Lecture Notes

Relativistic Quantum Mechanics

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1 Introduction

In this class, “Relativistic Quantum Mechanics”, we combine Quantum Mechanics with Special Relativity and develop a formalism to quantize fields in a Lorentz-invariant way.

We will recapitulate the Lagrange and Hamilton formalism for the treatment of classical point particles as well as the quantization of the harmonic oscillator through creation and annihilation operators.

Building on the former, we will briefly analyze the Lagrange formalism and the derivation of Euler-Lagrange equations of motion for a discrete system, before taking the continuum limit, resulting in the Lagrange formulation of field dynamics.

We will analyze free real and complex scalar fields in this formalism, and for the latter, we will find a symmetry – phase shifts of the fields – that leaves the Lagrangian invariant.

We will see that such invariances result in conserved currents and charges.

We will further exemplify the power of the formalism by constructing a Lagrange density for the electromagnetic fields and deriving Maxwell’s equations from it.

To quantize fields we will copy the steps known from single-particle systems, in particular the harmonic oscillator, and adapt it to the case of fields.

In so doing we effectively replace the role of position and momentum of the particle, and the corresponding operators, with the field and its conjugate momentum.

The resulting logic is to replace the functions describing fields and their conjugate momenta with field and momentum operators, and to demand suitable commutator relations for them.

This is called second quantization.

As a consequence of relativistic invariance, encoded in the quadratic energy-momentum relation of $E^2 - p^2 = m^2$, solutions with negative energy become possible.

Demanding a Hamiltonian with an energy spectrum that is bounded from below, i.e. a physically meaningful ground state or vacuum, necessitates their interpretation as anti-particles.

It also immediately implies we have arrived at a multi-particle theory, because pairs of particles and anti-particles with short lifetimes can be produced.

We will check, by explicit calculation, that the resulting theory maintains causality at a microscopic level, by asserting that commutators of causally disconnected fields always vanish and that they therefore cannot impact onto each other.

After second quantization of the simplest possible theory, a single free real scalar field, we analyze the structure of a free complex scalar field.

We will recover the current and charge stemming from the phase invariance of the Lagrangian and we will by explicit calculation show that the charge and the Hamilton operators commute, making charge conservation of the theory manifest.

After analyzing the free scalar or Klein-Gordon fields we will turn our attention to the treatment of spin-1/2 particles in the celebrated Dirac equation.

We will analyze its structure and ingredients – γ matrices and spinors – and their properties before second quantization of the theory.

Reflecting the fermionic nature of the particles, we will use anti-commutators $\{\cdot, \cdot\}$ instead of commutators $[\cdot,\cdot]$ for the quantization conditions.

Similar to the case of the complex scalar field, also the Lagrangian for free spinors enjoys invariance under phase transformations of the fields, and again this leads to a conserved charge.

We then turn our attention to the quantization of electrodynamics and the free electromagnetic fields.

There, we will encounter an interesting problem: the vector potential A^μ, on which we build the theory, naively speaking, has four degrees of freedom in its four-components, but the physical field has only two degrees of freedom, the well-known linear or circular polarization states of the photons, the quanta of electromagnetism.

This necessitates the imposition of additional conditions onto the theory, to correctly reflect its physical content.

In more formalized language, this problem is a result of the gauge invariance of the underlying theory, electromagnetism, which results in identical physical fields for different vector potentials.

It will become clear that the problem of the additional content will be fixed by fixing the gauge of the theory, and we will see how this is shapes the additional conditions we will impose on the theory.

Having quantized various free field theories and discussing some of their properties, we will start with developing a framework to analyze their dynamical behavior.

To this end we will build on the concept of Green's functions and construct the Green's functions of our quantized theories.

It will turn out that these "propagators" are the vacuum expectation values of time-ordered products of the field operators.

2 Recapitulation

In this section we recapitulate important concepts and properties of the objects we will use throughout the class.

The aim is not to explain in detail how things work or why, but to provide you with a unified notation and nomenclature.

If you need to learn something from scratch, then look at my older notes on my website, i.e Mathematical Methods(MM), IntroMech+Classical Mechanics, IntroEM+Electrodynamics, SR1, and AdvQM,

2.1 Natural Units

Throughout the class we will use "natural units",

$$\hbar = c = 1\,. \tag{1}$$

All quantities will be expressed in units of energy, i.e. electron Volts (eV), or their inverse.

One eV is the kinetic energy an electron gains when being accelerated from rest through an electric potential difference of 1 Volt in the vacuum.

To transform between quantities in different units, we will multiply or divide by combinations of $\hbar$ and c, as in Table 1.

In particular this means we have the electron and proton mass as $m_e \approx 511$ keV = 0.511 MeV and $m_p \approx 938$ MeV ≈ 1 GeV.

time	$\longleftrightarrow$	length	with	$c \approx 0.3 \cdot 10^9$ m/s
momentum	$\longleftrightarrow$	energy	with	c
mass	$\longleftrightarrow$	energy	with	c^2
time	$\longleftrightarrow$	1/energy	with	$\hbar \approx 6.5 \cdot 10^{-22}$ MeV s
length	$\longleftrightarrow$	1/energy	with	$\hbar c \approx 200$ MeV fm

Table 1: Transformations between physical quantities

2.2 Some mathematics

Fourier Transformation Throughout the class we will define Fourier transformations between position x and momentum k in a somewhat asymmetric form as

$$\begin{aligned} \tilde{f}(k) &= \int \frac{\mathrm{d}x}{(2\pi)}\, e^{-ikx}\, f(x) \\ f(x) &= \int \mathrm{d}k\, e^{ikx}\, \tilde{f}(k)\,. \end{aligned} \tag{2}$$

the extension to higher dimensions – for example for the Fourier transformation of three-vectors – is straightforward:

$$\begin{aligned} \tilde{f}(\underline{k}) &= \int \frac{\mathrm{d}^3x}{(2\pi)^3}\, e^{-i\underline{k}\cdot\underline{x}}\, f(\underline{x}) \\ f(\underline{x}) &= \int \mathrm{d}^3k\, e^{i\underline{k}\cdot\underline{x}}\, \tilde{f}(\underline{k})\,. \end{aligned} \tag{3}$$

δ-function The δ-function is defined through an integral relation as

$$\int_a^b \mathrm{d}x\, \delta(x-x_0)\, f(x) = \begin{cases} f(x_0) & \text{if } x_0 \in [a,\, b] \\ 0 & \text{otherwise.} \end{cases} \tag{4}$$

In addition, we have

$$\int \mathrm{d}x\, e^{-ix(k-q)} = (2\pi)\delta(k-q) \tag{5}$$

Again, the extension to more dimensions is straightforward.

2.3 Four-Vectors and Minkowski Space

Four Vectors Throughout the course we will use relativistic notation.

Time t and spatial position x = (x, y, z) are combined into a (contravariant) four-position

$$x^\mu = (t,\, x,\, y,\, z) = (t,\, \underline{x}) \qquad (6)$$

and similar, energy E and momentum $\underline{p}$ = (p_x, p_y, p_z) are combined into a (contravariant) four-momentum

$$p^\mu = (E,\, p_x,\, p_y,\, p_z) = (E,\, \underline{p})\,. \qquad (7)$$

We will use Greek indices μ, ν, ρ, ... to label components of four-objects and Latin indices i, j, k, ... to label the spatial or three-components.

Einstein Convention When not stated otherwise we will use Einstein's convention of summing over repeated indices, for example

$$\underline{p}^2 = p_i p_i = p_x^2 + p_y^2 + p_z^2. \qquad (8)$$

Metric Tensor For four-vectors this is a meaningful operation only when combining contravariant objects (where the index is a superscript) with covariant objects (where the index is a subscript).

The two sets of four-objects – contravariant and covariant – are connected through the metric tensor $g_{\mu\upsilon}$,

$$p_\mu = g_{\mu\nu} p^\nu \quad \text{and} \quad p^\mu = g^{\mu\nu} p_\nu \,, \tag{9}$$

where the Minkowski metric is given by

$$g_{\mu\nu} = g^{\mu\nu} = \text{diag}(1, -\underline{1}) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{10}$$

In other words, if $p^\mu = (E, p)$, $p_\mu = (E, -p)$.

From $p_\mu = g_\mu{}^\upsilon p_\upsilon$ we can easily infer that

$$g_\mu{}^\nu = g^\mu{}_\nu = \text{diag}(1, \underline{1}) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} . \tag{11}$$

Raising and Lowering Indices We have already seen, how the metric tensor is used to raise or lower indices of four-vectors, e.g.,

$$x_\mu = g_{\mu\nu} x^\nu \quad \text{and} \quad x^\mu = g^{\mu\nu} x_\nu \,, \tag{12}$$

which introduces a sign flip in the spatial coordinates:

$$\text{if } x^\mu = (t, \underline{x}) \text{ then } x_\mu = (t, -\underline{x}) \,. \tag{13}$$

For tensors with n indices, one metric tensor is necessary to raise or lower one index.

For example, for a tensor $F^{\mu\upsilon}$ of rank two, two metric tensors are necessary to lower both indices.

As an example, consider the field-strength tensor of electromagnetism, given by

$$F^{\mu\nu} = \begin{pmatrix} 0 & -E_x & -E_y & -E_z \\ E_x & 0 & -B_z & B_y \\ E_y & B_z & 0 & -B_x \\ E_z & -B_y & B_x & 0 \end{pmatrix} \tag{14}$$

Therefore,

$$F_{\mu\nu} = g_{\mu\mu'} g_{\nu'\nu} F^{\mu'\nu'} \, , \tag{15}$$

where, making the sequence of matrix multiplications explicit

$$\begin{aligned} F^{\mu}_{\nu} &= g_{\nu\nu'} F^{\mu'\nu'} = F^{\mu'\nu'} g_{\nu'\nu} \\ &= \begin{pmatrix} 0 & -E_x & -E_y & -E_z \\ E_x & 0 & -B_z & B_y \\ E_y & B_z & 0 & -B_x \\ E_z & -B_y & B_x & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \\ &= \begin{pmatrix} 0 & E_x & E_y & E_z \\ E_x & 0 & B_z & -B_y \\ E_y & -B_z & 0 & B_x \\ E_z & B_y & -B_x & 0 \end{pmatrix} \end{aligned} \tag{16}$$

and

$$
\begin{aligned}
F_{\mu\nu} &= g_{\mu\mu'} F^{\mu'}_{\nu'} \\
&= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & E_x & E_y & E_z \\ E_x & 0 & B_z & -B_y \\ E_y & -B_z & 0 & B_x \\ E_z & B_y & -B_x & 0 \end{pmatrix} \\
&= \begin{pmatrix} 0 & E_x & E_y & E_z \\ -E_x & 0 & -B_z & B_y \\ -E_y & B_z & 0 & -B_x \\ -E_z & -B_y & B_x & 0 \end{pmatrix};
\end{aligned} \tag{17}
$$

in other words, lowering *both* indices changed the sign in the 0-row and 0-column of the tensor – the mixed temporal-spatial entries – and left the temporal-temporal and spatial-spatial entries unchanged.

Scalar Product Scalar products of two four-vectors are then given by

$$
x \cdot p = x_\mu p^\mu = x^\mu p_\mu = x_0 p_0 - \underline{x} \cdot \underline{p} = x_0 p_0 - x_1 p_1 - x_2 p_2 - x_3 p_3 \tag{18}
$$

Derivatives Derivatives of a scalar or scalar product with respect to a vector are given by

$$
\frac{\partial a \cdot b}{\partial a_\mu} = \frac{\partial a_\mu \cdot b^\mu}{\partial a_\mu} = b^\mu\,, \tag{19}
$$

i.e., derivatives of a scalar quantity w.r.t a covariant vector yield a contravariant vector.

In particular it is customary to define

$$\partial_\mu = \frac{\partial}{\partial x^\mu} = (\partial/\partial t,\, \underline{\nabla})$$
$$\partial^\mu = \frac{\partial}{\partial x_\mu} = (\partial/\partial t,\, -\underline{\nabla})\ . \tag{20}$$

Note that the derivatives have a relative sign in the spatial coordinates!

Relativistic Energy-Momentum Relation In particular, the energy-momentum relation for a physical particle of (rest) mass m can be written as

$$\boxed{p^2 = E^2 - \underline{p}^2 = m^2} \tag{21}$$

Kronecker-δ and Levi-Civita Tensor Two important tensors in three dimensions are the Kronecker-δ,

$$\delta_{ij} = \delta^{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise,} \end{cases} \tag{22}$$

and the anti-symmetric Levi-Civita Tensor, given by

$$\epsilon_{ijk} = \epsilon^{ijk} = \begin{cases} 1 & \text{if } \{ijk\} = \text{cyclical permutation of 123} \\ -1 & \text{if } \{ijk\} = \text{anti-cyclical permeation of 123} \\ 0 & \text{otherwise.} \end{cases} \tag{23}$$

The latter is generalized to the *totally anti-symmetric tensor in four dimensions*, $\epsilon^{\mu\upsilon\rho\sigma}$ with

$$\epsilon^{\mu\nu\rho\sigma} = -\epsilon_{\mu\nu\rho\sigma} = \begin{cases} 1 & \text{if } \{\mu\nu\rho\sigma\} = \text{cyclical permutation of } 0123 \\ -1 & \text{if } \{\mu\nu\rho\sigma\} = \text{anti-cyclical permutation of } 0123 \\ 0 & \text{otherwise.} \end{cases} \tag{24}$$

2.4 Lorentz Transformations

General idea Lorentz transformations,

$$x^\mu \longrightarrow x'^\mu = \Lambda^\mu{}_\nu x^\nu \tag{25}$$

are *linear transformations* that connect four-vectors with each other.

The $\Lambda^\mu{}_\nu$ are usually divided into active transformations where the four-vector in question is moved while the reference system is fixed, and passive transformations, where the four-vector is fixed, but the reference system is changed.

The difference between active and passive transformations is encoded in a relative sign of the defining parameters.

In the context of this class, the idea of Lorentz transformations is generalized such that they contain both *boosts* $B^\mu{}_\nu$ and *rotations* $R^\mu{}_\nu$, where the former are defined by three velocities and the latter defined by three angles.

In fact, the rotation are the Galilei transformations, which are superseded by the Lorentz transformations.

Boosts The (active) boosts $B^\mu{}_\nu$ are defined by the three-velocity $\underline{v}$; for example for a boost long the z-axis with velocity $v = v_z$

$$B^\mu{}_\nu(v_z) = \gamma \begin{pmatrix} 1 & 0 & 0 & -v \\ 0 & 1/\gamma & 0 & 0 \\ 0 & 0 & 1/\gamma & 0 \\ -v & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \cosh\eta & 0 & 0 & -\sinh\eta \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -\sinh\eta & 0 & 0 & \cosh\eta \end{pmatrix} \tag{26}$$

where

$$\cosh\eta = \gamma = \frac{1}{\sqrt{1-v^2}} \tag{27}$$

is the Lorentz factor and η is the *rapidity*.

To construct the boost defined by a three-velocity $\underline{v}$, $B^\mu{}_\nu(\underline{v})$, it is advantageous to realize that the spatial dimensions can be decomposed into one component parallel to the boost-vector v, $x'_{||}$ and two perpendicular ones $\vec{x}_\perp$.

With $\underline{v} = v\,\underline{n}$ and $x_{||} = \underline{x}\cdot\underline{n}$, the transformations read

$$\begin{aligned} t' &= \gamma(t - \underline{x}\cdot\underline{v}) \\ x'_{||} &= \gamma(x_{||} - vt) \\ \vec{x}'_\perp &= \vec{x}_\perp\,, \end{aligned} \tag{28}$$

or, for the spatial components in more compact form

$$\underline{x}' = \underline{x} + (\gamma - 1)(\underline{n} \cdot \underline{x})\underline{n} - \gamma \underline{v} t \tag{29}$$

In matrix form this translates to

$$B^{\mu}{}_{\nu}(\underline{v}) = \begin{pmatrix} \gamma & -\gamma v_x & -\gamma v_y & -\gamma v_z \\ -\gamma v_x & 1 + (\gamma - 1)\frac{v_x^2}{v^2} & (\gamma - 1)\frac{v_x v_y}{v^2} & (\gamma - 1)\frac{v_x v_z}{v^2} \\ -\gamma v_y & (\gamma - 1)\frac{v_y v_x}{v^2} & 1 - (\gamma - 1)\frac{v_y^2}{v^2} & (\gamma - 1)\frac{v_y v_z}{v^2} \\ -\gamma v_z & (\gamma - 1)\frac{v_z v_x}{v^2} & (\gamma - 1)\frac{v_z v_y}{v^2} & 1 - (\gamma - 1)\frac{v_z^2}{v^2} \end{pmatrix} \tag{30}$$

Rotations Similar to the boosts, the (active) rotations $R^{\mu}{}_{\nu}$ are defined by three Euler angles; for example a rotation around the z-axis with angle θ is mediated by

$$R^{\mu}{}_{\nu}(\theta) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta & 0 \\ 0 & \sin\theta & \cos\theta & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{31}$$

Invariance of Norm of Four-Vectors The Lorentz transformations have been constructed such that the norm of a four vector is invariant under a boost or rotation.

To see how this works look at a four-vector x, boosted with velocity v.

The square of its norm is given by

$$\begin{aligned} (\|x'\|)^2 &= x'^2 = t'^2 - \vec{x}'^2_{\perp} - x'^2_{\parallel} \\ &= \gamma^2 \left[(1 - v^2)t^2 - (1 - v^2)x_{\parallel}^2\right] - \vec{x}^2_{\perp} = x^2 \end{aligned} \tag{32}$$

and therefore invariant.

Time-like vs. Space-like Distances Invariance of the norm of four-vectors implies that distances of two four-vectors, $\Delta x^\mu{}_{12} = x^\mu{}_1 - x^\mu{}_2$, which of course are four-vectors themselves, can be decomposed into three cases:

1. Time-like distances: $\Delta x^2{}_{12} > 0$. A boost can be found in such a way that $\Delta x^\mu{}_{12} = (\Delta t, \underline{0})$, or, in other words, the spatial positions of x_1 and x_2 are identical. Events at four-positions x_1 and x_2 can be causally connected.

2. Space-like distances: $\Delta x^2{}_{12} < 0$. A boost can be found in such a way that $\Delta x^\mu{}_{12} = (0, \underline{\Delta x})$, or, in other words, the temporal positions of x_1 and x_2 are identical. Events at four-positions x_1 and x_2 are not causally connected.

3. Light-like distances: $\Delta x^2{}_{12} = 0$. A boost can be found such that $\Delta x^\mu{}_{12} = (0, 0)$, and events at four-positions x_1 and x_2 are on the same *light-cone* and can be causally connected through an interaction acting with the speed of light.

The connection of distances with causal structures will become important at a later stage during the class.

Inverse Lorentz Transformations Inverse Lorentz transformations are given by using velocities and rotations with a negative sign with respect to the originals.

This can be used to construct inverse Lorentz Transformations by expressing the squares of transformed and original four-vectors in component form:

$$x'^2 = x'^\mu g'_{\mu\nu} x'^\nu = \Lambda^\mu{}_{\mu'} x^{\mu'} g'_{\mu\nu} \Lambda^\nu{}_{\nu'} x^{\nu'} = x^{\mu'} g_{\mu'\nu'} x^{\nu'} \qquad (33)$$

or

$$\Lambda^{\mu}{}_{\mu'} g'_{\mu\nu} \Lambda^{\nu}{}_{\nu'} = g_{\mu'\nu'} \,. \tag{34}$$

Since no system is preferred the metric tensor must be the same in all systems, i.e. $g'^{\mu\nu} = g_{\mu\nu}$ and therefore

$$\Lambda^{\mu}{}_{\mu'} g_{\mu\nu} \Lambda^{\nu}{}_{\nu'} = (\Lambda^T)_{\mu'}{}^{\mu} g_{\mu\nu} \Lambda^{\nu}{}_{\nu'} = g_{\mu'\nu'} \,. \tag{35}$$

This implies that

$$(\Lambda^{-1})^{\mu}{}_{\mu'} = (\Lambda^T)^{\mu}{}_{\mu'}) = \Lambda_{\mu}{}^{\mu'} \,, \tag{36}$$

i.e., transposition is the inverse of a Lorentz transformation.

2.5 Lagrange and Hamilton Formalism for Point Particles

Lagrange Function Consider a point particle with kinetic energy T and a set of generalized coordinates $q_i(t)$ and velocities $\dot{q}_i(t)$ = dq_i/dt that are suitable to describe its motion in a potential V.

The Lagrange function is given by

$$L(q_i(t), \dot{q}_i(t), t) = T - V \tag{37}$$

and gives rise to the action

$$S(t_1, t_0) = \int_{t_0}^{t_1} \mathrm{d}t L(q_i(t), \dot{q}_i(t), t) \,. \tag{38}$$

Principle of Least Action Minimizing the action by employing virtual small perturbations of the particle's path ϵ_i and $\dot{\epsilon}_i$, taken to be zero at the endpoints t_0 and t_1, will yield the *Euler-Lagrange Equations of Motion* (E.o.M.).

This is also known as *Hamilton's Principle or Principle of Least Action*.

Under the usual assumption of an explicitly time-independent Lagrange function and suppressing for a moment the time dependence of the generalized coordinates and velocities, this yields

$$\begin{aligned}\delta S &= \int_{t_0}^{t_1} \mathrm{d}t\, [L(q_i + \epsilon_i,\, \dot{q}_i + \dot{\epsilon}_i) - L(q_i,\, \dot{q}_i)] \\ &= \int_{t_0}^{t_1} \mathrm{d}t \left[\epsilon_i \frac{\partial L}{\partial q_i} + \dot{\epsilon}_i \frac{\partial L}{\partial \dot{q}_i}\right] = \int_{t_0}^{t_1} \mathrm{d}t \left[\epsilon_i \frac{\partial L}{\partial q_i} - \epsilon_i \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}_i}\right] + \left[\epsilon_i \frac{\partial L}{\partial \dot{q}_i}\right]_{t_0}^{t_1},\end{aligned} \tag{39}$$

where in the last step the term with $\dot{\epsilon}_i$ has been partially integrated.

Euler-Lagrange Equations of Motion Since the variations ϵ_i are assumed to vanish at the path's endpoint the last term vanishes, demanding that the integral reduces to zero for *arbitrary* perturbations yields the Euler-Lagrange E.o.M. for systems without explicit time dependence:

$$\boxed{\frac{\partial L}{\partial q_i} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}_i} = 0\,.} \tag{40}$$

Canonical Momentum and Hamilton Function Introducing the canonical momenta

$$p_i = \frac{\partial L}{\partial \dot{q}_i} \tag{41}$$

and expressing the generalized velocities through the canonical momenta p_i allows to construct the Hamilton function as

$$\boxed{H(p_i, q_i) = \dot{q}_i p_i - L(q_i, \dot{q}_i) = \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} - L(q_i, \dot{q}_i) = T + V\,,} \tag{42}$$

identical to the energy of the system if it is not explicitly time-dependent.

Hamilton Equations of Motion The Hamilton equations of motions are given by the two sets of coupled partial differential equations

$$\boxed{\begin{aligned} \dot{p}_i &= \frac{\mathrm{d}p_i}{\mathrm{d}t} = -\frac{\partial H}{\partial q_i} \\ \dot{q}_i &= \frac{\mathrm{d}q_i}{\mathrm{d}t} = +\frac{\partial H}{\partial p_i}\,. \end{aligned}} \tag{43}$$

Poisson Brackets Poisson brackets are another possibility to express the Hamilton E.o.M. they are defined by

$$\boxed{\{f, g\} = \frac{\partial f}{\partial q_i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_i}\,.} \tag{44}$$

They have some interesting properties, for example

- anti-commutivity:

$$\{f,\, g\} = -\,\{g,\, f\} \tag{45}$$

- bilinearity (a and b constants):

$$\{af + bg,\, h\} = a\,\{f,\, h\} + b\,\{g,\, h\} \tag{46}$$

- Jacobi identity:

$$\{f,\, \{g,\, h\}\} + \{g,\, \{h,\, f\}\} + \{h,\, \{f,\, g\}\} = 0 \tag{47}$$

In particular, the Poisson brackets for the canonical coordinates (positions and momenta) enjoy the following simple properties:

$$\begin{aligned} \{q_i,\, q_j\} = \{p_i,\, p_j\} = 0 \\ \{q_i,\, p_j\} = \delta_{ij}\,. \end{aligned} \tag{48}$$

Equations of motion can therefore be expressed as

$$\boxed{\begin{aligned} \dot{p}_i &= -\,\frac{\partial H}{\partial q_i} = \{p_i,\, H\} \\ \dot{q}_i &= +\,\frac{\partial H}{\partial p_i} = \{q_i,\, H\}\ . \end{aligned}} \tag{49}$$

The time evolution of any function $f(p_i, q_i, t)$ can be evaluated using the chain rule,

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial q_i}\dot{q}_i + \frac{\partial f}{\partial p_i}\dot{p}_i + \frac{\partial f}{\partial t} = \{f,\, H\} + \frac{\partial f}{\partial t}\,. \tag{50}$$

This translates into explicitly time-independent *f* are constant of motion, if their Poisson bracket with the Hamilton function vanishes.

Note the similarity of the Poisson brackets to the commutator in Quantum Mechanics.

It is, however, important to stress that the functions here are not operators acting on a Hilbert space, but just functions.

2.6 First Quantization of the Harmonic Oscillator

Hamilton operator In a first step, the Hamilton function is written in terms of the usual canonical position and momentum, and position, momentum, and Hamilton function are promoted to operators, resulting in

$$\hat{H} = \frac{1}{2m}\,\hat{p}^2 + \frac{m\omega^2}{2}\,\hat{x}^2\,. \tag{51}$$

Note that we have used natural units, setting $\hbar = 1$, and in the following we will also set m = 1 to ease the notation.

