Chapter 2
From Classical to Quantum Fields

We have learned how the consistency of quantum mechanics with special relativity forces us to abandon the single-particle interpretation of the wave function. Instead we have to consider quantum fields whose elementary excitations are associated with particle states, as we will see below. In this chapter we study the basics of field quantization using both the canonical formalism and the path integral method.

2.1 Particles and Quantum Fields

In any scattering experiment the only information available to us is the set of quantum numbers associated with the set of free particles in the initial and final states. Ignoring for the moment other quantum numbers like spin and flavor, one-particle states are labelled by the three-momentum $\mathbf{p}$ and span the single-particle Hilbert space $\mathscr{H}_1$

$$|\mathbf{p}\rangle \in \mathscr{H}_1, \quad \langle \mathbf{p}|\mathbf{p}'\rangle = \delta(\mathbf{p}-\mathbf{p}'). \tag{2.1}$$

The states $\{|\mathbf{p}\rangle\}$ form a basis of $\mathscr{H}_1$ and therefore satisfy the closure relation

$$\int d^3p|\mathbf{p}\rangle\langle\mathbf{p}| = \mathbf{1}. \tag{2.2}$$

The group of spatial rotations acts unitarily on the states $|\mathbf{p}\rangle$. This means that for every rotation $R \in \mathrm{SO}(3)$ there is a unitary operator $\mathscr{U}(R)$ such that

$$\mathscr{U}(R)|\mathbf{p}\rangle = |R\mathbf{p}\rangle \tag{2.3}$$

where $R\mathbf{p}$ represents the action of the rotation on the vector $\mathbf{p}$, $(R\mathbf{p})^i = R^i_{\ j}p^j$. Using a spectral decomposition, the momentum operator can be written as

$$\hat{P}^i = \int d^3p|\mathbf{p}\rangle p^i\langle\mathbf{p}|. \tag{2.4}$$

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With the help of Eq. (2.3) it is straightforward to check that the momentum operator transforms as a vector under rotations:

$$\mathscr{U}(R)^{-1}\hat{P}^i\mathscr{U}(R) = \int d^3p|R^{-1}\mathbf{p}\rangle p^i\langle R^{-1}\mathbf{p}| = R^i_j\hat{P}^j, \tag{2.5}$$

where we have used that the integration measure is invariant under SO(3).

Since, as argued above, we are forced to deal with multiparticle states, it is convenient to introduce creation-annihilation operators associated with a single-particle state of momentum $\mathbf{p}$

$$\left[\hat{a}(\mathbf{p}), \hat{a}^\dagger(\mathbf{p}')\right] = \delta(\mathbf{p}-\mathbf{p}'), \quad \left[\hat{a}(\mathbf{p}), \hat{a}(\mathbf{p}')\right] = \left[\hat{a}^\dagger(\mathbf{p}), \hat{a}^\dagger(\mathbf{p}')\right] = 0, \tag{2.6}$$

such that the state $|\mathbf{p}\rangle$ is created out of the Fock space vacuum $|0\rangle$ (normalized such that $\langle 0|0\rangle = 1$) by the action of a creation operator $\hat{a}^\dagger(\mathbf{p})$

$$|\mathbf{p}\rangle = \hat{a}^\dagger(\mathbf{p})|0\rangle, \quad \hat{a}(\mathbf{p})|0\rangle = 0 \quad \text{for all} \quad \mathbf{p}. \tag{2.7}$$

Covariance under spatial rotations is all we need if we are interested in a nonrelativistic theory. However in a relativistic quantum field theory we must preserve more that SO(3), we need the expressions to be covariant under the full Poincaré group ISO(1, 3) consisting of spatial rotations, boosts and space-time translations (see Sect. 3.1 and Appendix B). Therefore, in order to build the Fock space of the theory we need two key ingredients: first an invariant normalization for the states, since we want a normalized state in one reference frame to be normalized in any other inertial frame. And secondly a relativistic invariant integration measure in momentum space, so the spectral decomposition of operators is covariant under the full Poincaré group.

Let us begin with the invariant measure. Given an invariant function *f*(*p*) of the four-momentum p^μ of a particle of mass m with positive energy $p^0 > 0$, there is an integration measure which is invariant under proper Lorentz transformations[1]

$$\int \frac{d^4p}{(2\pi)^4}(2\pi)\delta(p^2-m^2)\theta(p^0)f(p), \tag{2.8}$$

where the factors of 2π are introduced for later convenience, and $\theta(x)$ is the Heaviside step function

$$\theta(x) = \begin{cases} 0 & x < 0 \\ 1 & x > 0 \end{cases}. \tag{2.9}$$

The integration over p^0 can be easily done using the delta function identity

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1 The identity $p^2 = m^2$ satisfied by the four-momentum of a real particle will be referred to in the following as the *on-shell* condition.

$$\delta[g(x)] = \sum_{x_i=\text{zeros of } g} \frac{1}{|g'(x_i)|}\delta(x-x_i), \tag{2.10}$$

valid for any function $g(x)$ with simple zeroes. In our case this implies

$$\delta(p^2-m^2) = \frac{1}{2p^0}\delta\left(p^0-\sqrt{\mathbf{p}^2+m^2}\right) + \frac{1}{2p^0}\delta\left(p^0+\sqrt{\mathbf{p}^2+m^2}\right). \tag{2.11}$$

The second term has support on states with negative energy and therefore does not contribute to the integral. We can write

$$\int \frac{d^4p}{(2\pi)^4}(2\pi)\delta(p^2-m^2)\theta(p^0)f(p) = \int \frac{d^3p}{(2\pi)^3}\frac{1}{2\sqrt{\mathbf{p}^2+m^2}}f\left(\sqrt{\mathbf{p}^2+m^2},\mathbf{p}\right). \tag{2.12}$$

Hence, the relativistic invariant measure is given by

$$\int \frac{d^3p}{(2\pi)^3}\frac{1}{2E_{\mathbf{p}}} \quad \text{with} \quad E_{\mathbf{p}} \equiv \sqrt{\mathbf{p}^2+m^2}. \tag{2.13}$$

Once we have an invariant measure the next step is to find an invariant normalization for the states. We work with a basis $\{|p\rangle\}$ of eigenstates of the four-momentum operator $\hat{P}^\mu$

$$\hat{P}^0|p\rangle = E_{\mathbf{p}}|p\rangle, \quad \hat{P}^i|p\rangle = \mathbf{p}^i|p\rangle. \tag{2.14}$$

Since the states $|p\rangle$ are eigenstates of the three-momentum operator we can express them in terms of the non-relativistic states $|\mathbf{p}\rangle$ introduced in Eq. (2.1)

$$|p\rangle = N(\mathbf{p})|\mathbf{p}\rangle \tag{2.15}$$

with $N(\mathbf{p})$ a normalization to be determined now. The states $\{|p\rangle\}$ form a complete basis, so they should satisfy the Lorentz invariant closure relation

$$\int \frac{d^4p}{(2\pi)^4}(2\pi)\delta(p^2-m^2)\theta(p^0)|p\rangle\langle p| = \mathbf{1}. \tag{2.16}$$

At the same time, this closure relation can be expressed, using Eq. (2.15), in terms of the nonrelativistic basis of states $\{|\mathbf{p}\rangle\}$ as

$$\int \frac{d^4p}{(2\pi)^4}(2\pi)\delta(p^2-m^2)\theta(p^0)|p\rangle\langle p| = \int \frac{d^3p}{(2\pi)^3}\frac{1}{2E_{\mathbf{p}}}|N(\mathbf{p})|^2|\mathbf{p}\rangle\langle\mathbf{p}|. \tag{2.17}$$

