4

From harmonic oscillators to fields

Summary Ensemble of harmonic oscillators. Field quantization and mode expansion. Vacuum energy. Schrödinger equation for quantum fields.

4.1 Quantum harmonic oscillators

A free field can be treated as a set of infinitely many harmonic oscillators. Therefore we quantize a scalar field by simply generalizing the method used to describe a finite set of oscillators.

The most general classical action describing N harmonic oscillators with generalized coordinates $q_1, \ldots, q_N$ is

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

where the matrix M_{ij} is symmetric and positive-definite.

By choosing an appropriate set of normal coordinates

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

the matrix M_{ij} can be diagonalized, $M_{ij} \to M_{\alpha\beta} = \delta_{\alpha\beta} \omega_\alpha^2$, and the oscillators "decoupled" from each other. In terms of these new coordinates the action (4.1) reduces to

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

where ω_α are the eigenfrequencies.

Exercise 4.1
Find a linear transformation which "decouples" the oscillators.

For brevity, we shall omit the tilde and write q_α instead of $\tilde{q}_\alpha$ below. The normal modes q_α are quantized (in the Heisenberg picture) by introducing the operators $\hat{q}_\alpha(t)$, $\hat{p}_\alpha(t)$ which satisfy the standard equal-time commutation relations:

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

In turn, the creation and annihilation operators $\hat{a}_\alpha^\pm(t)$, defined as

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

obey the equations similar to (3.5) and (3.6):

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

The general solution of these equations for each oscillator is

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

where ${}^{(0)}\hat{a}_\alpha^\pm$ are operator-valued constants of integration which satisfy the commutation relations

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

Below we shall use mostly *time-independent* operators ${}^{(0)}\hat{a}$, so we skip the cumbersome superscript ${}^{(0)}$ and denote them simply by $\hat{a}_\alpha^\pm$.

The Hilbert space for the system of oscillators is constructed, as usual, with the help of the operators $\hat{a}_\alpha^\pm$. In particular, the vacuum state $|0, \ldots, 0\rangle$ is the unique eigenvector of all annihilation operators $\hat{a}_\alpha^-$ with eigenvalue 0:

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

The state $|n_1, n_2, \ldots, n_N\rangle$ with occupation numbers n_α for each oscillator q_α is defined by

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

and the vectors $|n_1, \ldots, n_N\rangle$, with all possible choices of occupation numbers n_α, span the whole Hilbert space.

4.2 From oscillators to fields

A *classical field* is described by a function, $\phi(\mathbf{x}, t)$, characterizing the field strength at every moment t and at each point $\mathbf{x}$ in space. One can interpret a field as an infinite set of oscillators $q_i(t) \Longleftrightarrow \phi_\mathbf{x}(t)$ "attached" to each point $\mathbf{x}$. Note that the oscillator "position" $\phi_\mathbf{x}(t)$ "takes its values" in the configuration space, i.e. in the space of the field strength. The spatial coordinate $\mathbf{x}$ plays the role of index labeling the oscillators, similarly to the discrete index i for the oscillators q_i.

Using this analogy, we treat the scalar field $\phi(\mathbf{x}, t)$ as an infinite collection of oscillators. Replacing the sums over the discrete indices i by the integrals over the continuous indices $\mathbf{x}$ in (4.1) we find that the action for the scalar field must be of the form

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

where the function M is yet to be determined. This action must be invariant with respect to the Lorentz transformations and to the spacetime translations (the *Poincaré group*). The simplest Poincaré-invariant action for a real scalar field $\phi(\mathbf{x}, t)$ is obtained if we set

$$M(\mathbf{x}, \mathbf{y}) = \left[-\Delta_{\mathbf{x}} + m^2\right]\delta(\mathbf{x} - \mathbf{y}). \quad (4.4)$$

Then action (4.3) becomes

$$\begin{aligned} S[\phi] &= \frac{1}{2}\int d^4x \left[\eta^{\mu\nu}(\partial_\mu\phi)(\partial_\nu\phi) - m^2\phi^2\right] \\ &= \frac{1}{2}\int d^3\mathbf{x}\, dt \left[\dot{\phi}^2 - (\nabla\phi)^2 - m^2\phi^2\right], \end{aligned} \quad (4.5)$$

where $\eta^{\mu\nu} = \mathrm{diag}(1, -1, -1, -1)$, $x^0 \equiv t$ and $(x^1, x^2, x^3) \equiv \mathbf{x}$. It is obviously translationally invariant, and Lorentz invariance is the subject of the next exercise.