Commutator of Position and Momentum Quantization is achieved by demanding that the position and momentum operators have a non-vanishing commutator, namely

$$\boxed{[\hat{x},\,\hat{p}] \equiv \hat{x}\hat{p} - \hat{p}\hat{x} = i\,.} \tag{52}$$

Creation and Annihilation Operators To cast the Hamilton operator into a form better suited for analysis, creation and annihilation operators $\hat{a}^\dagger$ and $\hat{a}$ are introduced as

$$\begin{aligned} \hat{a} &= \frac{1}{\sqrt{2}}\left(\sqrt{\omega}\,\hat{x} + \frac{i}{\sqrt{\omega}}\,\hat{p}\right) \\ \hat{a}^\dagger &= \frac{1}{\sqrt{2}}\left(\sqrt{\omega}\,\hat{x} - \frac{i}{\sqrt{\omega}}\,\hat{p}\right)\,. \end{aligned} \tag{53}$$

Direct calculation shows the following commutation relations:

$$\boxed{\begin{aligned} [\hat{a},\,\hat{a}] = [\hat{a}^\dagger,\,\hat{a}^\dagger] &= 0 \\ [\hat{a},\,\hat{a}^\dagger] &= 1\,. \end{aligned}} \tag{54}$$

Hamilton Operator Expressing the Hamilton operator from Eq, (51) through the annihilation and creation operators yields

$$\begin{aligned} \hat{H} = \frac{1}{2}\,\hat{p}^2 + \frac{\omega^2}{2}\,\hat{x}^2 \;&=\; \frac{\omega}{4}\left[-(\hat{a} - \hat{a}^\dagger)^2 + (\hat{a} + \hat{a}^\dagger)^2\right] \\ = \frac{\omega}{2}\left(\hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a}\right) \;&=\; \frac{\omega}{2}\left(\left[\hat{a},\,\hat{a}^\dagger\right] + 2\hat{a}^\dagger\hat{a}\right) \;=\; \omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) \end{aligned} \tag{55}$$

Number Operator Rewriting the Hamilton operator as

$$\boxed{\hat{H} = \omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) = \omega\left(\hat{N} + \frac{1}{2}\right)} \tag{56}$$

with the number operator

$$\boxed{\hat{N} = \hat{a}^\dagger\hat{a}}. \tag{57}$$

It has commutator relations

$$[\hat{N}, \hat{a}^\dagger] = \hat{a}^\dagger \quad \text{and} \quad [\hat{N}, \hat{a}] = -\hat{a} \tag{58}$$

with the creation and annihilation operators.

Eigenstates Denote the energy eigenstates and eigenvalues with

$$\hat{H}\,|E\rangle = E\,|E\rangle \tag{59}$$

it is easy to check that $\hat{a}\,|E\rangle$ is also an eigenstate of the Hamilton operator,

$$\begin{aligned} \hat{H}\hat{a}\,|E\rangle &= \omega\left(\hat{N} + \frac{1}{2}\right)\hat{a}\,|E\rangle \\ &= \omega\left\{\left[\hat{N} + \frac{1}{2}, \hat{a}\right] + \hat{a}\left(\hat{N} + \frac{1}{2}\right)\right\}|E\rangle = (-\omega + E)\,\hat{a}\,|E\rangle \end{aligned} \tag{60}$$

with eigenvalue (energy) (E−ω).

Using the fact that eigenvalues of Hermitean operators, such as the position, momentum, and Hamilton operators, are real numbers and realizing that the Hamilton operator is made up from squares of Hermitean operators with squares of real numbers as eigenvalues, implies that there must be a smallest, non-negative energy with a corresponding lowest-energy ground state of the system.

Denoting this state as "vacuum", the only way to guarantee that there are on lower energy eigenvalues is to *demand* that the annihilation operators annihilate this state,

$$\hat{a}\,|0\rangle = 0\,, \tag{61}$$

thereby justifying once more the interpretation of $\hat{a}$ as annihilation operator.

Conversely, excited states are created by repeated application of the creation operator,

$$\hat{a}^\dagger\,|0\rangle = |1\rangle \tag{62}$$

and so on.

Applying the number operator suggests that the vacuum contains zero quanta, thereby justifying the notation of $|0\rangle$ and similarly that the first excited state contains one quantum:

$$\begin{aligned} \hat{N}\,|0\rangle &= 0 \\ \hat{N}\,|1\rangle &= \hat{a}^\dagger\hat{a}\hat{a}^\dagger\,|0\rangle = \hat{a}^\dagger\left(\left[\hat{a},\,\hat{a}^\dagger\right] + \hat{a}^\dagger\hat{a}\right)|0\rangle = 1\cdot\hat{a}^\dagger\,|0\rangle = 1\,|1\rangle\,. \end{aligned} \tag{63}$$

This suggests that the number operator enjoys the eigenvalue equation

$$\hat{N}\,|n\rangle = n\,|n\rangle \tag{64}$$

or eigenvectors (eigenkets) $|n\rangle$.

It is worth commenting here on the states.

They populate a Hilbert space - put in somewhat sloppy terms, this is a vector space with a finite or infinite number of dimensions, which has a meaningfully defined scalar product.

This scalar product allows to define a measure of distance and the length of a vector in it.

Hilbert spaces are complete as well, which means that we can safely define limits etc..

Eigenvalues and Eigenstates of the Hamilton Operator Eq. (56) results in the realization that the Hamilton and the number operator share the same eigenvectors/eigenstates, the $|n\rangle$.

Plugging in numbers allows to directly read off the ground-state energy E_0 as

$$\hat{H}\,|0\rangle = \frac{\omega}{2}\,|0\rangle = E_0\,|0\rangle\ , \tag{65}$$

and similarly

$$\hat{H}\,|n\rangle = \omega\left(n + \frac{1}{2}\right)|0\rangle = E_n\,|0\rangle \tag{66}$$

with eigenvalues (energies) $E_n = \omega(n + 1/2)$ for the energies of the excited states.

3 Classical Fields

In this section we re-derive the Lagrange functions for classical fields.

3.1 One-Dimensional Lattice

Setup Consider a system of massive particles with identical mass m, arranged in a one-dimensional lattice with positions ξ_i, and with their motion confined along the lattice direction.

The kinetic energy of the system is given by

$$T = \frac{m}{2} \sum_i \dot{\xi}_i^2(t) \tag{67}$$

Coupling the particles with springs with constants k yields the potential energy

$$V = \frac{k}{2} \sum_i \left(\xi_{i+1}(t) - \xi_i(t)\right)^2 , \tag{68}$$

and the Lagrange function

$$\begin{aligned} L &= \frac{1}{2} \sum_i \left[m\dot{\xi}_i^2(t) - k\left(\xi_{i+1}(t) - \xi_i(t)\right)^2 \right] \\ &= \frac{a^2}{2} \sum_i \left[m\left(\frac{\dot{\xi}_i(t)}{a}\right)^2 - k\left(\frac{\xi_{i+1}(t) - \xi_i(t)}{a}\right)^2 \right] , \end{aligned} \tag{69}$$

where a is the equilibrium separation between the particles.

Euler-Lagrange E.o.M. To arrive at the E.o.M. for a specific η_i we have to take into account that for the same index ithe displacement η_i shows up twice in the sum over the differences, and therefore

$$\begin{aligned} 0 &= ma^2\frac{\ddot{\xi}(t)}{a^2} - ka^2\left(\frac{\xi_{i+1}(t)-\xi_i(t)}{a^2} - \frac{\xi_i(t)-\xi_{i-1}(t)}{a^2}\right) \\ &= a\left[\mu\ddot{\xi}(t) - Y\left(\frac{\xi_{i+1}(t)-\xi_i(t)}{a^2} - \frac{\xi_i(t)-\xi_{i-1}(t)}{a^2}\right)\right] \end{aligned} \tag{70}$$

where the second line was obtained after factoring out one power of a, and by identifying μ= m/a as the mass density per unit length, and Y= ka as Young's modulus of the continuous rod.

Continuum Limit Going from discrete lattice distances to a continuum can be understood as replacing the index i with a position x, $\xi_i(t) \to \xi(x, t)$, and by taking the limit $a \to 0$ for the lattice spacing.

The ξ differences become

$$\lim_{a\to 0}\frac{\xi_{i+1}(t)-\xi_i(t)}{a} = \lim_{a\to 0}\frac{\xi(x+a,\, t)-\xi(x,\, t)}{a} = \frac{\partial\xi(x,\, t)}{\partial x} \tag{71}$$

Summation over i translates into an integral over x,

$$a\sum_i \to \mathrm{d}x \tag{72}$$

and the discrete Lagrange function of Eq. (69) turns into the Lagrangian

$$L = \frac{1}{2}\int \mathrm{d}x\left[\mu\dot{\xi}^2 - Y\left(\frac{\partial\xi}{\partial x}\right)\right] \tag{73}$$

for the continuous rod; from now on we suppress the arguments of the ξ.

Going back to the equation of motion, Eq. (69), and taking a closer look at the second term in the limit of vanishing spacing a

$$\begin{aligned}\left(\frac{\xi_{i+1}-\xi_i}{a^2}-\frac{\xi_i-\xi_{i-1}}{a^2}\right) &\longrightarrow \left(\frac{\xi(x+a)-\xi(x)}{a^2}-\frac{\xi(x)-\xi(x-a)}{a^2}\right) \\ &\overset{a\to 0}{\longrightarrow} \lim_{a\to 0}\frac{\partial\xi(x+a)/\partial x-\partial\xi(x)/\partial x}{a}=\frac{\partial^2\xi(x)}{\partial x^2},\end{aligned} \tag{74}$$

it is clear that this is a second derivative, and the E.o.M. for the continuous elastic rod therefore is given by

$$\mu\frac{\partial^2\xi}{\partial t^2}-Y\frac{\partial^2\xi}{\partial x^2}=0\,, \tag{75}$$

with longitudinal waves as solution.

Lagrange Density The previous considerations suggest that it is sensible to introduce a Lagrange density

$$\mathcal{L}(\xi,\,\partial\xi/\partial t,\,\partial\xi/\partial t,\,x,\,t)=\frac{\mu}{2}\left(\frac{\partial\xi}{\partial t}\right)^2-\frac{Y}{2}\left(\frac{\partial\xi}{\partial x}\right)^2 \tag{76}$$

which becomes the Lagrange function through integration over the (one-dimensional) space,

$$L=\int \mathrm{d}x\mathcal{L}(\xi,\,\partial\xi/\partial t,\,\partial\xi/\partial x,\,x,\,t) \tag{77}$$

and the action S, as usual, by integrating the Lagrange function over time,

$$S(t_0, t_1) = \int_{t_0}^{t_1} \mathrm{d}t \int_{x_0}^{x_1} \mathrm{d}x \, \mathcal{L} \, . \tag{78}$$

In the rest of the class we will assume that Lagrange densities depend on fields and their derivatives only and do not explicitly depend on position or time, i.e.,

$$\mathcal{L} = \mathcal{L}\left(\xi, \frac{\partial \xi}{\partial t}, \frac{\partial \xi}{\partial x}\right) . \tag{79}$$

Euler-Lagrange E.o.M. To arrive at the Euler-Lagrange equations of motion we will proceed as before, by minimizing the action with respect to virtual variations of the fields ξ and their derivatives,

$$\begin{aligned} \xi(x, t) &\rightarrow \xi'(x, t) = \xi(x, t) + \alpha\zeta(x, t) \\ \frac{\partial \xi(x, t)}{\partial t} &\rightarrow \frac{\partial \xi'(x, t)}{\partial t} = \frac{\partial \xi(x, t)}{\partial t} + \alpha \frac{\partial \zeta(x, t)}{\partial t} \\ \frac{\partial \xi(x, t)}{\partial x} &\rightarrow \frac{\partial \xi'(x, t)}{\partial x} = \frac{\partial \xi(x, t)}{\partial x} + \alpha \frac{\partial \zeta(x, t)}{\partial x} \, . \end{aligned} \tag{80}$$

Here α is a parameter that steers the size of the variation, while $\zeta(x, t)$ represents an arbitrary function which vanishes at the endpoints of the integral, i.e., at times t_0 and t_1.

Minimizing the action with respect to the variations is achieved by

$$0 \equiv \frac{\mathrm{d}S}{\mathrm{d}\alpha} = \int_{t_0}^{t_1} \mathrm{d}t \int_{x_0}^{x_1} \mathrm{d}x \left[\frac{\partial \mathcal{L}}{\partial \xi} \frac{\partial \xi}{\partial \alpha} + \frac{\partial \mathcal{L}}{\partial \left(\frac{\partial \xi}{\partial t}\right)} \frac{\partial \left(\frac{\partial \xi}{\partial t}\right)}{\partial \alpha} + \frac{\partial \mathcal{L}}{\partial \left(\frac{\partial \xi}{\partial x}\right)} \frac{\partial \left(\frac{\partial \xi}{\partial x}\right)}{\partial \alpha} \right] \tag{81}$$

Because the variation vanishes at the endpoints, integration by parts allows us to replace the last two terms by

$$\begin{aligned} \int_{t_0}^{t_1} \mathrm{d}t \frac{\partial \mathcal{L}}{\partial \left(\frac{\partial \xi}{\partial t}\right)} \frac{\partial}{\partial \alpha} \left(\frac{\partial \xi}{\partial t}\right) &= \int_{t_0}^{t_1} \mathrm{d}t \frac{\partial \mathcal{L}}{\partial \left(\frac{\partial \xi}{\partial t}\right)} \frac{\partial}{\partial t} \frac{\partial \xi}{\partial \alpha} = -\int_{t_0}^{t_1} \mathrm{d}t \frac{\partial}{\partial t} \frac{\partial \mathcal{L}}{\partial \left(\frac{\partial \xi}{\partial t}\right)} \frac{\partial \xi}{\partial \alpha} \\ \int_{x_0}^{x_1} \mathrm{d}x \frac{\partial \mathcal{L}}{\partial \left(\frac{\partial \xi}{\partial x}\right)} \frac{\partial}{\partial \alpha} \left(\frac{\partial \xi}{\partial x}\right) &= \int_{x_0}^{x_1} \mathrm{d}x \frac{\partial \mathcal{L}}{\partial \left(\frac{\partial \xi}{\partial x}\right)} \frac{\partial}{\partial x} \frac{\partial \xi}{\partial \alpha} = -\int_{x_0}^{x_1} \mathrm{d}x \frac{\partial}{\partial x} \frac{\partial \mathcal{L}}{\partial \left(\frac{\partial \xi}{\partial x}\right)} \frac{\partial \xi}{\partial \alpha} \end{aligned} \tag{82}$$

Putting it all together results in

$$0 \equiv \int_{t_0}^{t_1} \mathrm{d}t \int_{x_0}^{x_1} \mathrm{d}x \frac{\partial \xi}{\partial \alpha} \left[\frac{\partial \mathcal{L}}{\partial \xi} - \frac{\partial}{\partial t} \frac{\partial \mathcal{L}}{\partial \left(\frac{\partial \xi}{\partial t}\right)} - \frac{\partial}{\partial x} \frac{\partial \mathcal{L}}{\partial \left(\frac{\partial \xi}{\partial x}\right)} \right] \tag{83}$$

and, finally, the equations of motion

$$\boxed{\frac{\partial}{\partial t} \frac{\partial \mathcal{L}}{\partial \left(\frac{\partial \xi}{\partial t}\right)} + \frac{\partial}{\partial x} \frac{\partial \mathcal{L}}{\partial \left(\frac{\partial \xi}{\partial x}\right)} - \frac{\partial \mathcal{L}}{\partial \xi} = 0\,.} \tag{84}$$

This of course is relatively straightforward to extend to the case of two or three spatial dimensions, by essentially replacing the derivative w.r.t. x with a gradient, $\partial/\partial x \rightarrow \underline{\nabla}$, and by replacing the one-dimensional integral over x with an integral over full space, $\int dx \rightarrow \int d^3x$.

Lorentz-Invariant Formulation The treatment of the fields in the Lagrange formalism until now has not been Lorentz-invariant, and we are going to rectify this now.

The first thing to note is that in a Lorentz-invariant framework, the integration should not distinguish between time and space, suggesting to move

$$\int_{t_0}^{t_1} \mathrm{d}t \int_{\underline{x}_0}^{\underline{x}_1} \mathrm{d}^3 x \longrightarrow \int_{x_0^\mu}^{x_1^\mu} \mathrm{d}^4 x \,. \tag{85}$$

A simple calculation will show that the integral over the space-time volume is boost and hence Lorentz-invariant.

In a similar way, the two derivative terms in the Lagrange density in Eq. (79) will be amalgamated such that the Lorentz-invariant Lagrange density is given by

$$\mathcal{L} = \mathcal{L}\left(\xi,\, \partial_\mu \xi\right) \,. \tag{86}$$

There is one big caveat, however.

This Lagrange density must be a Lorentz-scalar; pictorially speaking, all indices must be contracted.

This implies that terms of the type $\partial_\mu \xi$ must come at least in squares, like, e.g. $(\partial_\mu \xi)(\partial^\mu \xi)$ such that the two Lorentz-indices are contracted off.

To obtain Euler-Lagrange equations of motion from the action

$$S = \int_{x_0^\mu}^{x_1^\mu} \mathrm{d}^4x \, \mathcal{L}\left(\xi, \, \partial_\mu \xi\right) \, , \tag{87}$$

steps similar to the one before will be necessary.

In particular, we will now demand that the virtual variations of the field vanish on the surface of the d^4x-integration, leading to

$$\begin{aligned} 0 \equiv \frac{\mathrm{d}S}{\mathrm{d}\alpha} &= \int_{x_0^\mu}^{x_1^\mu} \mathrm{d}^4x \left[\frac{\partial \mathcal{L}}{\partial \xi} \frac{\partial \xi}{\partial \alpha} + \frac{\partial \mathcal{L}}{\partial(\partial_\mu \xi)} \frac{\partial(\partial_\mu \xi)}{\partial \alpha} \right] \\ &= \int_{x_0^\mu}^{x_1^\mu} \mathrm{d}^4x \left[\frac{\partial \xi}{\partial \alpha} \left(\frac{\partial \mathcal{L}}{\partial \xi} - \partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \xi)} \right) + \partial_\mu \left(\partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \xi)} \frac{\partial \xi}{\partial \alpha} \right) \right] \, . \end{aligned} \tag{88}$$

The last term is a four-dimensional volume integral over a four-dimensional divergence, which vanishes with the vanishing virtual variations of the fields, and we are left with the Euler-Lagrange E.o.M. for relativistic fields

$$\boxed{\partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \xi)} - \frac{\partial \mathcal{L}}{\partial \xi} = 0\,.} \tag{89}$$

3.2 Scalar Fields: Real Scalars

Know Thy Equation of Motion! The desired equations of motion are a good starting point to construct Lagrange densities for realistic and physically relevant examples of relativistic field theories.

We will first consider the probably simplest case of a free real scalar field $\phi(x)$, i.e., a field that does not interact with other fields or with an external potential.

To see how this works, let us start with the well-known Schrodinger equation, where the starting point is the kinetic energy, given by $E = p^2/2m$.

Substituting derivatives for energy and momentum, $E \rightarrow i\partial_t$ and $p \rightarrow -i\underline{\nabla}$ or $p_j \rightarrow -i\partial_j$, we arrive at the E.o.M.,

$$i\frac{\partial}{\partial t}\phi(x) + \frac{1}{2}\frac{\partial^2}{\partial x_j^2}\phi(x) = 0\,. \tag{90}$$

In the same vein, we start with the relativistic energy-momentum relation, $E^2 = \underline{p}^2 + m^2$ and find the *Klein-Gordon Equation*

$$\boxed{\left(\frac{\partial^2}{\partial t^2} - \underline{\nabla}^2 + m^2\right)\phi(x) \;=\; \left(\partial_\mu\partial^\mu + m^2\right)\phi(x) \;=\; 0\,.} \tag{91}$$

Solutions to the Klein-Gordon Equation The solution to the Klein-Gordon Equation, Eq. (91) for a fixed momentum is given by

$$\phi(x) = a(\underline{k})\, e^{-ik\cdot x} + a^*(\underline{k})\, e^{ik\cdot x}\,, \tag{92}$$

where $a(\underline{k})$ and $a^*(\underline{k})$ are the (complex) amplitudes for the plane-wave solution for a fixed wave four-vector k, which satisfies the implicit "on-shell" condition $k^2 = k_0^2 - \underline{k}^2 = m^2$.

Of course, we could also sum over many such waves and we arrive at

$$\boxed{\phi(x) = \int \frac{\mathrm{d}^3k}{(2\pi)^3(2k_0)} \left[a(\underline{k})\, e^{-ik\cdot x} + a^*(\underline{k})\, e^{ik\cdot x}\right].} \tag{93}$$

A few comments are in order here:

1. In Eq. (92) we have directly used the continuum limit.

   This necessitates the integration over all momenta instead of a summation over a discrete set of eigenvalues for the momentum.

   The latter would be the case for example when second quantizing on a lattice with lattice spacing a, where the eigenvalues for the momentum are discrete and behave like $k_n = n/a$.

2. The measure of integration, that sums over the different wave vectors, should better be Lorentz-invariant.

It is not trivial to see immediately that $d^3k/(2k_0)$ fulfils this criterion.

To realize that this is indeed the case, let us start with a manifestly Lorentz-invariant integration measure,

$$\begin{aligned}\int \frac{\mathrm{d}^4k}{(2\pi)^4}(2\pi)\delta(k^2-m^2)\Theta(k_0) &= \int \frac{\mathrm{d}^3k}{(2\pi)^3}\left[\mathrm{d}k_0\delta(k_0^2-\underline{k}^2-m^2)\Theta(k_0)\right] \\ &= \int \frac{\mathrm{d}^3k}{(2\pi)^3}\sum_{k_0=\pm\sqrt{\underline{k}^2+m^2}}\left[\frac{1}{2k_0}\Theta(k_0)\right] \\ &= \int \frac{\mathrm{d}^3k}{(2\pi)^3(2k_0)}\,,\end{aligned} \tag{94}$$

where the d^4k obviously is a boost and rotation-invariant quantity, the factor $\delta(k^2 - m^2)$ encodes the (Lorentz-invariant) relativistic energy-momentum relation necessary to ensure that the quanta behave in a physically sensible way, and $\Theta(k_0)$ projects on positive-energy solutions.

In performing the k_0-integration we have used a property of the δ-function, namely

$$\int \mathrm{d}x\,\delta(f(x)) = \sum_{x_i:\,f(x_i)=0}\frac{\delta(x-x_i)}{f'(x_i)}\,, \tag{95}$$

which replaces the integral over the δ-function of a function $f(x)$ with an integral over a sum of its zeroes x_i(given by $f(x_i) = 0$), normalzed by the first derivative of the function at the zero.

Klein-Gordon Lagrange Density It is simple to show that this equation of motion, cf. Eq. (91), can be obtained from the Lagrange density

$$\boxed{\mathcal{L}(\partial_\mu\phi,\,\phi) \;=\; \frac{1}{2}(\partial_\mu\phi)(\partial^\mu\phi) - \frac{m^2}{2}\phi^2\,.} \tag{96}$$

Note that, wherever the dependence is self-evident, we will ignore the arguments of the fields from now on.

To see this, let us plug this Lagrange density into Eq. (89), with the obvious replacement $\xi \to \phi$.

$$\begin{aligned} 0 &= \partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu\phi)} - \frac{\partial \mathcal{L}}{\partial\phi} \\ &= \partial_\mu \frac{\partial[\frac{1}{2}(\partial_\mu\phi)(\partial^\mu\phi)]}{\partial(\partial_\mu\phi)} - \frac{\partial[\frac{m^2}{2}\phi^2]}{\partial\phi}\,, \end{aligned} \tag{97}$$

where we have replaced the Lagrange density in the first line with the relevant parts of Eq. (96) in the second one.

The first expression looks a bit tricky and, naively, it seems as if derivation w.r.t. $\partial_\mu\phi$ would only deliver $\frac{1}{2}\partial_\mu\phi$ – this however is wrong, and it is easy to see why.

Rewriting this part component by component we would arrive at terms like

$$\frac{1}{2}\frac{\partial}{\partial t}\frac{\partial\dot{\phi}^2}{\partial\dot{\phi}} = 2\cdot\frac{1}{2}\frac{\partial\dot{\phi}}{\partial t} = \frac{\partial^2\phi}{\partial t^2} \tag{98}$$

and similar for the spatial components.

Another way to see this is to rewrite the Lorentz-scalar of the derivatives with other indices – replacing the μ's with ν's in the Lagrangian (it doesn't matter, they get contracted anyway, so I can sum over μ's, ν's or any other symbol I chose as Lorentz index)

$$\begin{aligned}\frac{\partial}{\partial(\partial_\mu\phi)}\left[\frac{1}{2}(\partial^\nu\phi)(\partial_\nu\phi)\right] &= \frac{\partial}{\partial(\partial_\mu\phi)}\left[\frac{g^{\nu\rho}}{2}(\partial_\nu\phi)(\partial_\rho\phi)\right] \\ &= \frac{g^{\nu\rho}}{2}\left[(\partial_\nu\phi)\frac{\partial(\partial_\rho\phi)}{\partial(\partial_\mu\phi)} + (\partial_\rho\phi)\frac{\partial(\partial_\nu\phi)}{\partial(\partial_\mu\phi)}\right] \\ &= \frac{g^{\nu\rho}}{2}\left[(\partial_\nu\phi)\delta^\mu_\rho + (\partial_\rho\phi)\delta^\mu_\nu\right] = \partial^\mu\phi\end{aligned} \tag{99}$$

Taking into account of this insight, we ultimately arrive at

$$0 = \partial_\mu\partial^\mu\phi + m^2\phi\,, \tag{100}$$

as requested.

3.3 Scalar Fields: Complex Scalars

Two Real Scalars = One Complex Scalar Consider now two such free real scalar fields, ϕ_1 and ϕ_2.

