{2\hbar t}\right)\right] \tag{4.11}$$

$$= -\frac{1}{\sqrt{2}}\sqrt{\frac{m}{2\pi\hbar t}}^3 \left\{\left[\cos\left(\frac{m\,q^2}{2\hbar t}\right) - \sin\left(\frac{m\,q^2}{2\hbar t}\right)\right] + i\left[\cos\left(\frac{m\,q^2}{2\hbar t}\right) + \sin\left(\frac{m\,q^2}{2\hbar t}\right)\right]\right\} .$$

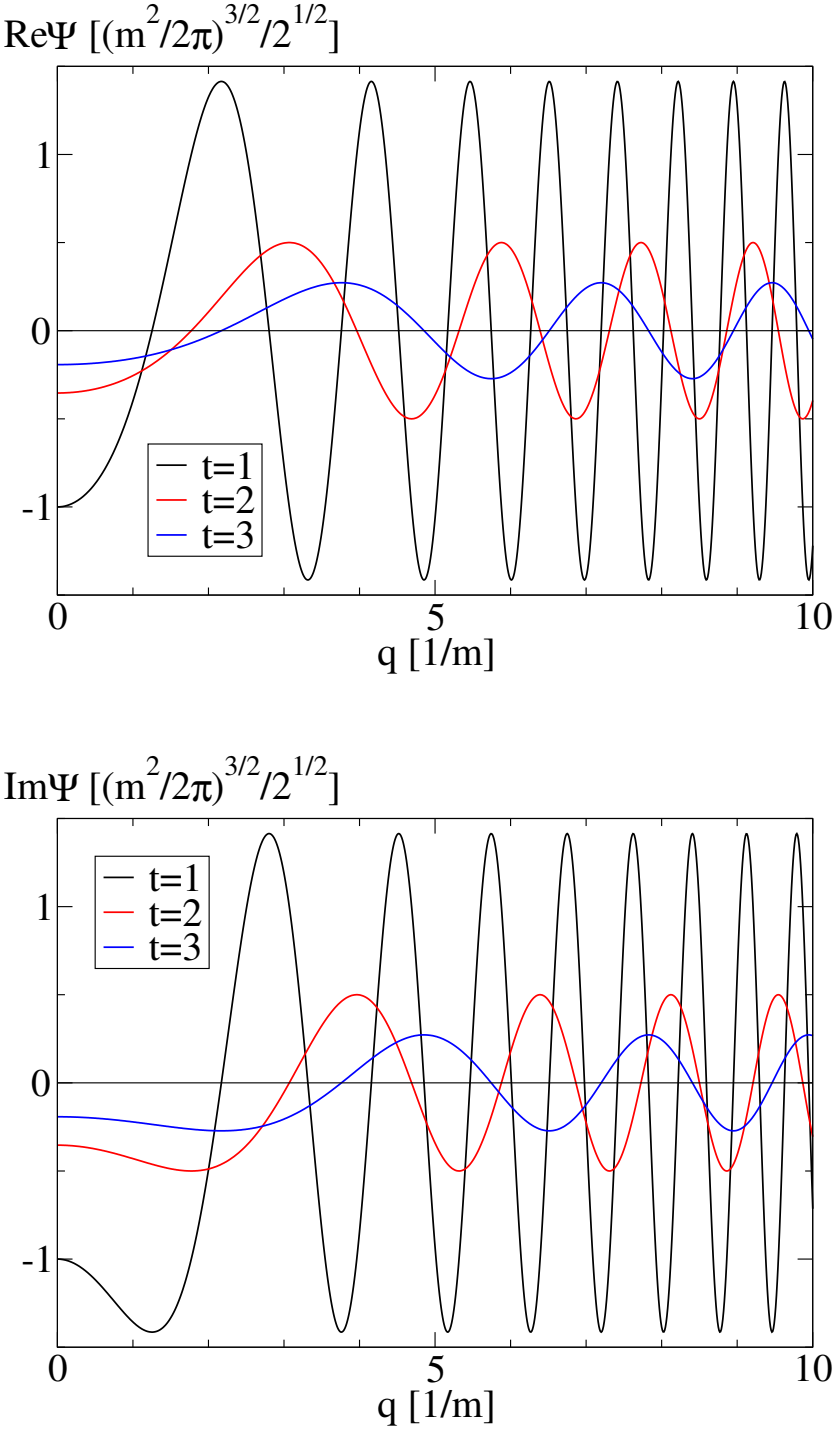


Figure 4.1: Real and imaginary part of the wave function (4.11) (in units of $[m^2/(2\pi)]^{3/2}/\sqrt{2}$) for times $t = 1$ (black), 2 (red), 3 (blue) (in units of $1/(\hbar m)$) as a function of spatial distance q (in units of $1/m$) from the origin.

Real and imaginary part are shown in Fig. 4.1 for a few exemplary values of t as function of q. One observes that the oscillation frequency increases with increasing distance q from

the origin and decreases with increasing time t. The amplitude decreases $\sim t^{-3/2}$.

The probability density

$$|\psi(\vec{q},t)|^2 = \left(\frac{m}{2\pi\hbar t}\right)^3 \tag{4.12}$$

to locate a particle somewhere in space is constant. At first sight, this is a surprising result, but it can be explained by the fact that the particle was exactly localized at $t = 0$. According to Heisenberg's uncertainty relation its momentum is then completely undetermined, i.e., all momenta $\vec{p}$ occur with the same probability. This also applies to arbitrarily large values of $\vec{p}$, which instantaneously transport the particle from $\vec{q} = 0$ to a spatial point which can be arbitrarily far away from the origin. (Causality problems are of no concern in a non-relativistic treatment.) On the other hand, the probability density (4.12) decreases at each point in space with time as t^{-3}. At first sight, this seems to contradict the normalization of the wave function. However, we have not yet properly normalized the latter. The wave function is normalized to one after an integration over the whole space,

$$\int_V \mathrm{d}^3\vec{q}\,|\psi(\vec{q},t)|^2 = V\,\left(\frac{m}{2\pi\hbar t}\right)^3 .$$

Therefore, the correctly normalized wave function still needs to be multiplied with a factor

$$\sqrt{\frac{1}{V}\left(\frac{2\pi\hbar t}{m}\right)^3} .$$

Then, the wave function is normalized to one, and the probability density no longer decays with time.

To have an exactly localized particle (which can then in principle have an arbitrarily large momentum) is, of course, hardly a realistic situation. Therefore, we consider the initial condition

$$\psi(\vec{r},0) = \frac{1}{\sqrt{2\pi\sigma}^{\,3}}\,\exp\left(-\frac{\vec{r}^{\,2}}{2\sigma}\right) , \tag{4.13}$$

i.e., a Gaussian wave packet of width σ. For $\sigma \to 0$ the wave packet becomes the delta function (4.9). Since the Fourier transform of a Gauss function is again a Gauss function, we can again have in principle arbitrarily large momenta $\vec{p} = \hbar\vec{k}$, but they become exponentially less probable with increasing $\vec{p}$,

$$\begin{aligned}
\tilde{\psi}(\vec{k},0) &= 2\pi \int \mathrm{d}^3\vec{r}\,e^{-i\vec{k}\cdot\vec{r}}\,\psi(\vec{r},0) \\
&= \frac{1}{\sqrt{2\pi\sigma^3}} \int \mathrm{d}^3\vec{r}\,\exp\left(-\frac{\vec{r}^{\,2}}{2\sigma} - i\vec{k}\cdot\vec{r}\right) \\
&= \frac{1}{\sqrt{2\pi\sigma^3}}\,\exp\left(-\frac{\sigma}{2}\,\vec{k}^{\,2}\right) \int \mathrm{d}^3\vec{r}\,\exp\left[-\frac{1}{2\sigma}\left(\vec{r} + i\sigma\vec{k}\right)^2\right] \\
&= 2\pi\,\exp\left(-\frac{\sigma}{2}\,\vec{k}^{\,2}\right) \equiv 2\pi\,\exp\left(-\frac{\sigma}{2\hbar^2}\,\vec{p}^{\,2}\right) .
\end{aligned} \tag{4.14}$$

According to Eq. (3.33) the wave function at a time $t > 0$ is

$$\psi(\vec{q},t) = \sqrt{\frac{m}{(2\pi)^2 i\hbar t\sigma}}^{\,3}\,\exp\left(\frac{im}{2\hbar t}\,q^2\right) \int \mathrm{d}^3\vec{r}\,\exp\left[-\frac{1}{2\sigma}\left(1 - \frac{im\sigma}{\hbar t}\right)\vec{r}^{\,2} - \frac{im}{\hbar t}\,\vec{q}\cdot\vec{r}\right] . \tag{4.15}$$

Completing the square yields

$$\begin{aligned} & -\frac{1}{2\sigma}\left(1-\frac{im\sigma}{\hbar t}\right)\vec{r}^{\,2}-\frac{im}{\hbar t}\,\vec{q}\cdot\vec{r} \\ = & -\frac{1}{2\sigma}\left(1-\frac{im\sigma}{\hbar t}\right)\left[\left(\vec{r}+\frac{im\sigma}{\hbar t-im\sigma}\,\vec{q}\right)^2-\left(\frac{im\sigma}{\hbar t-im\sigma}\right)^2 q^2\right] \\ = & -\frac{1}{2\sigma}\left(1-\frac{im\sigma}{\hbar t}\right)\vec{r}^{\,\prime\,2}-\frac{m^2}{2\hbar t}\,\frac{\sigma}{\hbar t-im\sigma}\,q^2\,, \end{aligned}$$

where we have employed the substitution

$$\vec{r}^{\,\prime}\equiv\vec{r}+\frac{im\sigma}{\hbar t-im\sigma}\,\vec{q}\,.$$

The Gaussian integral over $\vec{r}^{\,\prime}$ has the value

$$\sqrt{\frac{2\pi\hbar t\sigma}{\hbar t-im\sigma}}^{\,3}\,.$$

Inserting this into Eq. (4.15) gives

$$\begin{aligned} \psi(q,t) &= \sqrt{\frac{m}{2\pi i}\,\frac{1}{\hbar t-im\sigma}}^{\,3}\,\exp\left[-\frac{m}{2\hbar t}\left(\frac{m\sigma}{\hbar t-im\sigma}-i\right)q^2\right] \\ &= \sqrt{\frac{m}{2\pi i}\,\frac{1}{\hbar t-im\sigma}}^{\,3}\,\exp\left[\frac{i\,m}{2(\hbar t-im\sigma)}\,q^2\right]\,. \end{aligned} \tag{4.16}$$

In the limit $\sigma\to 0$ we again obtain the result (4.10). The decomposition into real and imaginary part is again possible, but yields a rather unwieldy expression. We therefore just show the result in Fig. 4.2. One observes very clearly how the initial Gaussian wave packet (dashed line in the plot for the real part) "dissolves" on account of the momentum uncertainty.

The probability density is

$$|\psi(\vec{q},t)|^2=\left(\frac{m}{2\pi\sqrt{(\hbar t)^2+(m\sigma)^2}}\right)^3\exp\left(-\frac{m^2\sigma}{(\hbar t)^2+(m\sigma)^2}\,q^2\right)\,. \tag{4.17}$$

It is not yet correctly normalized, since

$$\int \mathrm{d}^3\vec{q}\,|\psi(\vec{q},t)|^2=\frac{1}{\sqrt{4\pi\sigma}^{\,3}}\,.$$

The correctly (to unity) normalized probability density is shown in Fig. 4.3. Also here one observes a "dissolving" of the wave function as time evolves.

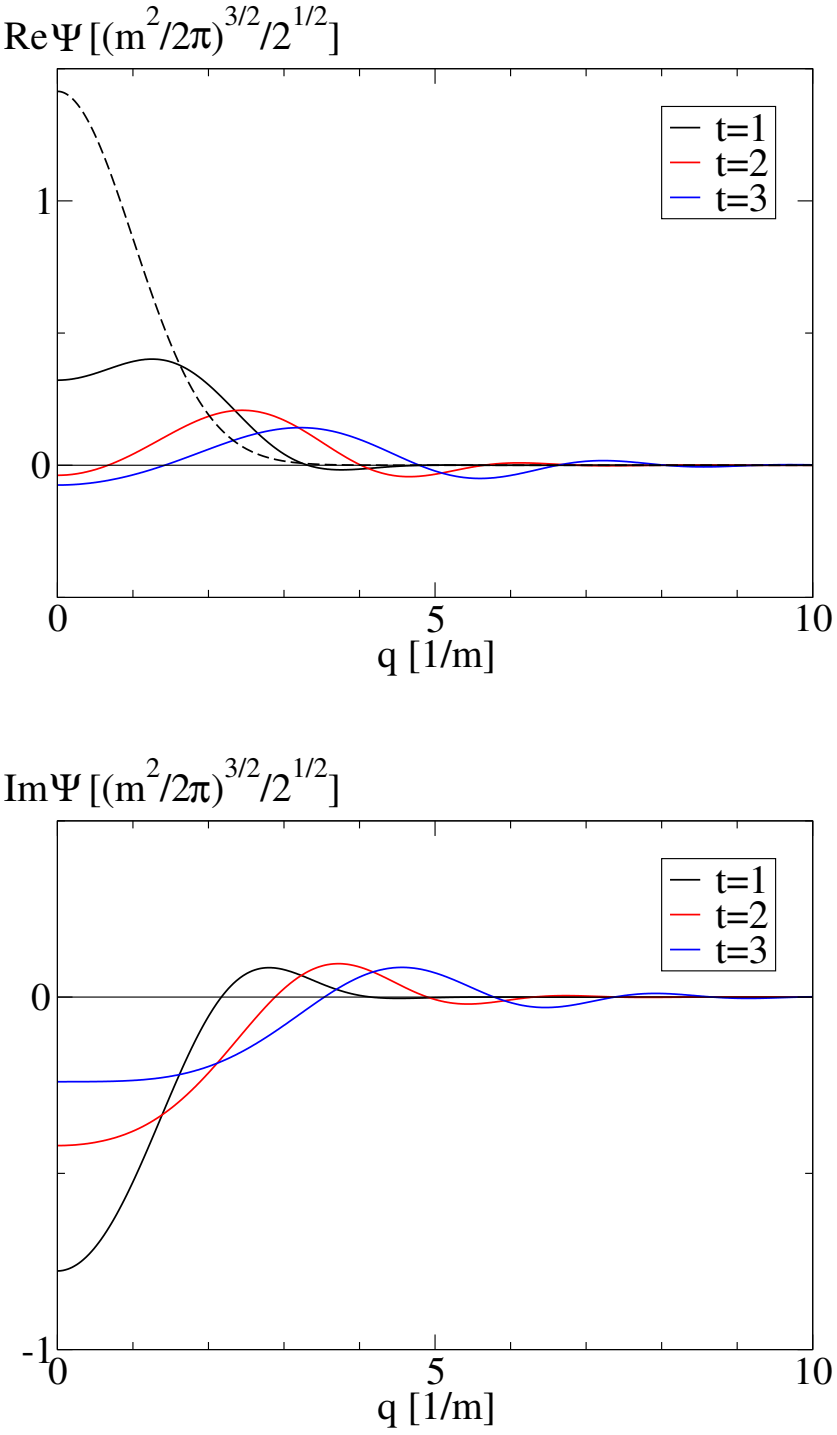


Figure 4.2: Real and imaginary part of the wave function (4.16) (in units of $[m^2/(2\pi)]^{3/2}/\sqrt{2}$) for times $t = 1$ (black), 2 (red), 3 (blue) (in units of $1/(\hbar m)$) as a function of spatial distance q (in units of $1/m$) from the origin. The initial width of the wave packet is $\sigma = 1$ (in units of $1/m^2$).

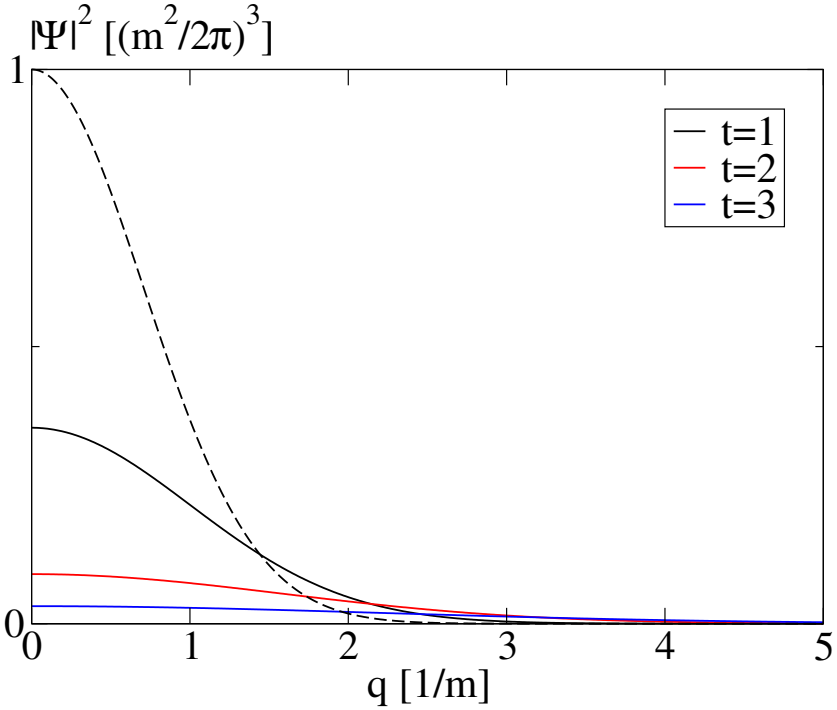


Figure 4.3: Probability density (in units of $[m^2/(2\pi)]^3$) for times $t = 1$ (black), 2 (red), 3 (blue) (in units of $1/(\hbar m)$) as a function of spatial distance q (in units of $1/m$) from the origin. The initial width of the wave function is $\sigma = 1$ (in units of $1/m^2$).

4.2 The double-slit experiment

The path-integral representation of the transition amplitude or propagator is a very natural and intuitive way to understand the interference pattern observed in the famous double-slit experiment. We first observe the following important **convolution property** of the transition amplitude,

$$\langle \vec{q}_b, t_b | \vec{q}_a, t_a \rangle = \int \mathrm{d}^3\vec{q}\, \langle \vec{q}_b, t_b | \vec{q}, t \rangle \langle \vec{q}, t | \vec{q}_a, t_a \rangle \;, \tag{4.18}$$

which simply follows from inserting a complete set of states (3.36). In terms of the propagator, this reads

$$G(\vec{q}_b, t_b; \vec{q}_a, t_a) = \int \mathrm{d}^3\vec{q}\, G(\vec{q}_b, t_b; \vec{q}, t)\, G(\vec{q}, t; \vec{q}_a, t_a) \;, \tag{4.19}$$

Here, t is an arbitrary intermediate time in the interval $[t_a, t_b]$. The situation is envisaged in Fig. 4.4. One should note that one has to integrate over all possible positions $\vec{q}$ at the intermediate time t, since the particle is can take any possible trajectory from its initial position $\vec{q}_a$ at time t_a to its final position $\vec{q}_b$ at time t_b.

The proof of the convolution property in terms of the path-integral representation of the transition amplitude is trivial. We start from Eq. (3.20) and select an intermediate

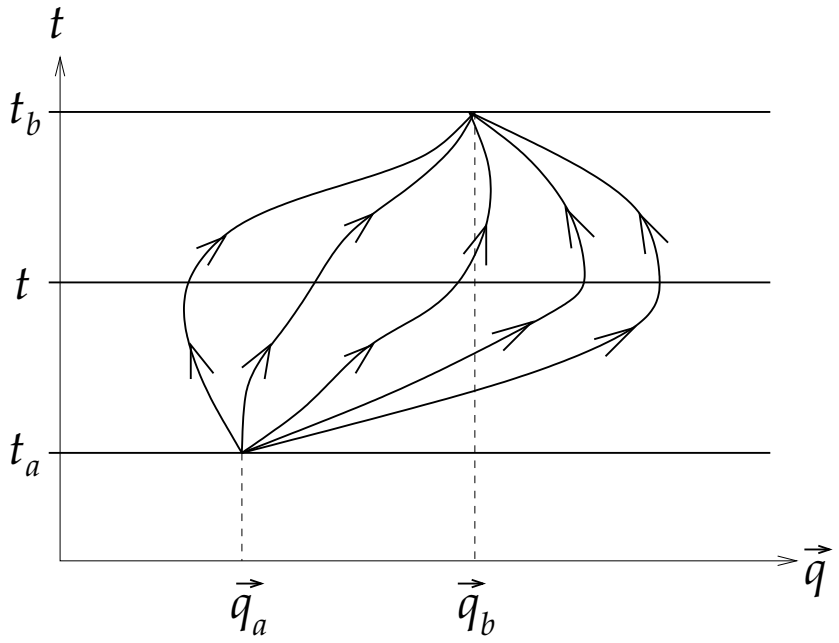


Figure 4.4: Visualization of the convolution property of the propagator in the space-time diagram.

spatial integral, say $\mathrm{d}^3\vec{q}_j$, pertaining to the intermediate time $t_j \in [t_a, t_b]$. We pull this particular spatial integration out of the product in Eq. (3.20) and factorize the remaining terms,

$$\begin{aligned}\langle \vec{q}_b, t_b | \vec{q}_a, t_a \rangle &= \int \mathrm{d}^3\vec{q}_j \\ &\times \sqrt{\frac{m}{2\pi i\tau\hbar}}^{3(N-j)} \int \prod_{m=j+1}^{N-1} \mathrm{d}^3\vec{q}_m \exp\left\{ \frac{i}{\hbar} \sum_{m=j+1}^{N} \tau \left[\frac{m}{2} \left(\frac{\vec{q}_m - \vec{q}_{m-1}}{\tau} \right)^2 - V(\vec{q}_m, t_{m-1} + \lambda\,\tau) \right] \right\} \\ &\times \sqrt{\frac{m}{2\pi i\tau\hbar}}^{3j} \int \prod_{n=1}^{j-1} \mathrm{d}^3\vec{q}_n \exp\left\{ \frac{i}{\hbar} \sum_{n=1}^{j} \tau \left[\frac{m}{2} \left(\frac{\vec{q}_n - \vec{q}_{n-1}}{\tau} \right)^2 - V(\vec{q}_n, t_{n-1} + \lambda\,\tau) \right] \right\} . \quad (4.20)\end{aligned}$$

In the limit $N \to \infty$, $\tau \to 0$, this becomes

$$\langle \vec{q}_b, t_b | \vec{q}_a, t_a \rangle = \int \mathrm{d}^3\vec{q}_j \, \langle \vec{q}_b, t_b | \vec{q}_j, t_j \rangle \, \langle \vec{q}_j, t_j | \vec{q}_a, t_a \rangle \, . \quad (4.21)$$

Relabelling $\vec{q}_j \to \vec{q}$, $t_j \to t$, this is identical with Eq. (4.18).

Finally, we can prove by a direct calculation that also the free propagator (4.7) fulfills the convolution property (4.18). We start from the right-hand side of this equation and

insert Eq. (4.7),

$$\begin{aligned}
&\int \mathrm{d}^3\vec{q}\,\langle\vec{q}_b,t_b|\vec{q},t\rangle\,\langle\vec{q},t|\vec{q}_a,t_a\rangle \\
&= \int \mathrm{d}^3\vec{q}\,\sqrt{\frac{m}{2\pi i\hbar(t_b-t)}}^{\,3}\,\exp\left[\frac{i\,m}{2\hbar(t_b-t)}\,(\vec{q}_b-\vec{q})^2\right] \\
&\times\sqrt{\frac{m}{2\pi i\hbar(t-t_a)}}^{\,3}\,\exp\left[\frac{i\,m}{2\hbar(t-t_a)}\,(\vec{q}-\vec{q}_a)^2\right] \\
&= \left[\frac{m}{2\pi i\hbar\sqrt{(t_b-t)(t-t_a)}}\right]^3\exp\left[\frac{i\,m}{2\hbar}\left(\frac{\vec{q}_b^{\,2}}{t_b-t}+\frac{\vec{q}_a^{\,2}}{t-t_a}\right)\right] \\
&\times\int \mathrm{d}^3\vec{q}\,\exp\left\{\frac{i\,m(t_b-t_a)}{2\hbar(t_b-t)(t-t_a)}\left[\vec{q}^{\,2}-2\vec{q}\cdot\frac{\vec{q}_b(t-t_a)+\vec{q}_a(t_b-t)}{t_b-t_a}\right]\right\}\,. \qquad (4.22)
\end{aligned}$$

Completing the square in the exponent,

$$\left[\vec{q}-\frac{\vec{q}_b(t-t_a)+\vec{q}_a(t_b-t)}{t_b-t_a}\right]^2-\left[\frac{\vec{q}_b(t-t_a)+\vec{q}_a(t_b-t)}{t_b-t_a}\right]^2\,, \qquad (4.23)$$

and performing a substitution of the integration variable

$$\vec{q}\longrightarrow\vec{q}\,'=\vec{q}-\frac{\vec{q}_b(t-t_a)+\vec{q}_a(t_b-t)}{t_b-t_a}\,, \qquad (4.24)$$

which has a Jacobi determinant of modulus unity, we can evaluate the (complex) Gauss integral over $\mathrm{d}^3\vec{q}\,'$ with the help of Eq. (3.19),

$$\begin{aligned}
&\int \mathrm{d}^3\vec{q}\,\langle\vec{q}_b,t_b|\vec{q},t\rangle\,\langle\vec{q},t|\vec{q}_a,t_a\rangle \\
&= \left[\frac{m}{2\pi i\hbar\sqrt{(t_b-t)(t-t_a)}}\right]^3\sqrt{\frac{2\pi i\hbar(t_b-t)(t-t_a)}{m(t_b-t_a)}}^{\,3} \\
&\times\exp\left\{\frac{im}{2\hbar}\left[\frac{\vec{q}_b^{\,2}}{t_b-t}\left(1-\frac{t-t_a}{t_b-t_a}\right)+\frac{\vec{q}_a^{\,2}}{t-t_a}\left(1-\frac{t_b-t}{t_b-t_a}\right)-\frac{2\vec{q}_a\cdot\vec{q}_b}{t_b-t_a}\right]\right\} \\
&= \sqrt{\frac{m}{2\pi i\hbar(t_b-t_a)}}^{\,3}\exp\left[\frac{im}{2\hbar}\frac{(\vec{q}_b-\vec{q}_a)^2}{t_b-t_a}\right]\equiv\langle\vec{q}_b,t_b|\vec{q}_a,t_a\rangle\,, \qquad (4.25)
\end{aligned}$$

as it should be.

Armed with the convolution property, we now discuss what happens in the double-slit experiment. The situation is depicted in Fig. 4.5. A source at $(\vec{q}_a,t_a)$ emits particles. We assume that they all have the same velocity. Then, at time t (which is supposed to be the one appearing in Eq. (4.19)) the particles hit the double slit. Finally, they reach the screen at time t_b. If we assume that the particles travel in z direction, both slits are supposed to have the same area $\Delta F=\Delta x\Delta y$. Furthermore, the thickness of the blind is Δz, such that the slits form a volume $\Delta V=\Delta F\Delta z$. The particles cannot pass the blind,

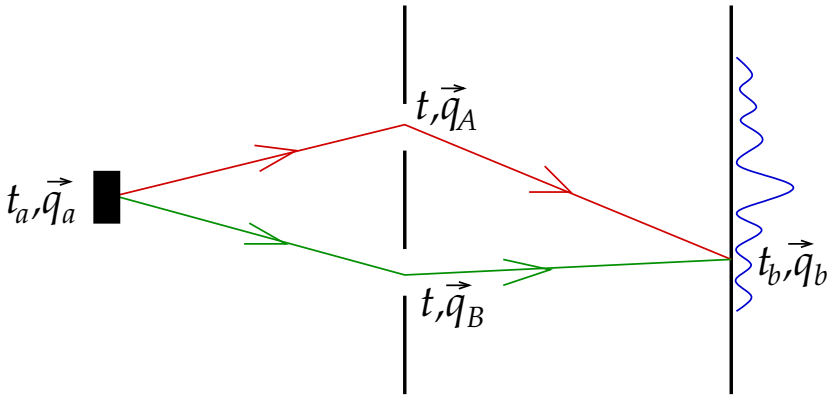


Figure 4.5: The double-slit experiment.

if they do not hit one of the two slits, either the one at $\vec{q}_A$ or the one at $\vec{q}_B$. Therefore, the volume integral in Eq. (4.19) reduces to

$$G(\vec{q}_b, t_b; \vec{q}_a, t_a) \simeq \Delta V \, \left[G(\vec{q}_b, t_b; \vec{q}_A, t) \, G(\vec{q}_A, t; \vec{q}_a, t_a) + G(\vec{q}_b, t_b; \vec{q}_B, t) \, G(\vec{q}_B, t; \vec{q}_a, t_a) \right] \, . \tag{4.26}$$

Here we have assumed that the product $G(\vec{q}_b, t_b; \vec{q}_A, t) \, G(\vec{q}_A, t; \vec{q}_a, t_a)$ does not change appreciably over the volume ΔV of the slit at $\vec{q}_A$, such that one can pull this factor out of the integral over $\mathrm{d}^3\vec{q}$, and similarly for the contribution of the slit at $\vec{q}_B$ to the integral. The quantum-mechanical probability for a particle emitted at the source at space-time point $(\vec{q}_a, t_a)$ to reach a point $\vec{q}_b$ at the screen at time t_b is then

$$\begin{aligned} P(\vec{q}_b, t_b; \vec{q}_a, t_a) &= |G(\vec{q}_b, t_b; \vec{q}_a, t_a)|^2 \\ &= \Delta V^2 \left\{ |G(\vec{q}_b, t_b; \vec{q}_A, t) \, G(\vec{q}_A, t; \vec{q}_a, t_a))|^2 + |G(\vec{q}_b, t_b; \vec{q}_B, t) \, G(\vec{q}_B, t; \vec{q}_a, t_a)|^2 \right. \\ &\quad \left. + 2 \, \mathrm{Re} \left[G(\vec{q}_b, t_b; \vec{q}_A, t) \, G(\vec{q}_A, t; \vec{q}_a, t_a) \, G^*(\vec{q}_b, t_b; \vec{q}_B, t) \, G^*(\vec{q}_B, t; \vec{q}_a, t_a) \right] \right\} \, . \end{aligned} \tag{4.27}$$

The last term is not positive semi-definite. It is the origin of the well-known quantum-mechanical interference effects, which lead to a diffraction pattern with maxima (constructive interference) and minima (destructive interference) on the screen.