Exercise 4.2

Verify that the action (4.5) does not change under the Lorentz transformations:

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

where the matrix Λ^μ_ν satisfies

$$\eta_{\mu\nu}\Lambda^\mu_\alpha\Lambda^\nu_\beta = \eta_{\alpha\beta}.$$

Calculating the functional derivative, we find that the scalar field satisfies the equation of motion

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

Exercise 4.3

Derive equation (4.7).

It is clear from (4.7) that the "oscillators" $\phi(\mathbf{x}, t) \equiv \phi_{\mathbf{x}}(t)$ are "coupled." To see this, note that the Laplacian $\Delta\phi$ contains the second derivatives of ϕ with respect to the spatial coordinates and, in particular,

$$\frac{\partial^2 \phi_x}{\partial x^2} \approx \frac{\phi_{x+\delta x} - 2\phi_x + \phi_{x-\delta x}}{(\delta x)^2}.$$

Therefore the behavior of the oscillator ϕ_x depends on the nearby oscillators at points $x \pm \delta x$.

To decouple the oscillators, we use the Fourier transform,

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

Substituting (4.8) into (4.7), we find that the complex functions $\phi_{\mathbf{k}}(t)$ satisfy the following ordinary differential equations,

$$\frac{d^2}{dt^2}\phi_{\mathbf{k}}(t) + \left(k^2 + m^2\right)\phi_{\mathbf{k}}(t) = 0, \tag{4.9}$$

and thus describe an infinite set of decoupled harmonic oscillators with frequencies

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

It is easy to verify that in terms of $\phi_{\mathbf{k}}(t)$ the action (4.5) takes the following form

$$S = \frac{1}{2}\int dt\, d^3\mathbf{k} \left(\dot{\phi}_{\mathbf{k}}\dot{\phi}_{-\mathbf{k}} - \omega_k^2 \phi_{\mathbf{k}}\phi_{-\mathbf{k}}\right). \tag{4.10}$$

Exercise 4.4

Show that for a real scalar field $\phi(\mathbf{x}, t)$ the relation $(\phi_{\mathbf{k}})^* = \phi_{-\mathbf{k}}$ must be satisfied.

4.3 Quantizing fields in a flat spacetime

To quantize the scalar field, we first need to reformulate the classical theory in the Hamiltonian formalism. Noting that the action is an integral of the Lagrangian only over the *time* (but not over space), we conclude that for the system described by the action (4.5) the Lagrangian is

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

where $\mathcal{L}$ is called the Lagrangian density. Taken at a given moment of time, the Lagrangian is a functional that depends on the field configuration. Therefore, the canonical momenta are defined as the functional derivatives of the Lagrangian with respect to the generalized "velocities" $\dot{\phi} \equiv \partial\phi/\partial t$,

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

The classical Hamiltonian is then

$$H = \int \pi(\mathbf{x},t)\,\dot{\phi}(\mathbf{x},t)\,d^3\mathbf{x} - L = \frac{1}{2}\int d^3\mathbf{x}\left[\pi^2 + (\nabla\phi)^2 + m^2\phi^2\right], \tag{4.11}$$

and the Hamilton equations of motion are

$$\frac{\partial\phi(\mathbf{x},t)}{\partial t} = \frac{\delta H}{\delta\pi(\mathbf{x},t)} = \pi(\mathbf{x},t),$$

$$\frac{\partial\pi(\mathbf{x},t)}{\partial t} = -\frac{\delta H}{\delta\phi(\mathbf{x},t)} = \Delta\phi(\mathbf{x},t) - m^2\phi(\mathbf{x},t). \tag{4.12}$$

Remark: Lorentz invariance We have noted previously that the Hamiltonian formalism is better suited for quantization. Although the Lorentz invariance is not manifest in the Hamiltonian formalism, this does not mean that the resulting quantum theory breaks this invariance. If the classical theory is relativistically invariant, then the resulting quantum theory is also relativistically invariant.