The Lagrange density reads

$$\mathcal{L} = \sum_{i=1}^{2} \frac{1}{2}(\partial_\mu \phi_i)(\partial^\mu \phi_i) - \frac{m_i^2}{2}\phi_i^2 \tag{101}$$

If both masses are equal, $m_1 = m_2$, the two real fields can be re-arranged into one complex one,

$$\phi = \frac{\phi_1 + i\phi_2}{\sqrt{2}} \quad \text{and} \quad \phi^* = \frac{\phi_1 - i\phi_2}{\sqrt{2}}, \tag{102}$$

or

$$\phi_1 = \frac{\phi + \phi^*}{\sqrt{2}} \quad \text{and} \quad \phi_2 = \frac{-i(\phi - \phi^*)}{\sqrt{2}} \tag{103}$$

The Lagrange density for the free complex scalar field then becomes

$$\boxed{\mathcal{L} = (\partial_\mu \phi^*)(\partial^\mu \phi) - m^2 \phi^* \phi\,.} \tag{104}$$

It is important to stress here that while the fields ϕ and ϕ^* are connected through complex conjugation, they still encode two independent degrees of freedom and therefore must be treated as independent quantities when analyzing the structure of the Lagrange density, or deriving E.o.M..

Equations of Motion The E.o.M. are obtained in the now familiar fashion as

$$
\begin{aligned}
0 = \partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} - \frac{\partial \mathcal{L}}{\partial \phi} &= \partial_\mu \partial^\mu \phi^* + m^2 \phi^* \\
0 = \partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi^*)} - \frac{\partial \mathcal{L}}{\partial \phi^*} &= \partial_\mu \partial^\mu \phi + m^2 \phi \,.
\end{aligned}
\tag{105}
$$

Note that, as we have two independent degrees of freedom (the two fields), we have two E.o.M., obtained by differentiating the Lagrangian with respect to each of the two fields.

A Simple Symmetry Inspection of the Lagrangian of Eq. (104) reveals an interesting invariance under rotations.

Transforming the fields as

$$
\phi \to \phi' = \exp(i\theta)\phi \,, \quad \phi^* \to \phi'^* = \exp(-i\theta)\phi^*
\tag{106}
$$

with a *constant* angle θ, we have

$$
\begin{aligned}
\mathcal{L} \to \mathcal{L}' &= (\partial_\mu \phi'^*)(\partial^\mu \phi') - m^2 \phi^{*\prime} \phi' \\
&= [\partial_\mu (e^{-i\theta} \phi^*)][\partial^\mu (e^{i\theta} \phi)] - m^2 (e^{-i\theta} \phi^*)(e^{i\theta} \phi) = \mathcal{L} \,.
\end{aligned}
\tag{107}
$$

Clearly, the Lagrangian and therefore the action are invariant under this set of transformations.

Conserved Current However, let us for a moment look at this from a different perspective, and *demand* invariance, by setting

$$
\begin{aligned}
0 &\equiv \delta S \\
&= \int \mathrm{d}^4x \left[\frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} \delta(\partial_\mu \phi) + \frac{\partial \mathcal{L}}{\partial \phi} \delta\phi + \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi^*)} \delta(\partial_\mu \phi^*) + \frac{\partial \mathcal{L}}{\partial \phi^*} \delta\phi^* \right]
\end{aligned} \tag{108}
$$

Realizing that, for example,

$$
\delta\phi = \phi' - \phi = (e^{i\theta} - 1)\phi \quad \Longrightarrow \quad \partial_\mu(\delta\phi) = \delta(\partial_\mu \phi) \tag{109}
$$

and using the by now familiar trick of integrating by parts, we arrive at

$$
\begin{aligned}
\delta S = \int \mathrm{d}^4x \Bigg\{ & i\theta\phi \left[\frac{\partial \mathcal{L}}{\partial \phi} - \partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} \right] - i\theta\phi^* \left[\frac{\partial \mathcal{L}}{\partial \phi^*} - \partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi^*)} \right] \\
& + i\theta\partial_\mu \left[\frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} \phi - \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi^*)} \phi^* \right] \Bigg\}.
\end{aligned} \tag{110}
$$

The first line of the result above equals 0, by virtue of the E.o.M. for both ϕ and ϕ^*, and in order for the second line to integrate to 0 we must have

$$
0 \equiv \partial_\mu \left[\frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi^*)} \phi^* - \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} \phi \right] = \partial_\mu \left[\phi^*(\partial^\mu \phi) - (\partial^\mu \phi^*)\phi \right] \tag{111}
$$

This implies the existence of a *conserved current*, i.e.

$$\boxed{\partial_\mu j^\mu = 0} \tag{112}$$

with the current obtained from the equation above

$$\boxed{j^\mu = \left[\phi^*(\partial^\mu \phi) - (\partial^\mu \phi^*)\phi\right] \equiv \phi^* \overleftrightarrow{\partial^\mu} \phi\,.} \tag{113}$$

Here, we have introduced the compact shorthand notation

$$a \overleftrightarrow{\partial^\mu} b = \left[a\,(\partial^\mu b) - (\partial^\mu a) b\right]\,. \tag{114}$$

Conserved Charge The current from Eq. (113) implies the existence of a conserved charge Q with dQ/dt = 0, constructed by integrating the temporal component over three-dimensional space,

$$\boxed{Q = \int \mathrm{d}^3x\, j^0\,.} \tag{115}$$

In the case of complex scalars this means that

$$\begin{aligned} \frac{\mathrm{d}Q}{\mathrm{d}t} &= \frac{\mathrm{d}}{\mathrm{d}t} \int \mathrm{d}^3x\, \frac{1}{2} \left[\phi^*(\partial_t \phi) - (\partial_t \phi^*)\phi\right] \\ &= \int \mathrm{d}^3x\, \frac{\partial j^0}{\partial t} = \int \mathrm{d}^3x\, \underline{\nabla} \cdot \underline{j} = 0 \end{aligned} \tag{116}$$

for the three-current vanishing because the fields are assumed to vanish for $|\underline{x}|\to\infty$.

Here, we have used the fact that the current is conserved,

$$\partial_\mu j^\mu = \partial_t j^t - \underline{\nabla}\cdot\underline{j} = 0 \quad\longrightarrow\quad \partial_t j^t - \underline{\nabla}\cdot\underline{j} \tag{117}$$

3.4 Vector Fields: Maxwell's Equations

A Little Game of Symmetry Assume you want to introduce two different three-vector fields.

From a (classical) symmetry point of view, they can be distinguished through parity, i.e., one of them is parity-odd – a "proper" vector – while the other one is parity-even – an axial-vector.

We call the parity odd fields (or 1^- in spin-parity notation) $\underline{E}$, and the parity even ones (or 1^+) $\underline{B}$.

Now let us assume that you only want to allow first derivatives of the fields, ∂_t and $\underline{\nabla}$ and scalar and pseudo-scalar charge densities $\rho_{E,B}$ and corresponding currents $j_{E,B}$.

Then you can sort resulting quantities by spin and parity as in Table 3.

name	J^P	allowed terms
scalars	0^+	$\underline{\nabla}\cdot\underline{E}$, ρ_E
pseudo-scalars	0^-	$\underline{\nabla}\cdot\underline{B}$, ρ_B
vectors	1^-	$\partial_t\underline{E}$, $\underline{\nabla}\times\underline{B}$, $\underline{j}_E$
axial-vectors	1^-	$\underline{\nabla}\times\underline{E}$, $\partial_t\underline{B}$, $\underline{j}_B$

Table 2: Terms in Maxwell's equations, by spin and parity

Symmetry to Dynamics Each of the four rows in Table 2 collects possible terms in one of the four equations defining the system, and this is where we will introduce data to the game.

First of all we identify E and B with electric and magnetic fields, respectively.

Then we realize that to date no magnetic monopoles have been found, and therefore there is no magnetic charge density of current, $\rho_B = 0$ and $\underline{j}_B = 0$.

Adding lastly that electrodynamics is a theory of light, and thereby fixing prefactors and signs we arrive at Maxwell's equations

$$\boxed{\begin{array}{rclrcl} \underline{\nabla} \cdot \underline{E} & = & 4\pi\rho_E & \underline{\nabla} \cdot \underline{B} & = & 0 \\ \underline{\nabla} \times \underline{B} - \partial_t \underline{E} & = & 4\pi \underline{j}_E & \underline{\nabla} \times \underline{E} + \partial_t \underline{B} & = & 0 \end{array}} \tag{118}$$

Note that we absorbed the usual factors of ϵ_0 and μ_0 into the definition of the charge and current, and we have used natural units with c = 1.

The Vector Potential The left column in Eq.(118) suggest to use a scalar potential Φ, which we denote as A_0, and a vector potential $\underline{A}$ and write

$$\underline{E} = -\underline{\nabla} A^0 - \partial_t \underline{A} \quad \text{and} \quad \underline{B} = \underline{\nabla} \times \underline{A}. \tag{119}$$

Of course this now forms a four-vector potential $A^\mu = (A^0, \underline{A})$, and we will continue the analysis of electrodynamics mainly based on this object.

Gauge Transformation and Gauge Invariance One of the first benefits of introducing the vector potential is that it is relatively easy to formulate *gauge transformations*.

To this end we introduce an *arbitrary* scalar gauge function, Λ(x), under which A(x) transforms as

$$\boxed{A^\mu \to A'^\mu = A^\mu - \partial^\mu \Lambda\,,} \tag{120}$$

and therefore

$$\begin{aligned} \underline{E} \to \underline{E}' = \; -\underline{\nabla}(A^0 - \partial^0\Lambda) - \partial_t(\underline{A} + \underline{\nabla}\cdot\Lambda) = -\underline{\nabla}A^0 - \partial_t\underline{A} = \underline{E} \\ \underline{B} \to \underline{B}' = \underline{\nabla} \times (\underline{A} + \underline{\nabla}\cdot\Lambda) = \underline{\nabla} \times \underline{A} = \underline{B}\,, \end{aligned} \tag{121}$$

where we have used that curl ·grad ($\underline{\nabla}$ x $\underline{\nabla}$) of a scalar function vanishes.

This suggest that it would be beneficial to express the theory in terms of gauge invariant quantities made from A^μ, to directly encode this symmetry.

The Field-Strength Tensor One such gauge-invariant quantity is the anti-symmetric field-strength tensor

$$\boxed{F^{\mu\nu} = \partial^\mu A^\nu - \partial^\nu A^\mu = \begin{pmatrix} 0 & -E_x & -E_y & -E_z \\ E_x & 0 & -B_z & B_y \\ E_y & B_z & 0 & -B_x \\ E_z & -B_y & B_x & 0 \end{pmatrix}}\,, \tag{122}$$

and another such tensor is its dual,

$$\tilde{F}^{\mu\nu} = \frac{1}{2}\epsilon^{\mu\nu\sigma\rho}F_{\rho\sigma} = \begin{pmatrix} 0 & -B_x & -B_y & -B_z \\ B_x & 0 & E_z & -E_y \\ B_y & -E_z & 0 & E_x \\ B_z & E_y & -E_x & 0 \end{pmatrix} \tag{123}$$

They allows to express the inhomogeneous and homogeneous Maxwell's equations, i.e. the left and right column of Eq. (118), as

$$\boxed{\partial_\mu F^{\mu\nu} = 4\pi j^\nu \ \text{ and } \ \partial_\mu \tilde{F}^{\mu\nu} = 0\,.} \tag{124}$$

Lagrange Density in Terms of the Fields There are various ways to express the Lagrange density; a typical version expresses it through the electric and magnetic fields and reads

$$\boxed{\mathcal{L} = \frac{E^2 - B^2}{8\pi} - \rho\phi + \underline{j} \cdot \underline{A}\,.} \tag{125}$$

The E.o.M. are obtained in terms of the potential ϕ and $\underline{A}$, using the fact that the electromagnetic fields are expressed through their derivatives.

This also fixes the two homogeneous Maxwell equations, i.e. the right column of Eqs. (118).

This also implies that we are left with the task to check if the Lagrange density above yields the correct inhomogenous equations – the left column of Eq. (118).

For example, for ϕ we have:

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \phi} &= -\rho \\ \frac{\partial \mathcal{L}}{\partial(\partial\phi/\partial x_k)} &= \frac{E_k}{4\pi}\frac{\partial E_k}{\partial(\partial\phi/\partial x_k)} = -\frac{E_k}{4\pi}, \end{aligned} \tag{126}$$

where

$$\frac{\partial E_k}{\partial(\partial\phi/\partial x_k)} = -1 \tag{127}$$

follows directly from Eq. (121).

Assembling all parts, and making the summation over repeated indices explicit therefore yields Gauss' law,

$$\sum_k \left[\frac{\partial}{\partial x_k}\frac{\partial \mathcal{L}}{\partial(\partial\phi/\partial x_k)}\right] - \frac{\partial \mathcal{L}}{\partial \phi} = -\frac{\underline{\nabla}\cdot\underline{E}}{4\pi} + \rho = 0\,. \tag{128}$$

Similarly, for an arbitrary component of $\underline{A}$, A_i we find

$$
\begin{aligned}
\frac{\partial \mathcal{L}}{\partial A_i} &= j_i \\
\frac{\partial \mathcal{L}}{\partial(\partial A_i/\partial t)} &= \frac{E_i}{4\pi}\frac{\partial E_i}{\partial(\partial A_i/\partial t)} = -\frac{E_i}{4\pi} \\
\frac{\partial \mathcal{L}}{\partial(\partial A_i/\partial x_j)} &= -\frac{B_k}{4\pi}\frac{\partial B_k}{\partial(\partial A_i/\partial x_j)} = -\epsilon_{ijk}\frac{B_k}{4\pi} \\
\frac{\partial \mathcal{L}}{\partial(\partial A_i/\partial x_k)} &= -\frac{B_j}{4\pi}\frac{\partial B_j}{\partial(\partial A_i/\partial x_k)} = -\epsilon_{ijk}\frac{B_j}{4\pi}\,,
\end{aligned}
\tag{129}
$$

where Eq. (121) has again been used, noting that, expressed in component notation

$$
\underline{B} = \underline{\nabla} \times \underline{A} \quad \longleftrightarrow \quad B_k = \epsilon_{ijk}\partial_i A_j\,. \tag{130}
$$

specializing i = 1 we are left with Ampere's law,

$$
\frac{1}{4\pi}\left(\frac{\partial B_3}{\partial x_2} - \frac{\partial B_2}{\partial x_3}\right) - \frac{1}{4\pi}\frac{\partial E_1}{\partial t} - j_1 = 0\,, \tag{131}
$$

or, in vector form,

$$
\underline{\nabla} \times \underline{B} - \frac{\partial E}{\partial t} = 4\pi \underline{j}\,. \tag{132}
$$

Lagrange Density in Terms of the Field Strength Tensor One obvious short-coming of the form of the the Lagrange density in Eq. (125) is that it is not manifestly gauge-invariant.

This can be overcome by reconstructing a Lagrange density not in terms of the electromagnetic fields but rather in terms of the field strength tensor.

Rearranging factors of 4π and introducing an overall sign we arrive at

$$\boxed{\mathcal{L} = -\frac{1}{4} F^{\mu\nu} F_{\mu\nu} - 4\pi j^{\mu} A_{\mu}\,.} \tag{133}$$

For the "source" term $j^{\mu} A_{\mu}$, which couples the potentials to charge and current densities, we have assumed the so-called "minimal coupling", typically of the form **`source·fields`**, in a Lorentz-invariant way.

This form also fixes the gauge transformation of the four-vector current j^{μ}.

The $(E^2 - B^2)$-term is replaced by a product of field-strength tensors, by realizing that

$$\begin{aligned}
F^{\mu\nu}F_{\mu\nu} &= \; -F^{\nu\mu}F_{\mu\nu} \\
&= \mathrm{Tr}\left[\begin{pmatrix} 0 & -E_x & -E_y & -E_z \\ E_x & 0 & -B_z & B_y \\ E_y & B_z & 0 & -B_x \\ E_z & -B_y & B_x & 0 \end{pmatrix}\begin{pmatrix} 0 & -E_x & -E_y & -E_z \\ E_x & 0 & B_z & -B_y \\ E_y & -B_z & 0 & B_x \\ E_z & B_y & -B_x & 0 \end{pmatrix}\right] \\
&= \mathrm{Tr}\left[\begin{pmatrix} -\underline{E}^2 & \bullet & \bullet & \bullet \\ \bullet & -E_x^2 + B_z^2 + B_y^2 & \bullet & \bullet \\ \bullet & \bullet & -E_y^2 + B_z^2 + B_x^2 & \bullet \\ \bullet & \bullet & \bullet & -E_z^2 + B_y^2 + B_x^2 \end{pmatrix}\right] \\
&= -2(\underline{E}^2 - \underline{B}^2)\,.
\end{aligned} \tag{134}$$

3.5 Hamiltonian Formulation

Hamilton Density In analogy to the case of point particles, momenta π_i conjugate to the fields ϕ_i are defined through

$$\boxed{\pi_i(x) = \frac{\partial \mathcal{L}(\phi_i,\, \partial_\mu \phi_i)}{\partial(\partial_t \phi_i)}} \tag{135}$$

and a Hamilton density is constructed as

$$\boxed{\mathcal{H} = \sum_i \pi_i \dot{\phi}_i - \mathcal{L}\,.} \tag{136}$$

The Hamilton function reads

$$H = \int \mathrm{d}^3x\, \mathcal{H}(\phi_i,\, \pi_i) = \int \mathrm{d}^3x \left(\frac{\partial \mathcal{L}}{\partial \dot{\phi}_i} \dot{\phi}_i - \mathcal{L} \right)\,. \tag{137}$$

Equations of Motion Similarly to the case of point particles, the Hamilton E.o.M. read

$$\frac{\partial \mathcal{H}}{\partial \phi_i} = -\dot{\pi}_i \quad \text{and} \quad \frac{\partial \mathcal{H}}{\partial \pi_i} = \dot{\phi}_i\,. \tag{138}$$

4 Second Quantization

You may have read the title above and asked yourself: What does second quantization actually mean?

Haven't we already quantized the theory?

The answer is that in "first quantization" we quantized the position and momentum of point particles.

This led to important properties related to our ability to measure them – the uncertainty principle – and to a crucial reassessment of the inner working of the world around us, replacing Laplace's demon of deterministic physics with a determinism of probabilities.

So while in this first quantization we replaced the real numbers x and p with operators $\hat{x}$ and $\hat{p}$ and constructed wave functions for the emerging states, in "second quantization" we quantize something else, namely the fields.

Consequently, x and p become "ordinary" numbers again, which serve as arguments of the field operators $\hat{\phi}$ and $\hat{\pi}$.

This step necessitates the introduction of a new state.

While, formally speaking, the states of Quantum Mechanics constitute a *Hilbert space*, the field operators act on objects in a more complicated *Fock space*, which is not labelled by eigen-positions or momenta, but by the number of field quanta of a given momentum.

We will, however, not discuss the properties of these vector spaces in this class.

Simply put: while first quantization quantized the point dynamics of Classical Mechanics, leading to Quantum Mechanics, second quantization produces a *Quantum Field Theory*.

4.1 A How-To Guide

Process Summary The process of second or field quantization follows the logic of the familiar first quantization program, with suitably replacing position and momentum with the field and its conjugate momentum, and by replacing the δ's of the commutators with δ-functions of the positions.

This proceeds in a relatively straight-forward "algorithmic" fashion, as outlined in Fig. 1.

The crucial part in it is to demand equal-time commutator relations between fields and their momenta, which also fixes a Lorentz frame in which the field quantization is performed.

Obviously, there are other choices for such a program, for example a quantization on the light-cone, which however is beyond the scope of the class here.

It is, nevertheless, important to stress that despite the implicit choice of a Lorentz frame during quantization, the resulting theory has the correct causal properties.

This will be shown towards the end of this section.

How-to: Second Quantisation

1. determine **conjugate momenta** of fields:

$$\pi = \partial\mathcal{L}/\partial(\partial_t\phi) = \partial\mathcal{L}/\partial\dot{\phi}$$

2. construct **Hamiltonian** as function of fields ϕ and their momenta π

$$H = \int \mathrm{d}^3x \left(\dot{\phi}\pi - \mathcal{L}\right)$$

3. promote fields and momenta to operators, $\phi \longrightarrow \hat{\phi}$, $\pi \longrightarrow \hat{\pi}$

4. demand **equal time commutators of fields and momenta**

$$\begin{aligned} \left[\hat{\phi}(t,\, \underline{x}),\, \hat{\pi}(t,\, \underline{y})\right] &= i\delta^3(\underline{x} - \underline{y}) \\ \left[\hat{\phi}(t,\, \underline{x}),\, \hat{\phi}(t,\, \underline{y})\right] &= \left[\hat{\pi}(t,\, \underline{x}),\, \hat{\pi}(t,\, \underline{y})\right] = 0 \end{aligned}$$

5. express fields as linear combination of plane waves and **annihilation and creation operators** (which will "inherit" commutator relations)

$$\hat{\phi}(x) = \sum_{\underline{k}} \left[\hat{a}(\underline{k})e^{-ik\cdot x} + \hat{a}^\dagger(\underline{k})e^{ik\cdot x}\right] ,$$

where summation is replaced with integration for continuous momenta k.

Figure 1: The steps performed during second quantization in form of an "algorithm". Details will be worked out and highlighted through examples during the class.

4.2 Second Quantization of the Real Scalar Field

Lagrangian: Fields and Conjugate Momenta Starting with the Lagrangian of Eq. (96),

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

the conjugate momentum reads

$$\pi = \frac{\partial\mathcal{L}}{\partial\dot{\phi}} = \dot{\phi} . \tag{139}$$

Hamiltonian The Hamilton function therefore is given by

$$\boxed{H = \int d^3x \left[\pi\dot{\phi} - \mathcal{L}\right] = \int d^3x \, \frac{1}{2}\left[\pi^2 + (\underline{\nabla}\phi)^2 + m^2\phi^2\right] .} \tag{140}$$

Field Operators and Commutators Promoting the field and its conjugate momentum to operators, $\phi(x) \rightarrow \hat{\phi}(x)$ and $\pi(x) \rightarrow \hat{\pi}(x)$, we *demand the equal-time* commutators,

$$\begin{aligned} \left[\hat{\phi}(t, \underline{x}), \hat{\pi}(t, \underline{y})\right] &= i\delta^3(\underline{x} - \underline{y}) \\ \left[\hat{\phi}(t, \underline{x}), \hat{\phi}(t, \underline{y})\right] &= \left[\hat{\pi}(t, \underline{x}), \hat{\pi}(t, \underline{y})\right] = 0 \end{aligned} \tag{141}$$

Creation and Annihilation Operators The field and the conjugate momentum is expressed through creation and annihilation operators as

$$\begin{aligned}\hat{\phi}(x) &= \int \frac{\mathrm{d}^3k}{(2\pi)^3 2k_0}\left[\hat{a}(\underline{k})\,e^{-ik\cdot x} + \hat{a}^\dagger(\underline{k})\,e^{ik\cdot x}\right]\\ \hat{\pi}(x) &= \int \frac{\mathrm{d}^3k}{(2\pi)^3 2k_0}\left[-ik_0\hat{a}(\underline{k})\,e^{-ik\cdot x} + ik_0\hat{a}^\dagger(\underline{k})\,e^{ik\cdot x}\right],\end{aligned} \tag{142}$$

where we have obtained the momentum operator through straightforward calculation of the derivative $\hat{\pi}(x) = \partial_t \hat{\phi}(x)$.

Comparing the expression for the field operator $\hat{\phi}(x)$ in the equation above with the solution to the Klein-Gordon equation for the classical field $\phi(x)$, Eq. (93), we recognize the same pattern of an expansion in amplitude factors and plane waves.

But while the amplitude factors for the classical field are merely numbers $a(\underline{k})$ and their complex conjugate $a^*(\underline{k})$, they become operators for the quantized fields, and the complex conjugation turns into an Hermitean conjugate.

The interpretation is clear.

While for classical fields every value of the amplitude is allowed, in quantized fields the amplitude is composed by adding finite quanta.

This “amplitude quantization” is reflected by using creation and annihilation operators from which the field “inherits” its quantized properties.

We will build on this in the following by expressing the Hamiltonian through these operators, by creating a number operator, and by analyzing their inherent properties.

Commutators of the Creation and Annihilation Operators To calculate the commutators it is necessary to express, in a first step, the creation and annihilation operators through the field and conjugate momentum operators.

To see how this works, let us first try to combine $\hat{\phi}$ and $\hat{\pi}$ in such a way that the annihilation operator $\hat{a}$ drops out.

Multiplying, inside the integral, the expression for $\hat{\phi}$ with k_0 and $\hat{\pi}$ with i and adding the expression for $\hat{\pi}$ we arrive at

$$\begin{aligned} \text{“}\left[k_0\hat{\phi}(x) - i\hat{\pi}(x)\right]\text{”} &= \int \frac{\mathrm{d}^3k}{(2\pi)^3}\frac{1}{2k_0}\left[2ik_0\hat{a}^\dagger(\underline{k})e^{ik\cdot x}\right] \\ &= \int \frac{\mathrm{d}^3k}{(2\pi)^3}\,\hat{a}^\dagger(\underline{k})e^{-i\underline{k}\cdot\underline{x}}e^{ik_0x_0}\,, \end{aligned} \tag{143}$$

which looks suspiciously like the Fourier transform of $\hat{a}^\dagger$ times a factor.