Using the expression (4.7) of the free propagator, we can evaluate Eq. (4.27) explicitly,

$$\begin{aligned} P(\vec{q}_b, t_b; \vec{q}_a, t_a) = & \frac{2 \Delta V^2 m^6}{(2\pi\hbar)^6 (t_b - t)^3 (t - t_a)^3} \\ & \times \left\{ 1 + \cos \left[\frac{m}{2\hbar} \, (\vec{q}_A - \vec{q}_B) \cdot \left(\frac{\vec{q}_A + \vec{q}_B - 2\vec{q}_b}{t_b - t} + \frac{\vec{q}_A + \vec{q}_B - 2\vec{q}_a}{t - t_a} \right) \right] \right\} \, . \end{aligned} \tag{4.28}$$

Further simplification is possible by assuming that the source is located in the origin of the coordinate system, $\vec{q}_a = 0$, that the particles are emitted at $t_a = 0$, and that the two slits have the same distance from the origin, $|\vec{q}_A| = |\vec{q}_B|$. Then,

$$P(\vec{q}_b, t_b; 0, 0) = \frac{2 \Delta V^2 m^6}{(2\pi\hbar)^6 (t_b - t)^3 t^3} \left\{ 1 + \cos \left[\frac{m}{\hbar (t_b - t)} \, (\vec{q}_A - \vec{q}_B) \cdot \vec{q}_b \right] \right\} \, . \tag{4.29}$$

Introducing the quantities defined in Fig. 4.6, we now have $|\vec{q}_A - \vec{q}_B| \equiv a$ and $x = q_b \sin\beta = l\tan\beta = d\tan\alpha$. From this we compute

$$(\vec{q}_A - \vec{q}_B)\cdot\vec{q}_b = aq_b\cos\left(\frac{\pi}{2}-\beta\right) = aq_b\sin\beta = ad\tan\alpha\ .$$

Furthermore, if v is the velocity of the particles, the distance from the double slit to

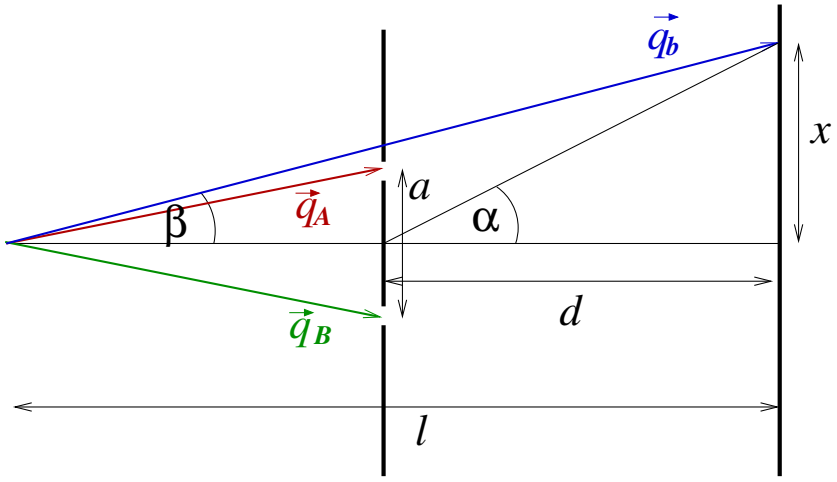


Figure 4.6: Geometry of the double-slit experiment.

the screen travelled by the particles is $v(t_b - t)$. If the screen is very far from the double slit, one can neglect the difference between the distance travelled from the slit at $\vec{q}_A$ and that travelled from the slit of $\vec{q}_B$. The average distance is then $v(t_b - t) \simeq d/\cos\alpha$. The argument of the cosine in Eq. (4.29) becomes

$$\frac{m}{\hbar(t_b-t)}\,(\vec{q}_A - \vec{q}_B)\cdot\vec{q}_b = \frac{mv}{\hbar v(t_b-t)}ad\tan\alpha \simeq \frac{k}{d}ad\sin\alpha = ka\sin\alpha\ ,$$

where we used that the momentum $p = mv = \hbar k$, where $k \equiv 2\pi/\lambda$ is the wave number associated with the de Broglie wave length λ of the particle. With $1 + \cos(2\varphi) = \cos^2\varphi$, the final result for the interference pattern is then

$$P(\vec{q}_b, t_b; 0, 0) \sim \cos^2\left(\frac{\pi}{\lambda}a\sin\alpha\right)\ , \tag{4.30}$$

which is shown in Fig. 4.7. Equation (4.30) is the standard result and is valid also for diffraction of light (massless photons) at the double slit. If we also consider the diffraction across the single slits, there is an additional modulation factor. For light waves, the result is

$$P(\vec{q}_b, t_b; 0, 0) \sim \cos^2\left(\frac{\pi}{\lambda}a\sin\alpha\right)\,\frac{\sin^2\left(\frac{\pi}{\lambda}\Delta x\sin\alpha\right)}{\left(\frac{\pi}{\lambda}\Delta x\sin\alpha\right)^2}\ , \tag{4.31}$$

where Δx is the width of the slit in the direction of $\vec{q}_A - \vec{q}_B$. However, for massive particles the result is more complicated and involves the so-called Fresnel integrals.

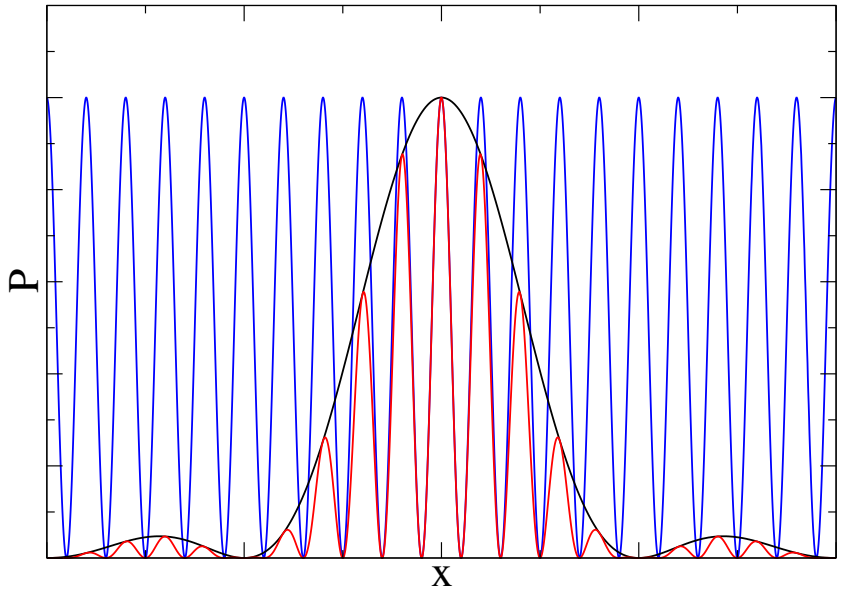


Figure 4.7: Diffraction pattern in the double-slit experiment, according to Eq. (4.30) (blue), the modulation factor alone (black), and the result (4.31) including the modulation factor (red).

4.3 Semiclassical approximation

Lecture 4

For an arbitrary potential $V(\vec{q},t)$ the path integral (3.21) can in general no longer be explicitly computed. An exception are potentials which are **quadratic** in $\vec{q}$, since then path integral over $\vec{q}$ is again a Gaussian integral (or more precisely, infinitely many of them). However, one can always apply the so-called **semiclassical approximation**, i.e., one expands the action $S[\vec{q}(t)]$ up to **quadratic order** in $\vec{q}(t)$ around the **classical trajectory** $\vec{q}_{\rm cl}(t)$. This then leads to exactly solvable path integrals. We will make this observation more precise in the following.

The classical trajectory $\vec{q}_{\rm cl}(t)$ is given by the solution of the Euler–Lagrange equations (2.3) and the corresponding action is

$$S_{\rm cl} \equiv S[\vec{q}_{\rm cl}(t)] = \int_{t_a}^{t_b} {\rm d}t\, L(\vec{q}_{\rm cl}, \dot{\vec{q}}_{\rm cl}, t)\ .$$

We introduce the **variation** around the classical trajectory via

$$\vec{r}(t) \equiv \vec{q}(t) - \vec{q}_{\rm cl}(t)\ . \tag{4.32}$$

Obviously,

$$\vec{r}(t_a) = \vec{r}(t_b) \equiv 0\ ,$$

since for all trajectories in the path integral the initial point $\vec{q}_a = \vec{q}(t_a)$ and the final point $\vec{q}_b = \vec{q}(t_b)$ are identical, i.e., they are not subjected to a variation. We expand the

Lagrange function up to order $O(\vec{r}^{\,2})$ around the classical trajectory,

$$L(\vec{q},\dot{\vec{q}},t) \simeq L(\vec{q}_{\rm cl},\dot{\vec{q}}_{\rm cl},t) + \sum_i \left(r_i \left.\frac{\partial L}{\partial q_i}\right|_{\vec{q}=\vec{q}_{\rm cl}} + \dot{r}_i \left.\frac{\partial L}{\partial \dot{q}_i}\right|_{\vec{q}=\vec{q}_{\rm cl}} \right)$$
$$+ \quad \frac{1}{2}\sum_{i,j} \left(r_i\, r_j \left.\frac{\partial^2 L}{\partial q_i \partial q_j}\right|_{\vec{q}=\vec{q}_{\rm cl}} + 2\, r_i\, \dot{r}_j \left.\frac{\partial^2 L}{\partial q_i \partial \dot{q}_j}\right|_{\vec{q}=\vec{q}_{\rm cl}} + \dot{r}_i\, \dot{r}_j \left.\frac{\partial^2 L}{\partial \dot{q}_i \partial \dot{q}_j}\right|_{\vec{q}=\vec{q}_{\rm cl}} \right) , \quad (4.33)$$

where we denoted the components of $\vec{r}(t)$ by $r_i(t)$, $i = x, y, z$. In the following we use the fact that the mixed second derivatives of L vanish for Lagrange functions of the type (3.22). If we then insert Eq. (4.33) into the action, we obtain

$$\begin{aligned} S[\vec{q}(t)] \;&\simeq\; \int_{t_a}^{t_b} {\rm d}t \left[L(\vec{q}_{\rm cl},\dot{\vec{q}}_{\rm cl},t) + \sum_i \left(r_i \left.\frac{\partial L}{\partial q_i}\right|_{\vec{q}=\vec{q}_{\rm cl}} + \dot{r}_i \left.\frac{\partial L}{\partial \dot{q}_i}\right|_{\vec{q}=\vec{q}_{\rm cl}} \right) \right. \\ &\qquad \left. + \frac{1}{2}\sum_{i,j} \left(r_i\, r_j \left.\frac{\partial^2 L}{\partial q_i \partial q_j}\right|_{\vec{q}=\vec{q}_{\rm cl}} + \dot{r}_i\, \dot{r}_j \left.\frac{\partial^2 L}{\partial \dot{q}_i \partial \dot{q}_j}\right|_{\vec{q}=\vec{q}_{\rm cl}} \right) \right] \\ &=\; S_{\rm cl} + \int_{t_a}^{t_b} {\rm d}t \sum_i r_i \left(\frac{\partial L}{\partial q_i} - \frac{\rm d}{{\rm d}t}\frac{\partial L}{\partial \dot{q}_i} \right)_{\vec{q}=\vec{q}_{\rm cl}} \\ &\qquad + \int_{t_a}^{t_b} {\rm d}t \left[\frac{m}{2}\,\dot{\vec{r}}^{\,2} - \frac{1}{2}\,\vec{r}^{\,T} V''(\vec{q}_{\rm cl},t)\,\vec{r} \right] , \end{aligned} \quad (4.34)$$

where we have performed an integration by parts in the term $\sim O(\vec{r})$ and used the fact that the variation of $\vec{r}(t)$ vanishes at t_a and t_b. Furthermore, due to Eq. (3.22) we have used

$$\begin{aligned} \left.\frac{\partial^2 L}{\partial \dot{q}_i \partial \dot{q}_j}\right|_{\vec{q}=\vec{q}_{\rm cl}} &= m\,\delta_{ij} , \\ \left.\frac{\partial^2 L}{\partial q_i \partial q_j}\right|_{\vec{q}=\vec{q}_{\rm cl}} &= -\left.\frac{\partial^2 V(\vec{q},t)}{\partial q_i \partial q_j}\right|_{\vec{q}=\vec{q}_{\rm cl}} \equiv -V''_{ij}(\vec{q}_{\rm cl},t) . \end{aligned}$$

The last equation represents the (ij) element of the matrix V'' of second derivatives of the potential V with respect to the coordinates. The second term in Eq. (4.34) vanishes on account of the Euler–Lagrange equations (2.3) and we obtain

$$S[\vec{q}(t)] \simeq S_{\rm cl} + \int_{t_a}^{t_b} {\rm d}t \left[\frac{m}{2}\,\dot{\vec{r}}^{\,2} - \frac{1}{2}\,\vec{r}^{\,T} V''(\vec{q}_{\rm cl},t)\,\vec{r} \right] . \quad (4.35)$$

When inserting this into the path integral (3.21), we can factor out the contribution of the classical action from the integral, since it does not depend on the integration variables $\vec{q}_n$. Furthermore, we can substitute the latter by the variables $\vec{r}_n$ on account of Eq. (4.32). This substitution of variables has a Jacobi determinant which is unity, and it immediately follows that

$$\langle \vec{q}_b, t_b | \vec{q}_a, t_a \rangle \simeq \mathcal{N}\, e^{iS_{\rm cl}/\hbar} \int_{\vec{r}(t_a)=0}^{\vec{r}(t_b)=0} \mathcal{D}\vec{r}\, \exp\left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} {\rm d}t \left[\frac{m}{2}\,\dot{\vec{r}}^{\,2} - \frac{1}{2}\,\vec{r}^{\,T} V''(\vec{q}_{\rm cl},t)\,\vec{r} \right] \right\} . \quad (4.36)$$

The path integral is again of the type of a(n infinitely dimensional) Gaussian integral and can be exactly computed. We demonstrate this explicitly for the case of **one spatial dimension**. To this end we first write the path integral in Eq. (4.36) (including the normalization factor $\mathcal{N}$) in the form of Eq. (3.20), i.e., where integrate over $N-1$ variables r_n,

$$I(t_b,t_a) \equiv \sqrt{\frac{m}{2\pi i\tau\hbar}}^N \int \prod_{n=1}^{N-1} \mathrm{d}r_n \, \exp\left\{ \frac{i}{\hbar} \sum_{n=1}^{N} \tau \left[\frac{m}{2} \left(\frac{r_n - r_{n-1}}{\tau} \right)^2 - \frac{1}{2} V_n'' \, r_n^2 \right] \right\} \ , \quad (4.37)$$

where we abbreviated

$$V_n'' \equiv V''(q_{\mathrm{cl},n}, t_{n-1} + \lambda\tau) \ .$$

The exponent in Eq. (4.37) has the following form:

$$\begin{aligned} -\sum_{n=1}^{N} \left[\frac{m}{2i\tau\hbar} (r_n - r_{n-1})^2 + \frac{i\tau}{2\hbar} V_n'' \, r_n^2 \right] &= -\frac{m}{2i\tau\hbar} \big(r_0^2 - 2r_0 r_1 + r_1^2 + r_1^2 - 2r_1 r_2 + r_2^2 + \cdots \\ &\quad + r_{N-2}^2 - 2r_{N-2} r_{N-1} + r_{N-1}^2 + r_{N-1}^2 - 2r_{N-1} r_N + r_N^2 \big) \\ &\quad - \frac{i\tau}{2\hbar} \left(V_1'' r_1^2 + V_2'' r_2^2 + \cdots + V_N'' r_N^2 \right) \\ \equiv \ & -\frac{m}{2i\tau\hbar} \left(2r_1^2 - 2r_1 r_2 + 2r_2^2 + \cdots + 2r_{N-2}^2 - 2r_{N-2} r_{N-1} + 2r_{N-1}^2 \right) \\ - \ & \frac{i\tau}{2\hbar} \left(V_1'' r_1^2 + V_2'' r_2^2 + \cdots + V_{N-1}'' r_{N-1}^2 \right) \ , \end{aligned} \quad (4.38)$$

where we have used the fact that $r_0 \equiv r_a = 0$, $r_N \equiv r_b = 0$. The result can be written as a product of row vector, matrix, and column vector,

$$-\frac{m}{2i\tau\hbar} \sum_{n=1}^{N} \left[(r_n - r_{n-1})^2 - \frac{\tau^2}{m} V_n'' \, r_n^2 \right] \equiv -\frac{m}{2i\tau\hbar} \, \vec{r}^{\,T} \mathrm{A} \, \vec{r} \, , \quad (4.39)$$

where $\vec{r} \equiv (r_1,\, r_2,\, r_3,\, \ldots,\, r_{N-1})^T$ and

$$\mathrm{A} = \begin{pmatrix} 2+c_1 & -1 & 0 & \cdots & & 0 \\ -1 & 2+c_2 & -1 & 0 & \cdots & \vdots \\ 0 & -1 & 2+c_3 & -1 & 0 & 0 \\ \vdots & & & \ddots & & \vdots \\ 0 & \cdots & 0 & -1 & 2+c_{N-2} & -1 \\ 0 & & \cdots & 0 & -1 & 2+c_{N-1} \end{pmatrix} \ , \quad (4.40)$$

with $c_n \equiv -\tau^2 V_n''/m$. Equation (4.37) thus assumes the compact form

$$I(t_b,t_a) = \sqrt{\frac{m}{2\pi i\tau\hbar}}^N \int \mathrm{d}^{N-1}\vec{r} \, \exp\left(-\frac{m}{2i\tau\hbar} \, \vec{r}^{\,T} \mathrm{A} \, \vec{r} \right) \ .$$

The $[(N-1)\times(N-1)]-$Matrix A is symmetric, therefore one can **diagonalize it by means of an orthogonal transformation $\boldsymbol{O}$**, $O^T \equiv O^{-1}$ and $\det O = +1$,

$$\mathrm{D} \equiv \mathrm{diag}\,(a_1,\, a_2,\, \ldots,\, a_{N-1}) \equiv O \, \mathrm{A} \, O^T \ , \quad (4.41)$$

where a_n are the eigenvalues of A. Multiplying from the left with O^T and from the right with O yields

$$O^T \mathrm{D}\, O = \mathrm{A}\ ,$$

i.e.,

$$\begin{aligned} I(t_b,t_a) &= \sqrt{\frac{m}{2\pi i\tau\hbar}}^N \int \mathrm{d}^{N-1}\vec{r}\, \exp\left(-\frac{m}{2i\tau\hbar}\,\vec{r}^{\,T} O^T \mathrm{D}\, O\,\vec{r}\right) \\ &\equiv \sqrt{\frac{m}{2\pi i\tau\hbar}}^N \int \mathrm{d}^{N-1}\vec{s}\, \exp\left(-\frac{m}{2i\tau\hbar}\,\vec{s}^{\,T} \mathrm{D}\,\vec{s}\right) \\ &\equiv \sqrt{\frac{m}{2\pi i\tau\hbar}}^N \int \prod_{n=1}^{N-1} \mathrm{d}s_n\, \exp\left(-\frac{m}{2i\tau\hbar}\sum_{n=1}^{N-1} a_n\, s_n^2\right)\ , \end{aligned} \tag{4.42}$$

where we have substituted variables according to

$$\vec{s} \equiv O\,\vec{r}\,, \quad \vec{s}^{\,T} \equiv \vec{r}^{\,T} O^T\ .$$

The corresponding Jacobi determinant is $\mathcal{J} \equiv \det O = +1$, so that the integration measure does not change. The $N-1$ Gaussian integrals in Eq. (4.42) can again be computed with the formula (3.17), so that

$$I(t_b,t_a) = \sqrt{\frac{m}{2\pi i\tau\hbar}}^N \sqrt{\frac{2\pi i\tau\hbar}{m}}^{N-1} \prod_{n=1}^{N-1} a_n^{-1/2} \equiv \sqrt{\frac{m}{2\pi i\hbar}}\,(\tau \det \mathrm{A})^{-1/2}\ , \tag{4.43}$$

where, on account of Eq. (4.41) and $\det O \equiv \det O^T = +1$, we employed the identity

$$\det \mathrm{D} = \prod_{n=1}^{N-1} a_n = \det\left(O\,\mathrm{A}\,O^T\right) = \det O \det \mathrm{A} \det O^T = \det \mathrm{A}\ . \tag{4.44}$$

We now compute the determinant of the matrix (4.40) with the help of Laplace's theorem,

$$\varphi_{N-1} \equiv \tau \det \mathrm{A} = (2 + c_{N-1})\,\varphi_{N-2} - \varphi_{N-3}\ , \tag{4.45}$$

where

$$\varphi_{N-2} = \tau \begin{vmatrix} 2+c_1 & -1 & 0 & \cdots & & 0 \\ -1 & 2+c_2 & -1 & 0 & \cdots & \vdots \\ 0 & -1 & 2+c_3 & -1 & 0 & 0 \\ \vdots & & & \ddots & & \vdots \\ 0 & \cdots & 0 & -1 & 2+c_{N-3} & -1 \\ 0 & & \cdots & 0 & -1 & 2+c_{N-2} \end{vmatrix}\ ,$$

$$\begin{aligned}
\varphi_{N-3} &= -\tau \begin{vmatrix} 2+c_1 & -1 & 0 & \cdots & & 0 \\ -1 & 2+c_2 & -1 & 0 & \cdots & \vdots \\ 0 & -1 & 2+c_3 & -1 & 0 & 0 \\ \vdots & & & \ddots & & \vdots \\ 0 & \cdots & 0 & -1 & 2+c_{N-3} & 0 \\ 0 & & \cdots & 0 & -1 & -1 \end{vmatrix} \\
&\equiv \tau \begin{vmatrix} 2+c_1 & -1 & 0 & \cdots & 0 \\ -1 & 2+c_2 & -1 & 0 & \vdots \\ 0 & -1 & 2+c_3 & -1 & 0 \\ \vdots & & & \ddots & \vdots \\ 0 & \cdots & 0 & -1 & 2+c_{N-3} \end{vmatrix} .
\end{aligned}$$

From this follows the recursion formula

$$\varphi_{n+1} = (2 + c_{n+1})\,\varphi_n - \varphi_{n-1} \;, \quad n = 1, \ldots, N-2 \;, \tag{4.46}$$

where we set $\varphi_1 = \tau(2 + c_1)$ and $\varphi_0 = \tau$. Using the definition of the c_n, we can write this recursion formula as

$$\frac{\varphi_{n+1} - 2\,\varphi_n + \varphi_{n-1}}{\tau^2} = \frac{c_{n+1}}{\tau^2}\,\varphi_n \equiv -\frac{V''_{n+1}}{m}\,\varphi_n \;. \tag{4.47}$$

In the limit $\tau \to 0$ this becomes the **differential equation**

$$\frac{\mathrm{d}^2\varphi(t)}{\mathrm{d}t^2} = -\frac{V''(t)}{m}\,\varphi(t) \;. \tag{4.48}$$

In order to solve this equation, we need **initial conditions**, which read

$$\begin{aligned}
\varphi(t_a) &\equiv \lim_{\tau\to 0}\varphi_0 = \lim_{\tau\to 0}\tau \equiv 0 \;, \\
\frac{\mathrm{d}\varphi(t_a)}{\mathrm{d}t} &\equiv \lim_{\tau\to 0}\frac{\varphi_1 - \varphi_0}{\tau} = \lim_{\tau\to 0}\frac{\tau(2+c_1) - \tau}{\tau} = \lim_{\tau\to 0}\left(1 - \frac{\tau^2\,V_1''}{m}\right) \equiv 1 \;.
\end{aligned} \tag{4.49}$$

At this point, we can only proceed further if the potential $V(\vec{q}, t)$ is known. Then, the differential equation (4.48) can be explicitly solved until time t_b. This yields a function

$$f(t_b, t_a) \equiv \varphi(t_b) \equiv \lim_{\substack{N\to\infty \\ \tau\to 0}} \varphi_N = \lim_{\substack{N\to\infty \\ \tau\to 0}} \varphi_{N-1} = \lim_{\substack{N\to\infty \\ \tau\to 0}} (\tau \det \mathrm{A}) \;, \tag{4.50}$$

which depends on the initial conditions (4.49) at time t_a. These will be determined for the example of the one-dimensional harmonic oscillator in the next section.

Let us summarize the results of this section. With Eqs. (4.36), (4.43), and (4.50) the **transition amplitude (resp. the propagator) in the semiclassical approximation** reads

$$\langle \vec{q}_b, t_b | \vec{q}_a, t_a \rangle \equiv G(\vec{q}_b, t_b; \vec{q}_a, t_a) \simeq \sqrt{\frac{m}{2\pi i\hbar\, f(t_b, t_a)}}\, \exp\left(\frac{i}{\hbar}\, S_{\mathrm{cl}}\right) \;. \tag{4.51}$$

4.4 Propagator of the one-dimensional harmonic oscillator

The potential of the one-dimensional harmonic oscillator reads

$$V(q) = \frac{1}{2}\, m\omega^2\, q^2 \;, \tag{4.52}$$

where ω is the eigenfrequency of the oscillator. For this potential the semiclassical approximation discussed in the previous section is **exact**, because the expansion of the potential automatically terminates after the second order,

$$V'' = m\,\omega^2 = const. \;, \quad V''' \equiv 0 \;.$$

The differential equation (4.48) is simply the equation of motion of the harmonic oscillator,

$$\frac{\mathrm{d}^2\varphi(t)}{\mathrm{d}t^2} + \omega^2\,\varphi(t) = 0 \;, \tag{4.53}$$

with the well-known solution

$$\varphi(t) = A\,\cos(\omega t) + B\,\sin(\omega t) \;. \tag{4.54}$$

The initial conditions (4.49) yield

$$\begin{aligned} \varphi(t_a) &= A\,\cos(\omega t_a) + B\,\sin(\omega t_a) \equiv 0 \;, \\ \frac{\mathrm{d}\varphi(t_a)}{\mathrm{d}t} &= -\omega\, A\,\sin(\omega t_a) + \omega\, B\,\cos(\omega t_a) = 1 \;, \end{aligned}$$

from which we can determine the constants A and B:

$$\begin{aligned} A &= -B\,\tan(\omega t_a) \;, \\ B &= \frac{\cos(\omega t_a)}{\omega} \;, \end{aligned}$$

so that the solution at time t_b reads

$$\begin{aligned} f(t_b, t_a) \equiv \varphi(t_b) &= -B\,\tan(\omega t_a)\,\cos(\omega t_b) + B\,\sin(\omega t_b) \\ &= \frac{\cos(\omega t_a)}{\omega}\,[\sin(\omega t_b) - \tan(\omega t_a)\,\cos(\omega t_b)] \\ &= \frac{1}{\omega}\,[\sin(\omega t_b)\,\cos(\omega t_a) - \cos(\omega t_b)\,\sin(\omega t_a)] \\ &\equiv \frac{\sin[\omega(t_b - t_a)]}{\omega} \;. \end{aligned} \tag{4.55}$$

In order to determine the propagator (4.51) we still need to compute the action along the classical trajectory. This is possible without major difficulties, albeit a bit cumbersome. First, the classical trajectory is of course a solution of the Euler–Lagrange equation for the harmonic oscillator,

$$0 = \frac{\mathrm{d}}{\mathrm{d}t}\,\frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} = m\,\ddot{q} + m\omega^2 q \;,$$

or

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

The solution is well known,

$$q_{\rm cl}(t) = C\, \cos(\omega t) + D\, \sin(\omega t) \; . \tag{4.56}$$

The constants A and B are determined by the given initial and final conditions (which of course hold also for the classical trajectory)

$$\begin{aligned} q_a \equiv q_{\rm cl}(t_a) &= C\, \cos(\omega t_a) + D\, \sin(\omega t_a) \; , \\ q_b \equiv q_{\rm cl}(t_b) &= C\, \cos(\omega t_b) + D\, \sin(\omega t_b) \; . \end{aligned}$$

One can check that this yields

$$\begin{aligned} C &= \frac{q_a\, \sin(\omega t_b) - q_b\, \sin(\omega t_a)}{\sin\left[\omega(t_b - t_a)\right]} \; , \\ D &= \frac{q_b\, \cos(\omega t_a) - q_a\, \cos(\omega t_b)}{\sin\left[\omega(t_b - t_a)\right]} \; . \end{aligned} \tag{4.57}$$

Inserting this into Eq. (4.56) we obtain

$$q_{\rm cl}(t) = \frac{q_a\, \sin\left[\omega(t_b - t)\right] + q_b\, \sin\left[\omega(t - t_a)\right]}{\sin\left[\omega(t_b - t_a)\right]} \; . \tag{4.58}$$

The time derivative is

$$\dot{q}_{\rm cl}(t) = \omega\, \frac{q_b\, \cos\left[\omega(t - t_a)\right] - q_a\, \cos\left[\omega(t_b - t)\right]}{\sin\left[\omega(t_b - t_a)\right]} \; . \tag{4.59}$$

If we insert this into the Lagrange function, we get

$$\begin{aligned} L(q_{\rm cl}, \dot{q}_{\rm cl}, t) &= \frac{m}{2}\, \dot{q}_{\rm cl}^2 - \frac{m}{2}\, \omega^2\, q_{\rm cl}^2 \\ &= \frac{m\omega^2}{2 \sin^2\left[\omega(t_b - t_a)\right]} \Big\{ q_b^2\, \cos^2\left[\omega(t - t_a)\right] + q_a^2\, \cos^2\left[\omega(t_b - t)\right] \\ &\qquad - 2\, q_a\, q_b\, \cos\left[\omega(t - t_a)\right]\, \cos\left[\omega(t_b - t)\right] \\ &\qquad - q_b^2\, \sin^2\left[\omega(t - t_a)\right] - q_a^2\, \sin^2\left[\omega(t_b - t)\right] \\ &\qquad - 2\, q_a\, q_b\, \sin\left[\omega(t - t_a)\right]\, \sin\left[\omega(t_b - t)\right] \Big\} \\ &= \frac{m\omega^2}{2 \sin^2\left[\omega(t_b - t_a)\right]} \Big\{ q_b^2\, \cos\left[2\omega(t - t_a)\right] + q_a^2\, \cos\left[2\omega(t_b - t)\right] \\ &\qquad - 2\, q_a\, q_b\, \cos\left[\omega(t_b + t_a - 2t)\right] \Big\} \; . \end{aligned} \tag{4.60}$$

Inserting this into the action integral, we need to compute the following three integrals:

$$\begin{aligned} \int_{t_a}^{t_b} {\rm d}t\, \cos\left[2\omega(t - t_a)\right] &= \int_0^{t_b - t_a} {\rm d}z\, \cos(2\omega z) = \frac{1}{2\omega}\, \sin\left[2\omega(t_b - t_a)\right] \; , \\ \int_{t_a}^{t_b} {\rm d}t\, \cos\left[2\omega(t_b - t)\right] &= -\int_{t_b - t_a}^{0} {\rm d}z\, \cos(2\omega z) = \frac{1}{2\omega}\, \sin\left[2\omega(t_b - t_a)\right] \; , \\ \int_{t_a}^{t_b} {\rm d}t\, \cos\left[\omega(t_b + t_a - 2t)\right] &= -\frac{1}{2} \int_{t_b - t_a}^{t_a - t_b} {\rm d}z\, \cos(\omega z) = \frac{1}{\omega}\, \sin\left[\omega(t_b - t_a)\right] \; . \end{aligned}$$

Thus, the classical action reads

$$\begin{aligned} S_{\rm cl} &= \int_{t_a}^{t_b} \mathrm{d}t\, L(q_{\rm cl}, \dot{q}_{\rm cl}, t) \\ &= \frac{m\omega}{2\sin^2\left[\omega(t_b - t_a)\right]} \left\{ \frac{q_a^2 + q_b^2}{2} \sin\left[2\omega(t_b - t_a)\right] - 2\, q_a\, q_b \sin\left[\omega(t_b - t_a)\right] \right\} \\ &= \frac{m\omega}{2\sin\left[\omega(t_b - t_a)\right]} \left\{ (q_a^2 + q_b^2) \cos\left[\omega(t_b - t_a)\right] - 2\, q_a\, q_b \right\} . \end{aligned} \tag{4.61}$$

With this and with Eq. (4.55) the **propagator of the one-dimensional harmonic oscillator** reads

$$\begin{aligned} &\langle \vec{q}_b, t_b | \vec{q}_a, t_a \rangle \equiv G(\vec{q}_b, t_b; \vec{q}_a, t_a) \\ &= \sqrt{\frac{m\omega}{2\pi i\hbar \sin\left[\omega(t_b - t_a)\right]}} \exp\left\{ \frac{im\omega}{2\hbar} \frac{(q_a^2 + q_b^2) \cos\left[\omega(t_b - t_a)\right] - 2\, q_a\, q_b}{\sin\left[\omega(t_b - t_a)\right]} \right\} . \end{aligned} \tag{4.62}$$

Lecture 5

4.5 The anharmonic oscillator

The potential of the anharmonic oscillator contains an additional quartic term besides the quadratic term of the harmonic-oscillator potential (4.52),

$$V(q) = \frac{1}{2}\, m\omega^2\, q^2 + \frac{1}{4}\, \lambda\, q^4 . \tag{4.63}$$

In order to have potential which is bounded from below at large q, we have to choose $\lambda > 0$. For small q, this potential is very close to that of the harmonic oscillator, but for large q it increases more rapidly than the latter, i.e., it has "stiffer" walls than the harmonic oscillator, cf. Fig. 4.8.