Using Eq. (2.4) we get the expression (2.16) provided

$$|N(\mathbf{p})|^2 = (2\pi)^3(2E_{\mathbf{p}}). \tag{2.18}$$

Taking the overall phase in Eq. (2.15) so that $N(\mathbf{p})$ is real and positive, we define the Lorentz invariant states $|p\rangle$ as

$$|p\rangle = (2\pi)^{\frac{3}{2}}\sqrt{2E_{\mathbf{p}}}|\mathbf{p}\rangle, \tag{2.19}$$

and given the normalization of $|\mathbf{p}\rangle$ we find the one of the relativistic states to be

$$\langle p|p'\rangle = (2\pi)^3(2E_{\mathbf{p}})\delta(\mathbf{p}-\mathbf{p}'). \tag{2.20}$$

It might not be obvious at first sight, but the previous normalization is Lorentz invariant. Although it is not difficult to show this in general, here we consider the simpler case of 1+1 dimensions where the two components (p^0, p^1) of the on-shell momentum $p^2 = m^2$ can be parametrized in terms of a single hyperbolic angle λ as

$$p^0 = m\cosh\lambda, \quad p^1 = m\sinh\lambda. \tag{2.21}$$

Now, the combination $2E_{\mathbf{p}}\delta(p^1 - p'^1)$ can be written as

$$2E_{\mathbf{p}}\delta(p^1 - p'^1) = 2m\cosh\lambda\,\delta(m\sinh\lambda - m\sinh\lambda') = 2\delta(\lambda-\lambda'), \tag{2.22}$$

where we have made use of the property (2.10) of the delta function. Lorentz transformations in 1+1 dimensions are labelled by a parameter $\xi \in \mathbb{R}$ and act on the momentum by shifting the hyperbolic angle $\lambda \to \lambda + \xi$. However, Eq. (2.22) is invariant under a common shift of λ and λ', so the whole expression is obviously invariant under Lorentz transformations.

To summarize what we did so far, we have succeeded in constructing a Lorentz covariant basis of states for the one-particle Hilbert space $\mathscr{H}_1$. The generators of space-time translations act on the basis states $|p\rangle$ as

$$\hat{P}^\mu|p\rangle = p^\mu|p\rangle, \tag{2.23}$$

whereas the action of Lorentz transformations is implemented by the unitary operator

$$\mathscr{U}(\Lambda)|p\rangle = |\Lambda^\mu{}_\nu p^\nu\rangle \equiv |\Lambda p\rangle \quad \text{with} \quad \Lambda \in \mathrm{SO}(1,3). \tag{2.24}$$

This transformation is compatible with the Lorentz invariant normalization (2.20),

$$\langle p|p'\rangle = \langle p|\mathscr{U}(\Lambda)^{-1}\mathscr{U}(\Lambda)|p'\rangle = \langle\Lambda p|\Lambda p'\rangle. \tag{2.25}$$

On $\mathscr{H}_1$ the operator $\hat{P}^\mu$ admits the following spectral representation

$$\hat{P}^\mu = \int\frac{d^3p}{(2\pi)^3}\frac{1}{2E_{\mathbf{p}}}|p\rangle p^\mu\langle p|. \tag{2.26}$$

Using (2.25) and the fact that the measure is invariant under Lorentz transformation, one can easily show that $\hat{P}^\mu$ transform covariantly under SO(1, 3)

$$\mathscr{U}(\Lambda)^{-1}\hat{P}^{\mu}\mathscr{U}(\Lambda) = \int \frac{d^3p}{(2\pi)^3}\frac{1}{2E_{\mathbf{p}}}|\Lambda^{-1}p\rangle p^{\mu}\langle\Lambda^{-1}p| = \Lambda^{\mu}{}_{\nu}\hat{P}^{\nu}. \tag{2.27}$$

A set of covariant creation-annihilation operators can be constructed now in terms of the operators $\hat{a}(\mathbf{p})$, $\hat{a}^{\dagger}(\mathbf{p})$ introduced above

$$\hat{\alpha}(\mathbf{p}) \equiv (2\pi)^{\frac{3}{2}}\sqrt{2E_{\mathbf{p}}}\hat{a}(\mathbf{p}), \quad \hat{\alpha}^{\dagger}(\mathbf{p}) \equiv (2\pi)^{\frac{3}{2}}\sqrt{2E_{\mathbf{p}}}\hat{a}^{\dagger}(\mathbf{p}). \tag{2.28}$$

with the Lorentz invariant commutation relations

$$\begin{aligned}\left[\hat{\alpha}(\mathbf{p}), \hat{\alpha}^{\dagger}(\mathbf{p}')\right] &= (2\pi)^3(2E_{\mathbf{p}})\delta(\mathbf{p}-\mathbf{p}'),\\ \left[\hat{\alpha}(\mathbf{p}), \hat{\alpha}(\mathbf{p}')\right] &= \left[\hat{\alpha}^{\dagger}(\mathbf{p}), \hat{\alpha}^{\dagger}(\mathbf{p}')\right] = 0.\end{aligned} \tag{2.29}$$

Particle states are created by acting with any number of creation operators $\alpha(\mathbf{p})$ on the Poincaré invariant vacuum state $|0\rangle$ satisfying

$$\begin{aligned}\langle 0|0\rangle &= 1,\\ \hat{P}^{\mu}|0\rangle &= 0,\\ \mathscr{U}(\Lambda)|0\rangle &= |0\rangle, \quad \text{for all } \Lambda \in \mathrm{SO}(1,3).\end{aligned} \tag{2.30}$$

A general one-particle state $|f\rangle \in \mathscr{H}_1$ can be written as

$$|f\rangle = \int \frac{d^3p}{(2\pi)^3}\frac{1}{2E_{\mathbf{p}}} f(\mathbf{p})\hat{\alpha}^{\dagger}(\mathbf{p})|0\rangle, \tag{2.31}$$

while a n-particle state $|f\rangle \in \mathscr{H}_1^{\otimes n}$ is

$$|f\rangle = \int \left[\prod_{i=1}^{n}\frac{d^3p_i}{(2\pi)^3}\frac{1}{2\omega_{p_i}}\right] f(\mathbf{p}_1,\ldots,\mathbf{p}_n)\hat{\alpha}^{\dagger}(\mathbf{p}_1)\ldots\hat{\alpha}^{\dagger}(\mathbf{p}_n)|0\rangle. \tag{2.32}$$

That these states are Lorentz invariant can be checked by noticing that from the definition of the creation-annihilation operators follows the transformation

$$\mathscr{U}(\Lambda)\hat{\alpha}(\mathbf{p})\mathscr{U}(\Lambda)^{\dagger} = \hat{\alpha}(\Lambda\mathbf{p}) \tag{2.33}$$

and the corresponding one for creation operators.

As we have argued above, the very fact that measurements have to be localized implies the necessity of introducing quantum fields. Here we will consider the simplest case of a quantum scalar field $\hat{\phi}(x)$ satisfying the following properties:

- *Hermiticity*

$$\hat{\phi}(x)^{\dagger} = \hat{\phi}(x). \tag{2.34}$$

- *Microcausality* Since measurements cannot interfere with each other when performed in causally disconnected points of space-time, the commutator of two fields has to vanish outside the relative light-cone

$$\left[\hat{\phi}(x), \hat{\phi}(y)\right] = 0, \quad (x-y)^2 < 0. \tag{2.35}$$

- *Translation invariance*

$$e^{i\hat{P}\cdot a}\hat{\phi}(x)e^{-i\hat{P}\cdot a} = \hat{\phi}(x-a). \tag{2.36}$$

- *Lorentz invariance*

$$\mathscr{U}(\Lambda)^{\dagger}\hat{\phi}(x)\mathscr{U}(\Lambda) = \hat{\phi}(\Lambda^{-1}x). \tag{2.37}$$

- *Linearity* To simplify matters we will also assume that $\phi(x)$ is linear in the creation-annihilation operators $\alpha(\mathbf{p}),\ \alpha^{\dagger}(\mathbf{p})$

$$\hat{\phi}(x) = \int \frac{d^3p}{(2\pi)^3}\frac{1}{2E_{\mathbf{p}}}\left[f(\mathbf{p},x)\hat{\alpha}(\mathbf{p}) + g(\mathbf{p},x)\hat{\alpha}^{\dagger}(\mathbf{p})\right]. \tag{2.38}$$