Therefore, Fourier-back-transforming yields

$$\begin{aligned}\int \mathrm{d}^3 x e^{i\underline{k}\cdot\underline{x}} \left[k_0\hat{\phi}(x) - i\hat{\pi}(x)\right] &= \int \mathrm{d}^3 x e^{i\underline{k}\cdot\underline{x}} \int \frac{\mathrm{d}^3 q}{(2\pi)^3} \hat{a}^\dagger(\underline{q}) e^{-i\underline{q}\cdot\underline{x}} e^{ik_0 x_0} \\ &= \int \frac{\mathrm{d}^3 q}{(2\pi)^3} \delta^3(\underline{k}-\underline{q}) \hat{a}^\dagger(\underline{q}) e^{ik_0 x_0} = \hat{a}^\dagger(\underline{k}) e^{ik_0 x_0} \, .\end{aligned} \tag{144}$$

After rearranging and repeating similar steps to extract the annihilation operator $\hat{a}$,

$$\begin{aligned}\hat{a}(\underline{k}) &= \int \mathrm{d}^3 x e^{ik\cdot x} \left[k_0\hat{\phi}(x) + i\hat{\pi}(x)\right] \\ \hat{a}^\dagger(\underline{k}) &= \int \mathrm{d}^3 x e^{-ik\cdot x} \left[k_0\hat{\phi}(x) - i\hat{\pi}(x)\right] \, .\end{aligned} \tag{145}$$

The equal-time commutators of the creation and annihilation operators can be readily calculated as

$$\begin{aligned}\left[\hat{a}(\underline{k}),\, \hat{a}(\underline{q})\right] &= \int \mathrm{d}^3 x \mathrm{d}^3 y e^{ik\cdot x + iq\cdot y} \left[k_0\hat{\phi}(x) + i\hat{\pi}(x),\, q_0\hat{\phi}(y) + i\hat{\pi}(y)\right] \\ &= \int \mathrm{d}^3 x \mathrm{d}^3 y e^{ik\cdot x + iq\cdot y} \left\{k_0 q_0 \left[\hat{\phi}(x),\, \hat{\phi}(y)\right] - \left[\hat{\pi}(x),\, \hat{\pi}(y)\right] \right. \\ &\qquad \left. + ik_0 \left[\hat{\phi}(x),\, \hat{\pi}(y)\right] + iq_0 \left[\hat{\pi}(x),\, \hat{\phi}(y)\right]\right\} \\ &= \int \mathrm{d}^3 x \mathrm{d}^3 y e^{ik\cdot x + iq\cdot y} \left\{0 - 0 - k_0\delta^3(\underline{x}-\underline{y}) + q_0\delta^3(\underline{y}-\underline{x})\right\} \\ &= \int \mathrm{d}^3 x e^{i(k+q)\cdot x} \left\{(q_0 - k_0)\right\} \\ &= e^{i(k_0+q_0)x_0} \left\{(q_0 - k_0)\right\} (2\pi)^3 \delta^3(\underline{k}+\underline{q}) = 0\end{aligned} \tag{146}$$

because $\underline{k} = -\underline{q}$ from the δ function implies that $\underline{k}^2 = \underline{q}^2$ and therefore $k_0 = q_0$.

Similarly, with the only difference being an ultimately inconsequential relative sign in front of *both* momentum operators and in *both* exponential factors

$$\left[\hat{a}^\dagger(\underline{k}),\, \hat{a}^\dagger(\underline{q})\right] \;=\; 0\,. \tag{147}$$

This leaves us with calculating

$$\begin{aligned}
\left[\hat{a}(\underline{k}),\, \hat{a}^\dagger(\underline{q})\right] \;&=\; \int \mathrm{d}^3x \mathrm{d}^3y e^{ik\cdot x - iq\cdot y}\left[k_0\hat{\phi}(x) + i\hat{\pi}(x),\, q_0\hat{\phi}(y) - i\hat{\pi}(y)\right] \\
&= \int \mathrm{d}^3x \mathrm{d}^3y e^{ik\cdot x - iq\cdot y}\left\{k_0 q_0\left[\hat{\phi}(x),\, \hat{\phi}(y)\right] + \left[\hat{\pi}(x),\, \hat{\pi}(y)\right]\right. \\
&\qquad\qquad\qquad\qquad \left. -ik_0\left[\hat{\phi}(x),\, \hat{\pi}(y)\right] + iq_0\left[\hat{\pi}(x),\, \hat{\phi}(y)\right]\right\} \\
&= \int \mathrm{d}^3x \mathrm{d}^3y e^{ik\cdot x - iq\cdot y}\left\{0 - 0 + k_0\delta^3(\underline{x} - \underline{y}) + q_0\delta^3(\underline{y} - \underline{x})\right\} \\
&= \int \mathrm{d}^3x e^{i(k-q)\cdot x}\left\{(k_0 + q_0)\right\} \\
&= e^{i(k_0 - q_0)x_0}\left\{k_0 + q_0)\right\}(2\pi)^3\delta^3(\underline{k} - \underline{q}) = 2k_0(2\pi)^3\delta^3(\underline{k} - \underline{q})
\end{aligned} \tag{148}$$

Putting it all together, we arrive at the following set of commutation relations between the creation and annihilation operators

$$\boxed{\begin{aligned} \left[\hat{a}(\underline{k}),\, \hat{a}^\dagger(\underline{q})\right] &= 2k_0(2\pi)^3\delta^3(\underline{k}-\underline{q}) \\ \left[\hat{a}(\underline{k}),\, \hat{a}(\underline{q})\right] &= \left[\hat{a}^\dagger(\underline{k}),\, \hat{a}^\dagger(\underline{q})\right] = 0\,. \end{aligned}} \tag{149}$$

Hamilton Operator In a next step in our analysis of the theory we express the Hamilton operator of Eq. (140) through the creation and annihilation operators.

A somewhat tricky part are the quadratic terms such as ϕ^2 and similar.

For them, we need to use the expansion of Eq. (142) for each factor, leading to two integrals over three-momenta $\underline{k}$ and k':

$$\begin{aligned} \hat{H} &= \int \mathrm{d}^3x\, \frac{1}{2}\left[\hat{\pi}^2 + (\underline{\nabla}\hat{\phi})^2 + m^2\hat{\phi}^2\right] \\ &= \frac{1}{2}\int \mathrm{d}^3x\, \frac{1}{2}\int \frac{\mathrm{d}^3k}{(2\pi)^3 2k_0}\frac{\mathrm{d}^3k'}{(2\pi)^3 2k_0'}\Bigg\{ \\ &\quad \hat{a}(\underline{k})\hat{a}(\underline{k}')\left[-k_0k_0' - \underline{k}\underline{k}' + m^2\right] e^{-i(k+k')\cdot x} \\ &\quad +\hat{a}(\underline{k})\hat{a}^\dagger(\underline{k}')\left[+k_0k_0'\underline{k}\underline{k}' + m^2\right] e^{-i(k-k')\cdot x} \\ &\quad +\hat{a}^\dagger(\underline{k})\hat{a}(\underline{k}')\left[+k_0k_0'\underline{k}\underline{k}' + m^2\right] e^{+i(k-k')\cdot x} \\ &\quad +\hat{a}^\dagger(\underline{k})\hat{a}^\dagger(\underline{k}')\left[-k_0k_0' - \underline{k}\underline{k}' + m^2\right] e^{+i(k+k')\cdot x} \Bigg\} \end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{2}\int \frac{\mathrm{d}^3k}{(2\pi)^3 2k_0}\frac{\mathrm{d}^3k'}{(2\pi)^3 2k'_0}\Big\{ \\
&\qquad (2\pi)^3\delta^3(+\underline{k}+\underline{k}')\, e^{-i(k_0+k'_0)x_0}\, \hat{a}(\underline{k})\hat{a}(\underline{k}')\, \left[-k_0k'_0 - \underline{kk}' + m^2\right] \\
&\quad + (2\pi)^3\delta^3(+\underline{k}-\underline{k}')\, e^{-i(k_0-k'_0)x_0}\, \hat{a}(\underline{k})\hat{a}^\dagger(\underline{k}')\, \left[+k_0k'_0 + \underline{kk}' + m^2\right] \\
&\quad + (2\pi)^3\delta^3(-\underline{k}+\underline{k}')\, e^{+i(k_0-k'_0)x_0}\, \hat{a}^\dagger(\underline{k})\hat{a}(\underline{k}')\, \left[+k_0k'_0 + \underline{kk}' + m^2\right] \\
&\quad + (2\pi)^3\delta^3(-\underline{k}-\underline{k}')\, e^{+i(k_0+k'_0)x_0}\, \hat{a}^\dagger(\underline{k})\hat{a}^\dagger(\underline{k}')\, \left[-k_0k'_0 - \underline{kk}' + m^2\right]\Big\} \\
&= \frac{1}{2}\int \frac{\mathrm{d}^3k}{(2\pi)^3 4k_0^2}\Big\{\ \hat{a}(\underline{k})\hat{a}(-\underline{k})e^{-2ik_0x_0}\left[-k_0^2+\underline{k}^2+m^2\right] \\
&\quad +\hat{a}(\underline{k})\hat{a}^\dagger(\underline{k})\left[+k_0^2+\underline{k}^2+m^2\right] + \hat{a}^\dagger(\underline{k})\hat{a}(\underline{k})\left[+k_0^2+\underline{k}^2+m^2\right] \\
&\quad +\hat{a}^\dagger(\underline{k})\hat{a}^\dagger(-\underline{k})e^{2ik_0x_0}\left[-k_0^2+\underline{k}^2+m^2\right]\Big\} \\
&= \frac{1}{2}\int \frac{\mathrm{d}^3k}{(2\pi)^3 4k_0^2}\Big\{\left[2k_0^2\right]\ \left[\hat{a}(\underline{k})\hat{a}^\dagger(\underline{k}) + \hat{a}^\dagger(\underline{k})\hat{(}\underline{k})\right]\Big\} \\
&= \frac{1}{2}\int \frac{\mathrm{d}^3k}{(2\pi)^3 2k_0}\, k_0\left[\hat{a}(\underline{k})\hat{a}^\dagger(\underline{k}) + \hat{a}^\dagger(\underline{k})\hat{(}\underline{k})\right],
\end{aligned}
\tag{150}
$$

where the δ functions in the first step emerge from the integral over x and where we have eliminated the terms $\hat{a}\hat{a}$ and $\hat{a}^\dagger\hat{a}^\dagger$ by realizing that due to the relativistic energy-momentum relation $k^2_0 = k^2 + m^2$.

Therefore, the Hamilton operator for the real scalar field is given by

$$\boxed{\hat{H} = \frac{1}{2} \int \frac{\mathrm{d}^3 k}{(2\pi)^3 2k_0} \, k_0 \left[\hat{a}(\underline{k}) \hat{a}^\dagger(\underline{k}) + \hat{a}^\dagger(\underline{k}) \hat{(}\underline{k}) \right]} \tag{151}$$

It suggests that the Quantum Field Theory for a real scalar field can be interpreted as a continuous sum of harmonic oscillators, permeating all space.

Simple States: Ground State and First Excited State Following the same logic already present in the harmonic oscillator in Quantum Mechanics we introduce a ground state – the "vacuum" – $|0\rangle$which is annihilated by any annihilation operator,

$$\hat{a}(\underline{k}) \, |0\rangle = 0 \quad \forall \underline{k} \, . \tag{152}$$

States containing fields (or particles) with momenta $\underline{k}_i$ are generated by repeated application of the corresponding creation operators

$$\begin{aligned} \hat{a}^\dagger(\underline{k}_1) \, |0\rangle \; &= \; |\underline{k}_1\rangle \\ \hat{a}^\dagger(\underline{k}_1) \hat{a}^\dagger(\underline{k}_2) \, |0\rangle \; &= \; |\underline{k}_1 \underline{k}_2\rangle \ldots . \end{aligned} \tag{153}$$

Normalization of States But here's a new problem.

Let us take a look at the norm of a one-field (one-particle) state $|\underline{k}\rangle$:

$$
\begin{aligned}
\langle \underline{k}|\underline{k}\rangle &= \left||\underline{k}\rangle\right|^2 = \left|\hat{a}^\dagger(\underline{k})\,|0\rangle\right|^2 = \left[\hat{a}^\dagger(\underline{k})\,|0\rangle\right]^\dagger \left[\hat{a}^\dagger(\underline{k})\,|0\rangle\right] \\
&= \langle 0|\hat{a}(\underline{k})\hat{a}^\dagger(\underline{k})|0\rangle = \left\langle 0\left|\left[\hat{a}(\underline{k})\hat{a}^\dagger(\underline{k}) - \hat{a}^\dagger(\underline{k})\hat{a}(\underline{k})\right]\right|0\right\rangle \\
&= \left\langle 0\left|2k_0(2\pi)^3\delta^3(\underline{k}-\underline{k})\right|0\right\rangle = \left\langle 0\left|2k_0(2\pi)^3\delta^3(\underline{0})\right|0\right\rangle \\
&= 2k_0(2\pi)^3\delta^3(\underline{0})\,,
\end{aligned}
\tag{154}
$$

where in the second line we have subtracted a 0 – remember that $\hat{a}\,|0\rangle = 0$, and where in the last step we used our normalization of the ground state, $\langle 0|0\rangle = 1$.

Using that

$$
(2\pi)^3\delta(\underline{k}) = \int \mathrm{d}^3x e^{i\underline{k}\cdot\underline{x}} \quad\longrightarrow\quad (2\pi)^3\delta(\underline{0}) = \int \mathrm{d}^3x
\tag{155}
$$

suggests that the normalization of the state equals the (infinite) spatial volume – a veritable divergence.

This is actually not a surprising finding, after all, the uncertainty principle tells you that a particle with completely fixed momentum has no localization.

Our particle here, with its fixed momentum represents a plane wave, filling all volume.

If the volume is infinite – which it is for us to have a continuous spectrum – such states have no normalization.

The solution to this conundrum is to "smear" the state with a modulating function $f(\mathrm{k})$, and to define

$$|\underline{k}\rangle \longrightarrow |\underline{k}\rangle_f = f(\underline{k})\hat{a}^\dagger(\underline{k})\,|0\rangle \tag{156}$$

which will lead to perfectly normalizable states, if

$$\int \mathrm{d}^3k\,|f(\underline{k})|^2 < \infty\,. \tag{157}$$

In this respect, states obtained through application of the creation operator on the vacuum, $\hat{a}^\dagger(\underline{k})\,|0\rangle$ are physically sensible only, if used together with a test function that smears them out.

A natural question to ask is: in what space do these new states live?

The answer is that they populate a Fock space, which is the sum of all n-particle Hilbert spaces plus, possibly, some symmetrization that takes care of the fact that identical particles are indistinguishable.

It also has a meaningful scalar product, again allowing the definition of a distance, which it "inherits" from the underlying Hilbert space.

Ground-State Energy The ground state $|0\rangle$is an eigenstate of the Hamiltonian; calculating its energy E_0 we arrive at

$$\begin{aligned} E_0 \;=\; \langle 0|\,\hat{H}\,|0\rangle \;&=\; \left\langle 0\left|\frac{1}{2}\int\frac{\mathrm{d}^3k}{(2\pi)^3 2k_0}k_0\left[\hat{a}(\underline{k})\hat{a}^\dagger(\underline{k})+\hat{a}^\dagger(\underline{k})\hat{a}(\underline{k})\right]\right|0\right\rangle \\ &= \frac{1}{2}\int\frac{\mathrm{d}^3k}{(2\pi)^3 2k_0}k_0\left\langle 0\left|\hat{a}(\underline{k})\hat{a}^\dagger(\underline{k})\right|0\right\rangle \\ &= \frac{1}{2}\int \mathrm{d}^3k k_0\delta^3(\underline{0}) = \infty\,, \end{aligned} \tag{158}$$

the product of the volume in both position and momentum space, infinity for a Quantum Field Theory in an infinite volume.

A simple solution is to just subtract the ground state energy, by redefining the Hamiltonian as

$$\hat{H} \longrightarrow \hat{H}' = \hat{H} - \langle 0| \hat{H} |0\rangle \ . \tag{159}$$

Normal Ordering Alternatively, we can define *normal-ordering* of the operators, indicated by colons around the operators as

$$:\hat{a}(\underline{k})\hat{a}^\dagger(\underline{k}): = :\hat{a}^\dagger(\underline{k})\hat{a}(\underline{k}): = \ \hat{a}^\dagger(\underline{k})\hat{a}(\underline{k}) \,, \tag{160}$$

and therefore we replace

$$\hat{H} \longrightarrow :\hat{H}: = \frac{1}{2}\int \frac{\mathrm{d}^3 k}{(2\pi)^3 2k_0} k_0 :\Big[\hat{a}(\underline{k})\hat{a}^\dagger(\underline{k}) + \hat{a}^\dagger(\underline{k})\hat{a}(\underline{k})\Big]: \tag{161}$$

and, finally,

$$\boxed{:\hat{H}: = \int \frac{\mathrm{d}^3 k}{(2\pi)^3 2k_0} k_0 \ \hat{a}^\dagger(\underline{k})\hat{a}(\underline{k}) \,.} \tag{162}$$

This obviously cures the divergence stemming from $\langle 0| \hat{a}(\underline{k})\hat{a}^\dagger(\underline{k}) |0\rangle$ in the ground state energy and similar observables.

In the remainder of this class we will always assume implicit normal ordering, if not stared otherwise.

4.3 A Little Detour: Causal Structure of the Theory

Commutator of Field Operators To guarantee the correct causal structure of the theory, we need to convince ourselves that fields in space-like distances cannot influence each other: they *must* commute for space-like distances.

To see this, define the commutator of two field operators at *arbitrary* four-positions x and y as

$$\begin{aligned} i\Delta(x-y) &= \left[\hat{\phi}(x),\, \hat{\phi}(y)\right] \\ &= \int \frac{\mathrm{d}^3k}{(2\pi)^3 2k_0} \frac{\mathrm{d}^3k'}{(2\pi)^3 2k_0'} \left\{\left[\hat{a}(\underline{k}),\, \hat{a}^\dagger(\underline{k}')\right] e^{-ik\cdot x+ik'\cdot y} \right. \\ &\qquad\qquad \left. + \left[\hat{a}^\dagger(\underline{k}),\, \hat{a}(\underline{k}')\right] e^{ik\cdot x-ik'\cdot y}\right\} \\ &= \int \frac{\mathrm{d}^3k}{(2\pi)^3 2k_0} \left\{e^{-ik\cdot(x-y)} - e^{ik\cdot(x-y)}\right\} \\ &= \Delta_+(x-y) - \Delta_-(x-y)\,, \end{aligned} \tag{163}$$

where we have used the commutator relations for the creation and annihilation operators to arrive at two δ-functions that allowed us to perform the k′-integration, and where we have also introduced the two terms $\Delta_\pm(x-y)$.

Properties of the Commutator The commutator has a number of properties, which are worthwhile to discuss:

1. it is manifestly Lorentz-invariant, i.e. its value will not change under Lorentz transformations such as boosts, rotations, or combinations of both. This is because it is given by a Lorentz-invariant integral over a function that only depends on scalar products k(x−y).

2. it manifestly encodes micro-causality, as it vanishes for all space-like distances of x and y. The easiest way to see this is by looking directly at the first line of the equation above, Eq. (163), where the argument of the integration depends on $[\hat{\phi}(x), \hat{\phi}(y)]$. We know that this commutator vanishes for equal times, cf. Eq. (141). Since for every space-like distance of four-positions (x−y) a Lorentz-boost can be found that reduces it to a space-like distance at equal times, (x̲−y̲), the commutator vanishes for all space-like distances. Hence, the theory is causal in the sense that fields at space-like distances are decoupled.

3. direct calculation reveals that Δ(x−y) is a solution of the Klein- Gordon equation,

$$
\begin{aligned}
0 &= \left(\partial^\mu \partial_\mu + m^2\right) \Delta(x-y) \\
&= \left(\partial^\mu \partial_\mu + m^2\right) \int \frac{\mathrm{d}^3 k}{(2\pi)^3 2k_0} \left[e^{-ik\cdot(x-y)} - e^{ik\cdot(x-y)}\right] \\
&= \int \frac{\mathrm{d}^3 k}{(2\pi)^3 2k_0} \left(\partial^\mu \partial_\mu + m^2\right) \left[e^{-ik\cdot(x-y)} - e^{ik\cdot(x-y)}\right] \\
&= \int \frac{\mathrm{d}^3 k}{(2\pi)^3 2k_0} \left(-k^2 + m^2\right) \left[e^{-ik\cdot(x-y)} - e^{ik\cdot(x-y)}\right]
\end{aligned}
\tag{164}
$$

where the term $k^2 - m^2$ in the last line guarantees that the overall expression vanishes.

4.4 Second Quantization of the Complex Scalar Field

Lagrangian and Hamilton and Field Operators Starting with the Lagrangian of Eq. (104),

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

the conjugate momenta to the two fields ϕ and ϕ^* are given by

$$\boxed{\pi = \frac{\partial \mathcal{L}}{\partial \dot{\phi}} = \dot{\phi}^* \text{ and } \pi^* = \frac{\partial \mathcal{L}}{\partial \dot{\phi}^*} = \dot{\phi}} \tag{165}$$

and the Hamilton operator density reads

$$\hat{\mathcal{H}} = \hat{\pi}^* \hat{\pi} + \underline{\nabla} \hat{\phi}^* \cdot \underline{\nabla} \hat{\phi} + m^2 \hat{\phi}^* \hat{\phi} \,, \tag{166}$$

after promoting fields and momenta to operators.

We demand the equal-time commutation relations

$$\boxed{\left[\hat{\phi}(t, \underline{x}), \hat{\pi}(t, \underline{y})\right] = \left[\hat{\phi}^*(t, \underline{x}), \hat{\pi}^*(t, \underline{y})\right] = i\delta^3(\underline{x} - \underline{y})} \tag{167}$$

with all other equal-time commutators vanishing.

Creation and Annihilation Operators The field operators can be expanded, as before, as products of plane waves and creation and annihilation operators

$$\boxed{\begin{aligned} \phi(x) &= \int \frac{\mathrm{d}^3k}{(2\pi)^3 2k_0} \left[\hat{a}(\underline{k})\, e^{-ik\cdot x} \;+\; \hat{b}^\dagger(\underline{k})\, e^{ik\cdot x}\right] \\ \phi^*(x) &= \int \frac{\mathrm{d}^3k}{(2\pi)^3 2k_0} \left[\hat{b}(\underline{k})\, e^{-ik\cdot x} \;+\; \hat{a}^\dagger(\underline{k})\, e^{ik\cdot x}\right] . \end{aligned}} \tag{168}$$

As before, momentum operators are obtained through straightforward derivation with respect to time.

Expressing the fields and operators through the annihilation and creation operators,

$$\begin{aligned} \hat{a}(\underline{k}) &= \int \mathrm{d}^3x e^{+ik\cdot x} \left[k_0 \hat{\phi}(x) + i\hat{\pi}^*(x)\right] \\ \hat{b}^\dagger(\underline{k}) &= \int \mathrm{d}^3x e^{-ik\cdot x} \left[k_0 \hat{\phi}(x) - i\hat{\pi}^*(x)\right] \\ \hat{b}(\underline{k}) &= \int \mathrm{d}^3x e^{+ik\cdot x} \left[k_0 \hat{\phi}^*(x) + i\hat{\pi}(x)\right] \\ \hat{a}^\dagger(\underline{k}) &= \int \mathrm{d}^3x e^{-ik\cdot x} \left[k_0 \hat{\phi}^*(x) - i\hat{\pi}(x)\right] , \end{aligned} \tag{169}$$

we arrive at commutator relations, for example,

$$\begin{aligned}\left[\hat{a}(\underline{k}),\, \hat{a}^\dagger(\underline{k}')\right] &= \int \mathrm{d}^3x\mathrm{d}^3x' e^{+ik\cdot x - ik'\cdot x'} \\ &\quad\times \left[k_0\hat{\phi}(t,\,\underline{x}) + i\hat{\pi}^*(t,\,\underline{x}),\, k_0'\hat{\phi}^*(t,\,\underline{x}') - i\hat{\pi}(t,\,\underline{x}')\right] \\ &= \int \mathrm{d}^3x\mathrm{d}^3x' e^{+ik\cdot x - ik'\cdot x'} \Big\{-ik_0\left[\hat{\phi}(t,\,\underline{x}),\,\hat{\pi}(t,\,\underline{x}')\right] \\ &\qquad + ik_0'\left[\hat{\pi}^*(t,\,\underline{x}),\,\hat{\phi}^*(t,\,\underline{x}')\right]\Big\} \\ &= \int \mathrm{d}^3x\mathrm{d}^3x' e^{+ik\cdot x - ik'\cdot x'}\left[(k_0+k_0')\delta^3(\underline{x}-\underline{x}')\right] \\ &= \int \mathrm{d}^3x e^{+i(k-k')\cdot x}(k_0+k_0') = 2k_0(2\pi)^3\delta^3(\underline{k}-\underline{k}')\,,\end{aligned} \tag{170}$$

where we have used the definition of the δ function, as usual.

Therefore,

$$\boxed{\left[\hat{a}(\underline{k}),\, \hat{a}^\dagger(\underline{k}')\right] = \left[\hat{b}(\underline{k}),\, \hat{b}^\dagger(\underline{k}')\right] = 2k_0(2\pi)^3\delta^3(\underline{k}-\underline{k}')} \tag{171}$$

and all other commutators vanishing.

Hamilton and Number Operators The normal-ordered Hamilton operator is given by

$$\boxed{:\hat{H}: = \int \frac{\mathrm{d}^3k}{(2\pi)^3 2k_0}\, k_0\left[\hat{a}^\dagger(\underline{k})\hat{a}(\underline{k}) + \hat{b}^\dagger(\underline{k})\hat{b}(\underline{k})\right]\,,} \tag{172}$$

and it looks like the Hamilton operator for the sum of two free real scalar fields.

