Spin 0 quantisation

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From Quantum Mechanics to QFT

Quantum Mechanics:

- Fixed number of particles
- States: $\psi(\vec{x}, t)$

Quantum Field Theory:

- Particle number is not fixed
- Creation and annihilation processes
- Hilbert space $\rightarrow$ **Fock space**

States are labelled by particle content, not position

Fock Space

Definition:

Fock space is the direct sum of *n*-particle Hilbert spaces:

$$\mathcal{F} = \mathbb{C} \oplus \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \cdots$$

Interpretation:

- 0-particle sector: vacuum
- 1-particle sector
- 2-particle sector
- ...

Each sector describes a fixed number of particles.

Basis States

Momentum basis:

- One-particle:

$$|\vec{p}\,\rangle$$

- Two-particle:

$$|\vec{p}_1, \vec{p}_2\rangle$$

Bosons:

$$|\vec{p}_1, \vec{p}_2\rangle = |\vec{p}_2, \vec{p}_1\rangle$$

Fermions:

$$|\vec{p}_1, \vec{p}_2\rangle = -|\vec{p}_2, \vec{p}_1\rangle$$

Normalisation

One-particle states:

$$\langle \vec{p} | \vec{p}' \rangle = \delta^{(3)}(\vec{p} - \vec{p}')$$

Two-particle states (bosons):

$$\langle \vec{p}_1, \vec{p}_2 | \vec{p}_1', \vec{p}_2' \rangle = \delta^{(3)}(\vec{p}_1 - \vec{p}_1')\delta^{(3)}(\vec{p}_2 - \vec{p}_2')$$

$$+\delta^{(3)}(\vec{p}_1 - \vec{p}_2')\delta^{(3)}(\vec{p}_2 - \vec{p}_1')$$

Symmetrisation reflects particle indistinguishability.

Operators and Vacuum

Energy operator:

$$H|\vec{p}_1, \vec{p}_2\rangle = (\omega_1 + \omega_2)|\vec{p}_1, \vec{p}_2\rangle$$

Momentum operator:

$$\vec{P}|\vec{p}_1, \vec{p}_2\rangle = (\vec{p}_1 + \vec{p}_2)|\vec{p}_1, \vec{p}_2\rangle$$

Vacuum state:

$$\langle 0|0\rangle = 1, \quad H|0\rangle = 0, \quad \vec{P}|0\rangle = 0$$

Completeness and Structure

Resolution of identity:

$$\mathbb{I} = |0\rangle\langle 0| + \int d^3p \, |\vec{p}\rangle\langle\vec{p}|$$

$$+\frac{1}{2!}\int d^3p_1 d^3p_2 \, |\vec{p}_1, \vec{p}_2\rangle\langle\vec{p}_1, \vec{p}_2| + \cdots$$

- All states built from vacuum
- Leads naturally to:

$$a^\dagger(\vec{p}), \quad a(\vec{p})$$

Quantum Field Operator

Field as sum of modes:

$$\phi(x) = \int \frac{d^3k}{(2\pi)^3\, 2\omega_{\vec{k}}} \left(a_{\vec{k}} e^{-ik\cdot x} + a_{\vec{k}}^\dagger e^{ik\cdot x} \right)$$

Interpretation:

- $a_{\vec{k}}^\dagger$ creates a particle with momentum $\vec{k}$
- $a_{\vec{k}}$ annihilates a particle
- Field = superposition of all momentum modes

- A quantum field is an infinite collection of harmonic oscillators
- Particles are quanta of the field

Where we arrived:

$$\text{Classical field} \longrightarrow \text{Operator } \phi(x) \longrightarrow \text{Particles}$$

Particles in a Box → Discrete Modes

Setup:

- Particles in a cubic box of size L
- Momentum is quantised

$$\vec{k} = \left(\frac{2\pi n_x}{L}, \frac{2\pi n_y}{L}, \frac{2\pi n_z}{L}\right)$$

Occupation number basis:

$$|\{n(\vec{k})\}\rangle$$

$$H = \sum_{\vec{k}} \omega_{\vec{k}} N(\vec{k}), \quad \vec{P} = \sum_{\vec{k}} \vec{k}\, N(\vec{k})$$