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

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

$$\left[\hat{\phi}(\mathbf{x},t),\,\hat{\phi}(\mathbf{y},t)\right] = \left[\hat{\pi}(\mathbf{x},t),\,\hat{\pi}(\mathbf{y},t)\right] = 0.$$

Substituting

$$\hat{\phi}(\mathbf{x},t) = \int \frac{d^3\mathbf{k}}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot\mathbf{x}}\hat{\phi}_{\mathbf{k}}(t), \quad \hat{\pi}(\mathbf{y},t) = \int \frac{d^3\mathbf{k}'}{(2\pi)^{3/2}} e^{i\mathbf{k}'\cdot\mathbf{y}}\hat{\pi}_{\mathbf{k}'}(t) \tag{4.14}$$

into these commutation relations, after some algebra we find the following result for the mode operators:

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

Note that the plus sign in $\delta(\mathbf{k}+\mathbf{k}')$ indicates that the variable conjugate to $\hat{\phi}_{\mathbf{k}}$ is $\hat{\pi}_{-\mathbf{k}} = (\hat{\pi}_{\mathbf{k}})^\dagger$. This is also evident from the action (4.10).

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

Substituting (4.14) into the Hamilton equations (4.12) we obtain

$$\frac{d\hat{\phi}_{\mathbf{k}}}{dt} = \hat{\pi}_{\mathbf{k}}, \quad \frac{d\hat{\pi}_{\mathbf{k}}}{dt} = -\omega_k^2\hat{\phi}_{\mathbf{k}}. \tag{4.15}$$

Similarly to Section 4.1, it is convenient to introduce the creation and annihilation operators,

$$\hat{a}_{\mathbf{k}}^{-}(t) \equiv \sqrt{\frac{\omega_k}{2}}\left(\hat{\phi}_{\mathbf{k}} + \frac{i\hat{\pi}_{\mathbf{k}}}{\omega_k}\right);\ \hat{a}_{\mathbf{k}}^{+}(t) \equiv \left(\hat{a}_{\mathbf{k}}^{-}(t)\right)^{\dagger} = \sqrt{\frac{\omega_k}{2}}\left(\hat{\phi}_{-\mathbf{k}} - \frac{i\hat{\pi}_{-\mathbf{k}}}{\omega_k}\right), \quad (4.16)$$

which satisfy the commutation relations

$$\left[\hat{a}_{\mathbf{k}}^{-}(t), \hat{a}_{\mathbf{k}'}^{+}(t)\right] = \delta\left(\mathbf{k}-\mathbf{k}'\right), \quad \left[\hat{a}_{\mathbf{k}}^{-}(t), \hat{a}_{\mathbf{k}'}^{-}(t)\right] = \left[\hat{a}_{\mathbf{k}}^{+}(t), \hat{a}_{\mathbf{k}'}^{+}(t)\right] = 0, \quad (4.17)$$

and obey the equations

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

The general solution of these equations is

$$\hat{a}_{\mathbf{k}}^{\pm}(t) = {}^{(0)}\hat{a}_{\mathbf{k}}^{\pm} e^{\pm i\omega_k t}, \quad (4.18)$$

where the time-independent operators ${}^{(0)}\hat{a}_{\mathbf{k}}^{\pm}$ obviously also satisfy the commutation relations (4.17). Below we will mainly use these time-independent operators and will omit the superscript ${}^{(0)}$ for brevity.

The Hilbert space is built in the standard way. We postulate the existence of the vacuum state $|0\rangle$ which is annihilated by all operators $\hat{a}_{\mathbf{k}}^{-}$, that is, $\hat{a}_{\mathbf{k}}^{-}|0\rangle = 0$ for all $\mathbf{k}$. The state with the occupation numbers n_s in every mode $\mathbf{k}_s$ is

$$|n_1, n_2, \ldots\rangle = \left[\prod_s \frac{\left(\hat{a}_{\mathbf{k}_s}^{+}\right)^{n_s}}{\sqrt{n_s!}}\right]|0\rangle, \quad (4.19)$$

where $s = 1, 2, \ldots$ enumerates the excited modes and $|0\rangle \equiv |0, 0, \ldots\rangle$. The vector (4.19) corresponds to the quantum state in which n_1 particles have momentum $\mathbf{k}_1$, n_2 particles have momentum $\mathbf{k}_2$, etc. The vectors $|n_1, n_2, \ldots\rangle$ with all possible choices of n_s form the complete orthonormal basis in the Hilbert space.