The existence of a potential energy implies that the system is conservative, so the total energy

$$E = \frac{1}{2}\, m\dot{q}^2 + V(q) = \frac{1}{2}\, m\dot{q}^2 + \frac{1}{2}\, m\omega^2\, q^2 + \frac{1}{4}\, \lambda\, q^4 \tag{4.64}$$

is **conserved** and a **constant of motion** along the classical path. The turning points $\pm\bar{q}$ of the motion are determined by the condition $\dot{q} = 0$. Using Eq. (4.64), we can then express $\bar{q}$ as a function of the available energy E of the particle by solving

$$E = V(\bar{q}) = \frac{1}{2}\, m\omega^2\, \bar{q}^2 + \frac{1}{4}\, \lambda\, \bar{q}^4 \tag{4.65}$$

for $\bar{q}$. For a given energy $E = \text{const.}$, the turning points can thus be determined from

$$\bar{q}^2 = \frac{m\omega^2}{\lambda} \left(\sqrt{1 + \frac{4\lambda E}{(m\omega^2)^2}} - 1 \right) . \tag{4.66}$$

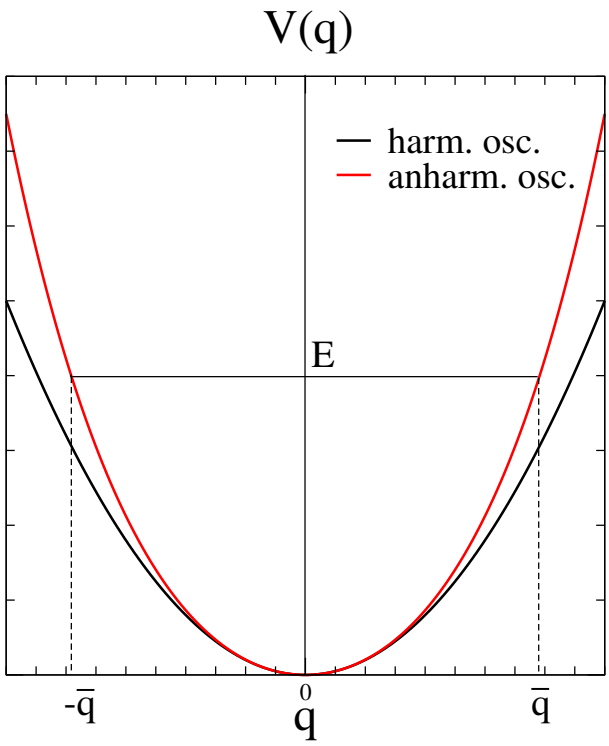


Figure 4.8: The anharmonic-oscillator potential (red) in comparison to the harmonic-oscillator potential (black).

In the limit $\lambda \to 0$, this becomes $\bar{q}^2 = 2E/(m\omega^2)$, which corresponds to the turning points of the harmonic-oscillator potential. As one can see from Fig. 4.8, $\bar{q}$ is smaller for the anharmonic-oscillator potential than for the harmonic-oscillator potential: the particle is "reflected" from the stiffer potential wall of the anharmonic potential at a smaller distance from the origin. Moreover, the force

$$m\ddot{q} = F = -\frac{\mathrm{d}V(q)}{\mathrm{d}q} = -m\omega^2\, q - \lambda\, q^3 \tag{4.67}$$

is at any distance q from the origin larger than that for the harmonic oscillator. Thus, when the particle hits the potential wall at the turning point of the motion, it will be accelerated more rapidly towards the origin than in the case of the harmonic oscillator. The semiclassical approximation discussed in the last section is no longer exact for the potential (4.63), but it is still useful and allows to gain some insights into the problem that are not possible by, e.g., perturbation theory in the "coupling constant" λ, as will be explored in the next chapter.

In order to proceed, the first task is to determine the action along the classical path. Equation (4.64) allows us to express the velocity in terms of the difference of energy and potential (as for the Kepler problem),

$$\dot{q} = \pm\sqrt{\frac{2}{m}\left[E - V(q)\right]}\,. \tag{4.68}$$

Thus, with $u \equiv q/\bar{q}$,

$$\begin{aligned} E - V(q) = V(\bar{q}) - V(q) &= \frac{1}{2}\, m\omega^2 \bar{q}^2 \left(1 - u^2\right) + \frac{1}{4}\, \lambda\, \bar{q}^4 \left(1 - u^4\right) \\ &= \left(1 - u^2\right) \left[\frac{1}{2}\, m\omega^2 \bar{q}^2 + \frac{1}{4}\, \lambda\, \bar{q}^4 \left(1 + u^2\right)\right] \\ &= \frac{1}{4}\, \lambda\, \bar{q}^4 \left(1 - u^2\right) \left(\kappa^2 + u^2\right) \ , \end{aligned} \tag{4.69}$$

where

$$\kappa^2 \equiv \frac{4E}{\lambda\, \bar{q}^4} = 1 + \frac{2m\omega^2}{\lambda\, \bar{q}^2} > 1 \ . \tag{4.70}$$

Using Eq. (4.68), the time $t_b - t_a$ that it takes the particle to move from $q(t_a) \equiv q_a$ to $q(t_b) \equiv q_b \geq q_a$ is then

$$t_b - t_a = \int_{t_a}^{t_b} \mathrm{d}t = \int_{q_a}^{q_b} \frac{\mathrm{d}q}{\dot{q}} = \pm\sqrt{\frac{2m}{\lambda}}\, \frac{1}{\bar{q}} \int_{u_a}^{u_b} \frac{\mathrm{d}u}{\sqrt{(1 - u^2)(\kappa^2 + u^2)}} \ , \tag{4.71}$$

where $u_{a,b} \equiv q_{a,b}/\bar{q}$. Now a trajectory starting at $u_a \in [-1, 1]$ and ending at $u_b \in [-1, 1]$ can always be decomposed into a linear combination of pieces starting from the origin, $u_a = 0$, and ending at some point $u_b \in [-1, 1]$. Therefore, for the sake of simplicity let us now simply consider such a piece starting at $u_a = 0$ at time $t_a = 0$ and ending at $0 < u_b \equiv v \leq 1$ at time $t_b \equiv t > 0$ (the case $u_b < 0$ can be treated analogously),

$$\begin{aligned} t &= \sqrt{\frac{2m}{\lambda}}\, \frac{1}{\bar{q}} \int_0^v \frac{\mathrm{d}u}{\sqrt{(1 - u^2)(\kappa^2 + u^2)}} \\ &\equiv \sqrt{\frac{2m}{\lambda}}\, \frac{1}{\bar{q}} \frac{1}{\sqrt{1 + \kappa^2}}\, F\left(\arcsin\left(v\sqrt{\frac{1 + \kappa^2}{v^2 + \kappa^2}}\right), \frac{1}{\sqrt{1 + \kappa^2}}\right) \ , \end{aligned} \tag{4.72}$$

where $F(\varphi, k)$ is the elliptic integral of the first kind (cf. Eq. (3.152.3) of Ref. [5]). If $v = 1$, or $q_b = \bar{q}$, the particle has completed one quarter of a period of oscillation, so the complete period is

$$T = 4\sqrt{\frac{2m}{\lambda}}\, \frac{1}{\bar{q}} \frac{1}{\sqrt{1 + \kappa^2}}\, F\left(\frac{\pi}{2}, \frac{1}{\sqrt{1 + \kappa^2}}\right) \equiv 4\sqrt{\frac{2m}{\lambda}}\, \frac{1}{\bar{q}} \frac{1}{\sqrt{1 + \kappa^2}}\, \mathbf{K}\left(\frac{1}{\sqrt{1 + \kappa^2}}\right) \ , \tag{4.73}$$

where $\mathbf{K}(k)$ is the complete elliptic integral of the first kind. Two limiting cases are of interest:

(i) $\lambda \to 0$: in this case,

$$\kappa^2 \longrightarrow \frac{2m\omega^2}{\lambda \bar{q}^2} \ , \quad \frac{1}{\sqrt{1 + \kappa^2}} \longrightarrow \sqrt{\frac{\lambda}{2m}}\, \frac{\bar{q}}{\omega} \ , \quad \mathbf{K}\left(\frac{1}{\sqrt{1 + \kappa^2}}\right) \longrightarrow \mathbf{K}\left(0\right) = \frac{\pi}{2} \ , \tag{4.74}$$

and

$$T \longrightarrow \frac{4}{\omega}\, \frac{\pi}{2} = \frac{2\pi}{\omega} \tag{4.75}$$

becomes identical to the oscillation period of the harmonic oscillator, as it should be when $\lambda \to 0$.

(ii) $\lambda \to \infty$: in this case, Eqs. (4.66) and (4.70) yield

$$\kappa^2 \longrightarrow 1 \,, \qquad \bar{q}^2 \longrightarrow \sqrt{\frac{4E}{\lambda}} \,. \tag{4.76}$$

The potential walls narrow so much that the turning points approach the origin as $\bar{q} \sim \lambda^{-1/4}$. Since

$$\mathbf{K}\left(\frac{1}{\sqrt{2}}\right) = \frac{1}{4\sqrt{\pi}}\left[\Gamma\left(\frac{1}{4}\right)\right]^2 \,,$$

see Eq. (8.129.1) of Ref. [5], we obtain for the period of oscillation

$$\begin{aligned}\lim_{\lambda\to\infty} T &= \lim_{\lambda\to\infty} 4\sqrt{\frac{2m}{\lambda}}\left(\frac{\lambda}{4E}\right)^{1/4}\frac{1}{\sqrt{2}}\frac{1}{4\sqrt{\pi}}\left[\Gamma\left(\frac{1}{4}\right)\right]^2 \\ &= \lim_{\lambda\to\infty}\left(\frac{m^2}{4\pi^2\lambda E}\right)^{1/4}\left[\Gamma\left(\frac{1}{4}\right)\right]^2 = 0 \,,\end{aligned} \tag{4.77}$$

The physical interpretation is that in this limit the potential walls become infinitely narrow so that the period of oscillation vanishes like $\sim \lambda^{-1/4}$. This behavior is in agreement with the decrease of $\bar{q}$ in this limit.

Solving Eq. (4.72) for v and computing $\bar{q}v(t) = \bar{q}u_b(t) = q_b(t)$ in principle gives the classical trajectory $q_b(t) \equiv q_{\rm cl}(t)$ of the particle as a function of time. With this in hand, one computes $V''(q_{\rm cl}(t)) \equiv m\omega^2 + 3\lambda\, q_{\rm cl}^2(t)$ on the classical trajectory and can then (in principle) also solve Eq. (4.48), which determines the prefactor $f(t_b, t_a)$ of the propagator (4.51). This is (at least as far as I know) no longer possible in closed analytic form. However, we can still compute the classical action $S_{\rm cl}$ in the exponent of Eq. (4.51).

To this end, we write with the help of Eqs. (4.64), (4.68) (for the sake of simplicity we suppress the index "cl" in the following)

$$\begin{aligned}S &= \int_{t_a}^{t_b} \mathrm{d}t\, L(\dot{q}, q, t) = \int_{t_a}^{t_b} \mathrm{d}t\, \left[\frac{1}{2}\, m\dot{q}^2 - V(q)\right] = \int_{q_a}^{q_b} \frac{\mathrm{d}q}{\dot{q}}\, \left[E - 2V(q)\right] \\ &= \pm\sqrt{\frac{m}{2}}\int_{q_a}^{q_b} \mathrm{d}q\, \left[\sqrt{E - V(q)} - \frac{V(q)}{\sqrt{E - V(q)}}\right] \,,\end{aligned} \tag{4.78}$$

where the + sign is for the case $q_a \le q_b$, while the − sign is for the case $q_a \ge q_b$. Similarly as in Eq. (4.72) we argue that we can write an arbitrary trajectory as a linear superposition of pieces starting at $q_a = 0$ and ending at $q_b \in [-\bar{q}, \bar{q}]$ and, for the sake of simplicity, we focus on the case $q_b \in [0, \bar{q}]$ in the following (the case $q_b \in [-\bar{q}, 0]$ can be treated similarly). Using the same variables as before ($u = q/\bar{q}$, $v = u_b = q_b/\bar{q}$, and κ^2 from Eq. (4.70) and employing Eqs. (4.63) and (4.69) we obtain

$$S = \frac{\bar{q}^3}{2}\sqrt{\frac{m\lambda}{2}}\int_0^v \mathrm{d}u\, \left[\sqrt{(1-u^2)(\kappa^2+u^2)} - \frac{(\kappa^2-1)u^2 + u^4}{\sqrt{(1-u^2)(\kappa^2+u^2)}}\right] \,. \tag{4.79}$$

The integrals are again standard elliptic integrals (cf. Eqs. (3.153.2), (3.154.2), and (3.155.4) in Ref. [5]). The final result is

$$S = \frac{\bar{q}^3}{6}\sqrt{\frac{m\lambda}{2}}\left[\frac{\kappa^2(2\kappa^2-1)}{\sqrt{1+\kappa^2}}\,F\left(\arcsin\left(v\sqrt{\frac{1+\kappa^2}{v^2+\kappa^2}}\right),\frac{1}{\sqrt{1+\kappa^2}}\right)\right.$$
$$-2\sqrt{1+\kappa^2}(\kappa^2-1)\,E\left(\arcsin\left(v\sqrt{\frac{1+\kappa^2}{v^2+\kappa^2}}\right),\frac{1}{\sqrt{1+\kappa^2}}\right)$$
$$\left.+\,2v(v^2+2\kappa^2-1)\sqrt{\frac{1-v^2}{\kappa^2+v^2}}\right]\ , \tag{4.80}$$

where $E(\varphi,k)$ is the elliptic integral of the second kind. Of particular interest is the case where the particle completes the way from the origin to the turning point. For this case, the above expression is taken for $v=1$,

$$S = \frac{\bar{q}^3}{6}\sqrt{\frac{m\lambda}{2}}\left[\frac{\kappa^2(2\kappa^2-1)}{\sqrt{1+\kappa^2}}\,\mathbf{K}\left(\frac{1}{\sqrt{1+\kappa^2}}\right)-2\sqrt{1+\kappa^2}(\kappa^2-1)\,\mathbf{E}\left(\frac{1}{\sqrt{1+\kappa^2}}\right)\right]\ , \tag{4.81}$$

where $\mathbf{E}(k)$ is the complete elliptic integral of the second kind.

Finally, we can make the following interesting observation. Irrespective of the length of the trajectory the particle travels in the potential, according to Eq. (4.72) the time behaves as

$$t = \sqrt{\frac{2m}{\lambda}}\frac{1}{\bar{q}}K_1\ , \tag{4.82}$$

where K_1 is some numerical factor resulting from evaluating the elliptic integral. Likewise, from Eq. (4.80) we see that the classical action behaves as

$$S = \frac{\bar{q}^3}{6}\sqrt{\frac{m\lambda}{2}}K_2\ , \tag{4.83}$$

where K_2 is again some numerical factor. Eliminating $\bar{q}$ by using Eq. (4.82) we see that

$$S = \frac{2m^2}{\lambda\,t^3}\,K_1K_2^3\ . \tag{4.84}$$

The fact that the action scales $\sim 1/\lambda$ is a typical **non-perturbative** feature of the semiclassical approximation, which will not appear, e.g., in a perturbative treatment of the problem to be discussed in the next chapter.

5 Perturbation Theory

Using the path-integral formalism, one obtains a physically intuitive interpretation of scattering processes. Scattering processes are a typically application for **perturbation theory**. In the following, we will first explain the concept of this approach.

5.1 The Born series

Consider the exponential function under the path integral in Eq. (3.21). We can factorize the part which contains the potential energy,

$$G(\vec{q}_b, t_b; \vec{q}_a, t_a) = \mathcal{N} \int_{\vec{q}(t_a)=\vec{q}_a}^{\vec{q}(t_b)=\vec{q}_b} \mathcal{D}\vec{q}\, \exp\left(\frac{i}{\hbar}\int_{t_a}^{t_b} \mathrm{d}t\, \frac{m}{2}\,\dot{\vec{q}}^{\,2}\right) \exp\left[-\frac{i}{\hbar}\int_{t_a}^{t_b} \mathrm{d}t\, V(\vec{q}, t)\right] \ . \quad (5.1)$$

We then multiply the potential energy $V(\vec{q}, t)$ with a number $\lambda > 0$. We first consider the case $\lambda \ll 1$, in order to mathematically justify to terminate the expansion of the exponential in powers of λ after a few terms. At the end of the calculation we will set $\lambda = 1$. The Taylor expansion of the exponential factor containing the potential energy reads

$$\begin{aligned} \exp\left[-\frac{i}{\hbar}\int_{t_a}^{t_b} \mathrm{d}t\, \lambda\, V(\vec{q}, t)\right] &= \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} \left[-\frac{i}{\hbar}\int_{t_a}^{t_b} \mathrm{d}t\, V(\vec{q}, t)\right]^n \\ &= 1 - \frac{i\,\lambda}{\hbar}\int_{t_a}^{t_b} \mathrm{d}t\, V(\vec{q}, t) - \frac{\lambda^2}{2\hbar^2}\int_{t_a}^{t_b} \mathrm{d}t\, \mathrm{d}t'\, V(\vec{q}, t)\, V(\vec{q}, t') + \dots \ . \end{aligned} \quad (5.2)$$

If we insert this into the propagator (5.1), we obtain the so-called **Born series**

$$G(\vec{q}_b, t_b; \vec{q}_a, t_a) = G_0(\vec{q}_b, t_b; \vec{q}_a, t_a) + \sum_{n=1}^{\infty} \lambda^n\, G_n(\vec{q}_b, t_b; \vec{q}_a, t_a) \ , \quad (5.3)$$

where

$$\begin{aligned} G_0(\vec{q}_b, t_b; \vec{q}_a, t_a) &= \int_{\vec{q}(t_a)=\vec{q}_a}^{\vec{q}(t_b)=\vec{q}_b} \mathcal{D}\vec{q}\, \exp\left(\frac{i}{\hbar}\int_{t_a}^{t_b} \mathrm{d}t\, \frac{m}{2}\,\dot{\vec{q}}^{\,2}\right) \\ &= \sqrt{\frac{m}{2\pi i\hbar(t_b - t_a)}}^{\,3} \exp\left[\frac{i\,m}{2\hbar(t_b - t_a)}\,(\vec{q}_b - \vec{q}_a)^2\right] \end{aligned} \quad (5.4)$$

is the **free propagator**, i.e., the propagator in the **non-interacting case** $V(\vec{q}, t) \equiv 0$, cf. Eq. (4.7).

In the following, we will restrict ourselves to the case of **causal propagation**, $t_b > t_a$. To this end, we multiply Eq. (5.4) with $\Theta(t_b - t_a)$,

$$G_0(\vec{q}_b, t_b; \vec{q}_a, t_a) = \sqrt{\frac{m}{2\pi i\hbar(t_b - t_a)}}^{\,3} \exp\left[\frac{i\,m}{2\hbar(t_b - t_a)}\,(\vec{q}_b - \vec{q}_a)^2\right] \Theta(t_b - t_a)\,. \tag{5.5}$$

The term of first order in the Born series reads

$$G_1(\vec{q}_b, t_b; \vec{q}_a, t_a) = -\frac{i}{\hbar}\,\mathcal{N} \int \mathcal{D}\vec{q} \exp\left(\frac{i}{\hbar}\int_{t_a}^{t_b} \mathrm{d}t\,\frac{m}{2}\,\dot{\vec{q}}^2\right) \int_{t_a}^{t_b} \mathrm{d}t\, V(\vec{q}, t)\,, \tag{5.6}$$

or in discretized form

$$\begin{aligned}
&G_1(\vec{q}_b, t_b; \vec{q}_a, t_a) \\
&\quad = -\frac{i}{\hbar}\sqrt{\frac{m}{2\pi\hbar\, i\tau}}^{\,3N} \sum_{\ell=1}^{N} \tau \int \prod_{n=1}^{N-1} \mathrm{d}^3\vec{q}_n \exp\left[\frac{i\,m}{2\hbar\tau}\sum_{n=1}^{N}(\vec{q}_n - \vec{q}_{n-1})^2\right] V(\vec{q}_\ell, t_\ell) \\
&\quad = -\frac{i}{\hbar}\sum_{\ell=1}^{N}\tau \int \mathrm{d}^3\vec{q}_\ell \left\{\sqrt{\frac{m}{2\pi\hbar\, i\tau}}^{\,3(N-\ell)} \int \prod_{n=\ell+1}^{N-1} \mathrm{d}^3\vec{q}_n \exp\left[\frac{i\,m}{2\hbar\tau}\sum_{n=\ell+1}^{N}(\vec{q}_n - \vec{q}_{n-1})^2\right]\right\} \\
&\qquad\qquad \times V(\vec{q}_\ell, t_\ell) \left\{\sqrt{\frac{m}{2\pi\hbar\, i\tau}}^{\,3\ell} \int \prod_{n=1}^{\ell-1} \mathrm{d}^3\vec{q}_n \exp\left[\frac{i\,m}{2\hbar\tau}\sum_{n=1}^{\ell}(\vec{q}_n - \vec{q}_{n-1})^2\right]\right\} \\
&\quad = -\frac{i}{\hbar}\sum_{\ell=1}^{N}\tau \int \mathrm{d}^3\vec{q}_\ell\, G_0(\vec{q}_b, t_b; \vec{q}_\ell, t_\ell)\, V(\vec{q}_\ell, t_\ell)\, G_0(\vec{q}_\ell, t_\ell; \vec{q}_a, t_a) \\
&\overset{\substack{N\to\infty \\ \tau\to 0}}{\longrightarrow} \quad -\frac{i}{\hbar}\int_{t_a}^{t_b}\mathrm{d}t \int \mathrm{d}^3\vec{q}\, G_0(\vec{q}_b, t_b; \vec{q}, t)\, V(\vec{q}, t)\, G_0(\vec{q}, t; \vec{q}_a, t_a) \\
&\quad = -\frac{i}{\hbar}\int_{-\infty}^{\infty}\mathrm{d}t \int \mathrm{d}^3\vec{q}\, G_0(\vec{q}_b, t_b; \vec{q}, t)\, V(\vec{q}, t)\, G_0(\vec{q}, t; \vec{q}_a, t_a)\,.
\end{aligned} \tag{5.7}$$

In the last step we have moved the integration boundaries to $\pm\infty$, since the intervals $(-\infty, t_a)$ and (t_b, ∞) do not contribute to integral due to the causality of the free propagator (5.5).

How can the result (5.7) be interpreted? The particle propagates **freely** from the space-time point $(\vec{q}_a, t_a)$ to the space-time point $(\vec{q}, t)$. There it is influenced by the potential $V(\vec{q}, t)$. Afterwards it again propagates **freely** to the space-time point $(\vec{q}_b, t_b)$. The situation is depicted in Fig. 5.1. Note that one integrates over all times t and positions $\vec{q}$, i.e., the potential can in principle act at **any** point t in time and at **any** position $\vec{q}$ on the particle, but only once. Before and after that instant in space and time, it propagates freely.

Quite analogously one derives the second term in the Born series,

$$\begin{aligned}
G_2(\vec{q}_b, t_b; \vec{q}_a, t_a) \;=\; &\left(-\frac{i}{\hbar}\right)^2 \int_{-\infty}^{\infty}\mathrm{d}t_1\,\mathrm{d}t_2 \int \mathrm{d}^3\vec{q}_1\,\mathrm{d}^3\vec{q}_2\, G_0(\vec{q}_b, t_b; \vec{q}_2, t_2)\, V(\vec{q}_2, t_2) \\
&\times G_0(\vec{q}_2, t_2; \vec{q}_1, t_1)\, V(\vec{q}_1, t_1)\, G_0(\vec{q}_1, t_1; \vec{q}_a, t_a)\,.
\end{aligned} \tag{5.8}$$

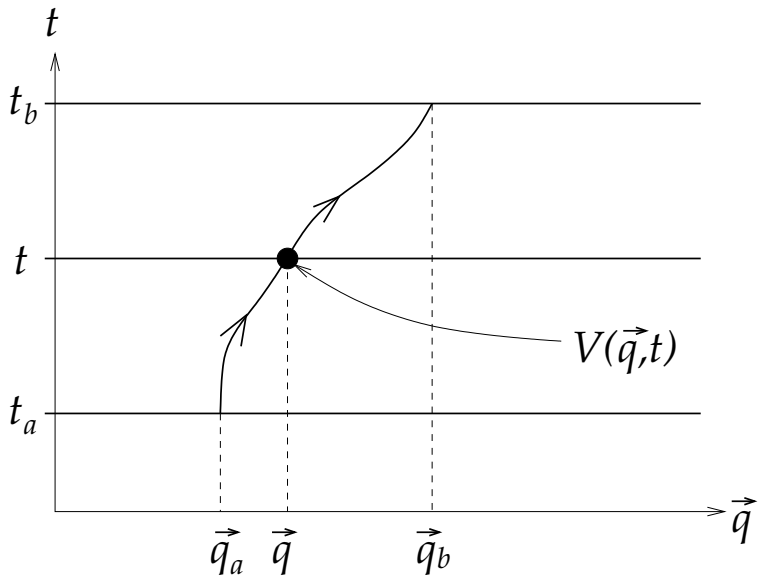


Figure 5.1: Graphical interpretation of the first-order term in the Born series.

Note that the factor 1/2 from the expansion of the exponential function cancels against a factor 2 which results from the fact that there are **two** possible orderings of the intermediate time points in the integral over t_1 and t_2: $t_2 \geq t_1$ and $t_1 \geq t_2$. Thus one obtains a contribution from the product $V(\vec{q}_2, t_2)\, V(\vec{q}_1, t_1)$ for $t_2 \geq t_1$ and another contribution $V(\vec{q}_2, t_2)\, V(\vec{q}_1, t_1)$ when $t_1 \geq t_2$. After relabelling the integration variables, $t_2 \leftrightarrow t_1$, $\vec{q}_2 \leftrightarrow \vec{q}_1$ both terms are identical. The second term in the Born series is graphically illustrated in Fig. 5.2. Now the potential acts twice on the particle, at the space-time points $(\vec{q}_1, t_1)$ and $(\vec{q}_2, t_2)$, in between it propagates freely. Again one has to integrate over all possible positions of these space-time points. The causality of the free propagator (5.5) always ensures that $t_a \leq t_1 \leq t_2 \leq t_b$.

We now consider Eq. (3.37),

$$\begin{aligned}\psi(\vec{q}_b, t_b) = \langle \vec{q}_b, t_b | \psi \rangle_H &= \int \mathrm{d}^3\vec{q}_a \, \langle \vec{q}_b, t_b | \vec{q}_a, t_a \rangle \, \langle \vec{q}_a, t_a | \psi \rangle_H \\ &= \int \mathrm{d}^3\vec{q}_a \, \langle \vec{q}_b, t_b | \vec{q}_a, t_a \rangle \, \psi(\vec{q}_a, t_a) \equiv \int \mathrm{d}^3\vec{q}_a \, G(\vec{q}_b, t_b; \vec{q}_a, t_a) \, \psi(\vec{q}_a, t_a) \; . \end{aligned} \tag{5.9}$$

In Sec. 3.3 we used it to prove the equivalence of the transition amplitude and the propagator for the free Schrödinger equation. However, as a matter of fact this equation holds not only for the free Schrödinger equation but also in the interacting case, since we did not make any further assumption about the complete set of time-evolved states $|\vec{q}_a, t_a\rangle$ that was inserted between $\langle \vec{q}_b, t_b|$ and $|\psi\rangle_H$. Inserting the Born series (5.3) for $\lambda = 1$ into

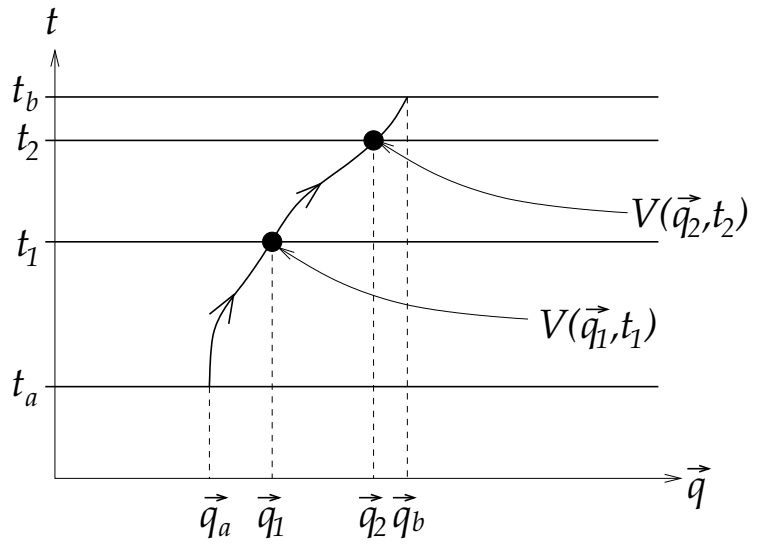


Figure 5.2: Graphical interpretation of the second-order term in the Born series.

this equation, we obtain

$$
\begin{aligned}
\psi(\vec{q}_b,t_b) &= \int \mathrm{d}^3\vec{q}_a\, G(\vec{q}_b,t_b;\vec{q}_a,t_a)\,\psi(\vec{q}_a,t_a) \\
&= \int \mathrm{d}^3\vec{q}_a\, G_0(\vec{q}_b,t_b;\vec{q}_a,t_a)\,\psi(\vec{q}_a,t_a) \\
&- \frac{i}{\hbar}\int_{-\infty}^{\infty}\mathrm{d}t \int \mathrm{d}^3\vec{q}\, G_0(\vec{q}_b,t_b;\vec{q},t)\,V(\vec{q},t) \int \mathrm{d}^3\vec{q}_a\, G_0(\vec{q},t;\vec{q}_a,t_a)\,\psi(\vec{q}_a,t_a) \\
&+ \left(-\frac{i}{\hbar}\right)\int_{-\infty}^{\infty}\mathrm{d}t \int \mathrm{d}^3\vec{q}\, G_0(\vec{q}_b,t_b;\vec{q},t)\,V(\vec{q},t)\left(-\frac{i}{\hbar}\right)\int_{-\infty}^{\infty}\mathrm{d}t_1 \int \mathrm{d}^3\vec{q}_1 \\
&\qquad \times G_0(\vec{q},t;\vec{q}_1,t_1)\,V(\vec{q}_1,t_1) \int \mathrm{d}^3\vec{q}_a\, G_0(\vec{q}_1,t_1;\vec{q}_a,t_a)\,\psi(\vec{q}_a,t_a) \\
&+ \dots \\
&= \int \mathrm{d}^3\vec{q}_q\, G_0(\vec{q}_b,t_b;\vec{q}_a,t_a)\,\psi(\vec{q}_a,t_a) \\
&- \frac{i}{\hbar}\int_{-\infty}^{\infty}\mathrm{d}t \int \mathrm{d}^3\vec{q}\, G_0(\vec{q}_b,t_b;\vec{q},t)\,V(\vec{q},t)\,\psi(\vec{q},t)\ . \qquad (5.10)
\end{aligned}
$$

Here the terms marked in red have been collected into the solution $\psi(\vec{q},t)$ of the Schrödinger equation.

5.2 The scattering matrix

Let us now consider a **scattering process**, where the particles are **non-interacting** at $t = \pm\infty$. For free particles the wave functions are eigenstates of momentum $\vec{p}$ and energy E, i.e., **plane waves**. For the initial state, i.e., the **incoming** particle the wave function

is then

$$\psi_{\text{in}}(\vec{q}_a, t_a) = \frac{1}{\sqrt{2\pi\hbar}^3} \exp\left[-\frac{i}{\hbar}\left(E_a t_a - \vec{p}_a \cdot \vec{q}_a\right)\right] \equiv \langle \vec{q}_a, t_a | \vec{p}_a \rangle_{\text{in}} \ , \tag{5.11}$$

where $E_a \equiv E(\vec{p}_a)$ is the energy of the incoming particle. The index "in" indicates that this is a state of the incoming particle. For the final state, i.e., the **outgoing** particle the respective wave function is

$$\psi_{\text{out}}(\vec{q}_b, t_b) = \frac{1}{\sqrt{2\pi\hbar}^3} \exp\left[-\frac{i}{\hbar}\left(E_b t_b - \vec{p}_b \cdot \vec{q}_b\right)\right] \equiv \langle \vec{q}_b, t_b | \vec{p}_b \rangle_{\text{out}} \ , \tag{5.12}$$

where $E_b \equiv E(\vec{p}_b)$ is the energy of the outgoing particle. The index "out" indicates that this is a state of the outgoing particle.