Each Mode = Harmonic Oscillator

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$$

Define operators:

$$[a, a^\dagger] = 1$$

$$H = \omega\left(a^\dagger a + \frac{1}{2}\right)$$

Energy ladder:

$$[H, a^\dagger] = \omega a^\dagger, \quad [H, a] = -\omega a$$

Fock Space Construction

Vacuum:

$$a|0\rangle = 0$$

n-particle states:

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle$$

$$N|n\rangle = n|n\rangle$$

Many modes:

$$[a_{\vec{k}}, a^\dagger_{\vec{k}'}] = \delta_{\vec{k},\vec{k}'}$$

Continuum Limit

Large box:

$$\sum_{\vec{k}} \to \int \frac{d^3k}{(2\pi)^3}$$

Commutation relations:

$$[a_{\vec{k}}, a^\dagger_{\vec{k}'}] = \delta^{(3)}(\vec{k} - \vec{k}')$$

Single-particle states:

$$\langle \vec{k} | \vec{k}' \rangle = \delta^{(3)}(\vec{k} - \vec{k}')$$

Relativistic Structure

Energy-momentum relation:

$$\omega_{\vec{k}} = \sqrt{\vec{k}^2 + m^2}, \qquad k^\mu = (\omega_{\vec{k}}, \vec{k})$$

Lorentz transformations:

$$k'^\mu = \Lambda^\mu{}_\nu k^\nu, \qquad k^2 = m^2 \text{ (invariant)}$$

Goal: construct Lorentz-invariant integrals over momentum space.

Invariant Measure from 4D Momentum Space

Start from the Lorentz-invariant measure:

$$d^4k$$

Restrict to on-shell momenta:

$$k^2 = m^2 \quad \Rightarrow \quad \delta(k^2 - m^2)$$

Select energy sign:

$$\mathrm{sgn}(k^0)$$

Invariant measure:

$$d^4k\,\delta(k^2 - m^2)\,\mathrm{sgn}(k^0)$$

Reduction to 3D Measure

Use:

$$\delta(k^2 - m^2) = \delta((k^0)^2 - \vec{k}^2 - m^2)$$

$$= \frac{1}{2\omega_{\vec{k}}}\left[\delta(k^0 - \omega_{\vec{k}}) + \delta(k^0 + \omega_{\vec{k}})\right]$$

Integrating over k^0:

$$\int d^4k\, \delta(k^2 - m^2)\, \mathrm{sgn}(k^0) = \int \frac{d^3k}{2\omega_{\vec{k}}}(\cdots)$$

Conclusion:

$$\boxed{\frac{d^3k}{2\omega_{\vec{k}}} \text{ is Lorentz invariant}}$$

Relativistic Normalisation of States

Define relativistically normalised states:

$$|k\rangle = \sqrt{(2\pi)^3 2\omega_{\vec{k}}}\, |\vec{k}\rangle$$

Normalisation:

$$\langle k|k'\rangle = (2\pi)^3 2\omega_{\vec{k}}\, \delta^{(3)}(\vec{k} - \vec{k}')$$

Invariant completeness relation:

$$\int \frac{d^3k}{(2\pi)^3 2\omega_{\vec{k}}}\, |k\rangle\langle k| = \mathbb{I}$$

Physical Interpretation

- Fields = infinite set of harmonic oscillators
- Each momentum mode $\vec{k}$ is one oscillator
- Particles = quanta of these modes

Lorentz invariance fixes:

- the integration measure
- the normalisation of states
- the structure of quantum fields

Heisenberg Picture: Time Evolution

Operator evolution:

$$O_H(t) = e^{iHt} O_S e^{-iHt}$$

Derivation of equation of motion:

$$\frac{d}{dt} O_H(t) = iHO_H(t) - iO_H(t)H = i[H, O_H(t)]$$

$$\Rightarrow \quad i\frac{d}{dt} O_H(t) = [O_H(t), H]$$

Interpretation:

- Direct analogue of classical Hamilton equations
- Commutator $\leftrightarrow$ Poisson bracket