The Hamiltonian (4.11) can be rewritten as

$$\hat{H} = \frac{1}{2}\int d^3\mathbf{k}\left[\hat{\pi}_{\mathbf{k}}\hat{\pi}_{-\mathbf{k}} + \omega_k^2\hat{\phi}_{\mathbf{k}}\hat{\phi}_{-\mathbf{k}}\right]. \quad (4.20)$$

Equivalently, we may express $\hat{H}$ in terms of the creation and annihilation operators:

$$\hat{H} = \int d^3\mathbf{k}\frac{\omega_k}{2}\left(\hat{a}_{\mathbf{k}}^{-}\hat{a}_{\mathbf{k}}^{+} + \hat{a}_{\mathbf{k}}^{+}\hat{a}_{\mathbf{k}}^{-}\right) = \int d^3\mathbf{k}\,\omega_k[\hat{a}_{\mathbf{k}}^{+}\hat{a}_{\mathbf{k}}^{-} + \frac{1}{2}\delta^{(3)}(0)]. \quad (4.21)$$

Exercise 4.5

Derive equations (4.20) and (4.21).

4.4 The mode expansion

Taking into account (4.18) we find from (4.16) that

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

Substituting this expression into (4.14) gives the following expansion of the field operator $\hat{\phi}(\mathbf{x}, t)$ in terms of the time-independent creation and annihilation operators,

$$\hat{\phi}(\mathbf{x}, t) = \int \frac{d^3\mathbf{k}}{(2\pi)^{3/2}} \frac{1}{\sqrt{2\omega_k}} \left[e^{-i\omega_k t + i\mathbf{k}\cdot\mathbf{x}} \hat{a}_{\mathbf{k}}^- + e^{i\omega_k t - i\mathbf{k}\cdot\mathbf{x}} \hat{a}_{\mathbf{k}}^+ \right], \tag{4.22}$$

where we have replaced $-\mathbf{k}$ by $\mathbf{k}$ in the second term. The obtained expression is called the *mode expansion* of the quantum field $\hat{\phi}(\mathbf{x}, t)$.

This observation suggests an alternative quantization procedure without explicitly introducing the operators $\hat{\phi}_{\mathbf{k}}$ and $\hat{\pi}_{\mathbf{k}}$. We can begin immediately with the field operator expansion

$$\hat{\phi}(\mathbf{x}, t) = \int \frac{d^3\mathbf{k}}{(2\pi)^{3/2}} \frac{1}{\sqrt{2}} \left[v_{\mathbf{k}}^*(t) e^{i\mathbf{k}\cdot\mathbf{x}} \hat{a}_{\mathbf{k}}^- + v_{\mathbf{k}}(t) e^{-i\mathbf{k}\cdot\mathbf{x}} \hat{a}_{\mathbf{k}}^+ \right], \tag{4.23}$$

and postulate the commutation relations for the time-independent operators $\hat{a}_{\mathbf{k}}^-$ and $\hat{a}_{\mathbf{k}}^+$:

$$\left[\hat{a}_{\mathbf{k}}^-, \hat{a}_{\mathbf{k}'}^+ \right] = \delta(\mathbf{k} - \mathbf{k}'); \quad \left[\hat{a}_{\mathbf{k}}^-, \hat{a}_{\mathbf{k}'}^- \right] = \left[\hat{a}_{\mathbf{k}}^+, \hat{a}_{\mathbf{k}'}^+ \right] = 0. \tag{4.24}$$

Because the field operator satisfies (4.7), the mode functions $v_{\mathbf{k}}(t)$ must obey the equation

$$\ddot{v}_{\mathbf{k}} + \omega_k^2 v_{\mathbf{k}} = 0, \tag{4.25}$$

where $\omega_k^2 = k^2 + m^2$. Substituting (4.23) together with

$$\hat{\pi}(\mathbf{y}, t) = \frac{\partial \hat{\phi}(\mathbf{y}, t)}{\partial t} = \int \frac{d^3\mathbf{k}}{(2\pi)^{3/2}} \frac{1}{\sqrt{2}} \left[\dot{v}_{\mathbf{k}}^*(t) e^{i\mathbf{k}\cdot\mathbf{y}} \hat{a}_{\mathbf{k}}^- + \dot{v}_{\mathbf{k}}(t) e^{-i\mathbf{k}\cdot\mathbf{y}} \hat{a}_{\mathbf{k}}^+ \right] \tag{4.26}$$