The last equality in Eqs. (5.11), (5.12) warrants some additional explanation. According to Eq. (3.9),

$$\langle \vec{q}_{a,b} | \vec{p}_{a,b} \rangle = \frac{1}{\sqrt{2\pi\hbar}^3} \exp\left(\frac{i}{\hbar}\, \vec{p}_{a,b} \cdot \vec{q}_{a,b}\right) \ . \tag{5.13}$$

The analogous relation for the time-evolved position states (2.10) reads

$$\begin{aligned} \langle \vec{q}_{a,b}, t_{a,b} | \vec{p}_{a,b} \rangle &= \langle \vec{q}_{a,b} | \hat{U}(t_{a,b}, t_0) | \vec{p}_{a,b} \rangle = \left\langle \vec{q}_{a,b} \left| \exp\left[-\frac{i}{\hbar}\hat{H}_0 (t_{a,b} - t_0)\right] \right| \vec{p}_{a,b} \right\rangle \\ &= \frac{1}{\sqrt{2\pi\hbar}^3} \exp\left\{-\frac{i}{\hbar}\left[E_{a,b}(t_{a,b} - t_0) - \vec{p}_{a,b} \cdot \vec{q}_{a,b}\right]\right\} \ . \end{aligned} \tag{5.14}$$

Here we have assumed that the particle is non-interacting in the time interval $[t_0, t_{a,b}]$, so that we can take the non-interacting Hamilton operator $\hat{H}_0$ in the time-evolution operator (2.9). Since $\hat{H}_0$ is not explicitly time-dependent, the time integral in the exponent can be immediately performed and the time-ordering operator is irrelevant. Since $\hat{H}_0 \equiv \frac{\hat{\vec{p}}^2}{2m}$, we have $\hat{H}_0 |\vec{p}_{a,b}\rangle = \frac{\vec{p}_{a,b}^{\,2}}{2m} |\vec{p}_{a,b}\rangle \equiv E_{a,b} |\vec{p}_{a,b}\rangle$, and the exponential can be factored out from the overlap $\langle \vec{q}_{a,b} | \vec{p}_{a,b} \rangle$. Setting $t_0 \equiv 0$ and using Eq. (5.13) we immediately obtain Eqs. (5.11), (5.12).

We now want to determine the quantum-mechanical amplitude for the scattering from the initial state $|\vec{p}_a\rangle_{\text{in}}$ into the final state $|\vec{p}_b\rangle_{\text{out}}$, the so-called **scattering matrix**,

$$\begin{aligned} S_{ba} &\equiv {}_{\text{out}}\langle \vec{p}_b | \vec{p}_a \rangle_{\text{in}} \\ &= \int \mathrm{d}^3\vec{q}_b \, {}_{\text{out}}\langle \vec{p}_b | \vec{q}_b, t_b \rangle \langle \vec{q}_b, t_b | \vec{p}_a \rangle_{\text{in}} \\ &= \int \mathrm{d}^3\vec{q}_b \, \mathrm{d}^3\vec{q}_a \, {}_{\text{out}}\langle \vec{p}_b | \vec{q}_b, t_b \rangle \langle \vec{q}_b, t_b | \vec{q}_a, t_a \rangle \langle \vec{q}_a, t_a | \vec{p}_a \rangle_{\text{in}} \\ &\equiv \int \mathrm{d}^3\vec{q}_b \, \mathrm{d}^3\vec{q}_a \, \psi^*_{\text{out}}(\vec{q}_b, t_b)\, G(\vec{q}_b, t_b; \vec{q}_a, t_a)\, \psi_{\text{in}}(\vec{q}_a, t_a) \\ &\equiv \int \mathrm{d}^3\vec{q}_b \, \psi^*_{\text{out}}(\vec{q}_b, t_b)\, \psi(\vec{q}_b, t_b) \ . \end{aligned} \tag{5.15}$$

Here we first inserted two complete sets of time-evolved position states and then used the equivalence of propagator and transition amplitude, as well as Eq. (5.9) for the time

evolution of the initial wave function $\psi_{\text{in}}(\vec{q}_a, t_a)$ to the space-time point $(\vec{q}_b, t_b)$,

$$\psi(\vec{q}_b, t_b) = \int \mathrm{d}^3\vec{q}_a \, G(\vec{q}_b, t_b; \vec{q}_a, t_a) \, \psi_{\text{in}}(\vec{q}_a, t_a) \; . \tag{5.16}$$

Note that we can now omit the index "in" at $\psi(\vec{q}_b, t_b)$, since the interaction occurring in the interval $[t_a, t_b]$ (which is taken into account in the full propagator $G(\vec{q}_b, t_b; \vec{q}_a, t_a)$) changes this wave function in a non-trivial manner. In particular, the initial momentum $\vec{p}_a$ will be changed due to the scattering processes occurring in this time interval.

The result (5.15) is the **quantum-mechanical overlap** of the solution $\psi(\vec{q}_b, t_b)$ of the full scattering problem (with given initial state $\psi_{\text{in}}(\vec{q}_a, t_a)$, where the particle has the fixed momentum $\vec{p}_a$) with the outgoing state $\psi_{\text{out}}(\vec{q}_b, t_b)$, which is an eigenstate of momentum with eigenvalue $\vec{p}_b$. Or in other words, the scattering matrix S_{ba} measures how much a plane wave with momentum $\vec{p}_b$ contributes to the final state $\psi(\vec{q}_b, t_b)$, which has evolved out of the initial state with fixed momentum $\vec{p}_a$.

If we insert the Born series (5.3) for the full propagator, we obtain

$$\begin{aligned} S_{ba} = & \int \mathrm{d}^3\vec{q}_b \, \mathrm{d}^3\vec{q}_a \, \psi^*_{\text{out}}(\vec{q}_b, t_b) \, G_0(\vec{q}_b, t_b; \vec{q}_a, t_a) \, \psi_{\text{in}}(\vec{q}_a, t_a) \\ & - \frac{i}{\hbar} \int \mathrm{d}^3\vec{q}_b \, \mathrm{d}^3\vec{q}_a \, \mathrm{d}t \, \mathrm{d}^3\vec{q} \, \psi^*_{\text{out}}(\vec{q}_b, t_b) \, G_0(\vec{q}_b, t_b; \vec{q}, t) \, V(\vec{q}, t) \, G_0(\vec{q}, t; \vec{q}_a, t_a) \, \psi_{\text{in}}(\vec{q}_a, t_a) \\ & + \; \ldots \; , \end{aligned} \tag{5.17}$$

where we only denoted the zeroth- and first-order terms of the Born series explicitly and inserted Eq. (5.7) for the latter.

In Exercise 5 one is supposed to prove that a plane wave which propagates without interaction from $(\vec{q}_a, t_a)$ to $(\vec{q}_b, t_b)$ is still a plane wave,

$$\int \mathrm{d}^3\vec{q}_a \, G_0(\vec{q}_b, t_b; \vec{q}_a, t_a) \, \psi_{\text{in}}(\vec{q}_a, t_a) \equiv \psi_{\text{in}}(\vec{q}_b, t_b) = \frac{1}{\sqrt{2\pi\hbar}^3} \, \exp\left[-\frac{i}{\hbar} \left(E_a t_b - \vec{p}_a \cdot \vec{q}_b \right) \right] \; . \tag{5.18}$$

Therefore, the first term in Eq. (5.17) is

$$\begin{aligned} \int \mathrm{d}^3\vec{q}_b \, \mathrm{d}^3\vec{q}_a \, \psi^*_{\text{out}}(\vec{q}_b, t_b) \, G_0(\vec{q}_b, t_b; \vec{q}_a, t_a) \, \psi_{\text{in}}(\vec{q}_a, t_a) &= \int \mathrm{d}^3\vec{q}_b \, \psi^*_{\text{out}}(\vec{q}_b, t_b) \, \psi_{\text{in}}(\vec{q}_b, t_b) \\ &= \frac{1}{(2\pi\hbar)^3} \int \mathrm{d}^3\vec{q}_b \, \exp\left\{ \frac{i}{\hbar} \left[(E_b - E_a) \, t_b - (\vec{p}_b - \vec{p}_a) \cdot \vec{q}_b \right] \right\} \\ &= \exp\left[\frac{i}{\hbar} \left(E_b - E_a \right) t_b \right] \, \delta^{(3)}(\vec{p}_b - \vec{p}_a) = \delta^{(3)}(\vec{p}_b - \vec{p}_a) \; , \end{aligned} \tag{5.19}$$

since on account of the delta function $E_b = E(\vec{p}_b) = E(\vec{p}_a) = E_a$.

We now abbreviate all higher-order terms in Eq. (5.17) with iT_{ba}, where the factor i is pure convention and T_{ba} represents the so-called **transition matrix**. While the delta function is the amplitude for the process where no scattering occurs, i.e., where the initial- and final-state momenta are identical, $\vec{p}_b = \vec{p}_a$, the term iT_{ba} is the amplitude for a process where scattering occurs, i.e., where the final-state momentum differs from that of the initial state, $\vec{p}_b \neq \vec{p}_a$. The scattering matrix (5.17) reads in compact notation

$$S_{ba} = \delta^{(3)}(\vec{p}_b - \vec{p}_a) + iT_{ba} \; . \tag{5.20}$$

Lecture 6

5.3 Feynman diagrams

There is a simple diagrammatic notation for the Born series (5.3) of the full propagator,

$$G(\vec{q}_b, t_b; \vec{q}_a, t_a) = G_0(\vec{q}_b, t_b; \vec{q}_a, t_a) - \frac{i}{\hbar} \int \mathrm{d}t\, \mathrm{d}^3\vec{q}\, G_0(\vec{q}_b, t_b; \vec{q}, t)\, V(\vec{q}, t)\, G_0(\vec{q}, t; \vec{q}_a, t_a) + \dots \,, \tag{5.21}$$

cf. Fig. 5.3.

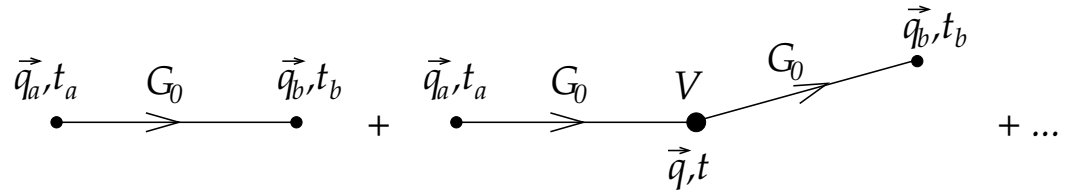


Figure 5.3: Diagrammatic representation of the Born series in terms of Feynman diagrams.

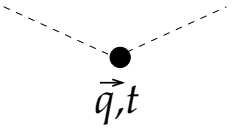
This notation was invented by R.P. Feynman, therefore these diagrams are called **Feynman diagrams**. With the help of the so-called **Feynman rules** for these diagrams, one can translate them back into mathematical formulas. The **Feynman rules in coordinate space** are:

(i) A **line** between two space-time points $(\vec{q}_1, t_1)$ and $(\vec{q}_2, t_2)$ symbolizes a free propagator,

$$G_0(\vec{q}_2, t_2; \vec{q}_1, t_1) =$$

(ii) A **vertex** at the space-time point $(\vec{q}, t)$ symbolizes a factor

$$-\frac{i}{\hbar}\, V(\vec{q}, t) =$$



An integration over all possible values $(\vec{q}, t)$ is implied.

One can formulate the Feynman rules also in **momentum space**. To this end, all objects have to be Fourier-transformed. The Fourier representation of the free propagator reads

$$\tilde{G}_0(\vec{p}_2, E_2; \vec{p}_1, E_1) = (2\pi\hbar)^4 \delta(E_2 - E_1) \delta^{(3)}(\vec{p}_2 - \vec{p}_1)\, \frac{i\hbar}{E_2 - \frac{\vec{p}_2^{\,2}}{2m} + i\epsilon} \,. \tag{5.22}$$

The proof of this equation is subject of Exercise 6(i). As will become clear in that exercise, the $i\epsilon$ in the denominator arises from the Θ function in Eq. (5.5). Without the Θ function, the propagator would have a pole on the real energy axis at $E_2 = \frac{\vec{p}_2^{\,2}}{2m}$. The $i\epsilon$ shifts this pole into the lower half of the complex-energy plane, $E_2 = \frac{\vec{p}_2^{\,2}}{2m} - i\epsilon$, cf. Fig. 5.4. This should

be familiar from Classical Electrodynamics, where the retarded propagator (or Green's function), i.e., the one which leads to causal wave propagation, has poles in the lower half of the complex-energy (or frequency) plane, while the advanced propagator (or Green's function), i.e., the one which leads to anticausal wave propagation, has poles in the upper half of the complex-energy plane. In general, propagators (or Green's functions) are only well-defined once a prescription of how to navigate poles is specified.

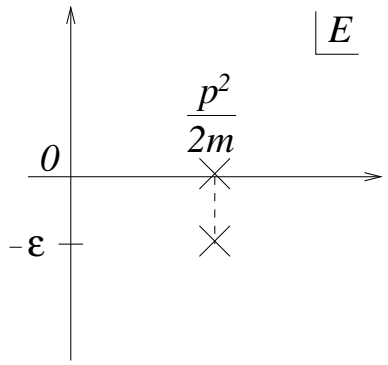


Figure 5.4: Shifting the pole of the propagator from the real axis into the lower half of the complex-energy plane leads to the causal propagator (5.5).

Without knowing the exact form of the potential $V(\vec{q},t)$ we can only quote the definition of the Fourier-transformed vertex,

$$\tilde{V}(\vec{p},\omega) = \int \mathrm{d}t\, \mathrm{d}^3\vec{q}\, V(\vec{q},t)\, \exp\left[\frac{i}{\hbar}\left(\omega t - \vec{p}\cdot\vec{q}\right)\right] \ . \tag{5.23}$$

If we insert this into the Born series (5.21) and identify the Fourier coefficients on the left- and right-hand sides of this equation, we obtain the following **Feynman rules in momentum space**:

(i) A **line** symbolizes a factor

$$\frac{i\hbar}{E - \frac{\vec{p}^{\,2}}{2m} + i\epsilon} = \qquad \vec{p},E$$

i.e., essentially the free propagator (5.22) in momentum space.

(ii) A **vertex** symbolizes a factor

$$-\frac{i}{\hbar}\tilde{V}(\vec{p},\omega) = \qquad \vec{p}_1,E_1 \qquad \vec{p}_2,E_2$$

At each vertex we have conservation of energy and momentum, i.e., the sum of all incoming energies and momenta are identical with those of the outgoing energies and momenta. This means that in the above expression we should use $\omega = E_2 - E_1$, $\vec{p} = \vec{p}_2 - \vec{p}_1$.

The proof of these rules is subject of Exercise 6(ii).

5.4 Green's functions revisited

In Sec. 3.3 we have already explained the relationship between transition amplitude, propagator, and Green's function. In this section we want to elaborate on this relationship from a somewhat different angle.

In principle, the method of Green's functions is applied to derive a **special solution** for an **inhomogeneous** differential equation. However, the Schrödinger equation is first of all a **homogeneous** differential equation. Nevertheless, we can put the term containing the potential energy to the other side,

$$\left(i\hbar\,\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\,\Delta_q\right)\psi(\vec{q},t) = V(\vec{q},t)\,\psi(\vec{q},t) \equiv j(\vec{q},t)\;. \tag{5.24}$$

Formally, this looks like a linear partial differential equation with the "inhomogeneous term" $j(\vec{q},t)$. Strictly speaking, this term depends by definition on the solution $\psi(\vec{q},t)$ of the differential equation, so rewriting the Schrödinger equation as in Eq. (5.24) appears to not gain anything. Nevertheless, let us ignore this for the moment and proceed towards the solution of the differential equation (5.24). The **general** solution of a linear, inhomogeneous differential equation is known to be a superposition of the **general** solution of the corresponding **homogeneous** differential equation and a **special** solution of the **inhomogeneous** differential equation. The **homogeneous** differential equation is simply the free Schrödinger equation,

$$\left(i\hbar\,\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\,\Delta_q\right)\psi_0(\vec{q},t) = 0\;, \tag{5.25}$$

and the **general** solution is a superposition of plane waves,

$$\psi_0(\vec{q},t) = \int \frac{\mathrm{d}^3\vec{p}}{(2\pi\hbar)^3}\,\tilde{\psi}_0(\vec{p})\,\exp\left[-\frac{i}{\hbar}\,(Et - \vec{p}\cdot\vec{q})\right]\;, \tag{5.26}$$

cf. Eq. (3.28). In comparison to that equation, we now choose a representation in terms of momentum $\vec{p} = \hbar\vec{k}$ and energy $E = \hbar\omega$ instead of wave number $\vec{k}$ and frequency ω. According to Eq. (3.26), the energy is given by the non-relativistic energy-momentum relation, $E = \frac{\vec{p}^{\,2}}{2m}$. Furthermore, we absorb the additional factor $1/(2\pi)$ in Eq. (3.28) into the definition of the Fourier coefficients $\tilde{\psi}_0(\vec{p})$.

As explained in Sec. 3.3, the Fourier coefficients $\tilde{\psi}_0(\vec{p})$ still need to be adapted to the initial and boundary conditions. Note that the choice

$$\tilde{\psi}_0(\vec{p}) \equiv \sqrt{2\pi\hbar}^3\,\delta^{(3)}(\vec{p}_a - \vec{p}) \tag{5.27}$$

just yields the incoming plane wave (5.11) with momentum $\vec{p}_a$ and energy $E_a = E(\vec{p}_a)$ in the discussion of the scattering matrix in Sec. 5.2.

A **special** solution of the **inhomogeneous** differential equation can be obtained with the method of Green's functions. The **Green's function** $\mathcal{G}_0(\vec{q},t;\vec{q}\,',t')$ of the homogeneous Schrödinger equation (5.25) is defined as the solution of the differential equation

$$\left(i\hbar\,\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\,\Delta_q\right)\mathcal{G}_0(\vec{q},t;\vec{q}\,',t') = \delta(t-t')\,\delta^{(3)}(\vec{q}-\vec{q}\,')\;, \tag{5.28}$$

and as such fulfills the inhomogeneous Schrödinger equation (5.24) with a (four-dimensional) delta function as inhomogeneity. A **special** solution of the **inhomogeneous** Schrödinger equation (5.24) is then given by

$$\psi_S(\vec{q},t) = \int \mathrm{d}t'\,\mathrm{d}^3\vec{q}'\,\mathcal{G}_0(\vec{q},t;\vec{q}',t')\,j(\vec{q}',t')\;, \tag{5.29}$$

since

$$\begin{aligned}\left(i\hbar\frac{\partial}{\partial t}+\frac{\hbar^2}{2m}\Delta_q\right)\psi_S(\vec{q},t) &= \int \mathrm{d}t'\,\mathrm{d}^3\vec{q}'\,\left(i\hbar\frac{\partial}{\partial t}+\frac{\hbar^2}{2m}\Delta_q\right)\mathcal{G}_0(\vec{q},t;\vec{q}',t')\,j(\vec{q}',t')\\ &= \int \mathrm{d}t'\,\mathrm{d}^3\vec{q}'\,\delta(t-t')\,\delta^{(3)}(\vec{q}-\vec{q}')\,j(\vec{q}',t')\\ &\equiv j(\vec{q},t)\;,\quad \text{q.e.d.}\end{aligned} \tag{5.30}$$

The **general** solution of the **inhomogeneous** Schrödinger equation (5.24) is then

$$\begin{aligned}\psi(\vec{q}_b,t_b) &= \psi_0(\vec{q}_b,t_b)+\psi_S(\vec{q}_b,t_b)\\ &= \psi_0(\vec{q}_b,t_b)+\int \mathrm{d}t\,\mathrm{d}^3\vec{q}\,\mathcal{G}_0(\vec{q}_b,t_b;\vec{q},t)\,V(\vec{q},t)\,\psi(\vec{q},t)\;.\end{aligned} \tag{5.31}$$

Compare this result with Eq. (5.10). Suppose that $\psi(\vec{q}_a,t_a)$ in that equation is a superposition of plane waves, analogous to the general solution (5.26) of the homogeneous Schrödinger equation. Then, according to Eq. (5.18), this superposition will simply be transported to the space-time point $(\vec{q}_b,t_b)$ via convolution with the free propagator $G_0(\vec{q}_b,t_b;\vec{q}_a,t_a)$, but it will stay a superposition of plane waves. Therefore, we can identify the first term in Eq. (5.10) wiht the first term $\psi_0(\vec{q}_b,t_b)$ in Eq. (5.31). But then also the second term in Eq. (5.10) has to be identical with the second term in Eq. (5.31). This in turn implies that

$$G_0(\vec{q},t;\vec{q}',t') \equiv i\hbar\,\mathcal{G}_0(\vec{q},t;\vec{q}',t')\;, \tag{5.32}$$

i.e., up to a factor $i\hbar$ propagator and Green's function are identical. In fact, we could have made them exactly identical, had we included a factor $1/(i\hbar)$ on the right-hand side of the defining equation (5.28) for the Green's function $\mathcal{G}_0$.

5.5 The generating functional for correlation functions

Conider the transition amplitude

$$\langle\vec{Q}',T'|\vec{Q},T\rangle^J = \mathcal{N}\int\mathcal{D}\vec{q}\,\exp\left\{\frac{i}{\hbar}\int_T^{T'}\mathrm{d}\tau\,\left[L(\vec{q},\dot{\vec{q}},\tau)+\hbar\,\vec{J}(\tau)\cdot\vec{q}(\tau)\right]\right\}\;, \tag{5.33}$$

i.e., the well-known transition amplitude (3.21), but now modified by the presence of an external **source** $\vec{J}(\tau)$, which couples to the position vector $\vec{q}(\tau)$. Without loss of generality we assume that the source $\vec{J}(\tau)$ is different from zero only in a time interval $[t,t']$, where $T<t$ and $t'<T'$, i.e., $[t,t']\subset[T,T']$. Later we will send $T\to-\infty$ and $T'\to+\infty$.

We now insert two complete sets of time-evolved position eigenstates on the left-hand side of Eq. (5.33),

$$\langle \vec{Q}\,', T'|\vec{Q}, T\rangle^J = \int \mathrm{d}^3\vec{q}'\,\mathrm{d}^3\vec{q}\,\langle \vec{Q}\,', T'|\vec{q}', t'\rangle\langle \vec{q}', t'|\vec{q}, t\,\rangle^J\langle \vec{q}, t\,|\vec{Q}, T\rangle\ . \tag{5.34}$$

Here we have omitted the superscript "J" at the first and the third overlap, since the source $\vec{J}(t)$ vanishes in the time intervals $[T, t]$ and $[t', T']$.

Using the definition of the time-evolved position eigenstates, we have

$$\langle \vec{Q}\,', T'|\vec{q}', t'\rangle = \langle \vec{Q}\,'|\,\hat{U}(T', 0)\,\hat{U}(0, t')\,|\vec{q}'\rangle = \langle \vec{Q}\,'|\,\hat{U}(T', t')\,|\vec{q}'\rangle\ . \tag{5.35}$$

Let us assume that the Hamilton operator does not explicitly depend on time in the time interval $[t', T']$. Then the time evolution operator assumes the simple form

$$\hat{U}(T', t') = e^{-\frac{i}{\hbar}\hat{H}(T'-t')}$$

and, after inserting a complete set of eigenfunctions of the Hamilton operator,

$$\mathbb{1} = \sum_m\!\!\!\!\!\!\int |m\rangle\langle m|\ , \quad \hat{H}\,|m\rangle = E_m\,|m\rangle\ , \tag{5.36}$$

it follows from Eq. (5.35) that

$$\begin{aligned}\langle \vec{Q}\,', T'|\vec{q}', t'\rangle &= \sum_m\!\!\!\!\!\!\int \langle \vec{Q}\,'|\,e^{-\frac{i}{\hbar}\hat{H}(T'-t')}\,|m\rangle\langle m|\vec{q}'\rangle = \sum_m\!\!\!\!\!\!\int \langle \vec{Q}\,'|m\rangle\langle m|\vec{q}'\rangle\,e^{-\frac{i}{\hbar}E_m(T'-t')} \\ &\equiv \sum_m\!\!\!\!\!\!\int \phi_m(\vec{Q}\,')\,\phi_m^*(\vec{q}')\,e^{-\frac{i}{\hbar}E_m(T'-t')}\ .\end{aligned} \tag{5.37}$$

Completely analogously it follows that

$$\langle \vec{q}, t\,|\vec{Q}, T\rangle = \sum_n\!\!\!\!\!\!\int \phi_n(\vec{q})\,\phi_n^*(\vec{Q})\,e^{-\frac{i}{\hbar}E_n(t-T)}\ . \tag{5.38}$$

Inserting Eqs. (5.37) and (5.38) into Eq. (5.34) we obtain

$$\begin{aligned}&\langle \vec{Q}\,', T'|\vec{Q}, T, \rangle^J \\ &= \sum_{m,n}\!\!\!\!\!\!\int \mathrm{d}^3\vec{q}'\,\mathrm{d}^3\vec{q}\,\phi_m(\vec{Q}\,')\,\phi_m^*(\vec{q}')\,\langle \vec{q}', t'|\vec{q}, t\,\rangle^J\phi_n(\vec{q})\,\phi_n^*(\vec{Q})\,e^{\frac{i}{\hbar}[E_m(t'-T')+E_n(T-t)]}\ .\end{aligned} \tag{5.39}$$

Now we "rotate" the time axis by a small angle $-\delta$, $\delta > 0$, in the **complex** time plane, cf. Fig. 5.5. This means that all times in the above formula are multiplied with a phase factor $e^{-i\delta}$, i.e.,

$$t' - T' \longrightarrow (t' - T')e^{-i\delta}\ , \quad T - t \longrightarrow (T - t)e^{-i\delta}\ .$$

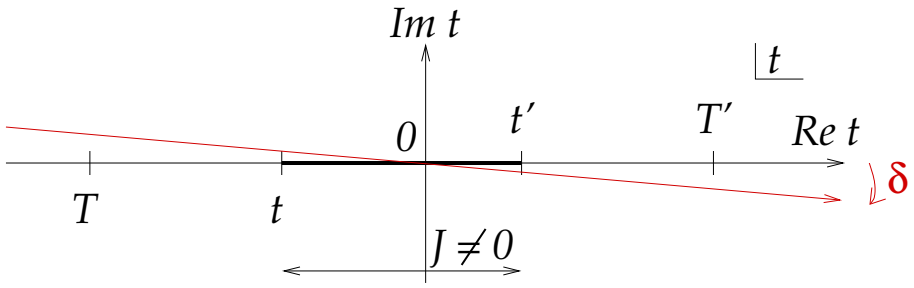


Figure 5.5: Rotation of the time axis in the complex time plane. We assumed without loss of generality that the origin of the real time axis lies in the interval $[t, t']$.

Then,

$$\mathrm{Re}\,\frac{i}{\hbar}\,E_m(t'-T') \longrightarrow \mathrm{Re}\,\frac{i}{\hbar}\,E_m(t'-T')e^{-i\delta} = \frac{E_m}{\hbar}\,(t'-T')\,\sin\delta \overset{T'\to+\infty}{\simeq} -\frac{E_m}{\hbar}\,T'\,\sin\delta < 0\,, \tag{5.40}$$

if we additionally assume that $E_m > 0\ \forall\ m$. Quite analogously it follows that

$$\mathrm{Re}\,\frac{i}{\hbar}\,E_n(T-t) \longrightarrow \mathrm{Re}\,\frac{i}{\hbar}\,E_n(T-t)e^{-i\delta} = \frac{E_n}{\hbar}\,(T-t)\,\sin\delta \overset{T\to-\infty}{\simeq} \frac{E_n}{\hbar}\,T\,\sin\delta < 0\,. \tag{5.41}$$

This in turn implies that, in the limit $T \to -\infty$, $T' \to +\infty$, **all** terms in Eq. (5.39) become **exponentially damped**. The dominant term is the one which is damped **to the least extent**, i.e., the one with the smallest argument of the exponential function. This is the term for $m = n = 0$, the **ground state**,

$$\lim_{\substack{T'\to+\infty\\ T\to-\infty}} \langle\vec{Q}', T'|\vec{Q}, T,\rangle^J \simeq \phi_0(\vec{Q}')\,\phi_0^*(\vec{Q})\,e^{-\frac{i}{\hbar}E_0(T'-T)}\int \mathrm{d}^3\vec{q}'\,\mathrm{d}^3\vec{q}\,\phi_0^*(t',\vec{q}')\,\langle\vec{q}', t'|\vec{q}, t\,\rangle^J\phi_0(t,\vec{q})\,, \tag{5.42}$$

where we have used

$$e^{-\frac{i}{\hbar}E_0t}\,\phi_0(\vec{q}) = e^{-\frac{i}{\hbar}E_0t}\,\langle\vec{q}|0\rangle = \langle\vec{q}|\,e^{-\frac{i}{\hbar}\hat{H}t}\,|0\rangle = \langle\vec{q}|\hat{U}(t,0)|0\rangle \equiv \langle\vec{q}, t\,|0\rangle \equiv \phi_0(\vec{q}, t)\,, \tag{5.43}$$

and analogously

$$\phi_0^*(\vec{q}')\,e^{\frac{i}{\hbar}E_0t'} = \langle 0|\vec{q}', t'\rangle = \phi_0^*(\vec{q}', t')\,. \tag{5.44}$$

Here we have assumed that $\hat{H}$ is not explicitly time-dependent. Equation (5.42) can be rearranged,

$$\begin{aligned}\lim_{\substack{T'\to+\infty\\ T\to-\infty}} \frac{\langle\vec{Q}', T'|\vec{Q}, T\rangle^J}{\phi_0(\vec{Q}')\,\phi_0^*(\vec{Q})\,e^{-\frac{i}{\hbar}E_0(T'-T)}} &= \int \mathrm{d}^3\vec{q}'\,\mathrm{d}^3\vec{q}\,\phi_0^*(\vec{q}', t')\,\langle\vec{q}', t'|\vec{q}, t\,\rangle^J\phi_0(\vec{q}, t)\\ &= \int \mathrm{d}^3\vec{q}'\,\mathrm{d}^3\vec{q}\,\langle 0|\vec{q}', t'\rangle\,\langle\vec{q}', t'|\vec{q}, t\,\rangle^J\langle\vec{q}, t\,|0\rangle \equiv \langle 0; t'|0; t\rangle^J\,.\end{aligned} \tag{5.45}$$

The bra $\langle 0; t'|$ is the **ground** or **vacuum state at time** t' and the ket $|0; t\rangle$ is the **vacuum state at time** t. Therefore, the overlap on the right-hand side is the **transition**

amplitude from the ground state or vacuum at t to the vacuum at t', the so-called **vacuum-to-vacuum transition amplitude**. Since t' can be chosen arbitrarily large (as long as $t' < T'$) and t arbitrarily small (as long as $T < t$), we can also write Eq. (5.45) as

$$\langle 0; +\infty | 0; -\infty \rangle^J \sim \lim_{\substack{T' \to +\infty \\ T \to -\infty}} \langle \vec{Q}', T' | \vec{Q}, T \rangle^J \; . \tag{5.46}$$

The denominator on the left-hand side of Eq. (5.45) was omitted, since it is just a numerical factor. Finally, we employ the path-integral representation (5.33) of the transition amplitude on the right-hand side and obtain (after relabelling the integration variable $\tau \to t$)

$$\langle 0; +\infty | 0; -\infty \rangle^J \sim \int \mathcal{D}\vec{q} \, \exp\left\{ \frac{i}{\hbar} \int_{-\infty}^{\infty} \mathrm{d}t \, \left[L(\vec{q}, \dot{\vec{q}}, t) + \hbar \, \vec{J}(t) \cdot \vec{q}(t) \right] \right\} \equiv Z[\vec{J}] \; . \tag{5.47}$$

The right-hand side is a **functional** of the source $\vec{J}(t)$. The functional $Z[\vec{J}]$ is the so-called **generating functional for correlation functions**. This entails that one can generate correlation function via **functional differentiation** of $Z[\vec{J}]$ with respect to the source $\vec{J}$. This will be explained in more detail in the following.

First, however, we need to remember the definition of a functional and clarify how to differentiate it. Let us consider the function

$$\begin{aligned} f \; : \; M \; &\longrightarrow \; N \; , \qquad M, N \subset \mathbb{R} \; , \\ x \; &\longmapsto \; f(x) \; , \quad x \in M \; , \; f(x) \in N \; . \end{aligned} \tag{5.48}$$

We denote the space of infinitely often differentiable functions f on the manifold $M \subset \mathbb{R}$ as $\mathcal{C}^\infty(M)$. A **functional**

$$\begin{aligned} F \; : \mathcal{C}^\infty(M) \; &\longrightarrow \; \mathbb{R} \; , \\ f \; &\longmapsto \; F[f] \; , \end{aligned} \tag{5.49}$$

maps an element $f \in \mathcal{C}^\infty(M)$ to a real number $F[f] \in \mathbb{R}$.