Since $\hat{\phi}(x)$ should be hermitian we are forced to take $g(\mathbf{p},x) = f(\mathbf{p},x)^*$. Moreover, $\phi(x)$ satisfies the equations of motion of a free scalar field, $(\partial_\mu\partial^\mu + m^2)\hat{\phi}(x) = 0$, only if $f(\mathbf{p},x)$ is a complete basis of solutions of the Klein–Gordon equation. These considerations leads to the expansion

$$\hat{\phi}(x) = \int \frac{d^3p}{(2\pi)^3}\frac{1}{2E_{\mathbf{p}}}\left[e^{-iE_{\mathbf{p}}t+i\mathbf{p}\cdot\mathbf{x}}\hat{\alpha}(\mathbf{p}) + e^{iE_{\mathbf{p}}t-i\mathbf{p}\cdot\mathbf{x}}\hat{\alpha}^{\dagger}(\mathbf{p})\right]. \tag{2.39}$$

It can be checked that $\hat{\phi}(x)$ and $\partial_t\hat{\phi}(x)$ satisfy the equal-time canonical commutation relations

$$\left[\hat{\phi}(t,\mathbf{x}), \partial_t\hat{\phi}(t,\mathbf{y})\right] = i\delta(\mathbf{x}-\mathbf{y}). \tag{2.40}$$

The general (non-equal time) commutator

$$\left[\hat{\phi}(x), \hat{\phi}(x')\right] = i\Delta(x-x') \tag{2.41}$$

can also be computed using the expression (2.39). The function $\Delta(x-y)$ is given by

$$\begin{aligned} i\Delta(x-y) &= -\mathrm{Im}\int \frac{d^3p}{(2\pi)^3}\frac{1}{2E_{\mathbf{p}}}e^{-iE_{\mathbf{p}}(t-t')+i\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')} \\ &= \int \frac{d^4p}{(2\pi)^4}(2\pi)\delta(p^2-m^2)\mathrm{sign}(p^0)e^{-ip\cdot(x-x')}, \end{aligned} \tag{2.42}$$

where the sign function is defined as

$$\text{sign}(x) \equiv \theta(x) - \theta(-x) = \begin{cases} 1 & x > 0 \\ -1 & x < 0 \end{cases}. \tag{2.43}$$

Using the last expression in Eq. (2.42) it is easy to show that $i\Delta(x - x')$ vanishes when x and x' are space-like separated. Indeed, if $(x - x')^2 < 0$ there is always a reference frame in which both events are simultaneous, and since $i\Delta(x - x')$ is Lorentz invariant we can compute it in this frame. In this case $t = t'$ and the exponential in the second line of (2.42) does not depend on p^0. Therefore, the integration over p^0 gives

$$\begin{aligned}
&\int_{-\infty}^{\infty} dp^0 \varepsilon(p^0)\delta(p^2 - m^2) \\
&\quad = \int_{-\infty}^{\infty} dp^0 \left[\frac{1}{2E_{\mathbf{p}}}\varepsilon(p^0)\delta(p^0 - E_{\mathbf{p}}) + \frac{1}{2E_{\mathbf{p}}}\varepsilon(p^0)\delta(p^0 + E_{\mathbf{p}})\right] \\
&\quad = \frac{1}{2E_{\mathbf{p}}} - \frac{1}{2E_{\mathbf{p}}} = 0.
\end{aligned} \tag{2.44}$$

So we have concluded that $i\Delta(x - x') = 0$ if $(x - x')^2 < 0$, as required by microcausality. Notice that the situation is completely different when $(x - x')^2 \geq 0$, since in this case the exponential depends on p^0 and the integration over this component of the momentum does not vanish.

2.2 Canonical Quantization

So far we have contented ourselves with requiring a number of properties from the quantum scalar field: existence of asymptotic states, locality, microcausality and relativistic invariance. With only these ingredients we have managed to go quite far. The previous results can also be obtained using canonical quantization. One starts with a classical free scalar field theory in the Hamiltonian formalism and obtains the quantum theory by replacing Poisson brackets by commutators. Since this quantization procedure is based on the use of the canonical formalism, which gives time a privileged role, it is important to check at the end of the calculation that the resulting quantum theory is Lorentz invariant. In the following we will briefly overview the canonical quantization of the Klein–Gordon scalar field.

The starting point is the action functional $S[\phi(x)]$ which, in the case of a free real scalar field of mass m is given by

$$S[\phi(x)] \equiv \int d^4x \mathscr{L}(\phi, \partial_\mu\phi) = \frac{1}{2}\int d^4x \Big(\partial_\mu\phi\partial^\mu\phi - m^2\phi^2\Big). \tag{2.45}$$

The equations of motion are obtained, as usual, from the Euler–Lagrange equations

$$\partial_\mu \left[\frac{\partial \mathscr{L}}{\partial(\partial_\mu \phi)}\right] - \frac{\partial \mathscr{L}}{\partial \phi} = 0 \quad \Longrightarrow \quad (\partial_\mu \partial^\mu + m^2)\phi = 0. \tag{2.46}$$

In the Hamiltonian formalism the physical system is described in terms of the field $\phi(x)$, its spatial derivatives and its canonically conjugated momentum

$$\pi(x) \equiv \frac{\partial \mathscr{L}}{\partial(\partial_0 \phi)} = \frac{\partial \phi}{\partial t}. \tag{2.47}$$

The dynamics of the system is determined by the Hamiltonian functional

$$H \equiv \int d^3x \left(\pi \frac{\partial \phi}{\partial t} - \mathscr{L}\right) = \frac{1}{2}\int d^3x \Big[\pi^2 + (\nabla\phi)^2 + m^2\Big]. \tag{2.48}$$

The canonical equations of motion can be written in terms of Poisson brackets. Given two functionals $A[\phi,\pi]$, $B[\phi,\pi]$ of the canonical variables

$$A[\phi,\pi] = \int d^3x \mathscr{A}(\phi,\pi), \quad B[\phi,\pi] = \int d^3x \mathscr{B}(\phi,\pi), \tag{2.49}$$

their Poisson bracket is defined by

$$\{A, B\}_{\mathrm{PB}} \equiv \int d^3x \left(\frac{\delta A}{\delta\phi}\frac{\delta B}{\delta\pi} - \frac{\delta A}{\delta\pi}\frac{\delta B}{\delta\phi}\right). \tag{2.50}$$

Here $\frac{\delta}{\delta\phi}$ denotes the functional derivative defined as

$$\frac{\delta A}{\delta\phi} \equiv \frac{\partial \mathscr{A}}{\partial\phi} - \partial_\mu\left[\frac{\partial \mathscr{A}}{\partial(\partial_\mu\phi)}\right]. \tag{2.51}$$

In particular, the canonically conjugated fields satisfy the following equal time Poisson brackets

$$\begin{aligned}\{\phi(t,\mathbf{x}), \phi(t,\mathbf{x}')\}_{\mathrm{PB}} &= \{\pi(t,\mathbf{x}), \pi(t,\mathbf{x}')\}_{\mathrm{PB}} = 0,\\ \{\phi(t,\mathbf{x}), \pi(t,\mathbf{x}')\}_{\mathrm{PB}} &= \delta(\mathbf{x}-\mathbf{x}'),\end{aligned} \tag{2.52}$$

The canonical equations of motion are

$$\partial_0\phi(x) = \{\phi(x), H\}_{\mathrm{PB}}, \quad \partial_0\pi(x) = \{\pi(x), H\}_{\mathrm{PB}}, \tag{2.53}$$

where H is the Hamiltonian of the system.