This further fortifies the idea that we are presented by two kinds of particles – those created and annihilated by $\hat{a}^\dagger$ and $\hat{a}$, and those created and annihilated by $\hat{b}^\dagger$ and $\hat{b}$, and that the vacuum is annihilated by both $\hat{a}$ and $\hat{b}$,

$$\hat{a}(\underline{k})\,|0\rangle \;=\; \hat{b}(\underline{k})\,|0\rangle \;=\; 0\,. \tag{173}$$

It is therefore natural to introduce two *number operators* for the two kinds of particles,

$$\begin{aligned} \hat{N}_a &= \int \frac{\mathrm{d}^3k}{(2\pi)^3 2k_0}\,\hat{a}^\dagger(\underline{k})\hat{a}(\underline{k}) \\ \hat{N}_b &= \int \frac{\mathrm{d}^3k}{(2\pi)^3 2k_0}\,\hat{b}^\dagger(\underline{k})\hat{b}(\underline{k})\,. \end{aligned} \tag{174}$$

It is easy to check that they are indeed number operators counting the number of a and b fields in a given state $|\psi\rangle$.

Denoting

$$\left|\underline{k}_1^{(a)}\underline{k}_2^{(a)}\ldots\underline{k}_{n_a}^{(a)}\underline{k}_1^{(b)}\underline{k}_2^{(b)}\ldots\underline{k}_{n_b}^{(b)}\right\rangle = \prod_{i=1}^{n_a}\left[\hat{a}^\dagger(\underline{k}_i)\right]\prod_{i=1}^{n_b}\left[\hat{b}^\dagger(\underline{k}_i)\right]|0\rangle\;, \tag{175}$$

it is easy to show that

$$\left\langle\underline{k}_1^{(a)}\underline{k}_2^{(a)}\ldots\underline{k}_{n_a}^{(a)}\underline{k}_1^{(b)}\underline{k}_2^{(b)}\ldots\underline{k}_{n_b}^{(b)}\right|\hat{N}_a\left|\underline{k}_1^{(a)}\underline{k}_2^{(a)}\ldots\underline{k}_{n_a}^{(a)}\underline{k}_1^{(b)}\underline{k}_2^{(b)}\ldots\underline{k}_{n_b}^{(b)}\right\rangle = n_a\,. \tag{176}$$

We leave this as part of a problem.

Current and Charge As noted in Sec. 3.3, the Lagrangian for the complex scalar field enjoys invariance under the "gauge transformation"

$$\phi \to \phi' = \exp(i\theta)\phi\,, \quad \phi^* \to \phi'^* = \exp(-i\theta)\phi^*\,,$$

cf. Eq. (106).

This leads to a conserved current given by Eq. (113)

$$j^\mu = i\left[\phi^*(\partial^\mu\phi) - (\partial^\mu\phi^*)\phi\right] \equiv i\phi^*\overleftrightarrow{\partial^\mu}\phi\,,$$

where we added a factor i to ensure that the current is a real number.

This factor, obviously, does not change the fact that $\partial_\mu j^\mu = 0$.

Of course the current can be promoted to a current operator by replacing the fields with field operators,

$$\hat{j}^\mu = i\hat{\phi}^*\overleftrightarrow{\partial^\mu}\hat{\phi}\,. \tag{177}$$

The spatial integral over the (normal-ordered) time-component of the current is the charge, given in operator form by

$$\begin{aligned} :\hat{Q}: &= \int \mathrm{d}^3x\ :\hat{j}_0: = i\int \mathrm{d}^3x\ :\hat{\phi}^*(\partial_t\hat{\phi}) - (\partial_t\hat{\phi}^*)\hat{\phi}: \\ &= \int \frac{\mathrm{d}^3k}{(2\pi)^3 2k_0}\left[\hat{a}^\dagger(\underline{k})\hat{a}(\underline{k}) - \hat{b}^\dagger(\underline{k})\hat{b}(\underline{k})\right] = \hat{N}_a - \hat{N}_b\,. \end{aligned} \tag{178}$$

This suggests that our two particle types a and b have opposite charged with

$$q_{a,b} = \pm 1 . \tag{179}$$

Conserved Charge To show that the charge is conserved, we need to verify that the charge operator

$$\boxed{:\hat{Q}: = \int \frac{\mathrm{d}^3 k}{(2\pi)^3 2k_0} \left[\hat{a}^\dagger(\underline{k})\hat{a}(\underline{k}) - \hat{b}^\dagger(\underline{k})\hat{b}(\underline{k})\right] = \hat{N}_a - \hat{N}_b} \tag{180}$$

commutes with the Hamiltonian, i.e. $[:\hat{H}:, :\hat{Q}:] = 0$.

This is indeed the case, and we leave this proof for the problems.

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5 Fermions

In this section we will get acquainted with the Dirac equation, which introduces not only fermions, but also provides insight into anti-particles.

The Dirac equation emerges through leariszation of the Klein-Gordon equation, after realizing that its quadratic form yields negative energy solutions.

Such a linearized form, however, only satisfies the original energy-momentum relation – essentially the kernel of the free Klein-Gordon equation – if the fields have an even number of components, at least two.

This proves to be a blessing, as it allows us to describe spin-1/2 particles, and the corresponding fields are dubbed “spinors”.

Insisting on maintaining that the spinors satisfy the Klein-Gordon equation for massive particles leads to spinors with four components - two more than necessary for spin-1/2 particles.

These additional degrees of freedom are identified with negative energy solutions and interpreted as anti-particles.

As before, in the case of the scalar fields, this implies that the energy spectrum of the theory is unbounded from below.

Consequently the vacuum is not empty, and in fact it contains short-lived quantum fluctuations of particle+anti-particle with opposite energy, momentum and spin.

5.1 The Dirac Equation

Short-comings of the Klein-Gordon Lagrangian Klein-Gordon equations of motion, Eq. (91) in Sec. 3.2,

$$\left(\frac{\partial^2}{\partial t^2} - \underline{\nabla}^2 + m^2\right)\phi(x) = \left(\partial_\mu\partial^\mu + m^2\right)\phi(x) = 0\,.$$

Fourier-transforming it into

$$(E^2 - \underline{p}^2 - m^2)\phi = 0 \quad \longrightarrow \quad E^2 = \underline{p}^2 + m^2 \tag{182}$$

we realize that, due to its quadratic form, nothing prevents us from constructing solutions with negative energies.

Assuming plane wave solutions for the fields, $\phi(x) \sim \exp(ikx)$ the charge or probability density for the complex scalar field is given by

$$\rho = j_0 = (\partial_t\phi^*)\phi - \phi^*(\partial_t\phi) = -2ik_0 \tag{183}$$

which can be translated into a real, unit-free quantity, that is more appropriate for a probability density.

This is achieved through a suitable normalization, for example

$$j^\mu \to \tilde{j}^\mu = \frac{i}{2m} j^\mu\,, \tag{184}$$

such that $\rho = k_0/m$.

For negative-energy solutions, though, this would result in negative probability densities, which are extremely hard to interpret.

Ultimately, the appearance of these solutions mean that the energy spectrum of the theory is not bound from below and there is no lowest energy ground-state.

In other words, there is nothing that prevents us from producing more and more particles, by pairing positive and negative energy solutions – clearly an unacceptable problem for the interpretation of the theory.

Ultimately this shows that it is impossible to produce a single-particle theory when imposing Lorentz-invariance as a construction paradigm.

Of course, we know by now that this issue can be completely circumnavigated by identifying the negative energy-solutions as anti-particles, particles with positive energy but opposite charge that propagate backwards in time.

However, when Dirac introduced his famous equation in 1928 this anti-particles were not discovered yet, and it was in fact his work that introduced anti-particles as a meaningful theoretical concept that emerges naturally when combining Quantum Mechanics and Special Relativity into Quantum Field Theory.

Linearizing the Klein-Gordon Equation Dirac's aim was to construct a linearized version of the Klein-Gordon equation such that the resulting E.o.M. are linear in ∂_t, and being Lorentz-invariant exhibit solutions that still satisfy the original equation.

Choosing an ansatz for the field ψ, that is first order in ∂_t and first order in ∇

$$\boxed{i\frac{\partial\psi(\underline{x},\, t)}{\partial t} = -i\underline{\alpha}\cdot\underline{\nabla}\psi(\underline{x},\, t) + \beta m\psi(\underline{x},\, t)\,,} \tag{185}$$

it becomes obvious that α_i and β must be matrices, and that ψ has at least two components.

The latter property in fact was seen as a nice bonus, because they could be identified with the two spin states (spin up and spin down) of the electrons that Dirac wanted to describe.

This identification of the components of the field ψ with spin states has led to the name for $\psi(x)$: *spinor* or *spinor field*.

Properties of the α_i and β matrices To guarantee that the equation above, Eq. (185), reduces to the Klein-Gordon E.o.M. when squaring the kernel

$$\left(\frac{\partial^2}{\partial t^2} - \underline{\nabla}^2 + m^2\right) \stackrel{!}{=} \left[i\partial_t + i\underline{\alpha}\cdot\underline{\nabla} - \beta m\right]^2 \tag{186}$$

α_i and β must satisfy the following relations

$$\boxed{\begin{aligned} \{\alpha_i,\, \alpha_j\} &= \alpha_i\alpha_j + \alpha_j\alpha_i = 2\delta_{ij} \\ \{\alpha_i,\, \beta\} &= 0 \\ \beta^2 &= \alpha_i^2 = 1 \\ \mathrm{Tr}(\alpha_i) &= \mathrm{Tr}(\beta) = 0\,. \end{aligned}} \tag{187}$$

This implies that the eigenvalues of α_i and β are ± 1, and the combination of them being traceless and having these eigenvalues suggests that they must be of an even dimension, i.e. $\dim(\alpha_i, \beta) = 2, 4, \ldots$.

Focusing on the case of lowest dimension, 2×2 matrices, we can see straightaway that the α_i can be identified with the Pauli matrices, $\alpha_i = \sigma_i$, where

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \text{ and } \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{188}$$

This however won't work for massive theories where $m \neq 0$: There is just no fourth candidate matrix for β that satisfies all the properties of Eq. (187).

This has two implications: First of all, for massless theories, we could stick with two-component fields ψ, also known as Weyl spinors.

And secondly, for massive theories like the ones we're going to pursue, we must use four-component fields – the Dirac spinors – and have four-dimensional α_i and β matrices:

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \text{ and } \quad \beta = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix}. \tag{189}$$

Here – and later in γ_0 – the 1 denotes 2×2 identity matrices.

γ Matrices and Their Properties For practical purposes, the α and β matrices proved a bit cumbersome, and they are usually replaced by the γ-matrices, defined by

$$\gamma^0 = \beta = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix} \quad \text{and} \quad \gamma^i = \beta\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix} . \tag{190}$$

Direct calculation shows that they enjoy the following anti-commutator relation

$$\{\gamma^\mu, \gamma^\nu\} = \gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2g^{\mu\nu} . \tag{191}$$

In addition, $\gamma^0 = \gamma^{0\dagger}$ is Hermitean with $\gamma^{02} = 1$, while the $\gamma^i = -\gamma^{i\dagger}$ are anti-Hermitean, with $(\gamma^i)^2 = -1$.

Dirac Equation Multiplying the Dirac equation, expressed through the α and β matrices, Eq. (185), from the left with γ^0 we arrive at

$$(i\gamma^\mu\partial_\mu - m\mathbf{1})_{\eta\xi}\, \psi_\xi = (i\partial\!\!\!/ - m)\psi = 0 . \tag{192}$$

In the equation above, Eq. (192) the components of the Dirac equation in "*spinor space*" have been made explicit, indicated by the indices η and ξ.

It is important to stress that this exhibits the fact that there are two spaces in the Dirac equation, namely the "normal" Minkowski space with index μ, incorporating the external Lorentz symmetry of space-time, and this spinor space.

The γ matrices and the spinor ψ have multiple components in this space, and the mass term is diagonal in this space, indicated by the **1**-symbol.

As before, the Lorentz indices μ etc. run from 0 to 3, while the Dirac or spinor indices run from 1 to 4.

Dirac Equation for $\psi^\dagger$ The nature of the equation above suggest that the Hermitean conjugate spinor $\psi^\dagger$ represents a second, independent field, similar to ϕ^* and ϕ.

Straightforward Hermitean conjugation of Eq. (185) results in

$$-i\frac{\partial\psi^\dagger(\underline{x},\,t)}{\partial t} = i\underline{\nabla}\psi^\dagger(\underline{x},\,t)\cdot\underline{\alpha}^\dagger + m\psi^\dagger(\underline{x},\,t)\beta^\dagger\,, \tag{193}$$

and multiplying from the right with $\beta^\dagger = \beta = \gamma^0$ yields

$$-i\psi^\dagger(\underline{x},\,t)\overleftarrow{\partial_\mu}\gamma^{\dagger\mu} = m\psi^\dagger(\underline{x},\,t)\,. \tag{194}$$

Using $\gamma^{02} = 1$ and $\underline{\gamma}^\dagger = (\beta\underline{\alpha})^\dagger = \underline{\alpha}\beta = \beta(\beta\underline{\alpha})\beta = \gamma^0\,\underline{\gamma}\gamma^0$ while defining the "barred" spinor $\overline{\psi} = \psi^\dagger\gamma^0$ allows us to find the E.o.M. for the barred spinor as

$$\boxed{\bar{\psi}(i\overleftarrow{\not\partial} + m) = 0\,.} \tag{195}$$

Lagrangian It is easy to check that the two E.o.M. for the spinors ψ and $\psi^\dagger$ can be obtained from the free Dirac Lagrangian

$$\boxed{\mathcal{L} = \bar{\psi}(x)\left(i\overleftrightarrow{\not\partial} - m\right)\psi(x)\,,} \tag{196}$$

where

$$a\overleftrightarrow{\partial}b = \frac{1}{2}\left[a(\partial b) - (\partial a)b\right]\,. \tag{197}$$

The E.o.M. for ψ ($\overline{\psi}$) are obtained, as usual, by varying the Lagrangian with respect to ψ ($\overline{\psi}$)

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \bar{\psi}} - \partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \bar{\psi})} &= -m\psi + \frac{1}{2}\left[i\partial\!\!\!/\psi - \partial_\mu(-i\gamma^\mu\psi)\right] = \left(i\overrightarrow{\partial\!\!\!/} - m\right)\psi = 0 \\ \frac{\partial \mathcal{L}}{\partial \psi} - \partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \psi)} &= -m\bar{\psi} - \frac{1}{2}\left[\bar{\psi}(i\overleftarrow{\partial\!\!\!/}) + \partial_\mu(i\bar{\psi}\gamma^\mu)\right] = -\bar{\psi}\left(i\overleftarrow{\partial\!\!\!/} + m\right) = 0\,. \end{aligned} \tag{198}$$

Conserved Current It is relatively straightforward to construct a conserved current from the two E.o.M. Eqs (192) and (195): multiply the former from the left with $\overline{\psi}$ and the latter from the right with ψ and add.

This results in

$$0 = \bar{\psi}\cdot(i\overrightarrow{\partial\!\!\!/} - m)\psi + \bar{\psi}\cdot(i\overleftarrow{\partial\!\!\!/} + m)\cdot\psi = i\bar{\psi}(\overrightarrow{\partial\!\!\!/} + \overleftarrow{\partial\!\!\!/})\psi \tag{199}$$

and we arrive at the conserved current

$$\boxed{\partial_\mu j^\mu = \partial_\mu\left[i\bar{\psi}\gamma^\mu\psi\right]\,.} \tag{200}$$

Solutions to the Dirac E.o.M.: Spinors at Rest To construct solutions for the Dirac equation, it is important to keep in mind that the ψ and $\overline{\psi}$ are objects with four components.

But, although they look like vectors because of the four-components, they differ from four-vectors in how they behave under Lorentz transformations.

Simply put: spinor index ≠ Lorentz index)

Let us for the moment describe the ψ as a product of advanced and retarded plane wave factors and polarization eigenstates u($\underline{p}$) and v($\underline{p}$),

$$\psi_\eta(x) = \int \frac{\mathrm{d}^3 p}{(2\pi)^3} \left[e^{-ip\cdot x} u_\eta(\underline{p}) + e^{ip\cdot x} v_\eta(\underline{p})\right] , \tag{201}$$

where we have made explicit the spinor index η.

This expansion moves the spinor index to the u and v spinors, i.e., they are objects with four entries, and the Dirac matrices act on these indices.

Positive and negative energy solutions $\psi_\pm$ are of course related to the wave factors such that

$$\psi_+ = e^{-ip\cdot x} u(\underline{p}) \;\; \text{and} \;\; \psi_- = e^{ip\cdot x} v(\underline{p}) ,$$

and we will recycle them later when quantizing the Dirac fields.

To construct them, it is sufficient to realize that the E.o.M. become a system of linear equations for the eigenstates u($\underline{p}$) and v($\underline{p}$).

Let us first solve this equation for a particle at rest, p = 0, p^0 = E = m, leading to

$$(E\gamma^0 - m)u(0) = m(\gamma^0 - 1)u(0) = 0 \;\; \text{and, similarly,} \; (\gamma^0 + 1)v(0) = 0 , \tag{202}$$

Inserting the (diagonal) form of

$$\gamma^0 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{203}$$

implies that the third and fourth component of u and the first and second component of v must be zero.

Both u and v therefore have two independent solutions each, and the corresponding eigenstates can be readily identified with the two spin states: $u^{(1/2)}$ describe positive-energy particles with spin up/down, and $v^{(1/2)}$ decibel negative-energy particles with spin up/down.

Choosing normalized "eigenvectors" then results in

$$\begin{aligned} u^{(1)}(\underline{0}) &= \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad u^{(2)}(\underline{0}) = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \\ v^{(1)}(\underline{0}) &= \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad v^{(2)}(\underline{0}) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}. \end{aligned} \tag{204}$$

Solutions to the Dirac E.o.M.: General Momenta To obtain solutions for general momenta, we use the fact that suitable multiplication of the kernels of the E.o.M. for u and v with terms $(\not{p} \pm m)$ encodes the energy-momentum relation for a massive particle,

$$(\not{p} - m)(\not{p} + m) = p^2 - m^2 = 0\,. \tag{205}$$

This means that, including normalization factors η(p), the transformed eigenstates

$$u^{(i)}(\underline{p}) = \eta^i(\not{p} + m)u^{(i)}(\underline{0})$$
$$v^{(i)}(\underline{p}) = \eta^i(-\not{p} + m)v^{(i)}(\underline{0}) \tag{206}$$

will satisfy the E.o.M. $(\not{p} - m)u = 0$ and $(\not{p} + m)v = 0$.

Introducing $p_\pm = p_x \pm ip_y$ of the momentum components the spinors and using

$$\not{p} \pm m = p_\mu\gamma^\mu \pm m = \begin{pmatrix} E \pm m & 0 & -p_z & -p_x + ip_y \\ 0 & E \pm m & -p_x - ip_y & p_z \\ p_z & p_x - ip_y & -E \pm m & 0 \\ p_x + ip_y & -p_z & 0 & -E \pm m \end{pmatrix} \tag{207}$$

we arrive at

$$\boxed{\begin{array}{ll} u^{(1)}(\underline{p}) = \eta \begin{pmatrix} 1 \\ 0 \\ \frac{p_z}{E+m} \\ \frac{p_+}{E+m} \end{pmatrix}, & u^{(2)}(\underline{p}) = \eta \begin{pmatrix} 0 \\ 1 \\ \frac{p_-}{E+m} \\ \frac{-p_z}{E+m} \end{pmatrix}, \\ v^{(1)}(\underline{p}) = \eta \begin{pmatrix} \frac{p_z}{E+m} \\ \frac{p_+}{E+m} \\ 1 \\ 0 \end{pmatrix}, & v^{(2)}(\underline{p}) = \eta \begin{pmatrix} \frac{p_-}{E+m} \\ \frac{-p_z}{E+m} \\ 0 \\ 1 \end{pmatrix}, \end{array}} \tag{208}$$

where the energy $E = \sqrt{\underline{p}^2 + m^2} > 0$ and the normalization is given by

$$\eta = \sqrt{E + m}\,. \tag{209}$$

Note that we have normalized the spinors such that, apart from the norm η the first component of the spinors equals 1.

What is left to do now is to explicitly check that the spinors indeed satisfy their equations of motion, i.e. that $(\not{p} - m)u^{(1,2)}(\underline{p})$ and $(\not{p} + m)v^{(1,2)}(\underline{p})$ vanish.

For example, for $u^{(1)}$ and $v^{(1)}$ we find

$$
\begin{aligned}
&(\not{p} - m)u^{(1)}(\underline{p}) \\
&\quad = \begin{pmatrix} E-m & 0 & -p_z & -p_- \\ 0 & E-m & -p_+ & p_z \\ p_z & p_- & -(E+m) & 0 \\ p_+ & -p_z & 0 & -(E+m) \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ \frac{p_z}{E+m} \\ \frac{p_+}{E+m} \end{pmatrix} \\
&\quad = \begin{pmatrix} E - m - \frac{\underline{p}^2}{E+m} \\ \frac{-p_+p_z + p_+p_z}{E+m} \\ -p_z + \frac{(E+m)p_z}{E+m} \\ -p_+ + \frac{(E+m)p_+}{E+m} \end{pmatrix} = 0\,;
\end{aligned}
$$

$$
\begin{aligned}
(\not{p}+m)v^{(1)}(\underline{p}) \\
&= \begin{pmatrix} E+m & 0 & -p_z & -p_- \\ 0 & E+m & -p_+ & p_z \\ p_z & p_- & -(E-m) & 0 \\ p_+ & -p_z & 0 & -(E-m) \end{pmatrix} \begin{pmatrix} \frac{p_z}{E+m} \\ \frac{p_+}{E+m} \\ 1 \\ 0 \end{pmatrix} \\
&= \begin{pmatrix} -\frac{(E+m)p_z}{E+m} + p_z \\ -\frac{(E+m)p_+}{E+m} + p_+ \\ \frac{\underline{p}^2}{E+m} - (E-m) \\ \frac{p_+p_z - p_+p_z}{E+m} \end{pmatrix} = 0 .
\end{aligned}
\tag{210}
$$

Similar calculations for $u^{(2)}$ and $v^{(2)}$ prove that the spinors indeed satisfy the equations of motion.

Spinor Products in Components The normalization has been chosen such that the spinors form a "nearly" ortho-normal basis,

$$
\boxed{\bar{u}^{(i)}(\underline{p})u^{(j)}(\underline{p}) = 2m\delta_{ij} = -\bar{v}^{(i)}(\underline{p})v^{(j)}(\underline{p}) .}
\tag{211}
$$

A simple calculation exemplifies how to calculate such spinor products.

For example for i = j = 1 we find

$$
\begin{aligned}
\bar{u}^{(i)}u^{(j)} = u^{(i)\dagger}\gamma^0 u^{(j)} &= \eta^2 \left(1 + 0 - \frac{p_z^2}{(E+m)^2} - \frac{p_+p_-}{(E+m)^2}\right) \\
&= \eta^2 \frac{E^2 + 2Em + m^2 - \underline{p}^2}{(E+m)^2} = \eta^2 \frac{2m(E+m)}{(E+m)^2} = \eta^2 \frac{2m}{E+m} ,
\end{aligned}
\tag{212}
$$

and plugging in our chosen normalization leads to the anticipated product of Eq. (211)

A similar calculation for the “daggered” instead of the “barred” spinors, i.e. ignoring the γ^0 yields

$$u^{(i)\dagger}u^{(j)} = \eta^2 \frac{E^2 + 2Em + m^2 + \underline{p}^2}{(E+m)^2} = \eta^2 \frac{2E(E+m)}{(E+m)^2} = \eta^2 \frac{2E}{E+m} = 2E\,. \tag{213}$$

Therefore,

$$\boxed{\begin{aligned} u^{(i)\dagger}(\underline{p})u^{(j)}(\underline{p}) = v^{(i)\dagger}(\underline{p})v^{(j)}(\underline{p}) = 2p_0\delta_{ij} \\ \bar{v}^{(i)}(\underline{p})u^{(j)}(\underline{p}) = \bar{u}^{(i)}(\underline{p})v^{(j)}(\underline{p}) = 0\,. \end{aligned}} \tag{214}$$

Completeness Relations Let us now reverse the order of multiplication and instead of calculating scalar products of a “row” spinor times a “column” spinor, $\bar{u}u,$ let us calculate the product of a “column” spinor times a “row” spinor, $u\bar{u}$.

This leads to the *completeness relations*

$$\boxed{\sum_{i=1}^{2} u_\alpha^{(i)}\bar{u}_\beta^{(i)} = (\not{p} + m)_{\alpha\beta}\ , \quad \sum_{i=1}^{2} v_\alpha^{(i)}\bar{v}_\beta^{(i)} = (\not{p} - m)_{\alpha\beta}\ .} \tag{215}$$

Using Eq. (207) and directly calculate the spinor products, i.e. the terms $u\bar{u}$ we see that this holds in fact true.

It is important to stress that the product of “column vector” and “row vector” is not a scalar product but generates a matrix.

Some Interpretations Before second quantizing Dirac theory, it is worth it to first analyze and interpret the structure of the solutions obtained above.

As before for the case of scalar fields we have plane waves moving in the “wrong direction” - the states that come with the v-spinors.

They can be interpreted either as states of negative energy moving forward in time or as states of positive energy moving backwards in time.

In any case, they describe anti-particles.

Of course, as before, their existence indicates that the energy states of the theory are not bound from below, so there is *a priori* no well-defined ground state.

Dirac circumnavigated this problem by demanding that the negative energy solutions are all filled, and that the v-states are “holes” in this otherwise full “sea” of negative energy solutions.

This obviously abandons any notion of the resulting Quantum Field Theory describing just one particle – which is possible in Quantum Mechanics.

Adding Special Relativity to the mix implies that the resulting Quantum Field Theory indeed can only be realized as a multi-particle theory.

It is then not surprising that the vacuum is not “empty”; instead it can have short-time quantum fluctuations of particle+anti-particle (hole), with opposite energy, momentum, and spin such that the overall quantum numbers (all 0) are conserved.

We will now move on to quantize this theory.