The **functional derivative** of $F[f]$ with respect to the function f (at the value y of its argument) is defined as

$$\frac{\delta F[f(x)]}{\delta f(y)} = \lim_{\epsilon \to 0} \frac{F[f(x) + \epsilon \, \delta(x-y)] - F[f(x)]}{\epsilon} \; . \tag{5.50}$$

In words, one calculates the functional F for a function, which is differs from f only by a delta function at $x = y$, multiplied by ϵ, and subtracts the functional $F[f]$. Subsequently one divides by ϵ and sends ϵ to zero. This definition of the functional derivative is very similar to the definition of the standard derivative of functions.

To practice functional differentiation, let us consider a few examples:

(i) $F[f] = \int_{-\infty}^{\infty} \mathrm{d}x \, f(x)$.

$$\begin{aligned} \Longrightarrow \; \frac{\delta F[f(x)]}{\delta f(y)} \; &= \; \lim_{\epsilon \to 0} \frac{1}{\epsilon} \left\{ \int_{-\infty}^{\infty} \mathrm{d}x \, [f(x) + \epsilon \, \delta(x-y)] - \int_{-\infty}^{\infty} \mathrm{d}x \, f(x) \right\} \\ &= \; \int_{-\infty}^{\infty} \mathrm{d}x \, \delta(x-y) \equiv 1 \; . \end{aligned} \tag{5.51}$$

(ii) $F_x[f] = \int_{-\infty}^{\infty} \mathrm{d}y\, G(x,y)\, f(y)$. Besides the function f, this functional also depends on the variable x. Therefore it is a **functional** of f and a **function** of x.

$$\begin{aligned} \Longrightarrow \frac{\delta F_x[f(y)]}{\delta f(z)} &= \lim_{\epsilon\to 0} \frac{1}{\epsilon} \left\{ \int_{-\infty}^{\infty} \mathrm{d}y\, G(x,y)\, [f(y) + \epsilon\, \delta(y-z)] - \int_{-\infty}^{\infty} \mathrm{d}y\, G(x,y)\, f(y) \right\} \\ &= \int_{-\infty}^{\infty} \mathrm{d}y\, G(x,y)\, \delta(y-z) \equiv G(x,z)\ . \end{aligned} \tag{5.52}$$

(iii) For the special choice $G(x,y) \equiv \delta(x-y)$ in the previous example we obtain $F_x[f] = \int_{-\infty}^{\infty} \mathrm{d}y\, \delta(x-y)\, f(y) \equiv f(x)$, from which follows

$$\Longrightarrow \frac{\delta F_x[f(y)]}{\delta f(z)} \equiv \frac{\delta f(x)}{\delta f(z)} \equiv \delta(x-z)\ . \tag{5.53}$$

A normal function f at the value x of its argument, $f(x)$, can therefore be functionally differentiated with respect to the same function at another value of its argument, say $f(z)$. The result is a delta function with support at $x = z$. This result generalizes the standard formula for the normal derivative of the ith with respect to the jth coordinate, $\mathrm{d}x_i/\mathrm{d}x_j \equiv \delta_{ij}$. For functions, which can be considered as "variables with continuous index", the delta function plays the same role as the Kronecker delta for variables with discrete index.

Let us now consider

$$\begin{aligned} \frac{\delta Z[\vec{J}]}{\delta J_k(t_1)} &= \lim_{\epsilon\to 0} \frac{1}{\epsilon} \left[\int \mathcal{D}\vec{q}\, \exp\left(\frac{i}{\hbar} \int_{-\infty}^{\infty} \mathrm{d}t \left\{ L(\vec{q},\dot{\vec{q}},t) + \hbar\, [J_j(t) + \epsilon\, \delta_{kj}\, \delta(t-t_1)]\, q_j(t) \right\} \right) \right. \\ &\qquad \left. - \int \mathcal{D}\vec{q}\, \exp\left(\frac{i}{\hbar} \int_{-\infty}^{\infty} \mathrm{d}t \left\{ L(\vec{q},\dot{\vec{q}},t) + \hbar\, J_j(t) q_j(t) \right\} \right) \right] \\ &= \lim_{\epsilon\to 0} \frac{1}{\epsilon} \left\{ \sum_{n=0}^{\infty} \frac{(i\,\epsilon)^n}{n!} \int \mathcal{D}\vec{q} \left[\int_{-\infty}^{\infty} \mathrm{d}t\, q_k(t)\, \delta(t-t_1) \right]^n e^{\frac{i}{\hbar}\int_{-\infty}^{\infty} \mathrm{d}t [L(\vec{q},\dot{\vec{q}},t) + \hbar\, \vec{J}(t)\cdot\vec{q}(t)]} \right. \\ &\qquad \left. - \int \mathcal{D}\vec{q}\, e^{\frac{i}{\hbar}\int_{-\infty}^{\infty} \mathrm{d}t [L(\vec{q},\dot{\vec{q}},t) + \hbar\, \vec{J}(t)\cdot\vec{q}(t)]} \right\} \\ &= i \int \mathcal{D}\vec{q}\, q_k(t_1)\, e^{\frac{i}{\hbar}\int_{-\infty}^{\infty} \mathrm{d}t [L(\vec{q},\dot{\vec{q}},t) + \hbar\, \vec{J}(t)\cdot\vec{q}(t)]}\ . \end{aligned} \tag{5.54}$$

From the first to the second equality we have expanded in terms of a Taylor series the part of the exponential function in the first path integral which is proportional to ϵ. The term $n = 0$ of this series cancels the second path integral. In the remaining series the term of order n is (after division by the factor ϵ in the denominator) proportional to ϵ^{n-1}. Thus, in the limit $\epsilon \to 0$ only the $n = 1$ term of the Taylor series survives.

Quite analogously one shows that

$$\frac{\delta^n Z[\vec{J}]}{\delta J_{k_1}(t_1) \cdots \delta J_{k_n}(t_n)} = i^n \int \mathcal{D}\vec{q}\, q_{k_1}(t_1) \cdots q_{k_n}(t_n)\, e^{\frac{i}{\hbar}\int_{-\infty}^{\infty} \mathrm{d}t [L(\vec{q},\dot{\vec{q}},t) + \hbar\, \vec{J}(t)\cdot\vec{q}(t)]}\ , \tag{5.55}$$

where the indices $k_1, \ldots, k_n = x, y,$ or z.

Let us now consider the transition amplitude

$$\langle \vec{q}_b, t_b |\, \hat{q}_k(t_j)\, | \vec{q}_a, t_a \rangle \ , \quad t_a < t_j < t_b \ , \quad k = x, y \text{ or } z \ . \tag{5.56}$$

We repeat the steps which we have taken in Sec. 3.1 to derive Eq. (3.12). First we partition the time interval $[t_a, t_b]$ in N pieces of length τ and insert complete sets of time-evolved position states,

$$\begin{aligned} \langle \vec{q}_b, t_b |\, \hat{q}_k(t_j)\, | \vec{q}_a, t_a \rangle \ &= \ \int \prod_{n=1}^{N-1} \mathrm{d}^3 \vec{q}_n \langle \vec{q}_b, t_b | \vec{q}_{N-1}, t_{N-1} \rangle \langle \vec{q}_{N-1}, t_{N-1} | \vec{q}_{N-2}, t_{N-2} \rangle \cdots \\ &\quad \times \langle \vec{q}_{j+1}, t_{j+1}, |\, \hat{q}_k(t_j)\, | \vec{q}_j, t_j \rangle \langle \vec{q}_j, t_j | \vec{q}_{j-1}, t_{j-1} \rangle \cdots \langle \vec{q}_1, t_1 | \vec{q}_a, t_a \rangle \ . \end{aligned} \tag{5.57}$$

The set

$$\mathbb{1} = \int \mathrm{d}^3 \vec{q}_j \, | \vec{q}_j, t_j \rangle \langle \vec{q}_j, t_j | \ ,$$

is the one which consists of eigenstates of the operator $\hat{q}_k(t_j)$,

$$\hat{q}_k(t_j)\, | \vec{q}_j, t_j \rangle = q_k(t_j)\, | \vec{q}_j, t_j \rangle \ . \tag{5.58}$$

This set will be inserted directly behind the operator $\hat{q}_k(t_j)$ in Eq. (5.57), such that the operator can be simply replaced by its eigenvalue. This eigenvalue is then just a numerical factor and can be pulled out of the overlap. The following steps mirror those of the derivation of Eq. (3.12). We obtain the final result

$$\langle \vec{q}_b, t_b |\, \hat{q}_k(t_j)\, | \vec{q}_a, t_a \rangle = \int \mathcal{D}\vec{q} \mathcal{D}\vec{p}\, q_k(t_j)\, e^{\frac{i}{\hbar} \int_{t_a}^{t_b} \mathrm{d}t \, [\vec{p} \cdot \dot{\vec{q}} - H(\vec{p}, \vec{q}, t)]} \ . \tag{5.59}$$

The object on the left-hand side is called **one-point correlation function**.

In complete analogy one derives for $t_a < t_1 < t_2 < t_b$

$$\langle \vec{q}_b, t_b |\, \hat{q}_{k_2}(t_2)\, \hat{q}_{k_1}(t_1)\, | \vec{q}_a, t_a \rangle = \int \mathcal{D}\vec{q} \mathcal{D}\vec{p}\, q_{k_1}(t_1)\, q_{k_2}(t_2)\, e^{\frac{i}{\hbar} \int_{t_a}^{t_b} \mathrm{d}t \, [\vec{p} \cdot \dot{\vec{q}} - H(\vec{p}, \vec{q}, t)]} \ . \tag{5.60}$$

Here we have to note that the operator $\hat{q}_{k_2}(t_2)$, which belongs to the **later** point in time t_2, is placed to the **left** of the operator $\hat{q}_{k_1}(t_1)$, which belongs to the **earlier** point in time t_1. The successive insertion of complete sets of time-evolved position states can therefore be performed without problems. However, this would not work if $t_2 < t_1$, since then the set which belongs to the earlier time would be inserted to the left of that belonging to the later time. This problem does not occur for the following amplitude for $t_a < t_2 < t_1 < t_b$,

$$\langle \vec{q}_b, t_b |\, \hat{q}_{k_1}(t_1)\, \hat{q}_{k_2}(t_2)\, | \vec{q}_a, t_a \rangle = \int \mathcal{D}\vec{q} \mathcal{D}\vec{p}\, q_{k_1}(t_1)\, q_{k_2}(t_2)\, e^{\frac{i}{\hbar} \int_{t_a}^{t_b} \mathrm{d}t \, [\vec{p} \cdot \dot{\vec{q}} - H(\vec{p}, \vec{q}, t)]} \ . \tag{5.61}$$

Obviously, the order of the factors $q_{k_1}(t_1)$ and $q_{k_2}(t_2)$ under the path integral on the right-hand side plays no role, therefore Eqs. (5.60) and (5.61) are identical. In order to summarize the left-hand sides of these equations in a single expression, we use the **time-ordering operator**,

$$\hat{T}\, [\hat{q}_{k_1}(t_1)\, \hat{q}_{k_2}(t_2)] = \begin{cases} \hat{q}_{k_1}(t_1)\, \hat{q}_{k_2}(t_2) & \text{for} \quad t_1 > t_2 \ , \\ \hat{q}_{k_2}(t_2)\, \hat{q}_{k_1}(t_1) & \text{for} \quad t_2 > t_1 \ , \end{cases} \tag{5.62}$$

such that we can write Eqs. (5.60) and (5.61) in the compact form

$$\langle \vec{q}_b, t_b | \, \hat{T} \left[\hat{q}_{k_1}(t_1) \, \hat{q}_{k_2}(t_2) \right] \, | \vec{q}_a, t_a \rangle = \int \mathcal{D}\vec{q} \mathcal{D}\vec{p} \, q_{k_1}(t_1) \, q_{k_2}(t_2) \, e^{\frac{i}{\hbar} \int_{t_a}^{t_b} \mathrm{d}t \, [\vec{p} \cdot \dot{\vec{q}} - H(\vec{p}, \vec{q}, t)]} \, . \tag{5.63}$$

This is the **two-point correlation function**. This result can be generalized to n points in time t_j, $j = 1, \ldots, n$,

$$\langle \vec{q}_b, t_b | \, \hat{T} \left[\hat{q}_{k_1}(t_1) \, \cdots \hat{q}_{k_n}(t_n) \right] \, | \vec{q}_a, t_a \rangle = \int \mathcal{D}\vec{q} \mathcal{D}\vec{p} \, q_{k_1}(t_1) \cdots q_{k_n}(t_n) \, e^{\frac{i}{\hbar} \int_{t_a}^{t_b} \mathrm{d}t \, [\vec{p} \cdot \dot{\vec{q}} - H(\vec{p}, \vec{q}, t)]} \, . \tag{5.64}$$

This is the n–**point correlation function**. For Hamilton functions which are quadratic in the momenta, cf. Eq. (3.15), one can again explicitly compute the path integral over the momenta and obtains

$$\langle \vec{q}_b, t_b | \, \hat{T} \left[\hat{q}_{k_1}(t_1) \, \cdots \hat{q}_{k_n}(t_n) \right] \, | \vec{q}_a, t_a \rangle = \mathcal{N} \int \mathcal{D}\vec{q} \, q_{k_1}(t_1) \cdots q_{k_n}(t_n) \, e^{\frac{i}{\hbar} \int_{t_a}^{t_b} \mathrm{d}t \, L(\vec{q}, \dot{\vec{q}}, t)} \, . \tag{5.65}$$

If we now send $t_a \to -\infty$ and $t_b \to +\infty$, we can shown in analogy to the derivation of Eq. (5.46) that

$$\begin{aligned} \lim_{\substack{t_b \to +\infty \\ t_a \to -\infty}} \langle \vec{q}_b, t_b | \, \hat{T} \left[\hat{q}_{k_1}(t_1) \, \cdots \hat{q}_{k_n}(t_n) \right] \, | \vec{q}_a, t_a \rangle &= \mathcal{N} \int \mathcal{D}\vec{q} \, q_{k_1}(t_1) \cdots q_{k_n}(t_n) \, e^{\frac{i}{\hbar} \int_{-\infty}^{\infty} \mathrm{d}t \, L(\vec{q}, \dot{\vec{q}}, t)} \\ &\sim \quad \langle 0; +\infty | \, \hat{T} \left[\hat{q}_{k_1}(t_1) \, \cdots \hat{q}_{k_n}(t_n) \right] \, | 0; -\infty \rangle \, . \end{aligned} \tag{5.66}$$

If we compare this with Eq. (5.55), we observe that $Z[\vec{J}]$ is the **generating functional** for $\boldsymbol{n}$**–point correlation functions in the ground state**,

$$\left. \frac{\delta^n Z[\vec{J}]}{\delta J_{k_1}(t_1) \cdots \delta J_{k_n}(t_n)} \right|_{\vec{J}=0} \sim i^n \langle 0; +\infty | \, \hat{T} \left[\hat{q}_{k_1}(t_1) \, \cdots \hat{q}_{k_n}(t_n) \right] \, | 0; -\infty \rangle \, , \tag{5.67}$$

i.e., via functional differentiation of $Z[\vec{J}]$ with respect to the source $\vec{J}$ (which is set to zero afterwards) we generate the n–point correlation functions.

Lecture 7

5.6 Addendum: Ehrenfest's theorem, canonical commutation relation

The concept of the functional derivative allows us to draw conclusions on how **Ehrenfest's theorem** and the **canonical commutation relation** appear in the path-integral formalism. We will restrict our considerations to one spatial dimension, the generalization to three spatial dimensions is straightforward. We first prove the following

Proposition: Let $G[q(s)]$ be a functional of the function $q(s)$. Then

$$\int \mathcal{D}q \, \frac{\delta G[q(s)]}{\delta q(t)} = 0 \, . \tag{5.68}$$

Proof: According to the definition (5.50), we have

$$\int \mathcal{D}q\ \frac{\delta G[q(s)]}{\delta q(t)} = \int \mathcal{D}q\ \lim_{\epsilon\to 0}\frac{1}{\epsilon}\left\{G[q(s)+\epsilon\delta(s-t)] - G[q(s)]\right\}$$
$$= \lim_{\epsilon\to 0}\frac{1}{\epsilon}\left\{\int \mathcal{D}q\ G[q(s)+\epsilon\delta(s-t)] - \int \mathcal{D}q\ G[q(s)]\right\}\ , \qquad (5.69)$$

where we assumed that we can exchange the order of the path integration and the limit $\epsilon \to 0$. In the path integral we integrate over **all** functions $q(s)$, in particular also over the function $q(s) + \epsilon\delta(s-t)$. We may therefore substitute the integration variable, $q'(s) = q(s) + \epsilon\delta(s-t)$ in the first path integral in Eq. (5.69). The Jacobi determinant of this substitution is equal to one, $\mathcal{D}q = \mathcal{D}q'$. Then, the first path integral in Eq. (5.69) is exactly equal to the second, and they cancel, even prior to taking the limit $\epsilon \to 0$, q.e.d.

Now let $F[q(s)]$ be a functional of a trajectory $q(s)$ of a quantum-mechanical particle in one dimension, and $S[q(s)]$ the corresponding action. If we use Eq. (5.68) for the particular choice $G[q(s)] \equiv F[q(s)] \exp\left\{\frac{i}{\hbar}S[q(s)]\right\}$, we obtain with the product rule (which is also valid for functional derivatives)

$$0 = \int \mathcal{D}q \left\{\frac{\delta F[q(s)]}{\delta q(t)} + \frac{i}{\hbar}\,F[q(s)]\,\frac{\delta S[q(s)]}{\delta q(t)}\right\} e^{\frac{i}{\hbar}S[q(s)]}\ . \qquad (5.70)$$

Let us introduce the short-hand notation

$$\langle A(q)\rangle_S \equiv \int \mathcal{D}q\ A(q)\, e^{\frac{i}{\hbar}S[q(s)]}\ , \qquad (5.71)$$

which has the meaning of an **average** of the quantity $A(q)$ over the ensemble of quantum-mechanical trajectories represented by the path integral. Then, Eq. (5.70) assumes the compact form

$$\left\langle \frac{\delta F[q(s)]}{\delta q(t)}\right\rangle_S = -\frac{i}{\hbar}\left\langle F[q(s)]\,\frac{\delta S[q(s)]}{\delta q(t)}\right\rangle_S\ . \qquad (5.72)$$

This is also valid for discretized variables, i.e., when the time interval $[s_a, s_b]$ is discretized, $s_b - s_a = N\tau$, $s_a \equiv s_0$, $s_j = s_a + j\tau$, $j = 1, \ldots, N-1$, $s_b \equiv s_N$, and the trajectory $q(s)$ is replaced by a discrete set of variables, $q_a \equiv q_0, q_1, \ldots, q_N \equiv q_b$, where $q_j \equiv q(s_j)$, $j = 0, \ldots, N$. In this case, the **functionals** $F[q(s)]$ and $S[q(s)]$ become ordinary **functions** of the variables $q_0, q_1, \ldots, q_N$,

$$F[q(s)] \longrightarrow F(q_0, q_1, \ldots, q_N)\ ,$$
$$S[q(s)] \longrightarrow S(q_0, q_1, \ldots, q_N) \equiv \sum_{n=1}^{N}\tau\left[\frac{m}{2}\left(\frac{q_n - q_{n-1}}{\tau}\right)^2 - V(q_n, s_n)\right]\ . \qquad (5.73)$$

The **functional derivative** with respect to $q(t)$ simply becomes the **partial derivative** with respect to the spatial coordinate q_ℓ at the particular time slice t_ℓ corresponding to

the time t in the continuum, i.e., $\delta/\delta q(t) \to \partial/\partial q_\ell$. Then, Eq. (5.72) reads

$$\begin{aligned}\left\langle \frac{\partial F(q_0,\ldots,q_N)}{\partial q_\ell} \right\rangle_S &= -\frac{i}{\hbar} \left\langle F(q_0,\ldots,q_N)\, \frac{\partial S(q_0,\ldots,q_N)}{\partial q_\ell} \right\rangle_S \\ &= -\frac{i}{\hbar} \left\langle F(q_0,\ldots,q_N)\, \left[m \left(\frac{q_\ell - q_{\ell-1}}{\tau} - \frac{q_{\ell+1} - q_\ell}{\tau} \right) - \tau \frac{\partial V(q_\ell, t_\ell)}{\partial q_\ell} \right] \right\rangle_S \\ &= \frac{i}{\hbar} \tau \left\langle F(q_0,\ldots,q_N)\, \left[m\, \frac{q_{\ell+1} - 2q_\ell + q_{\ell-1}}{\tau^2} + \frac{\partial V(q_\ell, t_\ell)}{\partial q_\ell} \right] \right\rangle_S . \end{aligned} \tag{5.74}$$

Interesting relations emerge by making various choices of F:

(i) $F = 1$. In this case, Eq. (5.74) becomes (omitting overall factors)

$$\left\langle m\, \frac{q_{\ell+1} - 2q_\ell + q_{\ell-1}}{\tau^2} \right\rangle_S = - \left\langle \frac{\partial V(q_\ell, t_\ell)}{\partial q_\ell} \right\rangle_S , \tag{5.75}$$

or, in the continuum limit, where $\tau \to 0$ and $q_\ell \to q(t) \equiv q$,

$$\langle m\, \ddot{q} \rangle_S = - \left\langle \frac{\partial V(q,t)}{\partial q} \right\rangle_S . \tag{5.76}$$

This is the path-integral version of **Ehrenfest's theorem**: on average (symbolized by the angular brackets $\langle \cdot \rangle_S$) the particle obeys Newton's equation of motion (remember that $F \equiv -\partial V/\partial q$).

(ii) $F = q_\ell$. In this case, Eq. (5.74) becomes

$$\langle 1 \rangle_S = -\frac{i}{\hbar} \left\langle \left[m \left(q_\ell\, \frac{q_\ell - q_{\ell-1}}{\tau} - \frac{q_{\ell+1} - q_\ell}{\tau}\, q_\ell \right) - \tau q_\ell \frac{\partial V(q_\ell, t_\ell)}{\partial q_\ell} \right] \right\rangle_S . \tag{5.77}$$

In the limit $\tau \to 0$, the last term can be omitted, while $q_\ell \to q(t)$ and

$$\frac{q_\ell - q_{\ell-1}}{\tau} \longrightarrow \dot{q}(t^-) , \qquad \frac{q_{\ell+1} - q_\ell}{\tau} \longrightarrow \dot{q}(t^+) . \tag{5.78}$$

Here $\dot{q}(t^\pm) \equiv \lim_{\tau \to 0} \dot{q}(t \pm \tau)$. Introducing the momentum $p(t) \equiv m\dot{q}(t)$, we then have

$$\langle i\hbar \rangle_S = \big\langle q(t)p(t^-) - p(t^+)q(t) \big\rangle_S . \tag{5.79}$$

This is the path-integral version of the standard **canonical commutation relation**

$$i\hbar = \hat{q}\hat{p} - \hat{p}\hat{q} \equiv [\hat{q}, \hat{p}] . \tag{5.80}$$

One has to note that, in order to translate this relation into the path-integral version, one has to assume that the operators are **time-ordered**, i.e., the operator on the right belongs to a (slightly) earlier time than the one on the left.

We close this section with a remark on a related problem. Suppose we would like to calculate the average of the kinetic energy,

$$\left\langle \frac{p^2}{2m} \right\rangle_S = \left\langle \frac{m}{2}\,\dot{q}^2 \right\rangle_S \,. \tag{5.81}$$

Here we run into the same "time-ordering" problem as before. In fact, the discretized expressions

$$\left\langle \frac{m}{2}\left(\frac{q_\ell - q_{\ell-1}}{\tau}\right)^2 \right\rangle_S \quad \text{or} \quad \left\langle \frac{m}{2}\left(\frac{q_{\ell+1} - q_\ell}{\tau}\right)^2 \right\rangle_S \tag{5.82}$$

give the wrong answer. The reason is that the squared displacement on a "Brownian motion-like" trajectory is $(q_\ell - q_{\ell-1})^2 \sim \tau$, as explained in Sec. 3.5. Therefore,

$$\left(\frac{q_\ell - q_{\ell-1}}{\tau}\right)^2 \sim \frac{1}{\tau}\,, \tag{5.83}$$

which diverges in the limit $\tau \to 0$. The correct way to calculate the kinetic energy is therefore

$$\left\langle \frac{m}{2}\,\frac{q_{\ell+1} - q_\ell}{\tau}\,\frac{q_\ell - q_{\ell-1}}{\tau} \right\rangle_S \longrightarrow \left\langle \frac{m}{2}\,\dot{q}(t^+)\dot{q}(t^-) \right\rangle_S \equiv \left\langle \frac{p(t^+)p(t^-)}{2m} \right\rangle_S \,. \tag{5.84}$$

Why does this solve the divergence problem of Eq. (5.82)? Naively, one would think that both displacements $q_{\ell+1} - q_\ell \sim \sqrt{\tau}$ and $q_\ell - q_{\ell-1} \sim \sqrt{\tau}$, so that we get the same $1/\tau$ divergence as before. However, this argument is incorrect, because the displacements on **successive** time steps are **uncorrelated**. In one dimension this means that it is as likely that the displacement $q_{\ell+1} - q_\ell$ of the next time step happens in the **same** direction as the one $q_\ell - q_{\ell-1}$ of the previous time step, as that it happens in the **opposite** direction. In three dimensions, it is even **highly unlikely** that the displacement $\vec{q}_{\ell+1} - \vec{q}_\ell$ happens in **exactly the same** direction as that in the previous time step. Only if it did, the product $(q_{\ell+1} - q_\ell)(q_\ell - q_{\ell-1})$ displaces the particle by a much larger distance $\sim \tau$ than the τ^2 behavior expected for "normal" smooth trajectories. If it does not, in one dimension it is as likely that the displacement $q_{\ell+1} - q_\ell$ **reverts** the displacement $q_\ell - q_{\ell-1}$ from the previous time step, and in three dimensions it is very likely that it reverts this displacement at least to some extent. Therefore $(q_{\ell+1} - q_\ell)(q_\ell - q_{\ell-1}) \sim \tau^2$, and the kinetic energy (5.84) is well-defined.

6 From Classical Particles to Classical Fields

In Chap. 2 we have considered the Classical Mechanics of a single particle. By extending this to a system of N particles, and then sending $N \to \infty$, we would like to generalize classical mechanics to a **continuous system**, i.e., we aim at deriving **continuum mechanics** in the Lagrange formalism, which is equivalent to the **Lagrange formalism for fields**.

6.1 The longitudinally oscillating chain

The most simple N–particle system which allows to make the transition to a continuum of degrees of freedom is the **longitudinally oscillating chain**. Consider a chain of N particles of (identical) mass m aligned along the x–direction, which are connected via (identical) springs with spring constant k and perform **longitudinal oscillations**, i.e., oscillations along the extension of the chain, cf. Fig. 6.1. Note that it is not necessary to assume that all masses and spring constants are equal, but it simplifies the following calculations.

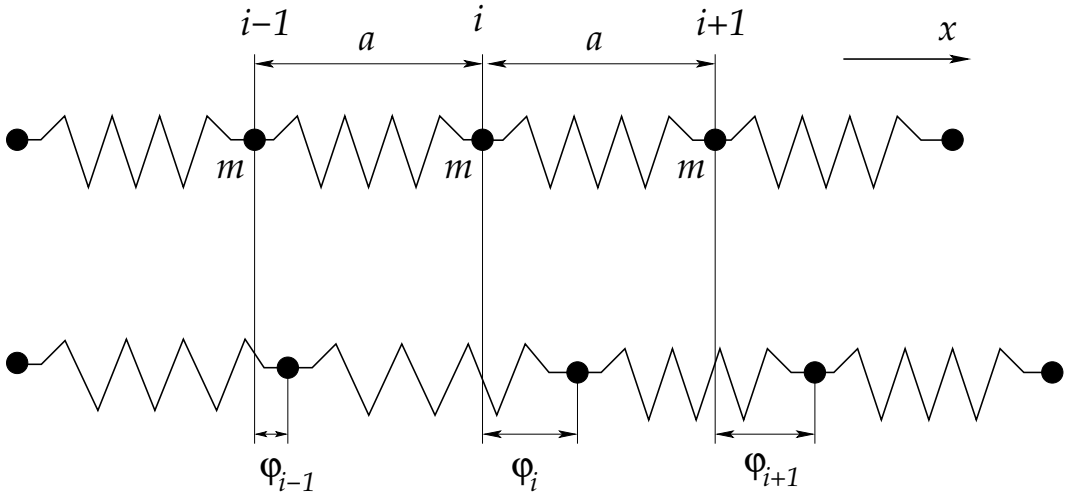


Figure 6.1: The longitudinally oscillating chain.

In their positions at rest the masses are supposed to be a distance a apart. When oscillating, the ith mass will be displaced by a distance φ_i from its position at rest. The

kinetic energy of the system is obviously

$$T = \frac{1}{2}\, m \sum_{i=1}^{N} \dot{\varphi}_i^2 \ . \tag{6.1}$$

The potential energy is

$$V = \frac{1}{2}\, k \sum_{i=1}^{N-1} \left(\varphi_{i+1} - \varphi_i\right)^2 \ . \tag{6.2}$$

We convince ourselves that this expression is correct by calculating the force which acts onto the jth mass,

$$F_j = -\frac{\partial V}{\partial \varphi_j} = -k\left(\varphi_j - \varphi_{j-1}\right) + k(\varphi_{j+1} - \varphi_j) \ , \quad j = 2, \ldots, N-1 \ . \tag{6.3}$$

The first term on the right-hand side corresponds to Hooke's law for the spring on the left-hand side of the jth mass. When this spring is extended, i.e., when $\varphi_j - \varphi_{j-1} > 0$, it will pull the jth mass back in the $-x$ direction. On the other hand, if the spring is compressed, $\varphi_j - \varphi_{j-1} < 0$, it will push the mass in the $+x$ direction. Therefore, this term has to have a negative sign. The second term on the right-hand side of Eq. (6.3) corresponds to Hooke's law for the spring on the right-hand side of the jth mass. Here one argues quite analogously, but since an elongation of this spring pulls the mass in $+x$ direction and a compression pushes it in $-x$ direction, the sign of the second term is just the opposite of that of the first. For $j = 1$ resp. $j = N$ we obtain the force by omitting the first resp. the last term in Eq. (6.3).

With Eqs. (6.1) and (6.2) the Lagrange function of the system reads

$$\begin{aligned} L = T - V &= \frac{1}{2} \sum_{i=1}^{N-1} \left[m\, \dot{\varphi}_i^2 - k\, \left(\varphi_{i+1} - \varphi_i\right)^2 \right] \\ &= \frac{1}{2} \sum_{i=1}^{N-1} a \left[\frac{m}{a}\, \dot{\varphi}_i^2 - ka \left(\frac{\varphi_{i+1} - \varphi_i}{a} \right)^2 \right] \\ &= \frac{1}{2} \sum_{i=1}^{N-1} a \left[\mu\, \dot{\varphi}_i^2 - \kappa \left(\frac{\varphi_{i+1} - \varphi_i}{a} \right)^2 \right] \equiv \sum_{i=1}^{N-1} a\, \mathcal{L}_i \ , \end{aligned} \tag{6.4}$$

where we have introduced the **mass per unit of length** $\mu \equiv m/a$, the **modulus of elasticity** $\kappa \equiv ka$, and the **Lagrange function per unit of length** $\mathcal{L}_i$. Furthermore, we have neglected the kinetic energy of the Nth mass. If $N \gg 1$, this is approximation is well justified, since the motion of a single mass cannot substantially influence the motion of the whole system.