into (4.13), we find that the canonical commutation relations are compatible with (4.24) only if the normalization conditions,

$$\dot{v}_{\mathbf{k}}(t) v_{\mathbf{k}}^*(t) - v_{\mathbf{k}}(t) \dot{v}_{\mathbf{k}}^*(t) = 2i, \tag{4.27}$$

are satisfied. The expression on the left-hand side is the Wronskian of the two independent complex solutions $v_{\mathbf{k}}(t)$ and $v_{\mathbf{k}}^*(t)$ of equation (4.25), and therefore does not depend on time. Substituting the general solution of equation (4.25),

$$v_{\mathbf{k}}(t) = \frac{1}{\sqrt{\omega_k}} \left(\alpha_{\mathbf{k}} e^{i\omega_k t} + \beta_{\mathbf{k}} e^{-i\omega_k t} \right), \tag{4.28}$$

into (4.27), we find that the constants of integration $\alpha_{\mathbf{k}}$ and $\beta_{\mathbf{k}}$ must obey

$$|\alpha_{\mathbf{k}}|^2 - |\beta_{\mathbf{k}}|^2 = 1. \tag{4.29}$$

This condition does not suffice to determine the two constants of integration, $\alpha_{\mathbf{k}}$ and $\beta_{\mathbf{k}}$. Therefore the operators $\hat{a}^-_{\mathbf{k}}$ and $\hat{a}^+_{\mathbf{k}}$ are not yet unambiguously defined. To resolve this ambiguity, let us calculate the Hamiltonian. Substituting (4.23) and (4.26) into (4.11), and using $v_{\mathbf{k}}(t)$ given in (4.28), we obtain

$$\hat{H} = \int d^3\mathbf{k}\,\omega_k \Big[\alpha^*_{\mathbf{k}}\beta^*_{\mathbf{k}}\hat{a}^-_{\mathbf{k}}\hat{a}^-_{-\mathbf{k}} + \alpha_{\mathbf{k}}\beta_{\mathbf{k}}\hat{a}^+_{\mathbf{k}}\hat{a}^+_{-\mathbf{k}}$$
$$+ \left(|\alpha_{\mathbf{k}}|^2 + |\beta_{\mathbf{k}}|^2\right)\left(\hat{a}^+_{\mathbf{k}}\hat{a}^-_{\mathbf{k}} + \tfrac{1}{2}\delta^{(3)}(0)\right)\Big], \tag{4.30}$$

where we have used $\alpha_{\mathbf{k}} = \alpha_{-\mathbf{k}}$ and $\beta_{\mathbf{k}} = \beta_{-\mathbf{k}}$. It is obvious from (4.30) that the vector $|0\rangle$, defined by the conditions $\hat{a}^-_{\mathbf{k}}|0\rangle = 0$ for all $\mathbf{k}$, is an eigenvector of the Hamiltonian only if $\alpha_{\mathbf{k}}\beta_{\mathbf{k}} = 0$. Combined with (4.29) this condition tells us that

$$\alpha_{\mathbf{k}} = e^{i\delta_{\mathbf{k}}}, \quad \beta_{\mathbf{k}} = 0,$$

where $\delta_{\mathbf{k}}$ are the irrelevant constant phase factors which we set to zero. Thus, the vector $|0\rangle$ can be interpreted as the vacuum state with the minimal energy only if the mode functions in the expansion (4.23) are taken as

$$v_k(t) = \frac{1}{\sqrt{\omega_k}} e^{i\omega_k t}. \tag{4.31}$$

The obtained result is in complete agreement with (4.22).

Remark: positive and negative frequency modes The modes $v^*_k(t) \propto e^{-i\omega_k t}$ and $v_k(t) \propto e^{i\omega_k t}$ are usually referred to as the positive and negative frequency modes respectively. Alternatively, these solutions are called positive and negative energy solutions. This rather confusing terminology has no particular meaning and is of historical origin. In "first quantized relativistic theory" the field was interpreted as the wave function of a relativistic particle. Therefore the solution $v^*_k(t) \propto e^{-i\omega_k t}$ was regarded as describing particles with positive energy,

$$\hat{H}v^*_k(t) = i\hbar\frac{\partial v^*_k(t)}{\partial t} = \hbar\omega_k v^*_k(t),$$

and the solution $v_k(t) \propto e^{i\omega_k t}$ as corresponding to negative-energy states. However, this interpretation does not make sense in a quantum field theory where particles always have positive energy.