Lagrangian and Conjugate Momenta Derivation of the Lagrange density of Eq. (196),

$$\mathcal{L} = \bar{\psi}(x)(i\partial\!\!\!/ - m)\psi(x)$$

with respect to the time-derivative of the two independent spinor fields ψ and $\psi^\dagger$ yields

$$\boxed{\begin{aligned} \pi &= \partial\mathcal{L}/\partial\dot{\psi} = \bar{\psi} i\gamma^0 = \frac{i}{2}\psi^\dagger \\ \pi^\dagger &= \partial\mathcal{L}/\partial\dot{\psi}^\dagger = -\frac{i}{2}\gamma^0\gamma^0\psi = -\frac{i}{2}\psi\,. \end{aligned}} \tag{216}$$

The Hamiltonian density then reads

$$\begin{aligned} \mathcal{H} &= \pi\dot{\psi} + \pi^\dagger\dot{\psi}^\dagger - \mathcal{L} = \frac{i}{2}\left(\psi^\dagger(\partial_0\psi) - \psi(\partial_0\psi^\dagger)\right) - \mathcal{L} \\ &= \bar{\psi}\left(i\gamma_0\overleftrightarrow{\partial_0} - i\gamma_0\overleftrightarrow{\partial_0} + i\underline{\gamma}\cdot\overleftrightarrow{\underline{\nabla}} + m\right)\psi \;=\; \bar{\psi}\left(i\underline{\gamma}\cdot\overleftrightarrow{\underline{\nabla}} + m\right)\psi \end{aligned} \tag{217}$$

It is worth noting here that our conjugate momenta differ from the usual form in textbooks by a factor of 1/2, stemming from our vey literal interpretation of the derivative of Eq. (197) in the Lagrangian, Eq. (196).

Anti-Commutators Quantization is achieved by promoting fields, momenta etc. to field operators and by demanding suitable commutation relations for them.

However, we know that spin-1/2 particles are fermions so we need to encapsulate Fermi-statistics into the quantization condition.

This necessitates to replace the equal-time commutators of fields and momenta with equal-time anti-commutators.

Using the relationship between fields and momenta from Eq. (216) they therefore read

$$\boxed{\begin{aligned} \left\{\hat{\psi}_\alpha(t,\underline{x}),\,\hat{\pi}^\dagger_\beta(t,\underline{y})\right\} &= \frac{i}{2}\left\{\hat{\psi}_\alpha(t,\underline{x}),\,\hat{\psi}^\dagger_\beta(t,\underline{y})\right\} = i\delta_{\alpha\beta}\delta^3(\underline{x}-\underline{y}) \\ \left\{\hat{\psi}_\alpha(t,\underline{x}),\,\hat{\psi}_\beta(t,\underline{y})\right\} &= \left\{\hat{\psi}^\dagger_\alpha(t,\underline{x}),\,\hat{\psi}^\dagger_\beta(t,\underline{y})\right\} = 0\,, \end{aligned}} \tag{216}$$

The Hamiltonian density then reads

$$\begin{aligned} \mathcal{H} = \pi\dot{\psi} + \pi^\dagger\dot{\psi}^\dagger - \mathcal{L} &= \frac{i}{2}\left(\psi^\dagger(\partial_0\psi) - \psi(\partial_0\psi^\dagger)\right) - \mathcal{L} \\ &= \bar{\psi}\left(i\gamma_0\overleftrightarrow{\partial_0} - i\gamma_0\overleftrightarrow{\partial_0} + i\underline{\gamma}\cdot\overleftrightarrow{\underline{\nabla}} + m\right)\psi = \bar{\psi}\left(i\underline{\gamma}\cdot\overleftrightarrow{\underline{\nabla}} + m\right)\psi \end{aligned} \tag{217}$$

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where the anti-commutator of two operators is defined by

$$\left\{\hat{A},\,\hat{B}\right\} = \hat{A}\hat{B} + \hat{B}\hat{A}\,, \tag{219}$$

and where we used that $\hat{\pi}_\beta = \hat{\psi}^\dagger_\beta$.

Creation and Annihilation Operators As before, we expand the fields in plane waves multiplied with creation and annihilation operators.

As we already have such plane waves for the “classical” fields, multiplied with the eigen-spinors u and v, we merely need to add one creation/annihilation operator for each such state and arrive at

$$\boxed{\begin{aligned}\psi(t,\,\underline{x}) &= \int \frac{\mathrm{d}^3p}{(2\pi)^3 2p_0} \sum_{i=1}^{2} \left[e^{-ip\cdot x}\hat{b}_i(\underline{p})u^{(i)}(\underline{p}) + e^{ip\cdot x}\hat{d}_i^\dagger(\underline{p})v^{(i)}(\underline{p})\right] \\ \psi^\dagger(t,\,\underline{x}) &= \int \frac{\mathrm{d}^3p}{(2\pi)^3 2p_0} \sum_{i=1}^{2} \left[e^{-ip\cdot x}\hat{d}_i(\underline{p})\bar{v}^{(i)}(\underline{p}) + e^{ip\cdot x}\hat{b}_i^\dagger(\underline{p})\bar{u}^{(i)}(\underline{p})\right]\gamma^0\end{aligned}} \tag{220}$$

With the following anti-commutation relations of the creation and annihilation operators,

$$\boxed{\left\{\hat{b}_\alpha(\underline{p}),\,\hat{b}_\beta^\dagger(\underline{q})\right\} = \left\{\hat{d}_\alpha(\underline{p}),\,\hat{d}_\beta^\dagger(\underline{q})\right\} = 2p_0(2\pi)^3\delta^3(\underline{p}-\underline{q})\delta_{\alpha\beta}\,,} \tag{221}$$

and all others vanishing, the anti-commutators of Eq. (218) are fulfilled.

For example:

$$\begin{aligned}&\left\{\hat{\psi}_\alpha(t,\,\underline{x}),\,\hat{\psi}_\beta^\dagger(t,\,\underline{y})\right\} \\ &= \int \frac{\mathrm{d}^3p}{(2\pi)^3 2p_0}\frac{\mathrm{d}^3q}{(2\pi)^3 2q_0}\Big[e^{-ip\cdot x-iq\cdot y}\left(\bar{v}^{(\beta)}(\underline{q})\gamma^0 u^{(\alpha)}(\underline{p})\right)\left\{\hat{b}_\alpha(\underline{p}),\,\hat{d}_\beta(\underline{q})\right\} \\ &\qquad +e^{-ip\cdot x+iq\cdot y}\left(\bar{u}^{(\beta)}(\underline{q})\gamma^0 u^{(\alpha)}(\underline{p})\right)\left\{\hat{b}_\alpha(\underline{p}),\,\hat{b}_\beta^\dagger(\underline{q})\right\} \\ &\qquad +e^{+ip\cdot x-iq\cdot y}\left(\bar{v}^{(\beta)}(\underline{q})\gamma^0 v^{(\alpha)}(\underline{p})\right)\left\{\hat{d}_\alpha^\dagger(\underline{p}),\,\hat{d}_\beta(\underline{q})\right\} \\ &\qquad +e^{+ip\cdot x+iq\cdot y}\left(\bar{u}^{(\beta)}(\underline{q})\gamma^0 v^{(\alpha)}(\underline{p})\right)\left\{\hat{d}_\alpha^\dagger(\underline{p}),\,\hat{b}_\beta^\dagger(\underline{q})\right\}\Big]\end{aligned}$$

$$
\begin{aligned}
&= \int \frac{\mathrm{d}^3 p}{(2\pi)^3 2p_0} \frac{\mathrm{d}^3 q}{(2\pi)^3 2q_0} \, 2p_0 \delta_{\alpha\beta} (2\pi)^3 \delta^3(\underline{p} - \underline{q}) \Big[\\
&\qquad e^{-ip\cdot x + iq\cdot y} \left(u^{(\beta)\dagger}(\underline{q}) u^{(\alpha)}(\underline{p}) \right) + e^{+ip\cdot x - iq\cdot y} \left(v^{(\beta)\dagger}(\underline{q}) v^{(\alpha)}(\underline{p}) \right) \Big] \\
&= \int \frac{\mathrm{d}^3 p}{(2\pi)^3 2p_0} \, \delta_{\alpha\beta} \left[e^{-ip\cdot(x-y)} u^{(\beta)\dagger}(\underline{p}) u^{(\alpha)}(\underline{p}) + e^{+ip\cdot(x-y)} v^{(\beta)\dagger}(\underline{p}) v^{(\alpha)}(\underline{p}) \right] \\
&= \int \frac{\mathrm{d}^3 p}{(2\pi)^3 2p_0} \, \delta_{\alpha\beta} 2p_0 \delta_{\alpha\beta} \left[e^{-ip_0\cdot(t-t) + i\underline{p}\cdot(\underline{x}-\underline{y})} + e^{+ip_0\cdot(t-t) - i\underline{p}\cdot(\underline{x}-\underline{y})} \right] \\
&= \int \frac{\mathrm{d}^3 p}{(2\pi)^3} \, \delta_{\alpha\beta} \left[e^{-i\underline{p}\cdot(\underline{x}-\underline{y})} + e^{+i\underline{p}\cdot(\underline{x}-\underline{y})} \right] = 2\delta_{\alpha\beta} \delta^3(\underline{x} - \underline{y}) \, , \qquad (222)
\end{aligned}
$$

in agreement with Eq. (218).

We realize that due to the equal times, the exponentials of the time differences vanish; in addition, because α and β are external parameters, we cannot use Einstein's convention of summing over repeated indices, since this would eliminate these parameters and the right-hand side of the anti-commutator would not depend on them.

Simply put, the α and β are not indices in some space but label the spin-states of the fermions and cannot be summed over.

Finally, we used that $\delta^3(\underline{x}-\underline{y}) = \delta^3(\underline{y}-\underline{x})$.

States To construct states with one and more particle states, we first realize that

- $\hat{b}^\dagger_{1,2}(\underline{p})/\hat{b}_{1,2}(\underline{p})$ creates/annihilates positive-energy electrons with spin up/down and momentum $\underline{p}$;

- $\hat{d}_{1,2}(\underline{p})/\hat{d}^\dagger_{1,2}(\underline{p})$ creates/annihilates negative-energy electrons – positrons with – spin up/down and momentum $\underline{p}$.

For example, a one-electron (positron) state with positive (negative) energy, spin-up (down) and momentum $\underline{p}$ is created by

$$\begin{aligned} \left|+,\, \underline{p},\, \uparrow\right\rangle &= b_1^\dagger(\underline{p})|0\rangle \\ \left|-,\, \underline{p},\, \downarrow\right\rangle &= d_2^\dagger(\underline{p})|0\rangle\,. \end{aligned} \tag{223}$$

While this looks straightforward, things become more interesting when considering two-electron states, both with positive energy, momentum $\underline{p}$, and one spin up and one spin down:

$$\left|+,\, \underline{p},\, \uparrow;\, +,\, \underline{p},\, \downarrow\right\rangle = b_1^\dagger(\underline{p})b_2^\dagger(\underline{p})\,|0\rangle = -b_2^\dagger(\underline{p})b_1^\dagger(\underline{p})\,|0\rangle\;, \tag{224}$$

where the sign is a reflection of the quantization through anti-commutators.

But if both electrons populate the same space in energy, momentum, and spin, for example

$$\left|+,\, \underline{p},\, \uparrow;\, +,\, \underline{p},\, \uparrow\right\rangle = b_1^\dagger(\underline{p})b_1^\dagger(\underline{p})\,|0\rangle = -b_1^\dagger(\underline{p})b_1^\dagger(\underline{p})\,|0\rangle = 0\,, \tag{225}$$

i.e., such states cannot be produced.

In fact double application of fermionic creation operators with identical momenta, energies and spins will annihilate any state.

Hamilton Operator To promote the Hamilton density of Eq. (217) to an operator it is suffcient to replace the fields with field operators.

Plugging in the expansion in terms of creation and annihilation operators, using $\overline{u}\gamma^0 = u^\dagger$ and $\overline{v}\gamma^0 = v^\dagger$, and integrating over space, we find

$$
\begin{aligned}
\hat{H} &= \int \mathrm{d}^3x \, \frac{\mathrm{d}^3p}{(2\pi)^3 2p_0} \frac{\mathrm{d}^3q}{(2\pi)^3 2q_0} \sum_{i,j=1}^{2} \Big[\\
&\quad \left(e^{-ip\cdot x} \hat{d}_i(\underline{p})\, \bar{v}^{(i)}(\underline{p}) + e^{ip\cdot x} \hat{b}_i^\dagger(\underline{p})\, \bar{u}^{(i)}(\underline{p}) \right) \left(i\underline{\gamma} \cdot \overleftrightarrow{\underline{\nabla}} + m \right) \\
&\qquad \times \left(e^{-iq\cdot x} \hat{b}_j(\underline{q}) u^{(j)}(\underline{q}) + e^{iq\cdot x} \hat{d}_j^\dagger(\underline{q}) v^{(j)}(\underline{q}) \right) \Big] \\
&= \int \mathrm{d}^3x \, \frac{\mathrm{d}^3p}{(2\pi)^3 2p_0} \frac{\mathrm{d}^3q}{(2\pi)^3 2q_0} \sum_{i,j=1}^{2} \Big\{ \\
&\quad e^{-i(p+q)\cdot x} \left(\hat{d}_i(\underline{p}) \hat{b}_j(\underline{q}) \right) \left[\bar{v}^{(i)}(\underline{p}) \left(\frac{1}{2}\underline{\gamma} \cdot (-\underline{p} + \underline{q}) + m \right) u^{(j)}(\underline{q}) \right] \\
&\quad + e^{-i(p-q)\cdot x} \left(\hat{d}_i(\underline{p}) \hat{d}_j^\dagger(\underline{q}) \right) \left[\bar{v}^{(i)}(\underline{p}) \left(\frac{1}{2}\underline{\gamma} \cdot (-\underline{p} - \underline{q}) + m \right) v^{(j)}(\underline{q}) \right] \\
&\quad + e^{+i(p-q)\cdot x} \left(\hat{b}_i^\dagger(\underline{p}) \hat{b}_j(\underline{q}) \right) \left[\bar{u}^{(i)}(\underline{p}) \left(\frac{1}{2}\underline{\gamma} \cdot (+\underline{p} + \underline{q}) + m \right) u^{(j)}(\underline{q}) \right] \\
&\quad + e^{+i(p+q)\cdot x} \left(\hat{b}_i^\dagger(\underline{p}) \hat{d}_j^\dagger(\underline{q}) \right) \left[\bar{u}^{(i)}(\underline{p}) \left(\frac{1}{2}\underline{\gamma} \cdot (+\underline{p} - \underline{q}) + m \right) v^{(j)}(\underline{q}) \right] \Big\}
\end{aligned}
$$

$$
\begin{aligned}
&= \int \frac{\mathrm{d}^3 q}{(2\pi)^3 4 q_0^2} \sum_{i,j=1}^{2} \Bigg\{ \\
&\qquad \left(\hat{d}_i(-\underline{q})\hat{b}_j(\underline{q})\right) \left[\bar{v}^{(i)}(-\underline{q})\left(+\underline{\gamma}\cdot\underline{q}+m\right)u^{(j)}(\underline{q})\right] e^{-2iq_0x_0} \\
&\quad + \left(\hat{d}_i(\underline{q})\hat{d}_j^{\dagger}(\underline{q})\right) \left[\bar{v}^{(i)}(\underline{q})\left(-\underline{\gamma}\cdot\underline{q}+m\right)v^{(j)}(\underline{q})\right] \\
&\quad + \left(\hat{b}_i^{\dagger}(\underline{q})\hat{b}_j(\underline{q})\right) \left[\bar{u}^{(i)}(\underline{q})\left(+\underline{\gamma}\cdot\underline{q}+m\right)u^{(j)}(\underline{q})\right] \\
&\quad + \left(\hat{b}_i^{\dagger}(-\underline{q})\hat{d}_j^{\dagger}(\underline{q})\right) \left[\bar{u}^{(i)}(-\underline{q})\left(-\underline{\gamma}\cdot\underline{q}+m\right)v^{(j)}(\underline{q})\right] e^{+2iq_0x_0} \Bigg\}, \qquad (226)
\end{aligned}
$$

where we the x-integration over space resulted in a δ-function, $\delta^3(\underline{p}-\underline{q})$, which in turn enabled the integration over $\underline{p}$.

Using the E.o.M. for the u and v spinors,

$$
\begin{aligned}
(\not{q}-m)u(\underline{q}) = 0 \quad &\longrightarrow \quad q_0\gamma_0 u(\underline{q}) = (\underline{q}\cdot\underline{\gamma}+m)u(\underline{q}) \\
(\not{p}+m)v(\underline{p}) = 0 \quad &\longrightarrow \quad q_0\gamma_0 v(\underline{q}) = (\underline{q}\cdot\underline{\gamma}-m)v(\underline{q})
\end{aligned} \qquad (227)
$$

and $\bar{u}\gamma_0 = u^{\dagger}$ and $\bar{v}\gamma_0 = v^{\dagger}$,

$$
\begin{aligned}
\hat{H} &= \frac{1}{2}\int \frac{\mathrm{d}^3 q}{(2\pi)^3 2q_0} \sum_{i,j=1}^{2} \Big\{ \Big(\hat{d}_i(-\underline{q})\hat{b}_j(\underline{q})\Big) \Big[v^{(i)\dagger}(-\underline{q})u^{(j)}(\underline{q})\Big]\, e^{-2iq_0x_0} \\
&\quad - \Big(\hat{d}_i(\underline{q})\hat{d}^\dagger_j(\underline{q})\Big) \Big[v^{(i)\dagger}(\underline{q})v^{(j)}(\underline{q})\Big] + \Big(\hat{b}^\dagger_i(\underline{q})\hat{b}_j(\underline{q})\Big) \Big[u^{(i)\dagger}(\underline{q})u^{(j)}(\underline{q})\Big] \\
&\quad + \Big(\hat{b}^\dagger_i(-\underline{q})\hat{d}^\dagger_j(\underline{q})\Big) \Big[u^{(i)\dagger}(\underline{q})v^{(j)}(-\underline{q})\Big]\, e^{+2iq_0x_0} \Big\}
\end{aligned}
$$

With the orthogonality relations of Eq. (214) and their counterparts for terms ,
$u^{(i)\dagger}(-\underline{q})v^{(j)}(\underline{q})$ and $v^{(i)\dagger}(-\underline{q})u^{(j)}(\underline{q})$, the first and the last term in the bracket above vanish.

We finally arrive at the Hamiltonian

$$
\hat{H} = \int \frac{\mathrm{d}^3 q}{(2\pi)^3 2q_0}\, q_0 \sum_{i=1}^{2} \Big[\hat{b}^\dagger_i(\underline{q})\hat{b}_i(\underline{q}) - \hat{d}_i(\underline{q})\hat{d}^\dagger_i(\underline{q})\Big]\,, \qquad \{228\}
$$

which exhibits the same problems with infinite ground state energy as its counterpart of the Klein-Gordon field, cf.. Sec. 4.2.

We cure this, again, by applying normal-ordering, Eq. (160) for bosons, which for fermion fields, however, comes with an extra minus sign to encode the Pauli exclusion principle,

$$
:\hat{d}^\dagger_i(\underline{q})\hat{d}_i(\underline{q}): = -\, :\hat{d}_i(\underline{q})\hat{d}^\dagger_i(\underline{q}): = \hat{d}^\dagger_i(\underline{q})\hat{d}_i(\underline{q})\,. \qquad (229)
$$

Therefore, the normal-ordered Hamiltonian is given by

$$\boxed{\hat{H} \;=\; \int \frac{\mathrm{d}^3 q}{(2\pi)^3 2q_0}\, q_0 \sum_{i=1}^{2} \left[\hat{b}_i^\dagger(\underline{q})\hat{b}_i(\underline{q}) \;+\; \hat{d}_i^\dagger(\underline{q})\hat{d}_i(\underline{q})\right] .} \tag{230}$$

Introducing number operators $\hat{N}_\pm$ for particles with positive and negative energy, electrons and positrons,

$$\hat{N}_+(\underline{q}) = \sum_{i=1}^{2} \hat{b}_i^\dagger(\underline{q})\hat{b}_i(\underline{q}) \quad \text{and} \quad \hat{N}_-(\underline{q}) = \sum_{i=1}^{2} \hat{d}_i^\dagger(\underline{q})\hat{d}_i(\underline{q})\,, \tag{231}$$

we see that the Hamiltonian merely sums the energies of these particles

$$:\hat{H}: = \int \frac{\mathrm{d}^3 q}{(2\pi)^3 2q_0}\, q_0 \left[\hat{N}_+(\underline{q}) \;-\; \hat{N}_-(\underline{q})\right] . \tag{232}$$

Conserved Charge In a similar way, we can construct the (normal-ordered) charge operator : $:\hat{Q}:$.

Promoting the fields in the 0-component of the current density Eq. (200) to field operators

$$:\hat{Q}:= \int \mathrm{d}^3 x \;:\!\left[i\hat{\bar{\psi}}(x)\gamma^0\hat{\psi}(x)\right]\!:\,, \tag{233}$$

we arrive at

$$\boxed{:\hat{Q}:= \int \frac{\mathrm{d}^3 q}{(2\pi)^3 2q_0} \sum_{i=1}^{2} \left[\hat{b}_i^\dagger(\underline{q})\hat{b}_i(\underline{q}) \;-\; \hat{d}_i^\dagger(\underline{q})\hat{d}_i(\underline{q})\right] .} \tag{234}$$

Expressed through the number operator this becomes

$$:\hat{Q}: = \int \frac{\mathrm{d}^3 q}{(2\pi)^3 2q_0} \left[\hat{N}_+(\underline{q}) - \hat{N}_-(\underline{q})\right] , \tag{235}$$

and the overall charge of the system is given by the difference of the total numbers of positively and negatively charged particles.

It is a straightforward exercise to show that the charge is conserved, by asserting that the commutator of the charge and Hamilton operator vanishes; we leave this as an exercise.

6 Electrodynamics

In this section we will quantisze electrodynamics, by quantizing the free vector potential that gives rise to the (free) electromagnetic fields.

It turns out that this results in a somewhat more involved procedure; while the vector potential has four components, which we would naively treat as four independent quantities – scalar fields – and quantize them accordingly, the gauge invariance of the fields implies that in fact there are only two physically meaningful degrees of freedom.

This means that, naively exercised, our algorithm of second quantization would lead to a degree of "over-quantization", i.e. trying to quantize objects that cannot and should not be quantized in a consistent and physically meaningful way.

The solution to this is to fix the gauge before quantizing the fields, which is nothing but the imposition of additional external conditions.

6.1 Gauge Invariance as Obstacle

Lagrangian and Gauge Invariance, once more Remember the (free) Lagrangian of Eqs. (125) and (133),

$$\mathcal{L} = \frac{E^2 - B^2}{2} = -\frac{1}{4}F^{\mu\nu}F_{\mu\nu}\,,$$

where we have set the current to zero, $j^\mu = 0$ and moved a factor of 4π into the vanishing $j^\mu A_\mu$ term in the first expression.

It is simple to show that under the gauge transformations of Eq. (120) ,

$$A^\mu \to A'^\mu = A^\mu - \partial^\mu \Lambda \,,$$

the field strength tensor $F^{\mu\nu}$ is a gauge-invariant quantity.

In fact it is a constant,

$$\begin{aligned} F^{\mu\nu} \to F'^{\mu\nu} &= \partial^\mu A'^\nu - \partial^\nu A'^\mu \;=\; \partial^\mu (A^\nu - \partial^\nu \Lambda) - \partial^\mu (A^\mu - \partial^\mu \Lambda) \\ &= \partial^\mu A^\nu - \partial^\nu A^\mu \;=\; F^{\mu\nu} \,. \end{aligned} \tag{236}$$

Reminding ourselves of the connection of the field strength tensor with the electric and magnetic fields E and B, Eq. (122), invariance of the fields under gauge transformations is manifest.

This has two implications, which are worth making explicit: First of all, although we will explicitly quantize the vector potential A^μ and only indirectly, through it, the fields, the latter are the physical quantities, measurable in every day life.

The impact of a finite vector potential in regions where the fields vanish is subject of the Aharonov-Bohm effect.

Secondly, and in the context of what follows more importantly, we may use special forms of the gauge transformation, Eq. (120), to eliminate some components of A^μ without impacting on the physics.

But this also implies that there are less than four physically meaningful degrees of freedom encoded in the vector potential, and we will have to deal with the problem of how to quantize a system that has less physical degrees of freedom than the field that is used for its description.

Fixing the Gauge Let us discuss now some of the conditions that can be imposed on A^μ, which effectively *fix the gauge*.

Looking at the form of the field strength tensor it is worth noting that $F^{00} = 0$, which implies that there is no conjugate momentum for the temporal component of A^μ.

Defining them, as before, through

$$\pi^\mu = \frac{\partial \mathcal{L}}{\partial \dot{A}^\mu} \tag{237}$$

and specializing on $\mu = 0$ yields

$$\pi^0 = \frac{\partial \mathcal{L}}{\partial \dot{A}^0} = 0\,. \tag{238}$$

This motivates us to use a temporal gauge defined by

$$\Lambda(t, \underline{x}) = \int_{-\infty}^{t} \mathrm{d}t' A^0(t', \underline{x}) \tag{239}$$

which results in $A^0{}_\Lambda = 0$.

Coulomb vs. Lorentz vs. Axial Gauge It turns out, however, that this does not yet entirely fix the gauge and an additional condition has to be applied.

Three types of gauge, with different calculational advantages and disadvantages in different situations are frequently found:

- *Coulomb gauge*, defined through

$$\underline{\nabla} \cdot \underline{A} = 0. \tag{240}$$

- *Lorentz gauge*, defined through

$$\partial_\mu A^\mu = 0. \tag{241}$$

- *Axial gauge*, defined through, e.g.

$$A_z = 0. \tag{242}$$

Polarization Vectors and Degrees of Freedom To build on this idea of gauge fixing, let us analyze in some more detail what this actually implies.