The displacements φ_i of the masses from their positions at rest represent the **degrees of freedom** of the system. The Euler–Lagrange equations for these degrees of freedom

read

$$\begin{aligned} 0 &= \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{\varphi}_j} - \frac{\partial L}{\partial \varphi_j} \\ \Longleftrightarrow \quad 0 &= \mu\,\ddot{\varphi}_j - \kappa\left(\frac{\varphi_{j+1}-\varphi_j}{a^2} - \frac{\varphi_j - \varphi_{j-1}}{a^2}\right) \\ &= \mu\,\ddot{\varphi}_j - \kappa\,\frac{\varphi_{j+1} - 2\,\varphi_j + \varphi_{j-1}}{a^2}\,. \end{aligned} \tag{6.5}$$

Let us now consider the limit $N \to \infty$ and $a \to 0$. Then, the chain of one-dimensional harmonic oscillators becomes a continuous **elastic rod**. When all of the (infinitely many) oscillators are in their rest positions, the length of the rod assumes the value ℓ. This value can change when the oscillators move: the rod can be elongated or compressed in x direction. The index i specifying the position of a mass assumes **continuous values**; we can replace it by the x coordinate,

$$\varphi_j(t) \quad \longrightarrow \quad \varphi(x,t)\,.$$

The distance a between the masses is replaced by the infinitesimal differential $\mathrm{d}x$, such that

$$\begin{aligned} \lim_{a\to 0}\frac{\varphi_{j+1}(t)-\varphi_j(t)}{a} &= \lim_{\mathrm{d}x\to 0}\frac{\varphi(x+\mathrm{d}x,t)-\varphi(x,t)}{\mathrm{d}x} \equiv \frac{\partial\varphi(x,t)}{\partial x}\,, \\ \lim_{a\to 0}\frac{\varphi_{j+1}(t)-2\,\varphi_j(t)+\varphi_{j-1}(t)}{a^2} &= \lim_{\mathrm{d}x\to 0}\frac{\varphi(x+\mathrm{d}x,t)-2\,\varphi(x,t)+\varphi(x-\mathrm{d}x,t)}{\mathrm{d}x^2} \\ &\equiv \frac{\partial^2\varphi(x,t)}{\partial x^2}\,. \end{aligned}$$

Note that we now have partial derivatives, due to the dependence of the displacement field $\varphi(t,x)$ on time **and** space. Thus, the usual differentiation of φ_i with respect to time must also be replaced by a partial derivative,

$$\dot{\varphi}_j \quad \longrightarrow \quad \frac{\partial\varphi(x,t)}{\partial t}\,, \qquad \ddot{\varphi}_j \quad \longrightarrow \quad \frac{\partial^2\varphi(x,t)}{\partial t^2}\,.$$

The Lagrange function (6.4) becomes

$$L = \lim_{a\to 0}\sum_{i=1}^{N-1} a\,\mathcal{L}_i \equiv \int_0^\ell \mathrm{d}x\;\mathcal{L}\,, \tag{6.6}$$

where ℓ is the length of the rod (as mentioned above, this is not necessarily constant, since the oscillations can lead to elongation or compression of the system) and

$$\mathcal{L} = \frac{\mu}{2}\left(\frac{\partial\varphi}{\partial t}\right)^2 - \frac{\kappa}{2}\left(\frac{\partial\varphi}{\partial x}\right)^2 \tag{6.7}$$

is the so-called **Lagrange density** or **Lagrangian**. The equation of motion (6.5) assumes the form

$$0 = \mu\,\frac{\partial^2\varphi}{\partial t^2} - \kappa\,\frac{\partial^2\varphi}{\partial x^2}\,. \tag{6.8}$$

This equation is of a type well-known from Classical Electrodynamics: it is a **wave equation**. Here, however, only a single spatial dimension appears (the one along the rod). In consequence, Eq. (6.8) describes the **one-dimensional**, i.e., **longitudinal** propagation of **sound waves** along the rod. These waves correspond to local maxima (compression of springs) or minima (elongation of springs) in mass density, which travel along the direction of the rod. If we divide Eq. (6.8) by κ, we can read off the **sound velocity**, which is the analogue of the velocity of light in the wave equation for electromagnetic fields,

$$c_S \equiv \sqrt{\frac{\kappa}{\mu}} \,. \tag{6.9}$$

6.2 Continuum Lagrange mechanics in three space and one time dimension

The consideration of the previous section can be easily generalized to a three-dimensional system. Equation (6.6) then reads

$$L \equiv \int_V \mathrm{d}^3\vec{x}\, \mathcal{L} \,, \tag{6.10}$$

where V is the spatial volume of the system under consideration. A closer inspection of Eq. (6.7) reveals that the **Lagrangian** $\mathcal{L}$ is not only a function of $\partial\varphi/\partial t$, but also depends on the spatial derivatives $\partial\varphi/\partial x$. In general, in three dimensions also partial derivatives with respect to y and z may appear. Furthermore, the Lagrangian can also depend on the field φ itself and may depend explicitly on time and space (i.e., not only implicitly through the dependence of φ on t and $\vec{x}$). Therefore, in general the Lagrangian can possess the following dependences:

$$\mathcal{L} = \mathcal{L}\left(\varphi(\vec{x},t), \frac{\partial\varphi(\vec{x},t)}{\partial t}, \vec{\nabla}\varphi(\vec{x},t); \vec{x}, t\right) \,. \tag{6.11}$$

Note that, in comparison to the Lagrange function $L(q,\dot{q};t)$, in the Lagrange **density** the field φ assumes the role of the generalized coordinate q, its derivatives $\frac{\partial\varphi}{\partial t}, \vec{\nabla}\varphi$ the role of the generalized velocity $\dot{q}$, and the explicit dependence on time t is extended to one on time t **and** spatial position $\vec{x}$. The spatial variable has no longer the meaning of a coordinate (or position) of a particle, it is simply a **continuous** index, similar to the index i enumerating the generalized coordinates (if one has a system with more than one such coordinate, $q \to \{q_1, q_2, \ldots\}$). In the Lagrange function, $q, \dot{q}$ were independent **degrees of freedom** of the system. In the Lagrangian the degrees of freedom are the field φ and its derivatives $\frac{\partial\varphi}{\partial t}, \vec{\nabla}\varphi$. Since these functions can assume distinct and (in principle) mutually independent values at **each** point $(\vec{x},t)$ in space-time, this is a system with **infinitely many** degrees of freedom.

For continuous systems the Lagrange density or Lagrangian plays the same role as the Lagrange function for discrete systems. Therefore, it should in principle be possible to derive the equation of motion (e.g., Eq. (6.8) for the previous example of the one-dimensional chain) for the field $\varphi(t,\vec{x})$ from the Lagrangian itself. This will be elaborated in the following.

Using Eq. (6.10) the action is defined as

$$S[\varphi(\vec{x},t)] = \int_{t_a}^{t_b} \mathrm{d}t \int_V \mathrm{d}^3\vec{x}\, \mathcal{L}\left(\varphi(\vec{x},t), \partial_t\varphi(\vec{x},t), \vec{\nabla}\varphi(\vec{x},t); \vec{x}, t\right) . \tag{6.12}$$

In principle, the equations of motion should follow from **Hamilton's principle**, which reads with Eq. (6.11)

$$\begin{aligned} 0 &= \delta S[\varphi] = S[\varphi+\delta\varphi] - S[\varphi] \\ &= \int_{t_a}^{t_b} \mathrm{d}t \int_V \mathrm{d}^3\vec{x}\, \left[\mathcal{L}\left(\varphi+\delta\varphi, \partial_t\varphi + \delta(\partial_t\varphi), \vec{\nabla}\varphi + \delta(\vec{\nabla}\varphi); \vec{x}, t\right) - \mathcal{L}\left(\varphi, \partial_t\varphi, \vec{\nabla}\varphi; \vec{x}, t\right)\right] , \end{aligned} \tag{6.13}$$

where we have omitted the arguments $(\vec{x},t)$ of the fields for the sake of brevity. Quite similar to the trajectory $q(t)$, which is not varied at the initial and final point in time, the field $\varphi(\vec{x},t)$ will **not** be varied at the **surface** ∂V_4 of the space-time volume $V_4 \equiv V \times [t_a, t_b]$,

$$\delta\varphi(\vec{x},t)\,|_{(\vec{x},t)\,\in\,\partial V_4} = 0 . \tag{6.14}$$

However, this constraint does not apply to the partial derivatives $\partial_t\varphi, \vec{\nabla}\varphi$ of the field, similar to the generalized velocity $\dot{q}$ which must not be held fixed at t_a and t_b (or like the generalized momentum p in the modified Hamilton's principle, which can vary freely at t_a and t_b, cf. Sec. 2.1.2).

If we assume infinitesimal variations of the field, $|\delta\varphi(\vec{x},t)| \ll |\varphi(\vec{x},t)|$, we can terminate the Taylor expansion of the first term under the integral in Eq. (6.13) after the order $O(\delta\varphi, \delta\partial_t\varphi, \delta\vec{\nabla}\varphi)$ and obtain

$$0 = \int_{t_a}^{t_e} \mathrm{d}t \int_V \mathrm{d}^3\vec{x}\, \left[\frac{\partial\mathcal{L}}{\partial\varphi}\,\delta\varphi + \frac{\partial\mathcal{L}}{\partial\left(\partial_t\varphi\right)}\,\delta\left(\partial_t\varphi\right) + \frac{\partial\mathcal{L}}{\partial(\vec{\nabla}\varphi)}\cdot\delta(\vec{\nabla}\varphi)\right] . \tag{6.15}$$

It furthermore holds that

$$\delta(\partial_t\varphi) \equiv \partial_t(\varphi+\delta\varphi) - \partial_t\varphi \equiv \partial_t\delta\varphi , \qquad \delta(\vec{\nabla}\varphi) \equiv \vec{\nabla}(\varphi+\delta\varphi) - \vec{\nabla}\varphi \equiv \vec{\nabla}\delta\varphi . \tag{6.16}$$

The second and third term in Eq. (6.15) can then be written as follows,

$$\begin{aligned} 0 = &\int_{t_a}^{t_e} \mathrm{d}t \int_V \mathrm{d}^3\vec{x}\, \left[\frac{\partial\mathcal{L}}{\partial\varphi} - \partial_t\frac{\partial\mathcal{L}}{\partial(\partial_t\varphi)} - \vec{\nabla}\cdot\frac{\partial\mathcal{L}}{\partial(\vec{\nabla}\varphi)}\right]\delta\varphi \\ &+ \int_{t_a}^{t_e} \mathrm{d}t \int_V \mathrm{d}^3\vec{x}\, \left\{\partial_t\left[\frac{\partial\mathcal{L}}{\partial(\partial_t\varphi)}\,\delta\varphi\right] + \vec{\nabla}\cdot\left[\frac{\partial\mathcal{L}}{\partial(\vec{\nabla}\varphi)}\,\delta\varphi\right]\right\} . \end{aligned} \tag{6.17}$$

The argument of second integral over the space-time volume $V \times [t_a, t_b]$ is basically a four-dimensional divergence

$$\partial_t\left[\frac{\partial\mathcal{L}}{\partial(\partial_t\varphi)}\,\delta\varphi\right] + \vec{\nabla}\cdot\left[\frac{\partial\mathcal{L}}{\partial(\vec{\nabla}\varphi)}\,\delta\varphi\right] \equiv \partial_\mu\left[\frac{\partial\mathcal{L}}{\partial(\partial_\mu\varphi)}\,\delta\varphi\right] , \tag{6.18}$$

where $\partial_\mu = (\partial_t, \vec{\nabla})$ is the four-dimensional gradient operator and a sum over μ is implied. The second integral can thus be converted with the help of Gauss' theorem in four dimensions into an integral over the closed surface ∂V_4 of that space-time volume,

$$\int_{t_a}^{t_e} \mathrm{d}t \int_V \mathrm{d}^3\vec{x}\, \partial_\mu \left[\frac{\partial \mathcal{L}}{\partial(\partial_\mu \varphi)}\, \delta\varphi \right] = \oint_{\partial V_4} \mathrm{d}\sigma_\mu \, \frac{\partial \mathcal{L}}{\partial(\partial_\mu \varphi)}\, \delta\varphi \equiv 0 \,, \tag{6.19}$$

since $\delta\varphi$ vanishes on ∂V_4, cf. Eq. (6.14). Here $\mathrm{d}\sigma_\mu$ is the μth component of the four-dimensional vector normal on ∂V_4.

Since the variation $\delta\varphi(\vec{x}, t)$ of the field is arbitrary at each space-time point $(\vec{x}, t)$, the term in brackets in the first integral in Eq. (6.17) must vanish,

$$0 = \frac{\partial \mathcal{L}}{\partial \varphi} - \partial_t \frac{\partial \mathcal{L}}{\partial(\partial_t \varphi)} - \vec{\nabla} \cdot \frac{\partial \mathcal{L}}{\partial(\vec{\nabla}\varphi)} \,. \tag{6.20}$$

This is the **Euler–Lagrange equation** for continuous systems, i.e., for the field φ, which represents the (infinitely many) degrees of freedom of such a continuous system. Equation (6.20) is a **classical** equation of motion for the field φ and as such exclusively determines the **classical field configuration**. According to Hamilton's principle (6.13), this configuration extremizes (minimizes) the action. We will see in the next chapter that in **quantum field theory** also all other possible field configurations appear and, similar to the path integral in quantum mechanics of a single particle, contribute with a weight $\exp\{iS[\varphi(\vec{x}, t)]/\hbar\}$) to physical observables.

We now convince ourselves that Eq. (6.20) gives the correct equation of motion for the field φ when applying it to the example of the elastic rod. In other words, we calculate the equation of motion (6.20) using the Lagrangian (6.7) and show that in this way we obtain the equation of motion (6.8).

The Lagrangian (6.7) contains only derivatives of the field, thus $\partial\mathcal{L}/\partial\varphi \equiv 0$. The derivative of $\mathcal{L}$ with respect to the partial derivative of the field with respect to time gives

$$\frac{\partial \mathcal{L}}{\partial\,(\partial_t \varphi)} = \mu \frac{\partial \varphi}{\partial t} \,,$$

and the derivative with respect to the partial derivative of the field with respect to the spatial coordinate x is

$$\frac{\partial \mathcal{L}}{\partial\,(\partial_x \varphi)} = -\kappa \frac{\partial \varphi}{\partial x} \,.$$

Since it is a one-dimensional problem, no dependences on, or derivatives with respect to, y or z appear. Inserting the above into the Euler–Lagrange equation (6.20) we obtain

$$0 = \frac{\partial}{\partial t}\left(\mu \frac{\partial \varphi}{\partial t}\right) + \frac{\partial}{\partial x}\left(-\kappa \frac{\partial \varphi}{\partial x}\right) \equiv \mu \frac{\partial^2 \varphi}{\partial t^2} - \kappa \frac{\partial^2 \varphi}{\partial x^2} \,,$$

which agrees with the previously derived equation of motion (6.8).

If we consider a system where not only one, but **many** fields appear, we enumerate them with an additional index,

$$\varphi_a(\vec{x}, t) \,, \quad a = 1, 2, \ldots \,.$$

Then **each** of these fields fulfills an Euler–Lagrange equation of the type (6.20),

$$0 = \partial_t \frac{\partial \mathcal{L}}{\partial \left(\partial_t \varphi_a\right)} + \vec{\nabla} \cdot \frac{\partial \mathcal{L}}{\partial (\vec{\nabla} \varphi_a)} - \frac{\partial \mathcal{L}}{\partial \varphi_a} \,, \quad a = 1, 2, \ldots \,. \tag{6.21}$$

7 Path Integrals in Quantum Field Theory

Lecture 8

As we have seen in the previous discussion, the path-integral formalism provides an alternative approach to solving the Schrödinger equation for the wave function of a quantum-mechanical particle. However, so far the discussion of path integrals was restricted to the dynamics of a **single** particle. This is still completely equivalent to solving a **classical** wave equation: the Schrödinger equation. Although the wave function resulting from the solution of this equation describes the quantum dynamics of a single particle, it is itself a purely **classical** object. If we want to describe the quantum mechanics of a system with (in principle) **infinitely many** degrees of freedom, such as contained in a field (as we have seen in the previous chapter), we have to devise a quantum-mechanical description for such a field. This leads to **quantum field theory**.

In principle, there are two different approaches to reach this goal. The first one is similar to the "second-quantization" approach known from the discussion of the harmonic oscillator in the introductory Quantum Mechanics lecture. There one introduces operators which allow to create and annihilate excitation quanta. The "second-quantization", or **canonical quantization** approach for quantum field theory extends this idea to a system of infinitely many degrees of freedom, which can be created or annihilated. Typically one formulates this in momentum space and introduces creation and annihilation operators for particles with a definite momentum, on-shell energy, as well other quantum numbers (e.g. spin, flavor, color, etc.). Since the momenta run over an uncountable infinite set of values, one deals with a system of infinitely many degrees of freedom.

The second approach is based on the path-integral formalism extended to fields, then sometimes also called **functional-integral formalism**. In the following, we will given an introduction to the latter. As an example, we consider the simplest possibility: a real scalar field.

7.1 The classical non-interacting Klein–Gordon field

The first attempt to establish a relativistic theory for the electron was made by Oskar Klein and Walter Gordon. It was bound to fail, since Klein and Gordon assumed the electron to be described by a **real scalar field** ϕ. As we know today, such a field describes **bosons with spin zero**, while the electron is a **fermion with spin 1/2**. The correct relativistic theory for the electron was found by Paul Adrien Maurice Dirac, but will not be subject of this lecture course.

The **Lagrangian** of **Klein–Gordon theory** has a striking similarity to that of the

elastic rod, cf. Eq. (6.7),

$$\mathcal{L} = \frac{1}{2}\left[\frac{1}{c^2}\left(\frac{\partial\phi}{\partial t}\right)^2 - (\vec{\nabla}\phi)\cdot(\vec{\nabla}\phi) - \left(\frac{mc}{\hbar}\right)^2\phi^2\right] . \tag{7.1}$$

The difference is that the velocity of light c appears instead of the sound velocity (6.9). Does this mean that waves of the Klein–Gordon field travel with light velocity? No, since there is also a so-called **mass term** $\sim (mc/\hbar)^2\phi^2$, which is absent in Eq. (6.7). As we will see below, points of constant phase travel with the **phase velocity** $v_{\text{phase}}(p) = E_{\vec{p}}/p$, while the **group velocity** is

$$v_{\text{group}}(p) = \frac{\mathrm{d}E_{\vec{p}}}{\mathrm{d}p} = \frac{pc^2}{E_{\vec{p}}} , \tag{7.2}$$

where $E_{\vec{p}} = c\sqrt{\vec{p}^2 + (mc)^2}$ is the relativistic energy of a particle with momentum $\vec{p}$. The group velocity of the Klein–Gordon field is then simply the velocity of a particle with energy $E_{\vec{p}}$ and momentum $\vec{p}$.

What is the classical equation of motion of the Klein–Gordon field? In order to determine this, we employ Eq. (6.20). From Eq. (7.1) we obtain

$$\frac{\partial\mathcal{L}}{\partial(\partial_t\phi)} = \frac{1}{c^2}\frac{\partial\phi}{\partial t} , \qquad \frac{\partial\mathcal{L}}{\partial(\vec{\nabla}\phi)} = -\vec{\nabla}\phi , \qquad \frac{\partial\mathcal{L}}{\partial\phi} = -\left(\frac{mc}{\hbar}\right)^2\phi , \tag{7.3}$$

so that the equation of motion, the so-called **Klein–Gordon equation**, reads

$$\left[\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \Delta + \left(\frac{mc}{\hbar}\right)^2\right]\phi \equiv \left[\Box + \left(\frac{mc}{\hbar}\right)^2\right]\phi = 0 , \tag{7.4}$$

where $\Delta \equiv \vec{\nabla}\cdot\vec{\nabla}$ is the Laplace operator and where we defined the **d'Alembert** or **wave operator**

$$\Box \equiv \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \Delta . \tag{7.5}$$

Like the Schrödinger equation (3.23), the Klein–Gordon equation (7.4) is a linear, homogeneous differential equation and the solution can be written as a superposition of plane waves. Thus, we make an Ansatz similar to Eq. (3.25),

$$\phi(\vec{x},t) = \int \frac{\mathrm{d}E\,\mathrm{d}^3\vec{p}}{(2\pi\hbar)^4}\,\tilde{\phi}(E,\vec{p})\,e^{-\frac{i}{\hbar}(Et-\vec{p}\cdot\vec{x})} . \tag{7.6}$$

Inserting this Ansatz into Eq. (7.4), we obtain

$$\begin{aligned}
0 &= \left[\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \Delta + \left(\frac{mc}{\hbar}\right)^2\right]\phi(\vec{x},t) \\
&= \int \frac{\mathrm{d}E\,\mathrm{d}^3\vec{p}}{(2\pi\hbar)^4}\,\tilde{\phi}(E,\vec{p})\,\left[\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \Delta + \left(\frac{mc}{\hbar}\right)^2\right]\,e^{-\frac{i}{\hbar}(Et-\vec{p}\cdot\vec{x})} \\
&= \int \frac{\mathrm{d}E\,\mathrm{d}^3\vec{p}}{(2\pi\hbar)^4}\,\tilde{\phi}(E,\vec{p})\,\left[-\frac{E^2}{(\hbar c)^2} + \frac{\vec{p}^2 + m^2c^2}{\hbar^2}\right]\,e^{-\frac{i}{\hbar}(Et-\vec{p}\cdot\vec{x})} \\
&= -\frac{1}{(\hbar c)^2}\int \frac{\mathrm{d}E\,\mathrm{d}^3\vec{p}}{(2\pi\hbar)^4}\,\tilde{\phi}(E,\vec{p})\,\left[E^2 - c^2\left(\vec{p}^2 + m^2c^2\right)\right]\,e^{-\frac{i}{\hbar}(Et-\vec{p}\cdot\vec{x})} .
\end{aligned} \tag{7.7}$$

Obviously, this is fulfilled if the energy fulfills the **relativistic energy-momentum relation**

$$E = \pm E_{\vec{p}}\,, \qquad E_{\vec{p}} = c\sqrt{\vec{p}^2 + (mc)^2}\,. \tag{7.8}$$

The fact that there are also solutions of negative energy is not a mathematical curiosity, it bears physical significance and is a hallmark of a relativistic theory. While positive-energy solutions describe **particles**, negative-energy solutions correspond to **antiparticles**. As we did for the Schrödinger equation in Eq. (3.27), we can incorporate the dispersion relation (7.8) into the Ansatz (7.6) by taking the Fourier coefficients as

$$\tilde{\phi}(E,\vec{p}) = 2\pi\hbar\,\delta(E - E_{\vec{p}})\,a^+_{\vec{p}} + 2\pi\hbar\,\delta(E + E_{\vec{p}})\,a^-_{\vec{p}}\,, \tag{7.9}$$

such that the **general solution** of the Klein–Gordon equation (7.4) becomes

$$\phi(\vec{x},t) = \int \frac{\mathrm{d}^3\vec{p}}{(2\pi\hbar)^3}\left[a^+_{\vec{p}}\,e^{-\frac{i}{\hbar}(E_{\vec{p}}t - \vec{p}\cdot\vec{x})} + a^-_{\vec{p}}\,e^{\frac{i}{\hbar}(E_{\vec{p}}t + \vec{p}\cdot\vec{x})}\right]\,. \tag{7.10}$$

Changing the integration variable $\vec{p} \to -\vec{p}$ in the last term yields

$$\phi(\vec{x},t) = \int \frac{\mathrm{d}^3\vec{p}}{(2\pi\hbar)^3}\left[a^+_{\vec{p}}\,e^{-\frac{i}{\hbar}(E_{\vec{p}}t - \vec{p}\cdot\vec{x})} + a^-_{-\vec{p}}\,e^{\frac{i}{\hbar}(E_{\vec{p}}t - \vec{p}\cdot\vec{x})}\right]\,. \tag{7.11}$$

Finally, we need to incorporate the fact that $\phi(\vec{x},t)$ is real-valued, which gives the condition

$$\phi^*(\vec{x},t) = \int \frac{\mathrm{d}^3\vec{p}}{(2\pi\hbar)^3}\left[\left(a^+_{\vec{p}}\right)^*\,e^{\frac{i}{\hbar}(E_{\vec{p}}t - \vec{p}\cdot\vec{x})} + \left(a^-_{-\vec{p}}\right)^*\,e^{-\frac{i}{\hbar}(E_{\vec{p}}t - \vec{p}\cdot\vec{x})}\right] \equiv \phi(\vec{x},t)\,. \tag{7.12}$$

The plane waves constitute a complete and orthogonal set of functions. Therefore, the Fourier coefficients in Eqs. (7.11) and (7.12) have to match,

$$\left(a^+_{\vec{p}}\right)^* = a^-_{-\vec{p}}\,, \qquad \left(a^-_{-\vec{p}}\right)^* = a^+_{\vec{p}}\,. \tag{7.13}$$

Therefore, $a^+_{\vec{p}}$ and $a^-_{\vec{p}}$ are not independent. It suffices to use $a^+_{\vec{p}} \equiv a_{\vec{p}}$ and one can write Eq. (7.11) in the final form

$$\phi(\vec{x},t) = \int \frac{\mathrm{d}^3\vec{p}}{(2\pi\hbar)^3}\left[a_{\vec{p}}\,e^{-\frac{i}{\hbar}(E_{\vec{p}}t - \vec{p}\cdot\vec{x})} + a^*_{\vec{p}}\,e^{\frac{i}{\hbar}(E_{\vec{p}}t - \vec{p}\cdot\vec{x})}\right]\,. \tag{7.14}$$

This is actually the starting point for the second-quantization procedure: one promotes the Fourier coefficients $a_{\vec{p}}$, $a^*_{\vec{p}}$ to annihilation and creation operators $\hat{a}_{\vec{p}}$, $\hat{a}^\dagger_{\vec{p}}$ for particles with momentum $\vec{p}$. This also makes the field operator-valued, $\phi(\vec{x},t) \to \hat{\phi}(\vec{x},t)$. We will not follow this approach further in this lecture series.

Let us also discuss phase and group velocity. For the sake of simplicity we consider a plane wave travelling in x direction, $e^{-\frac{i}{\hbar}(E_{\vec{p}}t - px)}$, where $\vec{p} = (p,0,0)^T$. The space-time points where the phase of the exponential function stays constant are given by $E_{\vec{p}}t - px = \text{const.}$. If we are sitting on a maximum of the wave at $x = t = 0$, i.e., where $E_{\vec{p}}t - px = 0$, this maximum will move with **phase velocity** $v_{\text{phase}}(p) = x/t = E_{\vec{p}}/p$ to the right. While

this velocity is larger than the velocity of light, it is **not** the velocity of a Klein–Gordon particle. The latter is determined from the **group velocity** of a wave packet. Consider a wave packet, which is a superposition of plane waves,

$$\phi(x,t) = \int \frac{\mathrm{d}p}{2\pi\hbar}\, \tilde{\phi}(p)\, e^{-\frac{i}{\hbar}(E_{\vec{p}}t - px)} + \text{c.c.}\,. \tag{7.15}$$

Furthermore, take the momentum spectrum $\tilde{\phi}(p)$ to be sharply peaked around a certain momentum p_0. In this case, we may linearize $E_{\vec{p}}$ around p_0,

$$E_{\vec{p}} = E_{p_0} + (p - p_0) v_{\text{group}}(p_0) + \mathcal{O}((p-p_0)^2)\,, \tag{7.16}$$

where the group velocity was introduced in Eq. (7.2). Inserting this into Eq. (7.15) we obtain

$$\phi(x,t) = e^{-\frac{i}{\hbar}(E_{p_0}t - p_0 x)} \int \frac{\mathrm{d}p}{2\pi\hbar}\, \tilde{\phi}(p)\, e^{\frac{i}{\hbar}(p-p_0)[x - v_{\text{group}}(p_0)t]} + \text{c.c.}\,. \tag{7.17}$$

The integral is the **envelope** of the wave packet. It only depends on the combination $x - v_{\text{group}}(p_0)t$, which means that the peak of the envelope moves with velocity $v_{\text{group}}(p_0)$, which is slower than the velocity of light.

For later use, we compute the **canonically conjugate field**

$$\Pi(\vec{x},t) \equiv c\,\frac{\partial \mathcal{L}}{\partial[\partial_t \phi(\vec{x},t)]} = \frac{1}{c}\frac{\partial \phi(\vec{x},t)}{\partial t}\,. \tag{7.18}$$

This field plays a role analogous to the **canonical momentum** $p \equiv \partial L/\partial \dot{q}$ in classical mechanics. We will also need the **Hamilton density**, which is the **Legendre transform** of the **Lagrangian** with respect to $\partial_t \phi/c$,

$$\begin{aligned}
\mathcal{H}(\phi, \Pi, \vec{\nabla}\phi; \vec{x}, t) &\equiv \Pi \frac{1}{c}\frac{\partial \phi}{\partial t} - \mathcal{L}(\phi, \partial_t\phi, \vec{\nabla}\phi; \vec{x}, t)\Big|_{\Pi = \partial_t\phi/c} \\
&= \Pi^2 - \frac{1}{2}\left[\Pi^2 - (\vec{\nabla}\phi)\cdot(\vec{\nabla}\phi) - \left(\frac{mc}{\hbar}\right)^2 \phi^2\right] \\
&= \frac{1}{2}\left[\Pi^2 + (\vec{\nabla}\phi)\cdot(\vec{\nabla}\phi) + \left(\frac{mc}{\hbar}\right)^2 \phi^2\right]\,.
\end{aligned} \tag{7.19}$$

This is the analogue of the Legendre transform (2.5) in Classical Mechanics.

7.2 The generating functional for correlation functions of the Klein–Gordon field

In this section we derive the quantum field-theoretical analogue of the quantum-mechanical vacuum-to-vacuum transition amplitude, or the generating functional for correlation functions, cf. Eq. (5.47). We will do this at hand of the example of the non-interacting Klein–Gordon field. For the sake of convenience, in this section we will use **natural units**, $\hbar = c = 1$.

In fact, there are only a few obvious changes to be made in comparison to the quantum-mechanical case:

(i) coordinates $\vec{q}(t)$ become **fields** $\phi(\vec{x}, t)$.

(ii) momenta $\vec{p}(t)$ become **canonically conjugate fields** $\Pi(\vec{x}, t) \equiv \partial\mathcal{L}/\partial[\partial_t\phi(t, \vec{x})]$, cf. Eq. (7.18).

(iii) position states $|\vec{q}\rangle$ become field states $|\phi(\vec{x})\rangle$. These are **eigenstates** of the (time-independent) **Schrödinger–picture field operator** $\hat{\phi}(\vec{x})$ at some arbitrary point in time, say $t = 0$,

$$\hat{\phi}(\vec{x})\,|\phi(\vec{x})\rangle = \phi(\vec{x})\,|\phi(\vec{x})\rangle\ . \tag{7.20}$$

Like the position states $|\vec{q}\rangle$, these states are **complete**,

$$\mathbb{1} = \int \prod_{\vec{x}} \mathrm{d}\phi(\vec{x})\,|\phi(\vec{x})\rangle\langle\phi(\vec{x})|\ . \tag{7.21}$$

Here, the integration measure $\prod_{\vec{x}} \mathrm{d}\phi(\vec{x})$ is a symbolic notation. The meaning is the following. We first discretize space as shown in Fig. 7.1. Then we obtain a set of discrete points $\{\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_r, \ldots\}$, which is countable and, in a finite volume $V < \infty$, also finite. Eventually we may take the continuum limit by sending the grid spacing to zero, and finally we may also send the volume $V \to \infty$. However, as long as we stay with a countable, finite set of points, the integration measure is well-defined: we have to integrate at each discrete point $\vec{x}_r$ in space over all values of the field $\phi_r \equiv \phi(\vec{x}_r)$. This gives the integration measure in the completeness relation (7.21). (For the sake of notational convenience, we omitted the index r.) For the sake of simplicity and convenience, we use the symbol $\prod_{\vec{x}} \mathrm{d}\phi(\vec{x})$ also in the continuum limit, i.e., when the grid spacing is sent to zero and, eventually, the spatial volume $V \to \infty$.

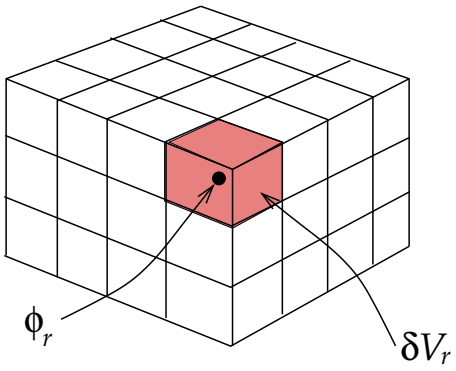


Figure 7.1: Discretization of the spatial volume.