Canonical Quantisation of Fields

Lagrangian density:

$$\mathcal{L} = \frac{1}{2}(\partial_\mu \phi \, \partial^\mu \phi - m^2 \phi^2)$$

Conjugate momentum:

$$\pi(x) = \frac{\partial \mathcal{L}}{\partial(\partial_0 \phi)} = \dot{\phi}(x)$$

Hamiltonian density:

$$\mathcal{H} = \pi \dot{\phi} - \mathcal{L} = \frac{1}{2}\left[\pi^2 + (\nabla \phi)^2 + m^2 \phi^2\right]$$

Equal-Time Commutation Relations

Canonical quantisation:

$$[\phi(\vec{x}, t), \pi(\vec{y}, t)] = i\delta^{(3)}(\vec{x} - \vec{y})$$

$$[\phi, \phi] = 0, \qquad [\pi, \pi] = 0$$

Interpretation:

- Field $\phi(\vec{x})$ = infinite set of coordinates
- $\pi(\vec{x})$ = conjugate momenta
- One harmonic oscillator per point in space

Mode Expansion at $t = 0$

We begin by expanding the field in Fourier modes:

$$\phi(\vec{x}, 0) = \int \frac{d^3k}{(2\pi)^3} \left[\alpha_{\vec{k}} e^{i\vec{k}\cdot\vec{x}} + \alpha^\dagger_{\vec{k}} e^{-i\vec{k}\cdot\vec{x}} \right] \quad (1)$$

Each momentum mode behaves like an independent harmonic oscillator.

Taking the time derivative:

$$\partial_0 \phi(\vec{x}, 0) = \int \frac{d^3k}{(2\pi)^3} (-i\omega_k) \left[\alpha_{\vec{k}} e^{i\vec{k}\cdot\vec{x}} - \alpha^\dagger_{\vec{k}} e^{-i\vec{k}\cdot\vec{x}} \right] \quad (2)$$

Extracting the Coefficients

To isolate $\alpha_{\vec{k}}$, we use Fourier orthogonality:

$$\int d^3x\, e^{-i(\vec{k}-\vec{k}')\cdot\vec{x}} = (2\pi)^3\delta^{(3)}(\vec{k}-\vec{k}')$$

Multiply by $e^{-i\vec{k}\cdot\vec{x}}$ and integrate:

$$\int d^3x\, \phi e^{-i\vec{k}\cdot\vec{x}} = \alpha_{\vec{k}} + \alpha^{\dagger}_{-\vec{k}} \tag{3}$$

$$\int d^3x\, \partial_0\phi e^{-i\vec{k}\cdot\vec{x}} = (-i\omega_k)(\alpha_{\vec{k}} - \alpha^{\dagger}_{-\vec{k}}) \tag{4}$$

Solving these equations gives:

$$\alpha_{\vec{k}} = \frac{1}{2}\int d^3x \left[\phi + \frac{i}{\omega_k}\partial_0\phi\right] e^{-i\vec{k}\cdot\vec{x}} \tag{5}$$

Canonical Quantisation

We now promote fields to operators.

Impose equal-time commutation relations:

$$[\phi(\vec{x}), \pi(\vec{y})] = i\delta^{(3)}(\vec{x} - \vec{y}) \tag{6}$$

where $\pi = \partial_0 \phi$.

This is the field-theory analogue of:

$$[x, p] = i$$

Commutation Relations of Modes

Insert the mode expansion into the canonical commutator.

After integrating over space, we obtain:

$$[\alpha_{\vec{k}}, \alpha^{\dagger}_{\vec{k}'}] = \frac{(2\pi)^3}{2\omega_k} \delta^{(3)}(\vec{k} - \vec{k}') \tag{7}$$

To simplify, define normalised operators:

$$a_{\vec{k}} = (2\pi)^{3/2} \sqrt{2\omega_k}\, \alpha_{\vec{k}}$$

Then:

$$[a_{\vec{k}}, a^{\dagger}_{\vec{k}'}] = \delta^{(3)}(\vec{k} - \vec{k}') \tag{8}$$

This is exactly the harmonic oscillator algebra.