Most transparently this can be done in Coulomb gauge.

For free fields, i.e., with $j = 0$ and, in particular the charge density $\rho = j^0 = 0$, A^0 is not a dynamical degree of freedom: its derivative w.r.t. time is not present in the free field Lagrangian and hence its conjugate momentum vanishes.

The temporal part of the gauge in Eq. (239) fixes this constant then to $A^0 = 0$, making the lack of dynamical relevance explicit.

This leaves only the spatial components of A, $\underline{A}$, and the field strength tensor is composed of the components of $\underline{\nabla} \times \underline{A}$, as $F^{ij} = \partial^i A^j - \partial^j A^i$.

But imposing the Coulomb gauge condition by demanding that the divergence of $\underline{A}$ vanishes, $\underline{\nabla}\cdot\underline{A}= 0$ we exposed that there is a longitudinal component of A, A_L.

By definition of it being longitudinal, $\underline{\nabla}$ x $\underline{A_L} = 0$.

The simplest way to see this is to assume a fixed longitudinal axis, for example the z-axis.

Then the photon momentum $\underline{k}$ is parallel to the z-axis, but, in addition, also A_z, the longitudinal component, is parallel to the z-axis.

Fourier-transforming the condition then yields $\underline{k}$ x $\underline{A_L} = 0$ and therefore $\underline{\nabla} \times \underline{A_L} = 0$.

This implies that yet another component of F vanishes, or, differently put, we see that also A_L is not dynamically relevant.

This shows that the Coulomb gauge is the one where the longitudinal degree of freedom vanishes, $A_L = 0$.

Not surprisingly, imposing two conditions on the four-vector A^μ eliminates two of its components, and we are left with two degrees of freedom.

The logic above, eliminating the temporal and longitudinal parts of A from the dynamical degrees of freedom means that we are left with two transverse degrees of freedom A_T.

To make the physics of this more explicit, let us see how this works out in practice.

Assume we want to describe a quantum of electromagnetism, a *photon*, with momentum $\underline{k}$.

It's four-momentum of course is given by

$$k^{\mu} = (\omega,\, \underline{k}) \quad \text{with} \;\; \omega = k_0 = \sqrt{\underline{k}^2}\,. \tag{243}$$

The relevant degrees of freedom for the photon are its two remaining polarizations.

They are usually denoted by $\lambda = \{1, 2\}$ and represented by polarization vectors $\epsilon^{\mu}_{(\lambda)}(k)$.

Fourier transformation of the gauge conditions above then become conditions on products of the three-momentum and the polarization three-vector; while the temporal gauge condition implies $\epsilon^0 = 0$ we have:

$$\underline{k} \cdot \underline{\epsilon}_{(\lambda)}(k) \;=\; 0 \quad \text{(no longitudinal polarisation)}\,. \tag{244}$$

Demanding additionally that the polarization vectors are real and orthonormal we have

$$\underline{\epsilon}_{(\lambda)}(k) \cdot \underline{\epsilon}_{(\kappa)}(k) = \delta_{\lambda\kappa}\,. \tag{245}$$

A simple way to guarantee this is to orient $\underline{k}$ along the z-axis.

Then

$$\epsilon_{(1)} = (1,\, 0,\, 0) \quad \text{and} \quad \epsilon_{(2)} = (0,\, 1,\, 0)\,. \tag{246}$$

6.2 Coulomb Gauge

Logic of the Procedure We will try to explicitly follow the algorithm for the second quantization of a field as summarized in Fig. 1, and highlight specifically, where this algorithm starts to crash.

Identifying the components of A^μ as the fields to be quantized, we have:

1. determine conjugate momenta π^ν

$$\pi^\nu = \frac{\partial L}{\partial \dot{A}^\nu} \Longrightarrow \begin{cases} \pi^0 = \dfrac{\partial L}{\partial \dot{A}^0} = 0 \\ \pi^i = \dfrac{\partial L}{\partial \dot{A}^i} = -E_i\,. \end{cases} \tag{247}$$

This makes the anticipated problem of vanishing conjugate momentum for A^0 manifest. Further down the line it will prevent us from quantising it, because we will not be able to produce a non-vanishing commutator between this field component and its conjugate momentum: for our choice of Lagrangian, it is guaranteed that $[A^0, \pi^0] = 0$ irrespective of what we try to do and therefore quantisation of A^0 is bound to fail.

2. construct the Hamiltonian
   As before, the Hamiltonian density expressed through the electric and magnetic fields is given by

$$\mathcal{H} = \dot{A}^\mu \pi_\mu - \mathcal{L} = \frac{\underline{E}^2 + \underline{B}^2}{2} + \underline{E} \cdot \underline{\nabla} A^0 \,, \tag{248}$$

   where the last term obviously vanishes if we set $A^0 = 0$.

3. promote fields to field operators

4. demand equal-time commutators of fields and conjugate momenta
   Due to $\pi^0 = 0$ we have only non-vanishing equal-time commutators for spatial components, namely

$$\boxed{\left[\hat{A}_i(t,\,\underline{x}),\,\hat{\pi}_j(t,\,\underline{y})\right] = i\delta_{ij}\delta^3(\underline{x}-\underline{y}) = -\left[\hat{A}_i(t,\,\underline{x}),\,\hat{E}_j(t,\,\underline{y})\right]\,.} \tag{249}$$

Dealing with A_0: Gauss' law To re-iterate: the fact that $\pi^0 = 0$ means that also the field operator vanishes and hence commutes with every field operator.

Therefore A_0 is not a dynamical variable, and $\dot{A}_0 = 0$.

This means that A_0 is not an operator but an ultimately inconsequential number in our construction of a quantum field theory.

However, there is a direct consequence of it being not dynamical:

$$\frac{\partial \mathcal{L}}{\partial A_0} = 0 \quad \longrightarrow \quad \underline{\nabla} \cdot \underline{E} = 0\,, \tag{250}$$

which is just Gauss' law in the absence of sources.

We would of course be tempted to implement this as a wonderfully physical constraint on the field operators.

But this would lead to yet another way to see the problem with the procedure.

Going back to the commutation relations, and forming a divergence we would arrive at, somewhat schematically,

$$\begin{aligned} &\sum_j \frac{\partial}{\partial y^j} \left[\hat{A}_i(t,\, \underline{x}),\, \hat{E}_j(t,\, \underline{y})\right] \\ &= \quad \left[\hat{A}_i(t,\, \underline{x}),\, \underline{\nabla} \cdot \underline{\hat{E}}_j(t,\, \underline{y})\right] \; = \; -i \sum_j \delta_{ij} \frac{\partial}{\partial y^j} \delta^3(\underline{x} - \underline{y})\,. \end{aligned} \tag{251}$$

This is difficult, because while the left hand side of the second line vanishes, due to Gauss' law, the right hand side doesn't.

This implies that we cannot implement Gauss' law as an operator equation.

Dealing with A_0: Conditions on the States Realizing that we cannot implement Gauss' law as a direct constraint on the field operators, we could try and rephrase it as a condition on the allowed states $|\psi\rangle$ forming the Fock space on which the operators then act.

We would proceed by demanding that all physical states $|\psi\rangle$satisfy

$$\underline{\nabla} \cdot \underline{\hat{E}} \, |\psi\rangle \;=\; 0 \tag{252}$$

and would classify all states that do not fulfill this criterion as unphysical and ignore them.

It is a bit cumbersome to show that this doesn't work either and in fact would also violate the commutation relations.

The next weaker constraint, however, works.

Demanding that for physical states Gauss' law is satisfied as expectation value,

$$\langle\psi| \, \underline{\nabla \hat{E}} \, |\psi\rangle \;=\; 0 \tag{253}$$

encapsulates this part of Maxwell's equation as an average.

We will come back to its implications at a somewhat later state.

Solving the Crisis: Transverse δ-function The solution to the problem of Gauss' law is to modify the commutation relation in such a way that they automatically encode it.

This is done by replacing the δ-function on the right hand side of the commutation relations of Eq. (255) with a *transverse* δ-function, δ^{tr}_{ij} defined as

$$\delta_{ij}\delta^3(\underline{x}-\underline{y}) \quad \longrightarrow \quad \boxed{\delta^{tr}_{ij}(\underline{x}-\underline{y}) \;=\; \int \frac{\mathrm{d}^3k}{(2\pi)^3}\, e^{i\underline{k}\cdot(\underline{x}-\underline{y})} \left(\delta_{ij} - \frac{k_i k_j}{\underline{k}^2}\right)\,.} \tag{254}$$

The modified commutators then read

$$\boxed{\left[\hat{A}_i(t,\,\underline{x}),\, \hat{\pi}_j(t,\,\underline{y})\right] \;=\; i\delta^{tr}_{ij}(\underline{x}-\underline{y}) \;=\; -\left[\hat{A}_i(t,\,\underline{x}),\, \hat{E}_j(t,\,\underline{y})\right]\,.} \tag{255}$$

It is easy to show that the gradient of the transverse δ-function with respect to x or y vanishes, because derivatives will produce a term $\pm k_i$ multiplying the rounded bracket, and

$$\sum_i k_i \left(\delta_{ij} - \frac{k_i k_j}{\underline{k}^2}\right) = k_j - \frac{k_j \underline{k}^2}{\underline{k}^2} = 0. \tag{256}$$

We can therefore safely set it to 0, asserting the validity of Gauss' law.

More Benefits of δ^{tr} As a byproduct, forming a divergence w.r.t to the x-position yield

$$\left[\underline{\nabla}\cdot\underline{\hat{A}}(t,\,\underline{x}),\, \hat{E}_j(t,\,\underline{y})\right] \;=\; 0\,, \tag{257}$$

and we recover the Coulomb gauge condition $\underline{\nabla}\cdot\underline{A} = 0$.

Non-Vanishing Commutator at Space-like Distances But there is a little snag.

Replacing the δ-function with its transverse modification implies that it is not guaranteed any more that the commutators $[\hat{A}_i,\, \hat{E}_j]$ vanish for space-like distances.

This looks like a severe problem with the causality structure of the theory.

However, there are two answers to the problem.

1. $\hat{A}$ is a gauge-dependent quantity and therefore essentially unphysical. It cannot directly be measured, and therefore, any potentially harmful a-causal behaviour may not have physical implications.

2. careful calculations reveals that while $[\hat{A}_i,\, \hat{E}_j]$ may not vanish for space-like distances, the commutators of the physical E and B fields and their components do vanish, irrespective of the use of the transverse δ function.

Creation and Annihilation Operators Reminding ourselves that we have set $A^0 = 0$, the field is expanded in terms of plane waves and creation and annihilation operators as

$$\underline{\hat{A}}(\underline{x},\, t) = \int \frac{\mathrm{d}^3 k}{(2\pi)^3 (2k_0)} \sum_{\lambda=1}^{2} \left[\underline{\epsilon}^{(\lambda)}(k) \hat{a}(\underline{k},\, \lambda) e^{-ik\cdot x} + \underline{\epsilon}^{*(\lambda)}(k) \hat{a}^\dagger(\underline{k},\, \lambda) e^{ik\cdot x} \right], \tag{259}$$

where the sum is over the two polarizations of the photons and, similar to the case of the Dirac spinors, we have “scalar” creation and annihilation operators for each of the polarization states.

As before, the creation and annihilation operators enjoy commutation relations, namely

$$\boxed{\left[\hat{a}(\underline{k},\, \lambda),\, \hat{a}^{\dagger}(\underline{q},\, \kappa)\right] \;=\; (2\pi)^3 2k_0\, \delta^3(\underline{k}-\underline{q})\, \delta_{\lambda\kappa}} \tag{260}$$

with all other commutators vanishing.

More on Polarizations Note that we now also allow complex polarization vectors, to capture, for example circular polarizations.

Assuming that the photon momentum is oriented along the positive z-axis, $\underline{k} = k\underline{e}_z$, we could use real polarization vectors for linear polarizations, as

$$\epsilon^{\mu(\lambda=1)}(\underline{k}) = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \quad \text{and} \quad \epsilon^{\mu(\lambda=2)}(\underline{k}) = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \tag{261}$$

while for circular polarizations we could write

$$\epsilon^{\mu(\lambda=1,2)}(\underline{k}) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ \pm i \\ 0 \end{pmatrix}. \tag{262}$$

Using four-vectors instead of three vectors means that we replace the transversality condition with $k^\mu \cdot \epsilon_\mu = 0$, keeping the ortho-normality condition of Eq. (245).

6.3 Lorentz Gauge

Modifying the Lagrangian One of the issues with the Coulomb gauge is that it is not Lorentz-invariant.

To achieve this invariance, though, we will need to demand commutator relations that fully reflect this symmetry,

$$\boxed{\left[\hat{A}_\mu(t,\, \underline{x}),\, \hat{\pi}_\nu(t,\, \underline{y})\right] \;=\; i g_{\mu\nu}\delta^3(\underline{x}-\underline{y})\,.} \tag{263}$$

This implies, obviously, that all four components of the vector potential have a conjugate momentum, and, in particular, that π^0 doesn't vanish.

Since π^0 emerges by differentiation of the Lagrangian w.r.t A^0, we must modify the Lagrangian such that this derivative does not vanish any more.

This is achieved by modifying the free-field Lagrange density,

$$\mathcal{L} = -\frac{1}{4}F^{\mu\nu}F_{\mu\nu} \quad\longrightarrow\quad \boxed{\mathcal{L} = -\frac{1}{4}F^{\mu\nu}F_{\mu\nu} - \frac{\alpha}{2}(\partial_\mu A^\mu)^2\,.} \tag{264}$$

Here, α is the, in principle, arbitrary gauge parameter, and physical results should not depend on its actual choice.

This kind of modification is not unknown from classical mechanics, where external conditions on the dynamics are often encoded through the method of Lagrange multipliers [15]
.

Modified Maxwell Equations and Feynman Gauge Adding a source term $4\pi\, j_\mu A^\mu$, the resulting Maxwell equations read

$$\partial_\mu \partial^\mu A^\nu - (1-\alpha)\partial^\nu(\partial \cdot A) = 4\pi j^\nu\,, \tag{265}$$

and it is suggestive to set $\alpha = 1$ to recover their original form.

This gauge choice is commonly referred to as *Feynman gauge*.

Conjugate Momenta As usual, the conjugate momenta are calculated by differentiation, and we have

$$\pi^\mu = \frac{\partial \mathcal{L}}{\partial \dot{A}_\mu} = F^{\mu 0} - \alpha g^{\mu 0}(\partial \cdot A) \longrightarrow \left\{ \begin{array}{lcl} \pi^0 & = & -\alpha(\partial \cdot A) \\ \pi^i & = & -E^i\,. \end{array} \right. \tag{266}$$

Clearly, the modification of the Lagrange density only modified π^0, which now is proportional to the gauge parameter α.

Imposing Lorentz Gauge We now have to decide how to impose the constraint $\partial \cdot A = 0$ which defines the Lorentz gauge that we chose at the beginning of this discussion.

Adjusting the commutators, like in the case of the Coulomb gauge, is not viable, because we have already postulated the commutation relations we would like to use, namely the ones in Eq. (263).

We also cannot impose the constraint $\partial \cdot A = 0$ as an operator equation, because this would imply that $\pi^0 = 0$, and we would not be able to recover our postulated commutator relations.

This means that we are forced down an avenue that we briefly considered in the case of the Coulomb gauge, by demanding that we implement the gauge condition as a condition on physical states.

We realize very quickly that it cannot be realized as a condition on physical states $|\psi\rangle$,

$$\partial \cdot \hat{A}\,|\psi\rangle = 0\,, \tag{267}$$

for the following reason.

Consider the expectation value of the commutator relation Eq. (263), specified for $\mu = \nu = 0$:

$$\langle\psi|\left[\hat{A}^0(t,\,\underline{x}),\,\hat{\pi}^0(t,\,\underline{y})\right]|\psi\rangle = i\delta^3(\underline{x}-\underline{y})\,\langle\psi|\psi\rangle\,. \tag{268}$$

But at the same time

$$\hat{\pi}^0\,|\psi\rangle = (\partial\cdot\hat{A})\,|\psi\rangle = 0 \tag{269}$$

enforces that the l.h.s. of Eq. (268) must vanish, while the r.h.s. does not.

This rules out the weaker constraint as a viable, consistent option.

This leaves us the only option to encode the gauge condition by demanding that it holds only true for expectation values of *physical states*, i.e., demanding that

$$\langle\psi|\,\partial\cdot\hat{A}\,|\psi\rangle = 0 \tag{270}$$

for physical states ψ.

To implement this, it is sufficient to demand that for the *positive energy/frequency* $\hat{A}_+$ part of the field operator we have

$$\partial \cdot \hat{A}_+ |\psi\rangle = 0\,, \tag{271}$$

because we can write

$$\begin{aligned} \langle\psi|\,\partial \cdot \hat{A}\,|\psi\rangle &= \langle\psi|\left(\partial \cdot \hat{A}_- + \partial \cdot \hat{A}_+\right)|\psi\rangle \\ &= \left(\partial \cdot \hat{A}_- |\psi\rangle\right)^\dagger |\psi\rangle + \langle\psi|\,\partial \cdot \hat{A}_+ |\psi\rangle = 0\,. \end{aligned} \tag{272}$$

We will use this after we defined polarization vectors and expanded the field operators in plane waves and creation and annihilation operators.

Field Operators The field operators are expanded as

$$\boxed{\hat{A}_\mu(x) = \int \frac{\mathrm{d}^3k}{(2\pi)^3 2k_0} \sum_{\lambda=0}^{3} \left[\epsilon_\mu^{(\lambda)}(\underline{k})\hat{a}_\lambda(\underline{k})e^{-ik\cdot x} + \epsilon_\mu^{*(\lambda)}(\underline{k})\hat{a}_\lambda^\dagger(\underline{k})e^{ik\cdot x}\right]}\,, \tag{273}$$

where we have chosen four linearly independent polarization vectors as

$$\epsilon^{(0)}(\underline{k}) = \begin{pmatrix}1\\0\\0\\0\end{pmatrix},\ \epsilon^{(1)}(\underline{k}) = \begin{pmatrix}0\\1\\0\\0\end{pmatrix},\ \epsilon^{(2)}(\underline{k}) = \begin{pmatrix}0\\0\\1\\0\end{pmatrix},\ \epsilon^{(3)}(\underline{k}) = \begin{pmatrix}0\\0\\0\\1\end{pmatrix} \tag{274}$$

For simplicity we assumed that the photon momentum is oriented along the positive z-axis, $\underline{k} \parallel \underline{e}_z$.

It is easy to check that the polarization vectors satisfy

$$\boxed{\epsilon^{(\lambda)}(\underline{k}) \cdot \epsilon^{*(\kappa)}(\underline{k}) = \epsilon^{(\lambda)\mu}(\underline{k})\epsilon^{*(\kappa)}_{\mu}(\underline{k})g_{\lambda\kappa} \,,} \tag{275}$$

where the differnence between labels (λ) for the polarization vectors and their components - the Lorentz index μ has been made explicit.

A simple calculation shows that the commutators of Eq. (263) are satisfied, if the only non-vanishing commutator of the creation and annihilation operators is given by

$$\boxed{\left[\hat{a}_\lambda(\underline{k}),\, \hat{a}^\dagger_\kappa(\underline{q})\right] = -(2\pi^3)(2k_0)g_{\lambda\kappa}\delta^3(\underline{k}-\underline{q})\,.} \tag{276}$$

Hamiltonian The resulting Hamiltonian density is given by

$$\boxed{:\hat{H}: = \int \frac{\mathrm{d}^3k}{(2\pi)^3 2k_0} k_0 \left[\sum_{\lambda=1}^{3} \left(\hat{a}^\dagger_\lambda(\underline{k})\hat{a}_\lambda(\underline{k})\right) - \hat{a}^\dagger_0(\underline{k})\hat{a}_0(\underline{k})\right] \,.} \tag{277}$$

The form of the Hamilton operator exhibits a potential problem: clearly, scalar photons, i.e. those with λ = 0, come with a negative sign, opposite to what we want and what we know how to deal with.

At first sight, this seems to signal that our attempt at quantizing the electromagnetic fields in Lorentz gauge failed, and that we arrived at a Hamiltonian describing an energy spectrum that is not bounded from below, despite the normal ordering.

The reason for this, of course, can be traced back to the use of the metric tensor in the quantization conditions, which enforces a state with a "wrong" sign.

However, careful inspection below will reveals that this is not a real problem and that the corresponding states are unphysical, motivating us to call them "ghosts".

Physical States So, let us now take a closer look at some of the states and their energies.

Start with the by now familiar assertion that the vacuum reduces to zero when the one of the annihilation operators is applied,

$$\hat{a}_\lambda(\underline{k})\,|0\rangle = 0 \;\; \forall\lambda\,. \tag{278}$$

Now, let us analyze one of the more tricky states: a scalar photon, modulated by some well-behaved function $f(\underline{k})$,

$$|1_S\rangle = \int \frac{\mathrm{d}^3k}{(2\pi)^3 2k_0}\, f(\underline{k})\hat{a}_0^\dagger(\underline{k})\,|0\rangle\;. \tag{279}$$

As already anticipated, the norm of this states is negative,

$$\begin{aligned}\langle 1_S|1_S\rangle &= \int \frac{\mathrm{d}^3k}{(2\pi)^3 2k_0}\int \frac{\mathrm{d}^3k'}{(2\pi)^3 2k_0} f(\underline{k}) f^*(\underline{k}')\langle 0|\hat{a}(\underline{k}',\,0)\hat{a}^\dagger(\underline{k},\,0)|0\rangle \\ &= -\,\langle 0|0\rangle \int \frac{\mathrm{d}^3k}{(2\pi)^3 2k_0}|f(\underline{k})|^2 < 0\,.\end{aligned} \tag{280}$$

The minus sign of course stems from the relative sign in the metric, or, when followed through, from the "-"-sign in front of the right-hand side of the commutator in Eq. (276).

Phrased differently, the combinations of positive and negative energy solutions that are still allowed destroys the positive definiteness of the norm.

So let us impose the gauge constraint $\partial\cdot \hat{A}_+ |\psi\rangle = 0$.

Evaluating $\partial\cdot \hat{A}_+$ we of course only take into account the positive energy solutions and arrive at

$$\partial \cdot \hat{A}_+ = -i \int \frac{\mathrm{d}^3 k}{(2\pi)^3 2k_0} \sum_{\lambda=0}^{3} \left[k^\mu \epsilon_\mu^{(\lambda)}(\underline{k}) \hat{a}_\lambda(\underline{k})\, e^{-ik\cdot x} \right] . \tag{281}$$

We can simplify this further by realizing that for $\lambda = \{1, 2\}$ the polarizations are orthogonal to the momentum, $\epsilon \perp k$ and therefore $k \cdot \epsilon = 0$.

This leaves us with two surviving polarizations, scalar ($\lambda = 0$) and longitudinal ($\lambda = 3$).

Our constraint on physical states $|\psi\rangle$ therefore becomes

$$\begin{aligned} 0 &= \partial \cdot \hat{A}_+ |\psi\rangle \\ &= -i \int \frac{\mathrm{d}^3 k}{(2\pi)^3 2k_0} \left[k \cdot \epsilon^{(0)}(\underline{k}) \hat{a}_0(\underline{k}) - k \cdot \epsilon^{(3)}(\underline{k}) \hat{a}_3(\underline{k}) \right] e^{-ik\cdot x} . \end{aligned} \tag{282}$$

For massless four-momenta – $k^2 = 0$ – longitudinal momentum and energy coincide, $k_\parallel = k = k_0$ and therefore $k \cdot \epsilon^{(0)} = -k \cdot \epsilon^{(3)}$.

This implies that the gauge constraint can be satisfied if

$$\left[\hat{a}_0(\underline{k}) - \hat{a}_3(\underline{k})\right] |\psi\rangle = 0 \tag{283}$$

for all physical states $|\psi\rangle$

the the the the the

7 Time-Ordered Products

Until now we have quantized various free elementary fields: real and complex scalars, Dirac-spinors, and the vector fields of electrodynamics.

The resulting structure in each case can be condensed into a sequence of algorithmic steps, which, starting from a Lagrange density, resulted in the expansion of field operators as products of plane waves and creation and annihilation operators, and we succeeded in expressing “static” global quantities such as the Hamilton or charge operators through the latter.

This implies an underlying causal structure if the theory: in non-relativistic field theories, which we do not discuss here, evolution is forward in time, and for the analysis of causality it is usually sufficient to concentrate on the positive–energy solutions only.

This changes in relativistic field theories, where both forward and backward evolution, and therefore positive and negative energy solutions, are included.

It is important to realize the interplay with causality requirements of the theory - the simplest one is that the commutator of two fields must vanish for space-like distances.

It turns out that in non-relativistic theory this cannot be achieved, which actually should not come as a surprise.

If you do not embed relativity in your formalism you cannot expect to obtain relativistically sensible results from it.

In the relativistic field theories we have discussed here, the positive and negative energy solutions could be arranged such that the commutator of two fields vanishes outside the light-cone, i.e. for space-like distances, but remains finite inside the light-cone

In this chapter we will build further on the logic and discussion started in Sec. 4.3, and we will analyze the propagation of particles.

This first step towards a dynamic picture of quantized field theories is deeply connected to the notion of Green's functions, which will return to us in this chapter, and called propagators.

They will fortify the notion of the negative-energy solutions as anti-particles, which travel backwards in time, with opposite charge.

We will also see how the wrong commutator (or anti-commutator) for a given statistics (Bose–Einstein vs. Fermi–Dirac) destroys the causality structure of the theory.