The field states are also **orthonormal**,

$$\langle\phi_a(\vec{x})|\phi_b(\vec{x})\rangle = \prod_{\vec{x}} \delta(\phi_a(\vec{x}) - \phi_b(\vec{x})) \equiv \delta\left[\phi_a - \phi_b\right]\ . \tag{7.22}$$

The delta function with argument in brackets is a **functional** delta function, i.e., the functions $\phi_a(\vec{x})$ and $\phi_b(\vec{x})$ must be identical at **all** points $\vec{x}$.

(iv) momentum states $|\vec{p}\rangle$ become canonically conjugate-field states $|\Pi(\vec{x})\rangle$, which are **eigenstates** of the **Schrödinger–picture field operator** $\hat{\Pi}(\vec{x})$ at time $t = 0$,

$$\hat{\Pi}(\vec{x})\,|\Pi(\vec{x})\rangle = \Pi(\vec{x})\,|\Pi(\vec{x})\rangle\ . \tag{7.23}$$

Also these states are **complete**,

$$\mathbb{1} = \int \prod_{\vec{x}} \frac{\mathrm{d}\Pi(\vec{x})}{2\pi}\,|\Pi(\vec{x})\rangle\langle\Pi(\vec{x})|\ , \tag{7.24}$$

and **orthonormal**,

$$\langle\Pi_a(\vec{x})|\Pi_b(\vec{x})\rangle = \prod_{\vec{x}} \delta(\Pi_a(\vec{x}) - \Pi_b(\vec{x})) \equiv \delta\left[\Pi_a - \Pi_b\right]\ . \tag{7.25}$$

The factor 2π in the denominator of the integration measure in Eq. (7.24) is purely conventional.

(v) The generalization of the quantum-mechanical overlap (3.9) is

$$\langle\phi(\vec{x})|\Pi(\vec{x})\rangle = \prod_{\vec{x}} \exp\left[i\mathrm{d}^3\vec{x}\,\Pi(\vec{x})\phi(\vec{x})\right] = \exp\left[i\int \mathrm{d}^3\vec{x}\,\Pi(\vec{x})\phi(\vec{x})\right]\ . \tag{7.26}$$

We now evolve the Schrödinger–picture state $|\phi(\vec{x})\rangle$ from time $t = 0$ to some later time t. In analogy to Eq. (2.10) we obtain

$$\hat{U}(0,t)\,|\phi(\vec{x})\rangle = |\phi(\vec{x}),t\rangle \equiv |\phi(\vec{x},t)\rangle\ . \tag{7.27}$$

As was the case for the time-evolved position states $|\vec{q},t\rangle$, also these time-evolved states are complete,

$$\begin{aligned}
\mathbb{1} &= \hat{U}(0,t_j)\,\hat{U}(t_j,0) = \hat{U}(0,t_j)\int \prod_{\vec{x}} \mathrm{d}\phi_j(\vec{x})\,|\phi_j(\vec{x})\rangle\langle\phi_j(\vec{x})|\,\hat{U}(t_j,0) \\
&= \int \prod_{\vec{x}} \mathrm{d}\phi_j(\vec{x})\,\hat{U}(0,t_j)\,|\phi_j(\vec{x})\rangle\langle\phi_j(\vec{x})|\,\hat{U}(t_j,0) \\
&= \int \prod_{\vec{x}} \mathrm{d}\phi_j(\vec{x})\,|\phi_j(\vec{x}),t_j\rangle\langle\phi_j(\vec{x}),t_j| \equiv \int \prod_{\vec{x}} \mathrm{d}\phi_j(\vec{x})\,|\phi_j(\vec{x},t_j)\rangle\langle\phi_j(\vec{x},t_j)|\ .
\end{aligned} \tag{7.28}$$

We now consider the quantum field-theoretical transition amplitude

$$\langle\phi_f(\vec{x}),t_f|\phi_i(\vec{x}),t_i\rangle \equiv \langle\phi_f(\vec{x},t_f)|\phi_i(\vec{x},t_i)\rangle\ , \tag{7.29}$$

and again partition the time interval $[t_i, t_f]$ into N pieces of equal length τ. We then insert $N-1$ complete sets (7.28) of field states, one each for the times $t_j = t_i + j\tau$, $j = 1,\ldots,N-1$,

$$\begin{aligned}
\langle\phi_f(\vec{x},t_f)|\phi_i(\vec{x},t_i)\rangle = \int \prod_{j=1}^{N-1}\prod_{\vec{x}} \mathrm{d}\phi_j(\vec{x})\,\langle\phi_f(\vec{x},t_f)|\phi_{N-1}(\vec{x},t_{N-1})\rangle \\
\times\,\langle\phi_{N-1}(\vec{x},t_{N-1})|\phi_{N-2}(\vec{x},t_{N-2})\rangle\cdots\langle\phi_1(\vec{x},t_1)|\phi_i(\vec{x},t_i)\rangle
\end{aligned} \tag{7.30}$$

Now we consider the factor

$$\begin{aligned}\langle\phi_{j+1}(\vec{x},t_{j+1})|\phi_j(\vec{x},t_j)\rangle &= \langle\phi_{j+1}(\vec{x})|\,\hat{U}(t_{j+1},0)\,\hat{U}(0,t_j)\,|\phi_j(\vec{x})\rangle \\ &= \langle\phi_{j+1}(\vec{x})|\,\hat{U}(t_{j+1},t_j)\,|\phi_j(\vec{x})\rangle\ . \end{aligned} \tag{7.31}$$

Here,

$$\hat{U}(t_{j+1},t_j) = \hat{T}\,\exp\left[-i\int_{t_j}^{t_{j+1}}\mathrm{d}t\,\hat{H}(t)\right] \equiv \hat{T}\,\exp\left[-i\int_{t_j}^{t_{j+1}}\mathrm{d}t\int_V \mathrm{d}^3\vec{x}\,\hat{\mathcal{H}}(\vec{x},t)\right] \tag{7.32}$$

is the time-evolution operator for the quantum field-theoretical system, cf. Eq. (2.9) for the quantum-mechanical analogue, with the **Hamilton–density operator** $\hat{\mathcal{H}}(\vec{x},t)$. The latter operator depends on field operators and canonically conjugate field operators (and potentially also explicitly on space and time),

$$\hat{\mathcal{H}}(\vec{x},t) \equiv \mathcal{H}(\hat{\phi}(\vec{x}),\hat{\Pi}(\vec{x}),\vec{\nabla}\hat{\phi}(\vec{x});\vec{x},t)\ . \tag{7.33}$$

In order to get rid of the dependence on operator-valued quantities, it is convenient to also insert complete sets (7.24) of canonically conjugate field states. Analogous steps which have lead to Eq. (3.10) then yield

$$\begin{aligned}\langle\phi_f(\vec{x},t_f)|\phi_i(\vec{x},t_i)\rangle &= \int\left[\prod_{j=1}^{N-1}\prod_{\vec{x}}\mathrm{d}\phi_j(\vec{x})\right]\left[\prod_{j=1}^{N}\prod_{\vec{x}}\frac{\mathrm{d}\Pi_j(\vec{x})}{2\pi}\right] \\ &\times\exp\left\{i\sum_{j=1}^{N}\tau\int_V\mathrm{d}^3\vec{x}\left[\Pi_j(\vec{x})\frac{\phi_j(\vec{x})-\phi_{j-1}(\vec{x})}{\tau}-\mathcal{H}(\phi_j(\vec{x}),\Pi_j(\vec{x}),\vec{\nabla}\phi_j(\vec{x});\vec{x},t_j)\right]\right\}\ . \end{aligned} \tag{7.34}$$

We now denote $\phi_j(\vec{x}) \equiv \phi(\vec{x},t_j)$, $\Pi_j(\vec{x}) \equiv \Pi(\vec{x},t_j)$. In the limit $N\to\infty$, $\tau\to 0$ we then obtain the final result

$$\begin{aligned}&\langle\phi_f(\vec{x},t_f)|\phi_i(\vec{x},t_i)\rangle \\ &= \int\mathcal{D}\phi(\vec{x},t)\,\mathcal{D}\Pi(\vec{x},t)\,\exp\left\{i\int_{t_i}^{t_f}\mathrm{d}t\int_V\mathrm{d}^3\vec{x}\left[\Pi(\vec{x},t)\,\partial_t\phi(\vec{x},t)-\mathcal{H}(\phi,\Pi,\vec{\nabla}\phi;\vec{x},t)\right]\right\}\ . \end{aligned} \tag{7.35}$$

For the Klein–Gordon field, we have $\Pi = \partial\mathcal{L}/\partial(\partial_t\phi) \equiv \partial_t\phi$. The Hamilton density for the Klein–Gordon field was already calculated in Eq. (7.19). In natural units,

$$\mathcal{H}(\phi,\Pi,\vec{\nabla}\phi) = \frac{1}{2}\left[\Pi^2+(\vec{\nabla}\phi)\cdot(\vec{\nabla}\phi)+m^2\phi^2\right]\ . \tag{7.36}$$

Therefore,

$$\Pi\partial_t\phi-\mathcal{H} = -\frac{1}{2}\left(\Pi-\partial_t\phi\right)^2+\frac{1}{2}\left[(\partial_t\phi)^2-(\vec{\nabla}\phi)\cdot(\vec{\nabla}\phi)-m^2\phi^2\right] = -\frac{1}{2}\left(\Pi-\partial_t\phi\right)^2+\mathcal{L}\ . \tag{7.37}$$

The functional integral over the canonically conjugate fields in Eq. (7.35) is now simply a shifted Gaussian integral and can be immediately performed. The result is a normalization constant, such that Eq. (7.35) reads

$$\langle \phi_f(\vec{x},t_f)|\phi_i(\vec{x},t_i)\rangle = \mathcal{N}\int \mathcal{D}\phi(\vec{x},t)\,\exp\left[i\int_{t_i}^{t_f}\mathrm{d}t\int_V \mathrm{d}^3\vec{x}\,\mathcal{L}(\phi,\partial_t\phi,\vec{\nabla}\phi;\vec{x},t)\right]\,. \tag{7.38}$$

The very same considerations which have lead to Eq. (5.47) now allow to derive the **generating functional for n–point correlation functions** for the Klein–Gordon field,

$$\begin{aligned} Z[J] &= \int \mathcal{D}\phi(\vec{x},t)\,\exp\left\{i\int_{-\infty}^{\infty}\mathrm{d}t\int \mathrm{d}^3\vec{x}\,\left[\mathcal{L}(\phi,\partial_t\phi,\vec{\nabla}\phi;\vec{x},t)+J(\vec{x},t)\phi(\vec{x},t)\right]\right\} \\ &\sim \langle 0;+\infty|0;-\infty\rangle^J\,. \end{aligned} \tag{7.39}$$

7.3 The generating functional of the non-interacting Klein–Gordon field

For the non-interacting Klein–Gordon field, the Lagrangian in the exponent in Eq. (7.39) is just that of Eq. (7.1). Apparently, this is quadratic in the field, so Eq. (7.39) is in essence a shifted Gaussian integral, which can be computed exactly. This calculation will be elaborated on in this section.

We first insert Eq. (7.1) into Eq. (7.39),

$$Z[J]=\int\mathcal{D}\phi\,\exp\left(i\int_{-\infty}^{\infty}\mathrm{d}t\int\mathrm{d}^3\vec{x}\,\left\{\frac{1}{2}\left[(\partial_t\phi)^2-(\vec{\nabla}\phi)\cdot(\vec{\nabla}\phi)-m^2\phi^2\right]+J\phi\right\}\right)\,, \tag{7.40}$$

and integrate the partial derivatives by parts,

$$\int_{-\infty}^{\infty}\mathrm{d}t\int\mathrm{d}^3\vec{x}\,\left[(\partial_t\phi)^2-(\vec{\nabla}\phi)\cdot(\vec{\nabla}\phi)\right]=-\int_{-\infty}^{\infty}\mathrm{d}t\int\mathrm{d}^3\vec{x}\,\phi\,\Box\phi\quad+\quad\text{surface terms}\,.$$

The surface terms vanish if we assume that the field vanishes at infinity. This then yields

$$Z[J]=\int\mathcal{D}\phi\,\exp\left\{-i\int\mathrm{d}^4X\,\left[\frac{1}{2}\,\phi\left(\Box+m^2\right)\phi-J\phi\right]\right\}\,, \tag{7.41}$$

where we have abbreviated the integration measure $\mathrm{d}^4X\equiv\mathrm{d}t\mathrm{d}^3\vec{x}$. As already mentioned, this is a shifted Gaussian integral and has an analytic solution in closed form.

There is a very useful generalization of Eq. (4.43) for the case of shifted Gaussian integrals. Let A be a symmetric, positive definite, non-singular $(N\times N)$ matrix and let $\vec{r}$, $\vec{b}$ be N dimensional vectors. Then

$$\int\mathrm{d}^N\vec{r}\,\exp\left(-\frac{1}{2}\,\vec{r}^{\,T}\mathrm{A}\,\vec{r}+\vec{b}^{\,T}\vec{r}\right)=(2\pi)^{N/2}(\mathrm{detA})^{-1/2}\,\exp\left(\frac{1}{2}\,\vec{b}^{\,T}\mathrm{A}^{-1}\vec{b}\right)\,. \tag{7.42}$$

Here we have used a compact notation, i.e., $\vec{r}^{\,T}\mathrm{A}\,\vec{r}=\sum_{i,j=1}^{N}r_i\,\mathrm{A}_{ij}\,r_j$ and $\vec{b}^{\,T}\vec{r}=\sum_{i=1}^{N}b_i\,r_i$. We now apply Eq. (7.42) to Eq. (7.41). We have to note that we should first discretize

space-time to obtain a finite, countable set of space-time points X_i, $i = 1, \ldots, N$, The integration variables $\phi_i \equiv \phi(X_i)$ at these space-time points then correspond to the components of the vector $\vec{r}$ in Eq. (7.42). At the end of the calculation we perform the continuum limit by sending the grid spacing (in space and time) to zero and the space-time volume to infinity.

Another point that one has to note is that the argument of the exponential function in Eq. (7.41) is purely **imaginary**. Although we know that Gaussian integrals also converge for complex-valued integrands, it is not immediately obvious that we can identify a matrix A with the properties necessary to apply Eq. (7.42). This problem will be solved by **analytically continuing** the real-valued time variable t to imaginary time.

We first insert a spurious four-dimensional delta function

$$\delta^{(4)}(X - Y) \equiv \delta(t_x - t_y)\delta^{(3)}(\vec{x} - \vec{y})$$

into the integrand in the argument of the exponential function in Eq. (7.41),

$$\begin{aligned} Z_0[J] &= \int \mathcal{D}\phi(X)\, \exp\left[-\frac{i}{2}\int \mathrm{d}^4X\, \mathrm{d}^4Y\, \phi(X)\left(\Box_x + m^2\right)\, \delta^{(4)}(X-Y)\, \phi(Y)\right. \\ &\qquad \left. + i\int \mathrm{d}^4X\, J(X)\phi(X)\right] \qquad (7.43) \\ &\equiv \int \mathcal{D}\phi(X)\, \exp\left[\frac{1}{2}\int \mathrm{d}^4X\, \mathrm{d}^4Y\, \phi(X)\, A(X,Y)\, \phi(Y) + i\int \mathrm{d}^4X\, J(X)\phi(X)\right]\,, \end{aligned}$$

with

$$A(X,Y) \equiv -i\left(\Box_x + m^2\right)\, \delta^{(4)}(X-Y)\,. \qquad (7.44)$$

Now we introduce the **imaginary time variable** τ, by **analytic continuation** of the real-valued time t,

$$t \longrightarrow -i\tau\,, \quad it \longrightarrow \tau\,. \qquad (7.45)$$

It is advantageous to collect this imaginary time variable together with the spatial position vector $\vec{x}$ into a four-dimensional vector

$$\bar{X} \equiv (\bar{X}_\mu) = (\tau, \vec{x})\,. \qquad (7.46)$$

The infinitesimal space-time volume element becomes

$$i\,\mathrm{d}^4X = i\,\mathrm{d}t\,\mathrm{d}^3\vec{x} \quad \longrightarrow \quad \mathrm{d}\tau\,\mathrm{d}^3\vec{x} = \mathrm{d}^4\bar{X}\,, \qquad (7.47)$$

from which follows

$$\mathrm{d}^4X\,\mathrm{d}^4Y \quad \longrightarrow \quad -\mathrm{d}^4\bar{X}\,\mathrm{d}^4\bar{Y}\,. \qquad (7.48)$$

The four-dimensional gradient operator with respect to the coordinates $\bar{X}_\mu$ reads

$$\left(\frac{\partial}{\partial \bar{X}_\mu}\right) = \left(\frac{\partial}{\partial\tau}, \vec{\nabla}\right)\,. \qquad (7.49)$$

The analytic continuation of the d'Alembert operator is therefore

$$\Box_x = \frac{\partial^2}{\partial t^2} - \Delta_x \quad \longrightarrow \quad -\frac{\partial^2}{\partial\tau^2} - \Delta_x \equiv -\overline{\Box}_x\,. \qquad (7.50)$$

The analytic continuation of the delta function in time is

$$\begin{aligned} -i\,\delta(t_x - t_y) &= -i\int \frac{\mathrm{d}k_0}{2\pi}\, e^{-ik_0(t_x-t_y)} = \int \frac{\mathrm{d}(-ik_0)}{2\pi}\, e^{-i(-ik_0)(it_x-it_y)} \\ &\longrightarrow \int \frac{\mathrm{d}\kappa}{2\pi}\, e^{-i\kappa(\tau_x-\tau_y)} \equiv \delta(\tau_x - \tau_y)\,. \end{aligned} \tag{7.51}$$

Here we have also analytically continued the energy variable k_0,

$$k_0 \longrightarrow i\kappa\,, \quad -ik_0 \longrightarrow \kappa\,. \tag{7.52}$$

Note that the analytic continuation of the energy requires the opposite sign as that of the time, cf. Eq. (7.45). From Eq. (7.51) now follows

$$-\,i\,\delta^{(4)}(X-Y) \longrightarrow \delta^{(4)}(\bar{X}-\bar{Y})\,. \tag{7.53}$$

Now we can also analytically continue the matrix (7.44). With Eqs. (7.50) and (7.51) this reads

$$A(X,Y) \longrightarrow A(\bar{X},\bar{Y}) = (-\bar{\Box}_x + m^2)\,\delta^{(4)}(\bar{X}-\bar{Y}) = \int \frac{\mathrm{d}^4\bar{K}}{(2\pi)^4}\, e^{-i\bar{K}\cdot(\bar{X}-\bar{Y})}\,(\bar{K}^2 + m^2)\,. \tag{7.54}$$

Here we have introduced the four-dimensional momentum vector

$$(\bar{K}_\mu) = (\kappa, \vec{k})\,, \tag{7.55}$$

with the energy variable κ from Eq. (7.52), the short notation $\bar{K}^2 \equiv \bar{K}\cdot\bar{K} = \kappa^2 + \vec{k}^{\,2}$, and the scalar product

$$\bar{K}\cdot\bar{X} = \kappa\tau_x + \vec{k}\cdot\vec{x}\,, \tag{7.56}$$

and used the Fourier representation of the four-dimensional delta function

$$\delta^{(4)}(\bar{X}-\bar{Y}) = \int \frac{\mathrm{d}^4\bar{K}}{(2\pi)^4}\, e^{-i\bar{K}\cdot(\bar{X}-\bar{Y})} = \int \frac{\mathrm{d}\kappa\,\mathrm{d}^3\vec{k}}{(2\pi)^4}\, e^{-i\kappa(\tau_x-\tau_y) - i\,\vec{k}\cdot(\vec{x}-\vec{y})}\,. \tag{7.57}$$

Since $\kappa \in \mathbb{R}$, we have $\bar{K}^2 = \kappa^2 + \vec{k}^{\,2} \geq 0$ and the Fourier transform of the matrix $A(\bar{X},\bar{Y})$ is **positive definite**, $\tilde{A}(\bar{K}) = \bar{K}^2 + m^2 > 0$ (for $m > 0$). Therefore $A(\bar{X},\bar{Y})$ is also positive definite. Furthermore, $A(\bar{X},\bar{Y})$ is **symmetric**, $A(\bar{X},\bar{Y}) = A(\bar{Y},\bar{X})$, as one immediately observes from Eq. (7.54) (substitute $\bar{K}_\mu \to -\bar{K}_\mu$). Finally, $A(\bar{X},\bar{Y})$ is **non-singular** (at least in discretized space-time, where $\delta^{(4)}(\bar{X}-\bar{Y}) \to a^{-4}\delta^{(4)}_{\bar{X},\bar{Y}}$, with the grid spacing a and the four-dimensional Kronecker delta). Therefore, all requirements are fulfilled to apply Eq. (7.42). With the identification

$$r_i \longrightarrow \phi(\bar{X})\,, \quad \mathrm{A}_{ij} \longrightarrow A(\bar{X},\bar{Y})\,, \quad b_i \longrightarrow J(\bar{X})\,, \tag{7.58}$$

and using Eqs. (7.47) and (7.48), Eq. (7.43) becomes

$$\begin{aligned} Z[J] &= \int \mathcal{D}\phi(\bar{X})\, \exp\left[-\frac{1}{2}\int \mathrm{d}^4\bar{X}\,\mathrm{d}^4\bar{Y}\,\phi(\bar{X})\,A(\bar{X},\bar{Y})\,\phi(\bar{Y}) + \int \mathrm{d}^4\bar{X}\,J(\bar{X})\phi(\bar{X})\right] \\ &= \mathcal{N}(\mathrm{detA})^{-1/2}\,\exp\left[\frac{1}{2}\int \mathrm{d}^4\bar{X}\,\mathrm{d}^4\bar{Y}\,J(\bar{X})\,A^{-1}(\bar{X},\bar{Y})\,J(\bar{Y})\right]\,. \end{aligned} \tag{7.59}$$

We now determine $A^{-1}(\bar{X},\bar{Y})$. With Eq. (7.54) it holds that

$$\begin{aligned}\delta^{(4)}(\bar{X}-\bar{Z}) &= \int \mathrm{d}^4\bar{Y}\, A(\bar{X},\bar{Y})\, A^{-1}(\bar{Y},\bar{Z}) \\ &= \int \mathrm{d}^4\bar{Y}\, (-\overline{\Box}_x + m^2)\, \delta^{(4)}(\bar{X}-\bar{Y})\, A^{-1}(\bar{Y},\bar{Z}) \\ &= (-\overline{\Box}_x + m^2)\, A^{-1}(\bar{X},\bar{Z})\ , \end{aligned} \tag{7.60}$$

i.e., $A^{-1}(\bar{X},\bar{Z})$ is the **Green's function** of the non-interacting Klein–Gordon equation (in imaginary time)!

The Fourier transform of $A^{-1}(\bar{X},\bar{Z})$ reads

$$A^{-1}(\bar{X},\bar{Z}) = \int \frac{\mathrm{d}^4\bar{K}\,\mathrm{d}^4\bar{Q}}{(2\pi)^8}\, e^{-i\bar{K}\cdot\bar{X}}\, \tilde{A}^{-1}(\bar{K},\bar{Q})\, e^{i\bar{Q}\cdot\bar{Z}}\ . \tag{7.61}$$

Note that we employed the Fourier transformation with respect to the second argument with the opposite sign in the argument of the exponential function. This is pure convention; also the usual choice of sign works, but would lead to respective changes of signs in the following. If we insert Eq. (7.61) into Eq. (7.60) we obtain

$$\int \frac{\mathrm{d}^4\bar{K}\,\mathrm{d}^4\bar{Q}}{(2\pi)^8}\, e^{-i\bar{K}\cdot\bar{X}}\, (\bar{K}^2+m^2)\, \tilde{A}^{-1}(\bar{K},\bar{Q})\, e^{i\bar{Q}\cdot\bar{Z}} = \int \frac{\mathrm{d}^4\bar{Q}}{(2\pi)^4}\, e^{-i\bar{Q}\cdot(\bar{X}-\bar{Z})}\ . \tag{7.62}$$

This equation is fulfilled if

$$\tilde{A}^{-1}(\bar{K},\bar{Q}) = (2\pi)^4\, \delta^{(4)}(\bar{K}-\bar{Q})\, \frac{1}{\bar{K}^2+m^2}\ . \tag{7.63}$$

If we insert this into Eq. (7.61) we obtain

$$A^{-1}(\bar{X},\bar{Z}) = \int \frac{\mathrm{d}^4\bar{K}}{(2\pi)^4}\, e^{-i\bar{K}\cdot(\bar{X}-\bar{Z})}\, \frac{1}{\bar{K}^2+m^2}\ . \tag{7.64}$$

Now we can revert the analytic continuation. With Eqs. (7.45) and (7.52), the abbreviation $\mathrm{d}^4K = \mathrm{d}k_0\mathrm{d}^3\vec{k}$, as well as $\bar{K}^2 = \kappa^2 + \vec{k}^{\,2} \longrightarrow -k_0^2 + \vec{k}^{\,2}$ we obtain

$$\begin{aligned} A^{-1}(\bar{X},\bar{Y}) \longrightarrow A^{-1}(X,Y) &= -i \int \frac{\mathrm{d}^4K}{(2\pi)^4}\, e^{-i(-ik_0)(it_x-it_y)-i\vec{k}\cdot(\vec{x}-\vec{y})}\, \frac{1}{-k_0^2+\vec{k}^{\,2}+m^2} \\ &= i \int \frac{\mathrm{d}^4K}{(2\pi)^4}\, e^{-i[k_0(t_x-t_y)+\vec{k}\cdot(\vec{x}-\vec{y})]}\, \frac{1}{k_0^2-E_{\vec{k}}^2} \\ &\equiv i\,\Delta(X-Y)\ . \end{aligned} \tag{7.65}$$

Using Eqs. (7.44) and (7.65), the thus defined $A^{-1}(X,Y)$ fulfills

$$\begin{aligned} &\int \mathrm{d}^4Y A(X,Y)A^{-1}(Y,Z) = \\ &= \int \mathrm{d}^4Y(-i)\left(\Box_x+m^2\right)\delta^{(4)}(X-Y)\int \frac{\mathrm{d}^4K}{(2\pi)^4}\, e^{-i[k_0(t_y-t_z)+\vec{k}\cdot(\vec{y}-\vec{z})]}\, \frac{1}{k_0^2-E_{\vec{k}}^2} \\ &= \left(\Box_x+m^2\right)\int \frac{\mathrm{d}^4K}{(2\pi)^4}\, e^{-i[k_0(t_x-t_z)+\vec{k}\cdot(\vec{x}-\vec{z})]}\, \frac{1}{k_0^2-E_{\vec{k}}^2} \equiv -\delta^{(4)}(X-Z)\ , \end{aligned} \tag{7.66}$$

i.e., it has the opposite sign compared to the corresponding relation (7.60) in imaginary time.

The generating functional (7.59) reads with Eq. (7.65)

$$Z[J] = \mathcal{N}'(\det\Delta)^{1/2} \exp\left[-\frac{i}{2}\int \mathrm{d}^4X\, \mathrm{d}^4Y\, J(X)\,\Delta(X-Y)\,J(Y)\right] , \tag{7.67}$$

where we again Eq. (7.48) and absorbed factors of i in the normalization constant (therefore now denoted with $\mathcal{N}'$).

Lecture 9

We had seen that $A^{-1}(X,Y) \equiv i\,\Delta(X-Y)$ is the Green's function of the non-interacting Klein–Gordon equation. The Fourier transform

$$\tilde{\Delta}(k_0,\vec{k}) = \frac{1}{k_0^2 - E_{\vec{k}}^2} \tag{7.68}$$

of the Green's function $\Delta(X-Y)$ has poles on the real k_0 axis at

$$k_0 = \pm\sqrt{\vec{k}^{\,2} + m^2} = \pm E_{\vec{k}} . \tag{7.69}$$

As usual for any Green's function, one needs to give a prescription how to circumvent these poles in the complex k_0 plane, cf. the discussion of the causal propagator (5.22). We choose the so-called **Feynman prescription**:

$$\tilde{\Delta}_F(k_0,\vec{k}) = \frac{1}{k_0^2 - E_{\vec{k}}^2 + i\eta} . \tag{7.70}$$

The poles will then be shifted into the complex k_0 plane, such that integrals along the real k_0 axis are well-defined. The poles are now at

$$k_0^2 = E_{\vec{k}}^2 - i\eta \implies k_0 = \pm\sqrt{E_{\vec{k}}^2 - i\eta} \simeq \pm E_{\vec{k}} \mp i\,\frac{\eta}{2E_{\vec{k}}} \equiv \pm E_{\vec{k}} \mp i\delta , \tag{7.71}$$

cf. Fig. 7.2.

We had clarified in Sec. 5.4 that Green's function are (up to constant factors) identical with **propagators**. Thus,

$$\Delta_F(X-Y) = \int \frac{\mathrm{d}^4K}{(2\pi)^4}\, e^{-i[k_0(t_x-t_y)+\vec{k}\cdot(\vec{x}-\vec{y})]}\, \frac{1}{k_0^2 - E_{\vec{k}}^2 + i\eta} \tag{7.72}$$

is called the **Feynman propagator** for the non-interacting Klein–Gordon field.

We now compute correlation functions from the generating functional (7.67). First we choose the normalization constant $\mathcal{N}'$ such that

$$Z[0] = 1 , \tag{7.73}$$

i.e.,

$$Z[J] = \exp\left[-\frac{i}{2}\int \mathrm{d}^4X\, \mathrm{d}^4Y\, J(X)\,\Delta_F(X-Y)\,J(Y)\right] . \tag{7.74}$$

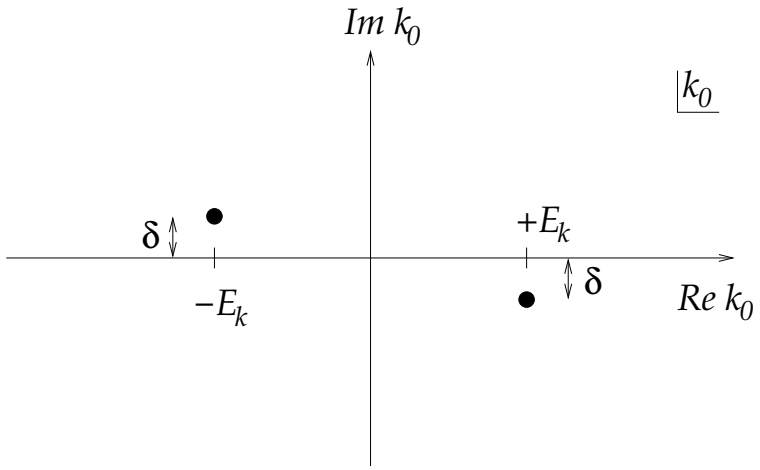


Figure 7.2: Feynman prescription for the shift of the poles into the complex k_0 plane.

On the other hand, from Eq. (7.39) follows that

$$Z[J] \sim \langle 0; +\infty | 0; -\infty \rangle^J \ . \tag{7.75}$$

We now show that the choice (7.73) implies that

$$Z[J] \equiv \langle 0; +\infty | 0; -\infty \rangle^J \ . \tag{7.76}$$

First, because of Eq. (7.75) we obviously have

$$Z[J] = \mathcal{N} \langle 0; +\infty | 0; -\infty \rangle^J \ , \tag{7.77}$$

with a yet to be determined normalization constant $\mathcal{N}$. In absence of external sources, $J(X) = 0$, this equation reads

$$Z[0] = \mathcal{N} \langle 0; +\infty | 0; -\infty \rangle \ . \tag{7.78}$$

But without external sources and without interactions nothing happens and the incoming vacuum is identical with the outgoing vacuum,

$$|0; -\infty\rangle \equiv |0; +\infty\rangle \equiv |0\rangle \implies \langle 0; +\infty | 0; -\infty \rangle \equiv \langle 0 | 0 \rangle = 1 \ , \tag{7.79}$$

i.e.,

$$Z[0] = \mathcal{N} \ . \tag{7.80}$$

But we had agreed upon that $Z[0] = 1$, cf. Eq. (7.73), therefore $\mathcal{N} \equiv 1$. This proves Eq. (7.76), q.e.d.