In the case of the scalar field, a general solution of the classical field equations (2.46) can be obtained by working with the Fourier transform of the equation of motion

$$(\partial_\mu\partial^\mu + m^2)\phi(x) = 0 \quad \Longrightarrow \quad (-p^2 + m^2)\tilde{\phi}(p) = 0, \tag{2.54}$$

whose general solution can be written as[2]

$$\begin{aligned}\phi(x) &= \int \frac{d^4p}{(2\pi)^4}(2\pi)\delta(p^2-m^2)\theta(p^0)\Big[\alpha(p)e^{-ip\cdot x}+\alpha(p)^* e^{ip\cdot x}\Big] \\ &= \int \frac{d^3p}{(2\pi)^3}\frac{1}{2E_{\mathbf{p}}}\Big[\alpha(\mathbf{p})e^{-iE_{\mathbf{p}}t+\mathbf{p}\cdot\mathbf{x}}+\alpha(\mathbf{p})^* e^{iE_{\mathbf{p}}t-\mathbf{p}\cdot\mathbf{x}}\Big]\end{aligned} \tag{2.55}$$

and we have required $\phi(x)$ to be real. The conjugate momentum is

$$\pi(x) = -\frac{i}{2}\int\frac{d^3p}{(2\pi)^3}\Big[\alpha(\mathbf{p})e^{-iE_{\mathbf{p}}t+\mathbf{p}\cdot\mathbf{x}}-\alpha(\mathbf{p})^* e^{iE_{\mathbf{p}}t-\mathbf{p}\cdot\mathbf{x}}\Big]. \tag{2.56}$$

Canonical quantization proceeds by replacing classical fields with operators and Poisson brackets with commutators according to the rule

$$i\{\cdot,\cdot\}_{\text{PB}} \longrightarrow [\cdot,\cdot]. \tag{2.57}$$

Now $\phi(x)$ and $\pi(x)$ are promoted to operators by replacing the functions $\alpha(\mathbf{p})$, $\alpha(\mathbf{p})^*$ by the corresponding operators

$$\alpha(\mathbf{p}) \longrightarrow \hat{\alpha}(\mathbf{p}), \quad \alpha(\mathbf{p})^* \longrightarrow \hat{\alpha}^\dagger(\mathbf{p}). \tag{2.58}$$

Moreover, demanding $[\phi(t,\mathbf{x}),\pi(t,\mathbf{x}')] = i\delta(\mathbf{x}-\mathbf{x}')$ forces the operators $\hat{\alpha}(\mathbf{p})$, $\hat{\alpha}(\mathbf{p})^\dagger$ to have the commutation relations found in Eq. (2.29). Therefore they are identified as a set of creation-annihilation operators creating states with well-defined momentum $\mathbf{p}$ out of the vacuum $|0\rangle$. In the canonical quantization formalism the concept of particle appears as a result of the quantization of a classical field.

From the expressions of $\hat{\phi}$ and $\hat{\pi}$ in terms of the creation-annihilation operators we can evaluate the Hamiltonian operator. After a simple calculation one arrives at

$$\begin{aligned}\hat{H} &= \frac{1}{2}\int\frac{d^3p}{(2\pi)^3}\Big[\hat{\alpha}^\dagger(\mathbf{p})\hat{\alpha}(\mathbf{p})+(2\pi)^3E_{\mathbf{p}}\delta(\mathbf{0})\Big] \\ &= \int\frac{d^3p}{(2\pi)^3}\frac{1}{2E_{\mathbf{p}}}E_{\mathbf{p}}\hat{\alpha}^\dagger(\mathbf{p})\hat{\alpha}(\mathbf{p})+\frac{1}{2}\int d^3p\,E_{\mathbf{p}}\delta(\mathbf{0}).\end{aligned} \tag{2.59}$$

The first integral has a simple physical interpretation: the integrand is the number operator of particles with momentum $\mathbf{p}$, weighted by the energy $E_{\mathbf{p}}$ of the particle and integrated using the Lorentz-invariant measure. The second term diverges and it is equal to the expectation value of the Hamiltonian in the ground state, $\langle 0|\hat{H}|0\rangle$. It measures the energy stored in the vacuum.

We should make sense of the divergent vacuum energy in Eq. (2.59). It has two sources of divergence. One is of infrared origin and it is associated with the delta

[2] In momentum space, the general solution to this equation is $\tilde{\phi}(p) = f(p)\delta(p^2-m^2)$, with $f(p)$ a completely general function of p^μ. The solution in position space is obtained by inverse Fourier transform. The step function $\theta(p^0)$ enforces positivity of the energy.

function evaluated at $\mathbf{p} = \mathbf{0}$, reflecting the fact that we work in infinite volume. The second one comes from the integration of $E_{\mathbf{p}}$ at large values of the momentum and it is then an ultraviolet divergence. The infrared divergence can be regularized by putting the system in a box of finite but large volume and replacing $\delta(\mathbf{0}) \sim V$. Since now the momentum gets discretized, we have

$$E_{\text{vac}} \equiv \langle 0|\hat{H}|0\rangle = \sum_{\mathbf{p}} \frac{1}{2} E_{\mathbf{p}}. \tag{2.60}$$

Written in this form the interpretation of the vacuum energy is straightforward. A free scalar quantum field can be seen as a infinite collection of harmonic oscillators per unit volume, each one labelled by $\mathbf{p}$. Even if those oscillators are not excited, they contribute to the vacuum energy with their zero-point energy, given by $\frac{1}{2}E_{\mathbf{p}}$. Due to the ultraviolet divergence, the vacuum contribution to the energy adds up to infinity even working at finite volume: there are modes with arbitrary high momentum contributing to the sum, $p_i \sim \frac{n_i}{L_i}$, with L_i the sides of the box of volume V and n_i an integer.

For many practical purposes we can shift the origin of energies and subtract the vacuum energy. This is done by replacing $\hat{H}$ by the normal-ordered Hamiltonian

$$:\hat{H}:\equiv \hat{H} - \langle 0|\hat{H}|0\rangle = \frac{1}{2}\int \frac{d^3p}{(2\pi)^3}\hat{\alpha}^\dagger(\mathbf{p})\hat{\alpha}(\mathbf{p}). \tag{2.61}$$

In spite of this, in the next section we will see that under certain conditions the vacuum energy has observable effects. In addition, in general relativity the energy of the vacuum is a source of the gravitational field and contributes to the cosmological constant (see Chap. 12).

All relevant information about the free scalar field theory is encoded in the time-ordered correlation functions

$$G_n(x_1, \ldots, x_n) = \langle 0|T\Big[\hat{\phi}(x_1)\ldots\hat{\phi}(x_n)\Big]|0\rangle. \tag{2.62}$$

The symbol T indicates that we have a time-ordered product, i.e. the noncommuting field operators are multiplied in the order in which they occur in time. For example, for the time-ordered product of two scalar fields we have

$$T\Big[\hat{\phi}(x_1)\hat{\phi}(x_2)\Big] = \theta\left(x_1^0 - x_2^0\right)\hat{\phi}(x_1)\hat{\phi}(x_2) + \theta\left(x_2^0 - x_1^0\right)\hat{\phi}(x_2)\hat{\phi}(x_1). \tag{2.63}$$

The generalization to monomials with more than two operators is straightforward: operators evaluated at earlier times always appear to the right.