4.5 Vacuum energy and vacuum fluctuations

Vacuum energy It is easy to see from (4.21) that the total energy of the field in the vacuum state $|0\rangle$ is

$$E_0 = \langle 0|\hat{H}|0\rangle = \frac{1}{2}\delta^{(3)}(0)\int d^3\mathbf{k}\,\omega_k. \tag{4.32}$$

This energy is divergent: there is an infinite multiplicative factor $\delta^{(3)}(0)$ in (4.32) and in addition the integral

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

diverges as k^4 at the upper limit of integration.

The origin of the divergent factor $\delta^{(3)}(0)$ is easy to understand: It is simply the infinite volume of space. Indeed, the factor $\delta^{(3)}(0)$ arises from the commutation relation (4.17) when we evaluate $\delta^{(3)}(\mathbf{k}-\mathbf{k}')$ at $\mathbf{k}=\mathbf{k}'$ (note that $\delta^{(3)}(\mathbf{k})$ has the dimension of 3-volume). For a field in a finite box of volume V, the vacuum energy is (see (1.11)):

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

Comparing this expression with (4.32), we find that the formally infinite factor $\delta^{(3)}(0)$ arises when the box volume V goes to infinity. In this limit, the vacuum energy density is equal to

$$\lim_{V\to\infty}\frac{E_0}{V} = \frac{1}{2}\int\frac{d^3\mathbf{k}}{(2\pi)^3}\omega_k, \tag{4.33}$$

and it also diverges at $|\mathbf{k}|\to\infty$. This *ultraviolet divergence* arises because the number of "oscillators" with large momentum grows as k^3 and each of them has zero-point energy $\omega_k/2 \approx k/2$.

In a flat spacetime there is a simple recipe to circumvent the problem of the vacuum energy divergence. The energy of an excited state $|n_1, n_2, \ldots\rangle$ can be computed using equations (4.17), (4.21) and taking into account that

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

As a result we obtain

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

Thus the total energy is always a sum of the divergent vacuum energy E_0 and a finite state-dependent contribution. The absolute value of the energy is relevant only for the gravitational field. If we neglect gravity, then the presence of the vacuum energy cannot be detected in experiments involving only transitions between the excited states. Therefore, we can postulate that the vacuum energy E_0 does not contribute to the gravitational field and simply subtract E_0 from the Hamiltonian. After this subtraction, the modified Hamiltonian becomes

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

and the vacuum is an eigenstate of the Hamiltonian with *zero* eigenvalue:

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

Vacuum fluctuations The subtraction of the vacuum energy density does not, however, remove the vacuum fluctuations of the quantum fields. To estimate the magnitude of fluctuations, let us calculate the correlation function

$$\xi_\phi(|\mathbf{x}-\mathbf{y}|) \equiv \langle 0|\,\hat{\phi}(\mathbf{x},t)\,\hat{\phi}(\mathbf{y},t)\,|0\rangle .$$

Substituting the mode expansion (4.22), we obtain

$$\xi_\phi(|\mathbf{x}-\mathbf{y}|) = \frac{1}{4\pi^2}\int \frac{k^3}{\omega_k}\frac{\sin(k|\mathbf{x}-\mathbf{y}|)}{k|\mathbf{x}-\mathbf{y}|}\frac{dk}{k},$$

where the integration over the angles was performed. It follows that the typical squared amplitude of the scalar field fluctuations on scales $L \sim 1/k$ is of order

$$\delta\phi_L^2 = \frac{1}{4\pi^2}\left.\frac{k^3}{\omega_k}\right|_{k\sim L^{-1}} \sim \frac{1}{L^2\sqrt{1+(mL)^2}}. \tag{4.34}$$

Thus, the amplitude of the vacuum fluctuations $\delta\phi_L$ decays as L^{-1} for $L < m^{-1}$ and as $L^{-3/2}$ for $L > m^{-1}$. This result is already familiar to us from Section 1.4 (see (1.13)).