According to Eq. (5.67) the **one-point correlation function**

$$\begin{aligned}
\langle 0;+\infty|\,\hat{\phi}(X)\,|0;-\infty\rangle &= -i\,\frac{\delta Z[J]}{\delta J(X)}\bigg|_{J=0} = -i\,\frac{\delta}{\delta J(X)}\,e^{-(i/2)\int \mathrm{d}^4U\,\mathrm{d}^4V\,J(U)\,\Delta_F(U-V)\,J(V)}\bigg|_{J=0} \\
&= -i\left[-\frac{i}{2}\int \mathrm{d}^4U\,\mathrm{d}^4V\,\frac{\delta J(U)}{\delta J(X)}\,\Delta_F(U-V)\,J(V)\right. \\
&\qquad \left. -\frac{i}{2}\int \mathrm{d}^4U\,\mathrm{d}^4V\,J(U)\,\Delta_F(U-V)\,\frac{\delta J(V)}{\delta J(X)}\right] Z[J]\bigg|_{J=0} \\
&= -i\left[-\frac{i}{2}\int \mathrm{d}^4V\,\Delta_F(X-V)\,J(V) - \frac{i}{2}\int \mathrm{d}^4U\,J(U)\,\Delta_F(U-X)\right] Z[J]\bigg|_{J=0} \\
&= (-i)^2\int \mathrm{d}^4V\,\Delta_F(X-V)\,J(V)\,Z[J]\bigg|_{J=0} \\
&= 0\,. \qquad (7.81)
\end{aligned}$$

Here we have made use of the four-dimensional generalization of Eq. (5.53),

$$\frac{\delta J(U)}{\delta J(X)} = \delta^{(4)}(U-X)\,, \qquad (7.82)$$

and we employed the symmetry of the Feynman propagator, $\Delta_F(X-Y) \equiv \Delta_F(Y-X)$.

The **two-point correlation function** reads according to Eq. (5.67)

$$\begin{aligned}
\langle 0;+\infty|\,\hat{T}\left[\hat{\phi}(X)\,\hat{\phi}(Y)\right]\,|0;-\infty\rangle &= (-i)^2\,\frac{\delta^2 Z[J]}{\delta J(X)\,\delta J(Y)}\bigg|_{J=0} \\
&= -i\,\frac{\delta}{\delta J(X)}\,(-i)^2\int \mathrm{d}^4V\,\Delta_F(Y-V)\,J(V)\,Z[J]\bigg|_{J=0} \\
&= (-i)^3\left[\Delta_F(Y-X) - i\int \mathrm{d}^4V\,\Delta_F(Y-V)\,J(V)\int \mathrm{d}^4U\,\Delta_F(X-U)\,J(U)\right] Z[J]\bigg|_{J=0} \\
&= i\,\Delta_F(X-Y) \qquad = \qquad Y \bullet\!\!-\!\!-\!\!-\!\!-\!\!-\!\!-\!\!-\!\!-\!\!-\!\!-\!\!\bullet X \qquad , \qquad (7.83)
\end{aligned}$$

where from the first to the second and from the second to the third line we made use of the intermediate result in the next-to-last line in Eq. (7.81). We also repeatedly employed the symmetry of the Feynman propagator. Apparently, the **two-point correlation function** is **identical** with the **Green's function** of the non-interacting Klein–Gordon equation, and (up to a factor of i) also identical with the **Feynman propagator**!

7.4 Interacting field theory: $\lambda\phi^4$ theory in perturbation theory

We now add a **local four-point interaction** to the Lagrangian of the Klein–Gordon field, Eq. (7.1), i.e., a term which is **proportional to the fourth power of the field**

$\phi(\vec{x},t)$,

$$\begin{aligned}\mathcal{L} &= \mathcal{L}_0 + \mathcal{L}_{\rm int}\ ,\\ \mathcal{L}_0 &= \frac{1}{2}\left[(\partial_t\phi)^2 - (\vec{\nabla}\phi)\cdot(\vec{\nabla}\phi) - m^2\phi^2\right]\ ,\\ \mathcal{L}_{\rm int} &= -\frac{\lambda}{4!}\,\phi^4\ .\end{aligned} \tag{7.84}$$

Here, λ is the **coupling constant** which determines the **strength** with which the field ϕ interacts with itself. The 4! in the denominator is purely conventional and simplifies the following expressions. Note that this theory looks rather similar to the anharmonic oscillator discussed in Sec. 4.5.

How does the generating functional for n–point correlation functions look like? Per definition, cf. Eq. (7.39), we would immediately write

$$Z[J] = \mathcal{N}\int\mathcal{D}\phi\,\exp\left\{iS[\phi] + i\int \mathrm{d}^4X\,J(X)\phi(X)\right\}\ , \tag{7.85}$$

with the classical action

$$S[\phi] = \int \mathrm{d}^4X\,\mathcal{L}\ . \tag{7.86}$$

$J(X)$ is the source term and the normalization constant $\mathcal{N}$ is chosen such that

$$Z[0] = 1\ , \tag{7.87}$$

i.e.,

$$\mathcal{N}^{-1} = \int\mathcal{D}\phi\,\exp\left\{iS[\phi]\right\}\ . \tag{7.88}$$

Using the classical action of the **non-interacting** Klein–Gordon field

$$S_0[\phi] = \int \mathrm{d}^4X\,\mathcal{L}_0\ , \tag{7.89}$$

we can **factorize** the part of the action which contains the **interaction term** in the generating functional (7.85),

$$Z[J] = \mathcal{N}\int\mathcal{D}\phi\,\exp\left[i\int \mathrm{d}^4X\,\mathcal{L}_{\rm int}(\phi)\right]\,\exp\left\{iS_0[\phi] + i\int \mathrm{d}^4X\,J(X)\phi(X)\right\}\ . \tag{7.90}$$

The first exponential function has the Taylor–series expansion

$$\exp\left[i\int \mathrm{d}^4X\,\mathcal{L}_{\rm int}(\phi)\right] = \sum_{n=0}^{\infty}\frac{i^n}{n!}\left[\int \mathrm{d}^4X\,\mathcal{L}_{\rm int}(\phi)\right]^n = \sum_{n=0}^{\infty}\frac{i^n}{n!}\left[-\frac{\lambda}{4!}\int \mathrm{d}^4X\,\phi^4(X)\right]^n\ , \tag{7.91}$$

where we have used Eq. (7.84). If we insert this into Eq. (7.90) we obtain

$$\begin{aligned}Z[J] &= \mathcal{N}\int\mathcal{D}\phi\,\sum_{n=0}^{\infty}\frac{(-i\lambda)^n}{(4!)^n n!}\left[\int \mathrm{d}^4X\,\phi^4(X)\right]^n e^{iS_0[\phi]+i\int \mathrm{d}^4X\,J(X)\phi(X)} \qquad (7.92)\\ &= \mathcal{N}\sum_{n=0}^{\infty}\frac{(-i\lambda)^n}{(4!)^n n!}\int \mathrm{d}^4X_1\cdots\mathrm{d}^4X_n\int\mathcal{D}\phi\,\phi^4(X_1)\cdots\phi^4(X_n)\,e^{iS_0[\phi]+i\int \mathrm{d}^4X\,J(X)\phi(X)}\ .\end{aligned}$$

It seems that we are now stuck with an unmanageably complicated expression. However, because of the source term in the exponent, each factor $\phi(X_i)$ in front ot the exponential function can be replaced by a **functional derivative** with respect to $J(X_i)$,

$$\phi(X_i)\, e^{iS_0[\phi]+i\int \mathrm{d}^4X\, J(X)\phi(X)} \equiv \frac{1}{i}\,\frac{\delta}{\delta J(X_i)}\, e^{iS_0[\phi]+i\int \mathrm{d}^4X\, J(X)\phi(X)} \,. \tag{7.93}$$

If we use this in Eq. (7.92) and pull the functional derivatives with respect to the sources out of the functional integral over the fields ϕ, we obtain

$$\begin{aligned} Z[J] \;&=\; \mathcal{N}\sum_{n=0}^{\infty}\frac{(-i\lambda)^n}{(4!)^n n!}\int \mathrm{d}^4X_1\cdots\mathrm{d}^4X_n \\ &\qquad\qquad \times\left[\frac{1}{i}\,\frac{\delta}{\delta J(X_1)}\right]^4\cdots\left[\frac{1}{i}\,\frac{\delta}{\delta J(X_n)}\right]^4\int \mathcal{D}\phi\, e^{iS_0[\phi]+i\int \mathrm{d}^4X\, J(X)\phi(X)} \\ &=\; \mathcal{N}'\sum_{n=0}^{\infty}\frac{i^n}{n!}\left\{-\frac{\lambda}{4!}\int \mathrm{d}X\,\left[\frac{1}{i}\,\frac{\delta}{\delta J(X)}\right]^4\right\}^n \mathcal{N}''\int \mathcal{D}\phi\, e^{iS_0[\phi]+i\int \mathrm{d}^4X\, J(X)\phi(X)} \\ &\equiv\; \mathcal{N}'\exp\left[i\int \mathrm{d}^4X\,\mathcal{L}_{\mathrm{int}}\left(\frac{1}{i}\,\frac{\delta}{\delta J(X)}\right)\right]\, Z_0[J]\,, \end{aligned} \tag{7.94}$$

where $\mathcal{N}\equiv\mathcal{N}'\mathcal{N}''$, where we wrote the Taylor–series again as an exponential function, and where we introduced the generating functional for the **non-interacting** Klein–Gordon field,

$$Z_0[J] = \mathcal{N}''\int \mathcal{D}\phi\, \exp\left\{iS_0[\phi]+i\int \mathrm{d}^4X\, J(X)\phi(X)\right\}\,, \quad \mathcal{N}''^{\,-1} = \int \mathcal{D}\phi\, \exp\left\{iS_0[\phi]\right\}\,, \tag{7.95}$$

which is normalized to one in the absence of sources. The latter we had already calculated in Eq. (7.74),

$$Z_0[J] = \exp\left[-\frac{i}{2}\int \mathrm{d}^4X\,\mathrm{d}^4Y\, J(X)\,\Delta_F(X-Y)\,J(Y)\right]\,, \tag{7.96}$$

with the Feynman propagator (7.72) for the non-interacting Klein–Gordon field. The normalization constant $\mathcal{N}'$ ensures that $Z[0]=1$, i.e.,

$$\mathcal{N}'^{\,-1} = \exp\left[i\int \mathrm{d}^4X\,\mathcal{L}_{\mathrm{int}}\left(\frac{1}{i}\,\frac{\delta}{\delta J(X)}\right)\right]\, Z_0[J]\Big|_{J=0}\,. \tag{7.97}$$

Equation (7.94) with Eq. (7.96) suggest a **calculation method** for the generating functional, which we had already encountered in other form in Chap. 5: we can expand the exponential in terms of a Taylor series and compute **the individual terms in this series explicitly**, at least up to some given order. Formally, this is equivalent to an expansion in **powers of the coupling constant** λ, i.e., to **perturbation theory**. Of course, we have to terminate the calculation of the series after a finite number of terms. However, if $\lambda \ll 1$ one may hope that the terms of higher order become successively smaller than those of lower order and the perturbation series in λ converges.

In the following we want to perform an exemplary calculation of the perturbation series in λ up to **first** order in λ. The Taylor series of the exponential function in Eq. (7.94) reads up to this order

$$\exp\left[i\int \mathrm{d}^4X\,\mathcal{L}_{\mathrm{int}}\left(\frac{1}{i}\frac{\delta}{\delta J(X)}\right)\right] = 1 - \frac{i\lambda}{4!}\int \mathrm{d}^4X\,\left[\frac{1}{i}\frac{\delta}{\delta J(X)}\right]^4 + O(\lambda^2)\,. \tag{7.98}$$

Inserting this into Eq. (7.94) and acting with it on $Z_0[J]$, the zeroth-order term in λ, the 1, just reproduces the generating functional $Z_0[J]$ of the non-interacting theory. To first order in λ we now have to compute the fourth functional derivative of $Z_0[J]$ with respect to the source term $J(X)$. We have

$$\begin{aligned}
\frac{1}{i}\frac{\delta}{\delta J(X)}\,Z_0[J] &= \frac{1}{i}\frac{\delta}{\delta J(X)}\,\exp\left[-\frac{i}{2}\int \mathrm{d}^4Y\,\mathrm{d}^4Z\,J(Y)\,\Delta_F(Y-Z)\,J(Z)\right] \\
&= \left[-\frac{1}{2}\int \mathrm{d}^4Z\,\Delta_F(X-Z)\,J(Z) - \frac{1}{2}\int \mathrm{d}^4Y\,J(Y)\,\Delta_F(Y-X)\right] Z_0[J] \\
&= -\int \mathrm{d}^4Z\,\Delta_F(X-Z)\,J(Z)\,Z_0[J]\,,
\end{aligned} \tag{7.99}$$

where we used the symmetry of the Feynman propagator, $\Delta_F(X-Y) \equiv \Delta_F(Y-X)$, and renamed the integration variable in the second term, $Y \to Z$. The second functional derivative is

$$\begin{aligned}
\left[\frac{1}{i}\frac{\delta}{\delta J(X)}\right]^2 Z_0[J] &= \frac{1}{i}\frac{\delta}{\delta J(X)}\left\{-\int \mathrm{d}^4Z\,\Delta_F(X-Z)\,J(Z)\,Z_0[J]\right\} \\
&= \left\{-\frac{1}{i}\,\Delta_F(0) - \int \mathrm{d}^4Z\,\Delta_F(X-Z)\,J(Z)\left[-\int \mathrm{d}^4U\,\Delta_F(X-U)\,J(U)\right]\right\} Z_0[J] \\
&= \left[i\,\Delta_F(0) + \int \mathrm{d}^4Z\,\mathrm{d}^4U\,\Delta_F(X-Z)\,\Delta_F(X-U)\,J(Z)\,J(U)\right] Z_0[J]\,.
\end{aligned} \tag{7.100}$$

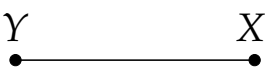
The third functional derivative is then

$$\begin{aligned}
&\left[\frac{1}{i}\frac{\delta}{\delta J(X)}\right]^3 Z_0[J] \\
&= \frac{1}{i}\frac{\delta}{\delta J(X)}\left\{\left[i\,\Delta_F(0) + \int \mathrm{d}^4Z\,\mathrm{d}^4U\,\Delta_F(X-Z)\,\Delta_F(X-U)\,J(Z)\,J(U)\right] Z_0[J]\right\} \\
&= \frac{1}{i}\left[\int \mathrm{d}^4U\,\Delta_F(0)\,\Delta_F(X-U)\,J(U) + \int \mathrm{d}^4Z\,\Delta_F(X-Z)\,\Delta_F(0)\,J(Z)\right] Z_0[J] \\
&\quad + \left[i\,\Delta_F(0) + \int \mathrm{d}^4Z\,\mathrm{d}^4U\,\Delta_F(X-Z)\,\Delta_F(X-U)\,J(Z)\,J(U)\right] \\
&\quad \times \left[-\int \mathrm{d}^4V\,\Delta_F(X-V)\,J(V)\right] Z_0[J] \\
&= \Big[-3\,i\,\Delta_F(0)\int \mathrm{d}^4Z\,\Delta_F(X-Z)\,J(Z) \\
&\quad - \int \mathrm{d}^4Z\,\mathrm{d}^4U\,\mathrm{d}^4V\,\Delta_F(X-Z)\,\Delta_F(X-U)\,\Delta_F(X-V)\,J(Z)\,J(U)\,J(V)\Big] Z_0[J]\,,
\end{aligned} \tag{7.101}$$

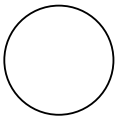
where we renamed several integration variables in order to collect the terms in a suitable manner. Finally, we also compute the fourth functional derivative,

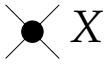
$$
\begin{aligned}
&\left[\frac{1}{i}\,\frac{\delta}{\delta J(X)}\right]^4 Z_0[J] \\
&\quad = \frac{1}{i}\,\frac{\delta}{\delta J(X)}\left\{\left[-3\,i\,\Delta_F(0)\int \mathrm{d}^4Z\,\Delta_F(X-Z)\,J(Z)\right.\right. \\
&\qquad \left.\left. -\int \mathrm{d}^4Z\,\mathrm{d}^4U\,\mathrm{d}^4V\,\Delta_F(X-Z)\,\Delta_F(X-U)\,\Delta_F(X-V)\,J(Z)\,J(U)\,J(V)\right] Z_0[J]\right\} \\
&\quad = \frac{1}{i}\left[-3\,i\,[\Delta_F(0)]^2 - 3\int \mathrm{d}^4Z\,\mathrm{d}^4U\,\Delta_F(X-Z)\,\Delta_F(X-U)\,\Delta_F(0)\,J(Z)\,J(U)\right] Z_0[J] \\
&\qquad + \left[-3\,i\,\Delta_F(0)\int \mathrm{d}^4Z\,\Delta_F(X-Z)\,J(Z)\right. \\
&\qquad \left. -\int \mathrm{d}^4Z\,\mathrm{d}^4U\,\mathrm{d}^4V\,\Delta_F(X-Z)\,\Delta_F(X-U)\,\Delta_F(X-V)\,J(Z)\,J(U)\,J(V)\right] \\
&\qquad \times\left[-\int \mathrm{d}^4W\,\Delta_F(X-W)\,J(W)\right] Z_0[J] \\
&\quad = \left\{-3\,[\Delta_F(0)]^2 + 6\,i\,\Delta_F(0)\int \mathrm{d}^4Z\,\mathrm{d}^4U\,\Delta_F(X-Z)\,\Delta_F(X-U)\,J(Z)\,J(U)\right. \\
&\qquad + \int \mathrm{d}^4Z\,\mathrm{d}^4U\,\mathrm{d}^4V\,\mathrm{d}^4W\,\Delta_F(X-Z)\,\Delta_F(X-U)\,\Delta_F(X-V)\,\Delta_F(X-W) \\
&\qquad\qquad \left.\times\,J(Z)\,J(U)\,J(V)\,J(W)\right\} Z_0[J]\,. \qquad (7.102)
\end{aligned}
$$

With the help of the following **Feynman rules** in space-time,

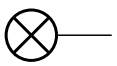
$$i\,\Delta_F(X-Y) \;=\;$$ 

, (7.103)

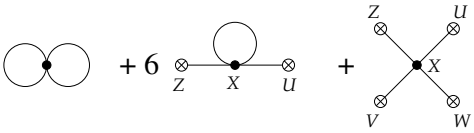
$$i\,\Delta_F(0) \;=\;$$ 
, (7.104)

$$-i\lambda\int \mathrm{d}^4X \;=\;$$ 

, (7.105)

$$i\int \mathrm{d}^4X\,J(X) \;=\;$$ 
, (7.106)

the space-time integral of Eq. (7.102), multiplied with $-i\lambda/4!$, can be written in terms of Feynman diagrams in the following way:

$$\int \mathrm{d}^4X\left\{-\frac{i\lambda}{4!}\left[\frac{1}{i}\,\frac{\delta}{\delta J(X)}\right]^4\right\} Z_0[J] = \frac{1}{4!}\left(\right.$$ 

$$\left.\right) Z_0[J]\,. \qquad (7.107)$$

8 Path Integrals in Statistical Field Theory

In the final chapter of this lecture series, we would like to give an outlook to the application of path integrals in Statistical Field Theory. Statistical Field Theory is the generalization of Statistical Mechanics of particles to that of fields, just like Quantum Field Theory is the generalization of Quantum Mechanics of particles to that of fields. The central object of Statistical Mechanics, as well as Statistical Field Theory, is the **partition function**, from which one can derive all thermodynamical properties of the system. We explain in this chapter how the partition function can be expressed in terms of a functional integral.

In Statistical Mechanics, the partition function of the so-called **canonical ensemble**, i.e., an ensemble of N particles in a given volume V, which is immersed in a heat bath that allows energy exchange with the system and keeps the system at a constant temperature T, is given by

$$\mathcal{Z} = \mathrm{Tr}\, e^{-\beta \hat{H}} \ . \tag{8.1}$$

Here, $\hat{H}$ is the Hamilton operator of the system and $\beta \equiv 1/(k_B T)$, where k_B is Boltzmann's constant. The trace runs over a complete set of states of the system. For instance, if we choose the set of eigenstates $\phi_0(\vec{x})$ of the Schrödinger–picture field operator $\hat{\phi}(\vec{x})$, cf. Eq. (7.20),

$$\mathcal{Z} = \mathrm{Tr}\, e^{-\beta \hat{H}} = \int \prod_{\vec{x} \in V} \mathrm{d}\phi_0(\vec{x}) \, \langle \phi_0 | \, e^{-\beta \hat{H}} \, | \phi_0 \rangle \ . \tag{8.2}$$

Note that the spatial coordinates of the fields must lie inside the volume V of the system. The matrix elements in the trace remind of the **quantum field-theoretical transition amplitude**

$$\langle \phi_f(\vec{x}, t_f) | \phi_i(\vec{x}, t_i) \rangle = \langle \phi_f | \, \hat{U}(t_f, 0) \hat{U}(0, t_i) \, | \phi_i \rangle = \langle \phi_f | \, \hat{U}(t_f, t_i) \, | \phi_i \rangle = \langle \phi_f | \, e^{-i\hat{H}(t_f - t_i)} \, | \phi_i \rangle \ , \tag{8.3}$$

cf. Eq. (7.30), with the following obvious replacements:

(i) $\phi_i = \phi_f = \phi_0$, initial and final state in the transition amplitude are identical,

(ii) $t_f - t_i \longrightarrow -i\beta$, the real time interval $[t_i, t_f]$ for the quantum-mechanical time evolution is replaced by an interval $[0, \beta]$ in **imaginary time**.

Because of the second point one also speaks of **Statistical Field Theory in imaginary-time formalism**. (There is also a version of Statistical Field Theory in the so-called real-time formalism, which is out of the scope of the present lecture.)

Point (ii) can be also be formulated as

(ii') $\hat{U}(t_f, t_i) \equiv e^{-i\hat{H}(t_f - t_i)} \longrightarrow e^{-\beta\hat{H}}$, the quantum-mechanical time-evolution operator is replaced by the so-called Gibbs operator of the canonical ensemble.

Just as demonstrated in Sec. 7.2, the matrix element (8.3) can be written in the form of a functional integral. We repeat the respective derivation, but immediately for the matrix element in Eq. (8.2). First we partition the interval $[0, \beta]$ into N pieces of length τ,

$$\beta \equiv N\tau \ ,$$

where we have in mind that, at the end of the calculation, we will perform the limit $N \to \infty$, $\tau \to 0$, with $N\tau = \beta = \text{const}$. The Gibbs operator can then be written as follows,

$$e^{-\beta\hat{H}} \equiv e^{-\hat{H}\tau N} \equiv \prod_{j=1}^{N} e^{-\hat{H}\tau} \ . \tag{8.4}$$

We insert this expression into the transition amplitude in Eq. (8.2) and insert in front of each factor $e^{-\hat{H}\tau}$ a complete set of eigenfunctions of the field operator, Eq. (7.21), and behind each factor a complete set of eigenfunctions of the canonically conjugate field operator, Eq. (7.24),

$$\begin{aligned}
\langle\phi_0|\, e^{-\beta\hat{H}}\, |\phi_0\rangle &= \langle\phi_0| \prod_{j=1}^{N} e^{-\hat{H}\tau} |\phi_0\rangle \\
&= \int \prod_{j=1}^{N} \prod_{\vec{x}\in V} \frac{\mathrm{d}\Pi_j(\vec{x})\mathrm{d}\phi_j(\vec{x})}{2\pi} \langle\phi_0|\phi_N\rangle\langle\phi_N|\, e^{-\hat{H}\tau}\, |\Pi_N\rangle\langle\Pi_N|\phi_{N-1}\rangle\langle\phi_{N-1}|\, e^{-\hat{H}\tau}\, |\Pi_{N-1}\rangle \cdots \\
&\qquad \cdots \langle\Pi_2|\phi_1\rangle\langle\phi_1|\, e^{-\hat{H}\tau}\, |\Pi_1\rangle\langle\Pi_1|\phi_0\rangle \ .
\end{aligned} \tag{8.5}$$

Here we have enumerated the various complete sets of eigenfunctions with an index j, in order to mutually distinguish them. We now use

(i) for the first factor under the integral the orthonormality (7.22) of the eigenstates $|\phi_j\rangle$,

$$\langle\phi_0|\phi_N\rangle = \delta[\phi_0 - \phi_N] \ , \tag{8.6}$$

(ii) for the factors $\langle\Pi_j|\phi_{j-1}\rangle$ Eq. (7.26), i.e.,

$$\langle\Pi_j|\phi_{j-1}\rangle = \exp\left[-i \int_V \mathrm{d}^3\vec{x}\, \Pi_j(\vec{x})\phi_{j-1}(\vec{x})\right] \ , \tag{8.7}$$

(iii) for the factors $\langle\phi_j|\, e^{-\hat{H}\tau}\, |\Pi_j\rangle$ the following consideration: in the limit $\tau \to 0$ we may terminate the Taylor–series expansion of the exponential function after the term linear in the (infinitesimally) small quantity τ,

$$\langle\phi_j|\, e^{-\hat{H}\tau}\, |\Pi_j\rangle = \langle\phi_j|\, 1 - \hat{H}\tau\, |\Pi_j\rangle + O(\tau^2) \ . \tag{8.8}$$

The Hamilton operator $\hat{H}$ can be written as a spatial integral over the Hamilton density,

$$\hat{H} \equiv \int_V \mathrm{d}^3\vec{x}\, \hat{\mathcal{H}} \,. \tag{8.9}$$

According to Eq. (7.33) $\hat{\mathcal{H}}$ is a function of the field $\hat{\phi}$ and $\hat{\Pi}$ (as well as gradients of $\hat{\phi}$; an explicit space and time dependence can be excluded for a system in global thermodynamical equilibrium). Between eigenstates $\langle\phi_j|$ and $|\Pi_j\rangle$ we can replace the field operators by their respective eigenvalues, i.e.,

$$\begin{aligned}\langle\phi_j|\,\hat{H}\,|\Pi_j\rangle &= \int_V \mathrm{d}^3\vec{x}\,\langle\phi_j|\mathcal{H}(\hat{\phi},\hat{\Pi},\vec{\nabla}\hat{\phi})|\Pi_j\rangle \\ &= \int_V \mathrm{d}^3\vec{x}\,\langle\phi_j|\mathcal{H}(\phi_j,\Pi_j,\vec{\nabla}\phi_j)|\Pi_j\rangle \equiv H_j\langle\phi_j|\Pi_j\rangle \,,\end{aligned} \tag{8.10}$$

where

$$H_j \equiv \int_V \mathrm{d}^3\vec{x}\,\mathcal{H}(\phi_j,\Pi_j,\vec{\nabla}\phi_j) \tag{8.11}$$

is the value of the Hamilton operator for the field eigenvalues ϕ_j, Π_j. If we insert Eq. (8.10) into Eq. (8.8) and reverse the expansion of the exponential function, we obtain

$$\begin{aligned}\langle\phi_j|\,e^{-\hat{H}\tau}\,|\Pi_j\rangle &= e^{-H_j\tau}\langle\phi_j|\Pi_j\rangle \\ &\equiv \exp\left\{\int_V \mathrm{d}^3\vec{x}\,\left[i\,\Pi_j(\vec{x})\phi_j(\vec{x}) - \tau\,\mathcal{H}(\phi_j,\pi_j,\vec{\nabla}\phi_j)\right]\right\} \,,\end{aligned} \tag{8.12}$$

where we have used Eq. (8.7).

Now we insert Eqs. (8.6), (8.7), and (8.12) into Eq. (8.5) and obtain

$$\begin{aligned}\langle\phi_0|\,e^{-\beta\hat{H}}\,|\phi_0\rangle = &\int \prod_{j=1}^{N}\prod_{\vec{x}\in V}\frac{\mathrm{d}\Pi_j(\vec{x})\mathrm{d}\phi_j(\vec{x})}{2\pi}\,\delta[\phi_0-\phi_N] \\ &\times\exp\left\{\sum_{k=1}^{N}\tau\int_V \mathrm{d}^3\vec{x}\,\left[i\,\Pi_k(\vec{x})\frac{\phi_k(\vec{x})-\phi_{k-1}(\vec{x})}{\tau} - \mathcal{H}(\phi_k,\Pi_k,\vec{\nabla}\phi_k)\right]\right\} \,.\end{aligned} \tag{8.13}$$

In the limit $N\to\infty$, $\tau\to 0$ the sum over k in the exponent becomes an integral over the variable τ. The finite difference of the fields becomes

$$\lim_{\tau\to 0}\frac{\phi_k(\vec{x})-\phi_{k-1}(\vec{x})}{\tau} = \frac{\partial\phi(\vec{x},\tau)}{\partial\tau} \,.$$

With the definitions

$$\mathcal{D}\phi(\vec{x},\tau) \equiv \lim_{N\to\infty}\prod_{j=1}^{N}\prod_{\vec{x}\in V}\mathrm{d}\phi_j(\vec{x}) \,, \quad \mathcal{D}\Pi(\vec{x},\tau) \equiv \lim_{N\to\infty}\prod_{j=1}^{N}\prod_{\vec{x}\in V}\frac{\mathrm{d}\Pi_j(\vec{x})}{2\pi} \,, \tag{8.14}$$

we obtain from Eq. (8.13) in the limit $N \to \infty$, $\tau \to 0$,

$$\begin{aligned} \langle \phi_0 | \, e^{-\beta \hat{H}} \, | \phi_0 \rangle &= \int \mathcal{D}\Pi(\vec{x},\tau) \int_{\phi(\vec{x},0)=\phi_0(\vec{x})}^{\phi(\vec{x},\beta)=\phi_0(\vec{x})} \mathcal{D}\phi(\vec{x},\tau) \\ &\quad \times \exp\left\{ \int_0^\beta \mathrm{d}\tau \int_V \mathrm{d}^3\vec{x} \left[\Pi(\vec{x},\tau)\, i\, \frac{\partial \phi(\vec{x},\tau)}{\partial \tau} - \mathcal{H}(\phi,\Pi,\vec{\nabla}\phi) \right] \right\} . \quad (8.15) \end{aligned}$$

Here we have indicated at the boundaries of the functional integral over the fields $\phi(\vec{x},\tau)$ that both the "initial state" at $\tau = 0$ as well as, due to the functional delta function $\delta[\phi_0 - \phi_N]$, the "final state" at $\tau = \beta$ are given by the field eigenvalue $\phi_0(\vec{x})$.

If we insert Eq. (8.15) into Eq. (8.2) we also integrate over all possible field eigenvalues $\phi_0(\vec{x})$. The only restriction of the functional integral over the fields ϕ is then that one has to integrate over all fields $\phi(\vec{x},\tau)$ which are **periodic** in the interval $[0,\beta]$. Thus, the **canonical partition function** has the following representation as a **functiona linteral**,

$$\begin{aligned} \mathcal{Z} &= \mathfrak{N} \int \mathcal{D}\Pi(\vec{x},\tau) \int_{\text{periodic}} \mathcal{D}\phi(\vec{x},\tau) \\ &\quad \times \exp\left\{ \int_0^\beta \mathrm{d}\tau \int_V \mathrm{d}^3\vec{x} \left[\Pi(\vec{x},\tau)\, i\, \frac{\partial \phi(\vec{x},\tau)}{\partial \tau} - \mathcal{H}(\phi,\Pi,\vec{\nabla}\phi) \right] \right\} . \quad (8.16) \end{aligned}$$

Here we have also introduced a normalization constant $\mathfrak{N}$, which accounts for the fact that the partition function must be a **dimensionless number**. This normalization is necessary because the fields $\Pi(\vec{x},\tau)$ and $\phi(\vec{x},\tau)$ in the integration measure are usually not dimensionless.

For Hamilton densities which are quadratic in Π, the functional integration over this field is again a shifted Gaussian integral and can be immediately performed. The result will then again be a functional integral over ϕ only, with the Lagrangian appearing in the argument in the exponent. For non-interacting field theories, the Lagrangian is a quadratic function of ϕ, i.e., the functional integral is again a Gaussian integral and can be explicitly computed. And here is where the fun starts: in contrast to Quantum Field Theory, where many prefactors could be neglected in the generating functional for n–point correlation functions, since the latter was normalized to one in the absence of sources, the partition function (8.16), which at first glance looks very similar to the generating functional in the absence of sources, is not one, but a number which determines the thermodynamics of the system. All factors resulting from the evaluation of the Gaussian integrals have to be carefully kept in order to obtain the correct result. But this is subject of a dedicated course on Statistical Field Theory and will not be elaborated further here.

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