In the case of our free scalar field theory the only independent time-ordered correlation function is the Feynman propagator $G_2(x_1, x_2)$. After some manipulations, it can be written as

$$\langle 0|T\Big[\hat{\phi}(x_1)\hat{\phi}(x_2)\Big]|0\rangle = \int \frac{d^4p}{(2\pi)^4}\frac{ie^{-ip\cdot(x_1-x_2)}}{p^2 - m^2 + i\varepsilon}. \tag{2.64}$$

The term $i\varepsilon$ in the denominator is a reminder of how to surround the poles in the integration over p^0. This is crucial to reproduce correctly the step functions in the time-ordered product (2.63). To calculate higher order correlation functions one uses a mathematical result known as Wick's theorem that allows to write a time-ordered product as a combination of normal-ordered products with coefficients given by the Feynman propagator $G_2(x_1, x_2)$. We will not give a general proof but state it for the case of three fields

$$\begin{aligned} T\Big[\hat{\phi}(x_1)\hat{\phi}(x_2)\hat{\phi}(x_3)\Big] &= :\hat{\phi}(x_1)\hat{\phi}(x_2)\hat{\phi}(x_3): + \wick{\c1{\hat{\phi}}(x_1)\c1{\hat{\phi}}(x_2)} :\hat{\phi}(x_3): \\ &+ \hat{\phi}(x_1) : \wick{\c1{\hat{\phi}}(x_2)\c1{\hat{\phi}}(x_3)} + \wick{\c1{\hat{\phi}}(x_1) : \hat{\phi}(x_2) : \c1{\hat{\phi}}(x_3)}. \end{aligned} \tag{2.65}$$

The pairs of operators connected by braces, called Wick contractions, have to be replaced by a Feynman propagator according to

$$\wick{\c1{\hat{\phi}}(x_i)\c1{\hat{\phi}}(x_j)} \longrightarrow G_2(x_i, x_j). \tag{2.66}$$

From this example we read the structure of the general case: the time-ordered product of n fields can be written as the sum of all monomials of n fields with any number of Wick contractions (from 0 to the integer part of $\frac{n}{2}$) done in all possible nonequivalent ways. In each of these monomial the product of those fields that are not Wick-contracted is always normal ordered.[3]

Using this result the correlation functions (2.62) can be easily computed. Since the vacuum expectation value of a normal ordered operator is zero, the only terms that contribute are those in which all fields are Wick-contracted among themselves. This automatically implies that all time-ordered correlation functions with an odd number of scalar fields are equal to zero. For correlation functions with an even number of insertion we illustrate how it works in the case of the four-point function, where there are three different contractions

$$\begin{aligned} G_4(x_1, \ldots, x_4) =& \langle 0|T\Big[\wick{\c1{\hat{\phi}}(x_1)\c1{\hat{\phi}}(x_2)\c2{\hat{\phi}}(x_3)\c2{\hat{\phi}}(x_4)}\Big]|0\rangle \\ &+\langle 0|T\Big[\wick{\c1{\hat{\phi}}(x_1)\c2{\hat{\phi}}(x_2)\c1{\hat{\phi}}(x_3)\c2{\hat{\phi}}(x_4)}\Big]|0\rangle + \langle 0|T\Big[\wick{\c1{\hat{\phi}}(x_1)\c2{\hat{\phi}}(x_2)\c2{\hat{\phi}}(x_3)\c1{\hat{\phi}}(x_4)}\Big]|0\rangle. \end{aligned} \tag{2.67}$$

---

[3] We remind the reader that in a normal-ordered product all annihilation operators appear to the right.

Replacing now each Wick contraction by the corresponding propagator according to (2.66), we find

$$G_4(x_1,\ldots,x_4) = G_2(x_1,x_2)G_2(x_3,x_4) + G_2(x_1,x_3)G_2(x_2,x_4) + G_2(x_1,x_4)G_2(x_2,x_3). \tag{2.68}$$

Any other correlation function is computed in terms of $G_2(x_1, x_2)$ following the same algorithm. In fact, this property is the defining feature of *any* free quantum field theory: the propagator completely determines all other correlation functions of the theory.

2.3 The Casimir Effect

The vacuum energy encountered in the quantization of the free scalar field is not exclusive of this theory. It is also present in other field theories and in particular in quantum electrodynamics. In 1948 Hendrik Casimir pointed out [1] that although a formally divergent vacuum energy would not be observable, any variation in this energy would be (see [2–4] for comprehensive reviews).

To show this he devised the following experiment. Consider a couple of infinite, perfectly conducting plates placed parallel to each other at a distance d (see Fig. 2.1). The plates fix the boundary condition of the vacuum modes of the electromagnetic field. These modes are discrete in between the plates (region II), while outside them they have a continuous spectrum (regions I and III). The vacuum energy of the electromagnetic field is equal to that of two massless scalar fields, corresponding to the two physical polarizations of the photon (see Sect. 4.2). Hence we can apply the formulae derived above.

A naive calculation of the vacuum energy in this system gives a divergent result. This infinity can be removed by subtracting the vacuum energy corresponding to the situation where the plates are removed

$$E(d)_{\text{reg}} = E(d)_{\text{vac}} - E(\infty)_{\text{vac}}. \tag{2.69}$$

This subtraction cancels the contribution of all the modes outside the plates. The boundary conditions of the electromagnetic field at the conducting plates dictate the quantization of the momentum modes perpendicular to them according to $p_\perp = \frac{n\pi}{d}$, with n a non-negative integer. When the size of the plates is much larger than their separation d, the momenta parallel to the plates $\mathbf{p}_\parallel$ can be treated as continuous. For $n > 0$ there are two polarizations for each vacuum mode of the electromagnetic field, each one contributing

$$\frac{1}{2}\sqrt{\mathbf{p}_\parallel^2 + p_\perp^2} \tag{2.70}$$

to the vacuum energy. When $p_\perp = 0$ (i.e., $n = 0$) the modes of the field are effectively (2+1)-dimensional and there is only one physical polarization. Taking all these

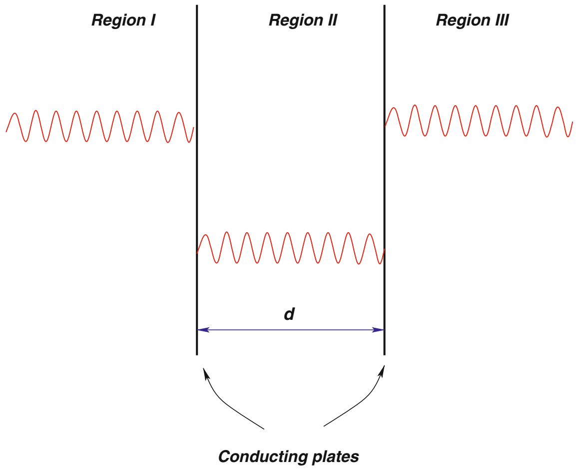

Fig. 2.1 Illustration of the Casimir effect. In regions I and II the spetrum of modes of the momentum $p_\perp$ is continuous, while in the space between the plates (region II) it is quantized in units of $\frac{\pi}{d}$

elements into account, we write

$$E(d)_{\text{reg}} = S\int \frac{d^2p_\parallel}{(2\pi)^2}\frac{1}{2}|\mathbf{p}_\parallel| + 2S\int \frac{d^2p_\parallel}{(2\pi)^2}\sum_{n=1}^{\infty}\frac{1}{2}\sqrt{\mathbf{p}_\parallel^2+\left(\frac{n\pi}{d}\right)^2} - 2Sd\int\frac{d^3p}{(2\pi)^3}\frac{1}{2}|\mathbf{p}|, \tag{2.71}$$

where S is the area of the plates. The factors of two count the two propagating degrees of freedom of the electromagnetic field, as discussed above.