4.6 The Schrödinger equation for a quantum field

So far we have been working in the Heisenberg picture. However, the fields can also be quantized using the Schrödinger picture. Let us begin with the Schrödinger equation for an ensemble of harmonic oscillators. Their Hamiltonian is obtained from action (4.1) in the standard way:

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

In the Schrödinger picture, the operators $\hat{p}_i$, $\hat{q}_i$ are time-*independent* and act on the time-dependent wave function $|\psi(t)\rangle$. The Hilbert space is spanned by the basis vectors $|q_1, \ldots, q_N\rangle$ which are the generalized eigenvectors of the coordinate operators $\hat{q}_i$. In this basis a state vector $|\psi(t)\rangle$ can then be decomposed as

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

where

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

The momentum operators $\hat{p}_i$ act on the wave function $\psi(q_1, \ldots, q_N, t)$ as derivatives $-i\partial/\partial q_i$. The Schrödinger equation then takes the form

$$i\frac{\partial\psi}{\partial t} = \hat{H}\psi = \frac{1}{2}\sum_{i,j}\left(-\delta_{ij}\frac{\partial^2}{\partial q_i \partial q_j} + M_{ij}q_i q_j\right)\psi. \tag{4.35}$$

To generalize this Schrödinger equation to the case of quantum scalar field, we replace the oscillator coordinates q_i by field values $\phi_{\mathbf{x}} \equiv \phi(\mathbf{x})$ and the wave function $\psi(q_1, \ldots, q_N, t)$ becomes a wave functional $\Psi[\phi(\mathbf{x}), t]$ defined in the space of the field configurations $\phi(\mathbf{x})$ (recall that the spatial coordinate $\mathbf{x}$ plays here the role of the index i). The wave functional has a simple physical interpretation, namely, the probability of measuring a particular spatial field configuration $\phi(\mathbf{x})$ at time t is proportional to $|\Psi[\phi(\mathbf{x}), t]|^2$.

The Schrödinger equation for the scalar field is obtained from (4.35) by replacing the partial derivatives $\partial/\partial q_i$ by functional derivatives $\delta/\delta\phi(\mathbf{x})$ and the sums over discrete indices i by an integral over the spatial coordinate $\mathbf{x}$:

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

For the kernel $M(\mathbf{x}, \mathbf{y})$ given in (4.4), this equation is relativistically invariant although this invariance is not immediately manifest from the form of the equation.

In quantum field theory, the wave functionals and the functional Schrödinger equation are rarely used. We wrote this equation here mainly for illustrative purposes and will proceed to use the Heisenberg picture and the basis of the Hamiltonian eigenstates in the following chapters.

Remark: canonical quantum gravity The use of the wave functional is inevitable in canonical nonperturbative quantum gravity. In this theory the metric is quantized and the role of generalized coordinates of the gravitational field is played by the spatial part of the metric $g_{ik}(\mathbf{x})$. In the coordinate basis, the wave functional Ψ depends on $g_{ik}(\mathbf{x})$ and the matter field configuration $\phi(\mathbf{x})$, that is, $\Psi[g_{ik}, \phi]$. This wave functional is constrained to respect three-dimensional diffeomorphism invariance. In addition, it obeys the Schrödinger-like equation which takes an unusual form,

$$\hat{H}\Psi[g_{ik}, \phi] = 0, \tag{4.36}$$

where $\hat{H}$ is a constraint quadratic in momenta conjugate to g_{ik}. This constraint generates the dynamics in classical gravity and therefore it plays the role of the Hamiltonian. One can crudely understand why the "Hamiltonian" vanishes by considering a closed universe where the positive energy of matter is exactly compensated by the "negative energy" of the gravitational field. Equation (4.36) is called the Wheeler–DeWitt equation.

The most remarkable feature of canonical quantum gravity is the disappearance of time in the fundamental theory and hence an explicit breaking of the spacetime diffeomorphism invariance. This invariance and the concept of time are recovered only at the quasiclassical level. Note that the time-dependent Schrödinger equation for the matter fields can be obtained from (4.36) assuming a quasi-classical background metric. The wave functional $\Psi[g_{ik}, \phi]$ describes the availability of the corresponding three-geometries, which are the "building blocks" for the four-dimensional quasiclassical spacetimes.

Unfortunately, at present the canonical quantum gravity remains only a formal scheme. In spite of many years of effort, this scheme has not yielded reliable physical results which could highlight the nonperturbative aspects of quantum geometry.