Field Expansion and Interpretation

The field becomes:

$$\phi(x) = \int \frac{d^3k}{(2\pi)^{3/2}\sqrt{2\omega_k}} \left[a_{\vec{k}} e^{-ikx} + a^\dagger_{\vec{k}} e^{ikx}\right] \tag{9}$$

Interpretation:

- $a^\dagger_{\vec{k}}$ creates a particle with momentum $\vec{k}$
- $a_{\vec{k}}$ annihilates a particle
- The field creates/annihilates quanta

Hamiltonian

Start from:

$$H = \frac{1}{2}\int d^3x \left[\pi^2 + (\nabla\phi)^2 + m^2\phi^2\right] \tag{10}$$

After inserting the mode expansion:

$$H = \int d^3k\, \omega_k \left(a^\dagger_{\vec{k}} a_{\vec{k}} + \frac{1}{2}\delta^{(3)}(0)\right) \tag{11}$$

Each mode contributes like a quantum harmonic oscillator.

Vacuum Energy

The term

$$\frac{1}{2}\delta^{(3)}(0)$$

represents an infinite constant.

Physically:

$$E_0 = \frac{1}{2}\int d^3k\,\omega_k \qquad (12)$$

To remove it, we define **normal ordering**:

$$: H := \int d^3k\,\omega_k\, a^\dagger_{\vec{k}} a_{\vec{k}}$$

Free Scalar Field and the Pauli–Jordan Function

For a free real scalar field,

$$\hat{\phi}(x) = \int \frac{d^3k}{(2\pi)^3} \frac{1}{\sqrt{2\omega_{\vec{k}}}} \left(\hat{a}_{\vec{k}}\, e^{-ik\cdot x} + \hat{a}^{\dagger}_{\vec{k}}\, e^{+ik\cdot x} \right), \qquad k^0 = \omega_{\vec{k}} = \sqrt{\vec{k}^{\,2} + m^2}.$$

Using the commutation relation

$$[\hat{a}_{\vec{k}}, \hat{a}^{\dagger}_{\vec{q}}] = (2\pi)^3 \delta^{(3)}(\vec{k} - \vec{q}),$$

one finds

$$[\hat{\phi}(x), \hat{\phi}(y)] = i\,\Delta(x - y),$$

where $\Delta(x)$ is the Pauli–Jordan function.

This result shows that the commutator of fields is a c-number function determined entirely by relativistic kinematics.

The Pauli–Jordan Function

A commonly used representation is

$$\Delta(x) = \int \frac{d^3k}{(2\pi)^3} \frac{1}{2\omega_{\vec{k}}} \left(e^{-ik\cdot x} - e^{+ik\cdot x} \right).$$

Equivalently, a manifestly Lorentz-invariant form is

$$\Delta(x) = \int \frac{d^4k}{(2\pi)^3} \, \delta(k^2 - m^2) \, \mathrm{sgn}(k^0) \, e^{-ik\cdot x}.$$

Property:

$$(x-y)^2 < 0 \quad \Longrightarrow \quad \Delta(x-y) = 0.$$

This property will be crucial for ensuring causality in the quantum theory.

Microcausality

From the previous result, we obtain

$$[\hat{\phi}(x), \hat{\phi}(y)] = 0 \quad \text{for space-like separation.}$$

Physical interpretation:

- Observables at space-like separated points commute
- Measurements performed at such points cannot influence one another

Conclusion: relativistic quantum field theory is consistent with causality.

This condition is known as **microcausality**.

Why Does $\Delta(x) = 0$ Outside the Light Cone?

- $\Delta(x)$ is Lorentz invariant
- For space-like x, we can go to a frame where $x^\mu = (0, \vec{r})$

In this frame,

$$\Delta(0, \vec{r}) = \int \frac{d^3p}{(2\pi)^3} \frac{1}{2\omega_{\vec{p}}} \left(e^{+i\vec{p}\cdot\vec{r}} - e^{-i\vec{p}\cdot\vec{r}} \right).$$

The integrand is odd under $\vec{p} \to -\vec{p}$, and the integration domain is symmetric.

Therefore,

$$\Delta(0, \vec{r}) = 0.$$

Conclusion: the vanishing of the commutator outside the light cone follows directly from Lorentz invariance and the structure of the field expansion.