The integrals and the infinite sum in Eq. (2.71) are divergent. In order to define them we insert an exponential damping factor[4]

$$E(d)_{\text{reg}} = \frac{1}{2}S\int\frac{d^2p_\perp}{(2\pi)^2}e^{-\frac{1}{\Lambda}|\mathbf{p}_\parallel|}|\mathbf{p}_\parallel| + S\sum_{n=1}^{\infty}\int\frac{d^2p_\parallel}{(2\pi)^2}e^{-\frac{1}{\Lambda}\sqrt{\mathbf{p}_\parallel^2+(\frac{n\pi}{d})^2}}\sqrt{\mathbf{p}_\parallel^2+\left(\frac{n\pi}{d}\right)^2} - Sd\int_{-\infty}^{\infty}\frac{dp_\perp}{2\pi}\int\frac{d^2p_\parallel}{(2\pi)^2}e^{-\frac{1}{\Lambda}\sqrt{\mathbf{p}_\parallel^2+p_\perp^2}}\sqrt{\mathbf{p}_\parallel^2+p_\perp^2}, \tag{2.72}$$

where Λ is an ultraviolet cutoff. It is now straightforward to see that in terms of the function

[4] Alternatively, one could introduce any cutoff function $f(p_\perp^2+p_\parallel^2)$ going to zero fast enough as $p_\perp,\ p_\parallel\to\infty$. The result is independent of the particular function used in the calculation.

$$F(x) = \frac{1}{2\pi}\int_0^\infty y\,dy\,e^{-\frac{1}{\Lambda}\sqrt{y^2+(\frac{x\pi}{d})^2}}\sqrt{y^2+\left(\frac{x\pi}{d}\right)^2}$$
$$= \frac{1}{4\pi}\int_{(\frac{x\pi}{d})^2}^\infty dz\,e^{-\frac{\sqrt{z}}{\Lambda}}\sqrt{z} \tag{2.73}$$

the regularized vacuum energy can be written as

$$E(d)_{\rm reg} = S\left[\frac{1}{2}F(0) + \sum_{n=1}^{\infty}F(n) - \int_0^\infty dx\,F(x)\right]. \tag{2.74}$$

This expression can be evaluated using the Euler-MacLaurin formula [5]

$$\sum_{n=1}^{\infty}F(n) - \int_0^\infty dx\,F(x) = -\frac{1}{2}\left[F(0)+F(\infty)\right] + \frac{1}{12}\left[F'(\infty) - F'(0)\right]$$
$$-\frac{1}{720}\left[F'''(\infty) - F'''(0)\right] + \cdots \tag{2.75}$$

Our function satisfies $F(\infty) = F'(\infty) = F'''(\infty) = 0$ and $F'(0) = 0$, whereas higher derivative terms give contributions that go to zero as the cutoff is sent to infinity. Hence the value of $E(d)_{\rm reg}$ is determined by $F'''(0)$. Computing this term and taking the limit $\Lambda \to \infty$ we find the result

$$E(d)_{\rm reg} = \frac{S}{720}F'''(0) = -\frac{\pi^2 S}{720 d^3}. \tag{2.76}$$

This shows that the vacuum energy between the two plates decreases when their separation is reduced. Therefore there should be a force per unit area between the plates given by

$$P_{\rm Casimir} = -\frac{\pi^2}{240}\frac{1}{d^4}. \tag{2.77}$$

The minus sign indicates that the force is attractive. This is called the Casimir effect. It was experimentally measured for the first time in 1958 by Sparnaay [6] and since then the Casimir effect has been checked with better and better precision in a variety of situations [2–4].

2.4 Path Integrals

The canonical quantization formalism relies in the Hamiltonian formulation of the theory. It has the obvious disadvantage of singling out time from the spatial coordinates, making Lorentz covariance nonexplicit. This could be avoided if quantization could be carried out directly in the Lagrangian formalism, where Lorentz covariance is explicit. This is achieved by the path integral quantization method introduced by Feynman [7, 8]. In addition, when applied to the quantization of fields, path integral quantization presents many advantages over canonical quantization.

To describe the main ideas of path integral quantization we will not enter into technical details that can be found in many available textbooks [9–12]. Also, to make the discussion more transparent, we first illustrate the method in the case of nonrelativistic quantum mechanical system with a single degree of freedom denoted by q and Lagrangian $L(q, \dot{q})$. To quantize this theory we only need to know its propagator defined by

$$K(q, q'; \tau) = \langle q'; \tau | q; 0 \rangle. \tag{2.78}$$

Here we have used the Heisenberg representation where the time-independent eigenstates of the time-dependent operator $q(t)$ are denoted by $|q; t\rangle$. Physically, $K(q, q'; \tau)$ represents the amplitude for the system to "propagate" from q to q' in a time τ. That the knowledge of the propagator is enough to solve the quantum system can be seen by noticing that the Schrödinger wave function $\psi(t, q)$ at any time can be written in terms of the initial data as

$$\psi(t, q') = \int_{-\infty}^{\infty} dq \, K(q, q'; t) \psi(0, q). \tag{2.79}$$

This equation follows from the fact that $K(q, q'; \tau)$ is the Green function of the time-dependent Schrödinger wave equation.

Another physically meaningful quantity is the fixed-energy propagator, defined in terms of (2.78) by[5]

$$G(q, q'; E) = \int_{0}^{\infty} d\tau \, e^{\frac{i}{\hbar} E \tau} K(q, q'; \tau). \tag{2.80}$$

This propagator is the Green function for the time-independent Schrödinger problem $(\hat{H} - E)\psi(t, q) = 0$. In fact, $G(q, q'; E)$ contains all the information about the spectrum of the theory codified in the structure of its singularities in the complex E plane.

Both $K(q, q'; \tau)$ and $G(q, q'; E)$ can be calculated using canonical quantization. Here instead we would rather follow the Lagrangian formalism and use of the following observation due to Dirac [13]

$$\langle q + \delta q; t + \delta t | q; t \rangle \sim \exp\left[\frac{i}{\hbar} \delta t \, L\left(q, \frac{\delta q}{\delta t}\right)\right]. \tag{2.81}$$

[5] For the remaining of this chapter we restore the powers of $\hbar$.

It states that the amplitude for the propagation of the system between q and $q+\delta q$ in an infinitesimal time δt can be expressed in terms of the Lagrangian function of the system. We justify this equation in the case of a particle moving in one dimension in the presence of a potential *V(q)*,

$$\begin{aligned}\langle q+\delta q; t+\delta t|q; t\rangle &= \langle q+\delta q|e^{-\frac{i}{\hbar}\delta t\hat{H}}|q\rangle \\ &= \langle q+\delta q|e^{-\frac{i}{\hbar}\delta t\left[\frac{\hat{p}^2}{2m}+V(\hat{q})\right]}|q\rangle. \end{aligned} \tag{2.82}$$

The kinetic and potential energy in the exponent can be taken to commute up to terms of order $(\delta t)^2$. Hence, to linear order in δt, the exponential can be split into two terms depending respectively on $\hat{q}$ and $\hat{p}$. Inserting between them the completeness relation for the momentum eigenstates we find

$$\langle q+\delta q; t+\delta t|q; t\rangle = \int\limits_{-\infty}^{\infty} dp e^{\frac{i}{\hbar}p\delta q-\frac{i}{\hbar}\delta t\left[\frac{p^2}{2m}-V(q)\right]}. \tag{2.83}$$

We complete now the square and perform the Gaussian integration over the momentum to arrive at

$$\langle q+\delta q; t+\delta t|q; t\rangle = \sqrt{\frac{m}{2\pi i\hbar\delta t}}e^{\frac{i}{\hbar}\left[\frac{1}{2}m\left(\frac{\delta q}{\delta t}\right)^2-V(q)\right]}. \tag{2.84}$$

This calculation shows that the proportionality constant omitted in Eq. (2.81) does not depend on the value of the coordinate q.

To compute the propagator (2.78) we split the time interval τ in $N+1$ subintervals of duration δt and insert the identity, $\int dq|q; n\delta t\rangle\langle q; n\delta t| = 1$ for $n = 1,\ldots,N$, at each intermediate time

$$K(q,q';\tau) = \left(\int\limits_{-\infty}^{\infty}\prod_{i=1}^{N}dq_i\right)\langle q';\tau|q_N;N\delta t\rangle\ldots\langle q_1;\delta t|q;0\rangle. \tag{2.85}$$

This representation of the propagator can be interpreted as a summation over continuous discretized paths defined by $q_n = q(n\delta t)$ and satisfying the boundary conditions $q(0) = q,\ q(\tau) = q$. We can go now to the continuous limit of the path by taking $\delta t \to 0$ and $N \to \infty$ while keeping $N\delta t = \tau$ fixed. Then, each overlap inside the integral can be evaluated using Eq. (2.81) and the result defines the path integral

$$\langle q';\tau|q;0\rangle = \mathcal{N}\int\limits_{\substack{q(0)=q\\ q(\tau)=q'}}\mathscr{D}q(t)\exp\left[\frac{i}{\hbar}\int\limits_0^{\tau}dt L(q,\dot{q})\right], \tag{2.86}$$

where $\mathscr{N}$ is a normalization constant. This equation is a shorthand to indicate that the quantum mechanical amplitude (2.78) is obtained by summing over *all* possible trajectories $q(t)$ joining the points q and q' in a time τ, each one weighted by a phase given by the action of the corresponding trajectory measured in units of $\hbar$.

From a purely technical point of view, the path integral formulation of quantum mechanics does not present any important advantage over other quantization methods, notably canonical quantization. It is however in quantum field theory that path integrals show their real power. Path integrals for quantum field theories can be constructed by looking at a quantum field $\phi(t, \mathbf{x})$ as a quantum mechanical system with one degree of freedom per point of space $\mathbf{x}$. In other words, $\mathbf{x}$ is treated as a (continuous) label counting the number of degrees of freedom of the system. Now, as in the quantum mechanical case, path integrals can be used to write the amplitude for the system to evolve from the field configuration $\phi_0(\mathbf{x})$ at $t = 0$ to $\phi_1(\mathbf{x})$ at $t = \tau$.

$$\langle\phi_1(\mathbf{x}); \tau|\phi_0(\mathbf{x}); 0\rangle = \mathscr{N} \int\limits_{\substack{\phi(0,\mathbf{x})=\phi_0(\mathbf{x}) \\ \phi(\tau,\mathbf{x})=\phi_1(\mathbf{x})}} \mathscr{D}\phi(t, \mathbf{x}) e^{\frac{i}{\hbar}S[\phi(t,\mathbf{x})]}, \tag{2.87}$$

where $S[\phi(t, \mathbf{x})]$ is the action functional of the theory. As above, this expression states that the amplitude is obtained by summing over all field configurations interpolating between the boundary values at $t = 0$, and $t = \tau$, each one multiplied by the phase factor $\exp\{\frac{i}{\hbar}S[\phi(t, \mathbf{x})]\}$.

Far more interesting, however, than the amplitudes (2.87) are the time-ordered correlation functions of fields that we already studied in the case of a free scalar field. For an interacting theory they are generalized to

$$G_n(x_1, \ldots, x_n) = \langle\Omega|T\Big[\hat{\phi}(x_1)\ldots\hat{\phi}(x_n)\Big]|\Omega\rangle. \tag{2.88}$$

where $|\Omega\rangle$ is the ground state of the theory. In Chap. 6 we will explain how the correlation functions (2.88) are related to scattering amplitudes. Here we only want to point out that they admit the following path integral representation[6]

$$\langle\Omega|T\Big[\hat{\phi}(x_1)\ldots\hat{\phi}(x_n)\Big]|\Omega\rangle = \frac{\int\mathscr{D}\phi(x)\phi(x_1)\ldots\phi(x_n)e^{\frac{i}{\hbar}S[\phi(x)]}}{\int\mathscr{D}\phi(x)e^{\frac{i}{\hbar}S[\phi(x)]}}. \tag{2.89}$$

In the left-hand side of this expression $\hat{\phi}(x)$ is the field operator, while in the right-hand side $\phi(x)$ represents a commuting function of the space-time coordinates. Unlike Eq. (2.87), here the functional integration is performed over *all* field configurations irrespective of any boundary conditions. Moreover, given that (2.89) contains the quotient of two path integrals the overall numerical normalization $\mathscr{N}$ cancels

6 Here we focus on bosonic fields. Path integrals for fermions will be discussed in Chap. 3 (see page 43).

out. A salient feature of path integrals to be noticed here is that they automatically implement time ordering.

Path integrals are not easy to evaluate. In fact they cannot be computed exactly in most cases. This notwithstanding, path integrals provide an extremely useful tool in quantum field theory. They can be formally manipulated to obtain results whose derivation using canonical quantization methods would be much harder. The only path integrals that can be computed exactly are the so-called *Gaussian integrals* where the action functional of the theory is at most quadratic in the fields. This is the case, for example, of the free scalar field theory whose canonical quantization we studied in Sect. 2.2.

2.5 The Semiclassical Limit

One of the most interesting aspects of the application of the path integral formalism to quantum mechanics is that it clarifies how the classical laws of motion emerge from quantum dynamics. In the limit $\hbar \to 0$ the phase $\exp\left(\frac{i}{\hbar}S\right)$ varies wildly when going from a path to a neighboring one. The consequence is that the contributions from these paths to the propagator tend to cancel each other. There is however one important exception to this that are those trajectories making the action stationary. Since the linear perturbation of the action around these paths vanishes, these are the only ones contributing to the functional integral (2.86) in the classical limit. This is the way in which the classical laws of mechanics are recovered.

It is kind of remarkable how the principle of least action can be seen in this light as a residual effect of quantum physics. What from the point of view of classical mechanics is just an elegant principle to derive the Newtonian equations of motion is in fact hinting at the existence of an underlying theory.

We can make this qualitative discussion more precise by looking at the case of a nonrelativistic quantum particle moving in one dimension in the presence of a potential $V(q)$. The Lagrangian function of the system is

$$L(q, \dot{q}) = \frac{1}{2}m\dot{q}^2 - V(q). \tag{2.90}$$

We have argued that in the limit $\hbar \to 0$ the path integral (2.86) is dominated by paths around the classical solution $q_{\rm cl}(t)$ that solves the equations of motion with the appropriate boundary conditions. Thus, the propagator $K(q, q'; \tau)$ can be computed in the semiclassical limit by considering only the contribution to the path integral coming from paths that are "close" to the classical one. In technical terms this means that we write

$$q(t) = q_{\rm cl}(t) + \sqrt{\hbar}\delta q(t) \tag{2.91}$$

and integrate over the perturbation $\delta q(t)$ keeping in the action only terms that are at most linear in $\hbar$

$$S[q] = S_{\rm cl}[q, q'; \tau] + \frac{\hbar}{2}\int_0^\tau dt\Big[m(\delta\dot{q})^2 - V''(q_{\rm cl})(\delta q)^2\Big] + \mathscr{O}(\hbar^3). \tag{2.92}$$

Here $S_{\rm cl}[q, q'; \tau]$ is the action evaluated on the classical trajectory with the boundary conditions $q(0) = q$ and $q(\tau) = q'$. Since $q_{\rm cl}(t)$ satisfies the classical equations of motion, the term linear in the perturbation vanishes.

With this prescription, the semiclassical propagator is given by

$$\begin{aligned} K(q, q'; \tau) &\overset{\hbar\to 0}{\approx} \mathscr{N} e^{\frac{i}{\hbar}S_{\rm cl}[q,q';\tau]} \int\limits_{\substack{\delta q(0)=0\\ \delta q(\tau)=0}} \mathscr{D}(\delta q)\, e^{\frac{i}{2}\int_0^\tau dt\left[m(\delta\dot{q})^2 - V^n\left(q_{cl}(\delta q)^2\right)\right]} \\ &= \mathscr{N}\sqrt{\frac{i}{2\pi\hbar}\frac{\partial^2 S_{\rm cl}[q, q'; \tau]}{\partial q\,\partial q'}}\, e^{\frac{i}{\hbar}S_{\rm cl}[q,q';\tau]}. \end{aligned} \tag{2.93}$$

Since the classical solution $q_{\rm cl}(t)$ satisfies the boundary conditions, the perturbation $\delta q(t)$ has to vanish at both $t = 0$ and $t = \tau$. The path integral over the fluctuations is Gaussian and can be computed exactly for any potential $V(q)$. Its evaluation is however nontrivial. The details of the calculation can be found in the literature [9–12].

A similar analysis can be applied to the computation of the semiclassical limit of the fixed-energy propagator $G(q, q'; E)$ defined in Eq. (2.80). Using the semiclassical expression for the full propagator (2.93) we are left with the integral

$$G(q, q'; E) \overset{\hbar\to 0}{\approx} \mathscr{N}\int_0^\infty d\tau \sqrt{\frac{i}{2\pi\hbar}\frac{\partial^2 S_{\rm cl}[q, q'; \tau]}{\partial q\,\partial q'}}\, e^{\frac{i}{\hbar}\{E\tau + S_{\rm cl}[q,q';\tau]\}}, \tag{2.94}$$

that has to be evaluated using the stationary phase method. The value $\tau = \tau_c$ that makes the phase stationary is the one solving the equation

$$E + \frac{\partial}{\partial\tau}S_{\rm cl}[q, q'; \tau]\bigg|_{\tau=\tau_c} = 0. \tag{2.95}$$

In this expression we recognize the Hamilton-Jacobi equation for a particle with constant energy E. Hence, the path dominating the path integral in the semiclassical computation of $G(q, q'; E)$ is the one solving the classical equation of motion

$$\dot{q}_{\rm cl}(\tau)^2 = \frac{2}{m}\Big[E - V(q_{\rm cl})\Big]. \tag{2.96}$$

and connecting the points q and q'. The calculation of τ_c reduces to the following quadrature

$$\tau_c = \sqrt{\frac{m}{2}} \int_q^{q'} \frac{dz}{\sqrt{E - V(z)}}. \tag{2.97}$$

The calculation of the semiclassical propagators requires some extra care in situations where quantum tunneling can occur. This is the case, for example, of a particle propagating in a barrier potential where the points q and q' are on different sides of the barrier. The calculation of $K(q, q'; \tau)$ in the limit $\hbar \to 0$ can be done in this case following the steps we have described, since there is always an above-the-barrier classical trajectory joining the points q and q' in a time τ that dominates the path integral.

The problem comes in the computation of $G(q, q'; E)$ when E is lower that the maximum of the barrier, $E < \max[V(q)]$. In this case there are no classical trajectories going through the classically forbidden region and therefore no saddle point value for the integral (2.94) is found in the domain of integration.

The key to solving the problem lies in performing an analytic continuation on the integrand of (2.94) and deforming the integration contour to capture the saddle points that occur for complex values of τ. For simplicity we concentrate on the case shown on the left panel of Fig. 2.2 where q and q' correspond to the classical turning points of a trajectory with energy E. Now, to compute the saddle point values of τ we have to continue the integrand of (2.97) and deform the contour of integration to surround the branch cut joining q and q'. As it happens, there is an infinite number of critical values given by[7]

$$\tau_n = -i(2n+1)\sqrt{\frac{m}{2}} \int_q^{q'} \frac{dx}{\sqrt{V(x) - E}}, \quad n = 0, 1, \ldots \tag{2.98}$$

Here n is the number of times the contour surrounds the branch cut before reaching the endpoint. As a matter of fact we only need to consider the saddle point with $n = 0$, since the remaining ones give contributions to the semiclassical limit of $G(q, q'; E)$ that are exponentially suppressed with respect to it.

This analysis shows that the quantum tunneling under a barrier proceeds semiclassically *as if* the particle is propagating in imaginary time. A look at Eq. (2.94) leads to a nice interpretation of this fact. This expression says that there are infinitely many classical trajectories connecting the points q and q' that contribute to the fixed-energy propagator describing the tunneling process. As we explained above, all these real-time trajectories have energies above the height of the barrier. However, when $E < \max\{V(q)\}$ and in the limit $\hbar \to 0$, the coherent effect of all these paths is "resummed" into a single imaginary-time trajectory with an energy below the maximum of the barrier. This is called an *instanton*.

[7] There is a global sign ambiguity associated with the sense in which the integration contour surrounds the branch cut. Here we take it clockwise.

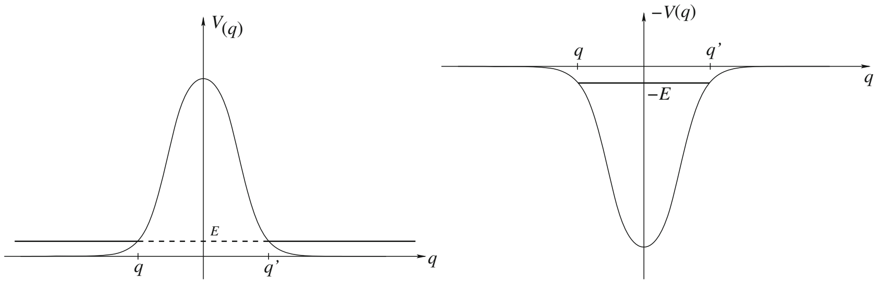

Fig. 2.2 On the left picture the tunneling of a particle with energy E from q to q' through the potential barrier is represented. In the right panel we have depicted the Euclidean trajectory describing this semiclassical tunneling

In fact, the imaginary-time trajectory that is found to dominate the path integral computation of $G(q, q'; E)$ in the semiclassical limit is a solution of the equations of motion derived from the Euclidean action $S_E[q]$, obtained by analytically continuing the action of the system to imaginary times

$$S[q] \overset{\tau\to -i\tau}{\to} \quad iS_E[q] = i\int_0^{\tau} dt\left[\frac{1}{2}m\dot{q}^2 + V(q)\right] \tag{2.99}$$

and the equations of motion of the Euclidean trajectories of energy E are

$$\dot{q}_{\rm cl}^2 = \frac{2}{m}\Big[-E + V(q_{\rm cl})\Big]. \tag{2.100}$$

Heuristically these equations can be interpreted as those of a "real" particle with energy $-E$ in the inverted potential $-V(q)$ (see the right panel of Fig. 2.2). From this point of view, the infinite number of saddle points trajectories found above correspond to this particle bouncing n times in the inverted potential before reaching the endpoint at q'. It should be clear, however, that the time parameter in Eq. (2.100) does not have any meaning as a physical time.

The previous discussion carries over to field theory. By the same arguments used above, the path integrals in (2.87) and (2.89) are dominated in the limit $\hbar \to 0$ by those field configurations making the action stationary, that is, satisfying the Euler–Lagrange equations. The semiclassical approximation is obtained by expanding around these classical field solutions to second order in the perturbations and carrying out the resulting Gaussian integral.

Field theories can have many vacua separated by energy barriers. For example, a scalar field theory

$$S[\phi] = \int d^4x\left[\frac{1}{2}\eta^{\mu\nu}\partial_\mu\phi\partial_\nu\phi - V(\phi)\right]. \tag{2.101}$$

has as many vacua as local minima of the potential $V(\phi)$, that we assume to be bounded from below. The spectrum of excitations around each vacuum can be computed using perturbation theory in powers of the corresponding coupling constant. The perturbative analysis, however, is blind to transitions between different vacua due to quantum tunneling.

The lesson we have learned in quantum mechanics can now be used to study the semiclassical tunneling between different vacua in a field theory by means of an analytic continuation to imaginary times. Letting $t \to -it$, the Minkowski spacetime transforms in Euclidean space

$$ds^2 = \eta_{\mu\nu}dx^\mu dx^\nu \quad \Longrightarrow \quad ds^2 = -\delta_{\mu\nu}dx^\mu dx^\nu. \tag{2.102}$$

In the example of the scalar field theory discussed above, this analytical continuation to imaginary time leads to the Euclidean action

$$S_E[\phi] = \int d^4x \left[\frac{1}{2}\delta^{\mu\nu}\partial_\mu\phi\partial_\nu\phi + V(\phi)\right]. \tag{2.103}$$

Instantons, i.e. the solution to the field equations derived from this action, are interpreted in quantum field theory as representing semiclassical tunneling between the different vacua of the theory. In Chap. 4 we will study field theory instantons in some more detail in the case of nonabelian gauge theories, where their existence has important physical consequences.

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