7.1 Greens Functions: Non-Relativistic Quantum Mechanics

What is the Green's Function? Consider the time-dependent Schrodinger equation for a point particle,

$$\left(\frac{i\partial}{\partial t} - \hat{H}\right)|\psi(t)\rangle \;=\; \left(\frac{i\partial}{\partial t} + \frac{\nabla^2}{2m} - \hat{V}\right)|\psi(t)\rangle \;=\; 0\,. \tag{284}$$

It is formally solved through the introduction of Green's function, $G(t, \underline{x}; t, \underline{x}')$:

$$\psi(t, \underline{x}) \;=\; \langle \underline{x}|\psi(t)\rangle \;=\; \int \mathrm{d}^3x'\, G(t, \underline{x}; t', \underline{x}')\psi(t', \underline{x}')\,. \tag{285}$$

The interpretation is clear: the wave function $\psi(t, \underline{x})$ at time t and position $\underline{x}$ in position space is constructed as the superposition of all wave functions at all positions $\underline{x}'$ at an earlier time t', and the Green's function parameterizes the "strength" of the connection.

Because it this has been couched in the framework of non-relativistic Quantum Mechanics the maximal velocity of causation (speed of light in relativistic physics) is infinite, and the connection is instantaneous.

The Green's function G is also called the (*retarded*) *propagator*.

Construction of the Green's Function The interpretation of the Green's function above suggests that it is the solution of

$$\boxed{\left(\frac{i\partial}{\partial t} - \hat{H}\right) G(t,\, \underline{x};\, t',\, \underline{x}') \;=\; \delta(t - t')\delta^3(\underline{x} - \underline{x}')\,,} \tag{286}$$

with the boundary condition that it vanishes for $t' > t$.

This allows to rewrite it as

$$G(t,\, \underline{x};\, t',\, \underline{x}') \;=\; K(t,\, \underline{x};\, t',\, \underline{x}')\, \Theta(t - t')\,, \tag{287}$$

where $K(t, \underline{x}; t', \underline{x}')$ is the transition amplitude

$$\langle \underline{x},\, t | \underline{x}',\, t' \rangle \;=\; \langle \underline{x} |\, \hat{U}(t,\, t')\, | \underline{x}' \rangle \tag{288}$$

and

$$\hat{U}(t, t') = \exp\left[-i \int_{t'}^{t} \mathrm{d}\tau \, \hat{H}(\tau)\right] \longrightarrow \exp\left[-i\hat{H}(t - t')\right] \tag{289}$$

is the unitary time-evolution operator, well-known from Quantum Mechanics, which reduces to the second expression if $\hat{H}$ does not explicitly depend on time.

Free-Particle Propagator: Direct Solution in Momentum Space As a simple example consider a free point particle in Quantum Mechanics.

Its propagator (Green's function) G_0 is a solution to

$$\begin{aligned} \left(\frac{i\partial}{\partial t} - \hat{H}_0\right) G_0(t, \underline{x}; t', \underline{x}') &= \\ \left(\frac{i\partial}{\partial t} + \frac{\nabla^2}{2m}\right) G_0(t, \underline{x}; t', \underline{x}') &= \delta(t - t')\delta^3(\underline{x} - \underline{x}') \,. \end{aligned} \tag{290}$$

A simple way to solve this equation is by Fourier-transforming on, resulting in

$$\left(\omega - \frac{\underline{p}^2}{2m}\right) G_0(\omega, \underline{p}) = 1 \tag{291}$$

and therefore

$$\boxed{G_0(\omega, \underline{p}) = \frac{1}{\omega - \underline{p}^2/2m}} \,. \tag{292}$$

Position Space The back-transformation into position space is formally achieved by

$$G_0(t, \underline{x}; t', \underline{x}') = \int \frac{d^3p}{(2\pi)^3} \frac{d\omega}{2\pi} \frac{\exp[i\underline{p} \cdot (\underline{x} - \underline{x}') - i\omega(t - t')]}{\omega - \underline{p}^2/(2m)} . \tag{293}$$

This however does come with two interesting problems:

1. the integral obviously diverges for $\omega = \underline{p}^2/2m$, and
2. the propagator G_0 does not satisfy the (causal) boundary condition, *i.e.* it does not vanish for $t' > t$.

There is a way, however, to solve simultaneously both problems.

And this is how it works, we deform the energy integration by shifting the pole on $\omega = p^2/2m$ by a minimal amount of $-i\epsilon^+$ into the imaginary plane – here and in the following, ϵ^+ represents an infinitesimal positive number.

This yields the *retarded Greens function*

$$G_0^{(R)}(t, \underline{x}; t', \underline{x}') = \int \frac{d^3p}{(2\pi)^3} \frac{d\omega}{2\pi} \frac{\exp[i\underline{p} \cdot (\underline{x} - \underline{x}') - i\omega(t - t')]}{\omega - \underline{p}^2/(2m) - i\epsilon^+} . \tag{294}$$

Cauchy's theorem asserts that the energy integral yields

$$\boxed{\int \frac{d\omega}{2\pi} \frac{\exp[-i\omega(t - t')]}{\omega - \underline{p}^2/(2m) - i\epsilon^+} = \Theta(t - t') \exp\left[-\frac{i\underline{p}^2(t - t')}{2m}\right] .} \tag{295}$$

Therefore the overall result is given by

$$
\begin{aligned}
G_0^{(R)}(t, \underline{x}; t', \underline{x}') &= \int \frac{\mathrm{d}^3 p}{(2\pi)^3}\, \Theta(t-t')\, \exp\left[-\frac{i\underline{p}^2(t-t')}{2m} + i\underline{p}\cdot(\underline{x}-\underline{x}')\right] \\
&= \prod_{i=1}^{3} \int \frac{\mathrm{d}p_i}{(2\pi)^3}\, \Theta(t-t')\, \exp\left[-\frac{ip_i^2(t-t')}{2m} + ip_i(x_i - x_i')\right] \\
&= \Theta(t-t') \prod_{i=1}^{3} \int \frac{\mathrm{d}p_i}{2\pi}\, \exp\left[-\frac{i(t-t')}{2m}\left(p_i - \frac{m(x_i-x_i')}{t-t'}\right)^2 \right. \\
&\qquad\qquad \left. + \frac{im(x_i-x_i')^2}{2(t-t')}\right] \\
&= \Theta(t-t') \prod_{i=1}^{3} \frac{1}{2\pi}\sqrt{\frac{2m\pi}{i(t-t')}}\, \exp\left[\frac{im(x_i-x_i')^2}{2(t-t')}\right] \\
&= \Theta(t-t') \sqrt{\frac{-im}{2\pi(t-t')}}^{\,3} \exp\left[\frac{im}{2(t-t')}\sum_{i=1}^{3}(x_i-x_i')^2\right] \\
&= \Theta(t-t') \left[\frac{-im}{2\pi(t-t')}\right]^{\frac{3}{2}} \exp\left[\frac{im(\underline{x}-\underline{x}')^2}{2(t-t')}\right].
\end{aligned}
\tag{296}
$$

We have made use of the fact that we can write this integral as a product of three integrals, one for each spatial component of p, then completed the squares in each component of p, rendering this a product of three Gaussian integrals.

Propagator from Position Space Transition Amplitude An alternative way to arrive at the same result rests on the identification of the propagator with the transition amplitude times the boundary condition, Eq. (287).

Using the free particle Hamiltonian in Eq. (288) we have

$$
\begin{aligned}
K(t,\underline{x};t',\underline{x}') &= \left\langle \underline{x} \middle| \exp\left[-\frac{i\hat{\underline{p}}^2}{2m}(t-t')\right] \middle| \underline{x}' \right\rangle \\
&= \int \frac{\mathrm{d}^3p}{(2\pi)^3}\frac{\mathrm{d}^3p'}{(2\pi)^3} \left\langle \underline{p} \middle| \exp\left[i\underline{p}\cdot\underline{x}\right] \exp\left[-\frac{i\hat{\underline{p}}^2}{2m}(t-t')\right] \exp\left[-i\underline{p}'\cdot\underline{x}'\right] \middle| \underline{p}' \right\rangle \\
&= \int \frac{\mathrm{d}^3p}{(2\pi)^3}\frac{\mathrm{d}^3p'}{(2\pi)^3} \left\langle \underline{p} \middle| \underline{p}' \right\rangle \exp\left[i\underline{p}\cdot\underline{x}\right] \exp\left[-\frac{i\underline{p}^2}{2m}(t-t')\right] \exp\left[-i\underline{p}'\cdot\underline{x}'\right] \\
&= \int \frac{\mathrm{d}^3p}{(2\pi)^3} \exp\left[-\frac{i\underline{p}^2}{2m}(t-t') + i\underline{p}\cdot(\underline{x}-\underline{x}')\right] . \qquad (297)
\end{aligned}
$$

In going from the first to the second line we have use the fact that momentum and position space kets are connected through a Fourier transform,

$$
|\underline{x}\rangle = \int \frac{\mathrm{d}^3p}{(2\pi)^3}\, e^{-i\underline{p}\cdot\underline{x}} \left|\underline{p}\right\rangle , \qquad (298)
$$

and in going to the third line we have replaced the operator $\hat{\underline{p}}^2$ with the eigenvalues p corresponding to its eigenkets $\left|\underline{p}\right\rangle$.

Of course, they form an ortho-normal base, such that their scalar product is a δ function,

$$\langle \underline{p} | \underline{p}' \rangle = (2\pi)^3 \delta^3 (\underline{p} - \underline{p}') \,. \tag{299}$$

Including the Θ-function which connects the transition amplitude with the restarted propagator, this is exactly the same result we already obtained with the more direct method in momentum space.

7.2 Propagators in Quantum Field Theory: Scalar Fields

Scalar Theories The Green's function for the Klein-Gordon equation, i.e., the propagator of the free scalar field is defined by

$$\left(\Box + m^2\right) G_0(x, x') \;=\; i\delta^4(x - x') \,. \tag{300}$$

Fourier transformation results in

$$\left(-p^2 + m^2\right) G_0(p) \;=\; i \quad \longrightarrow \quad \boxed{G_0(p) \;=\; \frac{-i}{p^2 - m^2}} \,. \tag{301}$$

As before, the Green's function exhibits a pole when the energy-momentum relation is satisfied, that is, when the particle goes "on its mass-shell" or "on-shell", and as before this is repaired by shifting the pole in the complex plane by an infinitesimally small amount of $i\epsilon^+$ away from the real axis.

Time-Ordered Products and Green's Functions In what follows we will show that the Green's function is also given by the vacuum expectation value of a time-ordered product,

$$\boxed{\begin{aligned} G_0(x,\, x') &= \langle 0|\, T\hat{\phi}(x)\hat{\phi}(x')\, |0\rangle \\ &= \Theta(t-t')\, \langle 0|\, \hat{\phi}(x)\hat{\phi}(x')\, |0\rangle \,+\, \Theta(t'-t)\, \langle 0|\, \hat{\phi}(x')\hat{\phi}(x)\, |0\rangle\ . \end{aligned}} \tag{302}$$

When expanding these products in terms of the creation and annihilation operators, it is worth noting that $\hat{a}\,|0\rangle = \langle 0|\,\hat{a}^\dagger = 0$ and that we thereforecan replace products $\hat{a}\hat{a}^\dagger$ with the commutators of the two operators, when they are sandwiched between vacuum states.

This leads to

$$\begin{aligned} G_0(x, x') &= \langle 0|\, T\hat{\phi}(x)\hat{\phi}(x')\, |0\rangle \\ &= \Theta(t-t') \int \frac{\mathrm{d}^3k}{(2\pi^3)2k_0} \frac{\mathrm{d}^3k'}{(2\pi^3)2k_0'} e^{-ik\cdot x + ik'\cdot x'}\, \langle 0|\, \hat{a}(\underline{k})\hat{a}^\dagger(\underline{k}')\, |0\rangle \\ &\quad + \Theta(t'-t) \int \frac{\mathrm{d}^3k}{(2\pi^3)2k_0} \frac{\mathrm{d}^3k'}{(2\pi^3)2k_0'} e^{+ik\cdot x - ik'\cdot x'}\, \langle 0|\, \hat{a}(\underline{k}')\hat{a}^\dagger(\underline{k})\, |0\rangle \\ &= \Theta(t-t') \int \frac{\mathrm{d}^3k}{(2\pi^3)2k_0} \frac{\mathrm{d}^3k'}{(2\pi^3)2k_0'} e^{-ik\cdot x + ik'\cdot x'}\, \langle 0|\, \left[\hat{a}(\underline{k}),\, \hat{a}^\dagger(\underline{k}')\right] |0\rangle \\ &\quad + \Theta(t'-t) \int \frac{\mathrm{d}^3k}{(2\pi^3)2k_0} \frac{\mathrm{d}^3k'}{(2\pi^3)2k_0'} e^{+ik\cdot x - ik'\cdot x'}\, \langle 0|\, \left[\hat{a}(\underline{k}'),\, \hat{a}^\dagger(\underline{k})\right] |0\rangle \\ &= \int \frac{\mathrm{d}^3k}{(2\pi^3)2k_0} \left[\Theta(t-t')\, e^{-ik\cdot(x-x')} \,+\, \Theta(t'-t)\, e^{+ik\cdot(x-x')}\right] \\ &= \Theta(t-t')\, \Delta_+(x-x') \,+\, \Theta(t'-t)\, \Delta_-(x-x')\, . \end{aligned} \tag{303}$$

The similarity with the vacuum expectation value is striking – it is given by

$$\begin{aligned} \Delta(x-y) &= \int \frac{\mathrm{d}^3 k}{(2\pi^3)2k_0} \left[e^{-ik\cdot(x-x')} - e^{+ik\cdot(x-x')}\right] \\ &= \Delta_+(x-x') - \Delta_-(x-x'), \end{aligned} \tag{304}$$

cf. Eq. (163), where in both cases the sign indicates whether the energies, i.e. the k_0 come with the correct or wrong sign for a wave the evolves in positive or negative time direction.

This means that the propagator is composed of two components: a +-component of forward propagation, and a–component of backward propagation of a particle with four-momentum k.

$i\epsilon^+$**-Prescription** To finish the discussion of how to arrive at the correct Green's function, let us remember the property

$$\Theta(t) = \lim_{\epsilon\to 0^+} \int \frac{\mathrm{d}\omega}{2\pi} \frac{-ie^{i\omega t}}{\omega - i\epsilon}. \tag{305}$$

We plug this into the result for the time-ordered product above and close the contour integral above or below the real k_0-axis for $t - t' > 0$ and $t - t' < 0$.

We also introduce a "dummy" energy $\omega_k = \sqrt{\underline{k}^2 + m^2}$ which we will identify with the "proper" k_0 at some convenient point of the calculation.

With all these steps we arrive at

$$\begin{aligned}
G(x,\,x') \;&=\; \lim_{\epsilon\to 0^+}\int \frac{\mathrm{d}\omega\mathrm{d}^3k}{(2\pi)^4 2k_0}\,\frac{-i}{\omega+i\epsilon}\,\Big[e^{i(\omega-k_0)(t-t')+i\underline{k}(\underline{x}-\underline{x}')} \\
&\qquad\qquad + e^{-i(\omega-k_0)(t-t')-i\underline{k}(\underline{x}-\underline{x}')}\Big] \\
&= \lim_{\epsilon\to 0^+}\int \frac{\mathrm{d}\omega_k\mathrm{d}^3k}{(2\pi)^4}\,\frac{-ie^{-ik\cdot(x-x')}}{2k_0}\left[\frac{1}{k_0-\omega_k-i\epsilon}+\frac{1}{k_0+\omega_k-i\epsilon}\right] \\
&= \lim_{\epsilon\to 0^+}\int \frac{\mathrm{d}\omega_k\mathrm{d}^3k}{(2\pi)^4}\,\frac{-ie^{-ik\cdot(x-x')}}{k_0^2-\omega_k^2+i\epsilon} \\
&= \lim_{\epsilon\to 0^+}\int \frac{\mathrm{d}k_0\mathrm{d}^3k}{(2\pi)^4}\,\frac{-ie^{-ik\cdot(x-x')}}{k_0^2-(\underline{k}^2+m^2)+i\epsilon} \\
&= \int \frac{\mathrm{d}^4k}{(2\pi)^4}\,e^{-ik\cdot(x-x')}\,\frac{-i}{k^2-m^2+i\epsilon^+} \\
&= \int \frac{\mathrm{d}^4k}{(2\pi)^4}\,e^{-ik\cdot(x-x')}\,\Delta_F(k) \;=\; \Delta_F(x-x')\,. \qquad (306)
\end{aligned}$$

This is obviously the Fourier transform of our propagator from Eq. (301), and it confirms that indeed propagators are time-ordered products.

It is also called the *Feynman propagator* of the theory.

7.3 Fermion Propagator

Direct Solution As before for the Klein-Gordon equation, the propagator for the free Dirac field is defined by

$$(i\partial\!\!\!/ - m)\, G_0(x, x') = i\delta^4(x - x'), \tag{307}$$

or, in momentum space,

$$(p\!\!\!/ - m)\, G_0(p) = i \quad \longrightarrow \quad G_0(p) = \frac{i}{p\!\!\!/ - m} = i\frac{p\!\!\!/ + m}{p^2 - m^2}. \tag{308}$$

In the last step we have used that $p\!\!\!/ p\!\!\!/ = p^2$.

There are a couple of things worth noting of this propagator.

As before, it exhibits a pole for on-shell particles, where $p^2 = m^2$, and, as before, we will cure this by shifting the pole in the complex plane by $i\epsilon^+$.

This is in complete analogy to the case of scalar particles.

In addition we realize that the numerator, $(p\!\!\!/ + m)$, represents a matrix in Dirac space.

This is not a surprise, as the propagator connects two Dirac spinors and their components.

What is structurally more interesting is that this matrix is the completeness relation for the u-spinors from Eq. (215), and we will see the emergence of analogous terms later when we discuss the propagator of the photon field.

However, to build more confidence into our interpretation of the propagator we will now check if we can recover it as a time-ordered product of two spinor fields.

Time-Ordered Product The starting point to building a time-ordered product for fermions is to construct the transition amplitude for a positive-energy fermion to move from x to y, naively

$$\langle f^{(+)}(y)|f^{(+)}(x)\rangle \;=\; \langle 0|\,\hat{\psi}(y)\hat{\psi}^{\dagger}(x)\,|0\rangle\;. \tag{309}$$

But we must also include the opposite case of a negative-energy fermion to go from y to x, taking into account Fermi statistics.

Making time-ordering explicit through Θ-functions we therefore arrive at

$$iS_F(y,\,x)\gamma^0 \;=\; \langle 0|\,\hat{\psi}(y)\hat{\psi}^{\dagger}(x)\,|0\rangle\;\Theta(y_0-x_0)\;-\;\langle 0|\,\hat{\psi}^{\dagger}(x)\hat{\psi}(y)\,|0\rangle\;\Theta(x_0-y_0)\,, \tag{310}$$

or, in a more compact form

$$\boxed{iS_F(y,\,x) \;=\; \langle 0|\,T\hat{\psi}(y)\hat{\bar{\psi}}(x)\,|0\rangle\;.} \tag{311}$$

Since $\hat{\psi}$ and $\hat{\bar{\psi}}$ are spinors, S_F is a matrix in spinor space, as already anticipated.

Let us now include the expansion of the fermion fields in place waves and creation and annihilation operators.

Making spinor indices explicit, using the fact that $\hat{b}\,|0\rangle = \hat{d}\,|0\rangle = 0$ and $\bar{0}\hat{b}^\dagger = \langle 0|\,\hat{d}^\dagger,$, and taking into account that $[\hat{b},\,\hat{d}] = [\hat{b}^\dagger,\,\hat{d}^\dagger] = 0$, which makes their products vanish, we arrive at

$$
\begin{aligned}
iS_F(y,\,x)_{\beta\alpha} &= \langle 0|\,T\hat{\psi}_\beta(y)\hat{\bar{\psi}}_\alpha(x)\,|0\rangle \\
&= \left\langle 0\right|\int \frac{\mathrm{d}^3k}{(2\pi)^3 2k_0}\frac{\mathrm{d}^3q}{(2\pi)^3 2q_0}\sum_{i,j=1}^{2} \\
&\qquad \Big[e^{-ik\cdot y+iq\cdot x}\hat{b}_i(\underline{k})\hat{b}_j^\dagger(\underline{q})u_\beta^{(i)}(\underline{k})\bar{u}_\alpha^{(j)}(\underline{q})\Theta(y_0-x_0) \\
&\qquad -e^{+ik\cdot y-iq\cdot x}\hat{d}_j(\underline{q})\hat{d}_i^\dagger(\underline{k})v_\beta^{(i)}(\underline{k})\bar{v}_\alpha^{(j)}(\underline{q})\Theta(x_0-y_0)\Big]\left|0\right\rangle \\
&= \left\langle 0\right|\int \frac{\mathrm{d}^3k}{(2\pi)^3 2k_0}\sum_{i,j=1}^{2}\Big[e^{-ik\cdot(y-x)}u_\beta^{(i)}(\underline{k})\bar{u}_\alpha^{(j)}(\underline{k})\Theta(y_0-x_0) \\
&\qquad -e^{+ik\cdot(y-x)}v_\beta^{(i)}(\underline{k})\bar{v}_\alpha^{(j)}(\underline{k})\Theta(x_0-y_0)\Big]\left|0\right\rangle \\
&= \left\langle 0\right|\int \frac{\mathrm{d}^3k}{(2\pi)^3 2k_0}\Big[e^{-ik\cdot(y-x)}(\not{k}+m)_{\beta\alpha}\,\Theta(y_0-x_0) \\
&\qquad -e^{+ik\cdot(y-x)}(\not{k}-m)_{\beta\alpha}\,\Theta(x_0-y_0)\Big]\left|0\right\rangle . \qquad (312)
\end{aligned}
$$

Repeating the same steps of replacing the Θ functions with integrals, suitably closing the contours and keeping track of the relative signs in the replacement of the "dummy" energy with the real energy, we arrive at

$$\boxed{iS_F(y,\, x)_{\beta\alpha} \;=\; \int \frac{\mathrm{d}^4 k}{(2\pi)^4}\, e^{-ik\cdot(y-x)} \left[i\frac{\not{k}+m}{k^2-m^2+i\epsilon^+}\right]_{\beta\alpha}\,,} \tag{313}$$

the Fourier transform of Eq. (311), modified by the now familiar iϵ prescription.

7.4 Photon Propagator As before, the E.o.M. for the field will provide the kernel for the Green's function. In the case of the free electromagnetic field we have to realize that

- the propagator will have two Lorentz indices, to become a matrix in Minkowski space. This is necessary, because it connects two photon fields and their components, which are labelled by Lorentz indices.
- we need to cast the homogeneous ($j = 0$)Maxwell's equations for the vector potential from Eq. (265) into a suitable form such that it has two Lorentz indices that can be contracted with the two indices from the propagator.

We therefore arrive at

$$[\partial^\rho \partial_\rho g_{\mu\nu} - (1-\alpha)\partial_\nu \partial_\mu]\, G_0^{\nu\rho}(x,\, x') \;=\; i\delta^4(x-x')g_\mu^\rho\,, \tag{314}$$

and Fourier transformation results in

$$\left[p^2 g_{\mu\nu} - (1-\alpha)p_\mu p_\nu\right]\, G_0^{\nu\rho}(p) \;=\; -ig_\mu^\rho\,, \tag{315}$$

or

$$\left[g_{\mu\nu} - \frac{(1-\alpha)p_\mu p_\nu}{p^2}\right] G_0^{\nu\rho}(p) = -\frac{ig_\mu^\rho}{p^2}. \tag{316}$$

To arrive at a solution we realize that there are only two possible tensors without any mass dimension and two Lorentz indices and make the *ansatz*

$$G_0^{\nu\rho}(p) = -i\frac{g^{\nu\rho} - \kappa\frac{p^\nu p^\rho}{p^2}}{p^2}. \tag{317}$$

We solve this by realizing that this implies that

$$\left[g_{\mu\nu} - \frac{(1-\alpha)p_\mu p_\nu}{p^2}\right]\left[g^{\nu\rho} - \kappa\frac{p^\nu p^\rho}{p^2}\right] = g_\mu^\rho \tag{318}$$

and therefore $\kappa = (1-\alpha)/\alpha$.

Therefore the photon propagator, including the $i\epsilon^+$ term reads

$$\boxed{D^{\mu\nu}(k) = -i\,\frac{g^{\mu\nu} - \frac{1-\alpha}{\alpha}\frac{k^\mu k^\nu}{k^2}}{k^2 + i\epsilon^+},} \tag{319}$$

which in Feynman gauge reduces to the simpler form

$$\boxed{D^{\mu\nu}(k) \;=\; \frac{-ig^{\mu\nu}}{k^2+i\epsilon^+}\,.} \tag{320}$$

Time-Ordered Product To arrive at the same expression using time-ordered products we employ the Feynman gauge from the beginning, where the completeness relation for the polarization vectors is given by

$$\sum_{\lambda=0}^{3} \epsilon_\mu^{(\lambda)}(\underline{k})\epsilon_\nu^{*(\lambda)}(\underline{k}) \;=\; g_{\mu\nu} \tag{321}$$

Using the by now usual $\hat{a}\,|0\rangle = 0$ relation allows to simplify the time-ordered product and the propagator reads

$$\begin{aligned}
D_{\mu\nu}(x,\,y) \;&=\; -i\,\langle 0|\,T A_\mu(x)A_\nu(y)\,|0\rangle \\
&= i\int \frac{\mathrm{d}^3k}{(2\pi)^3 2k_0}\frac{\mathrm{d}^3q}{(2\pi)^3 2q_0} \\
&\qquad \sum_{\lambda,\kappa=0}^{3}\Big\langle 0\Big|\Big[\Theta(x_0-y_0)e^{-ik\cdot x+iq\cdot y}\,\hat{a}_\lambda(\underline{k})\hat{a}_\kappa^\dagger(\underline{q})\epsilon_\mu^{(\lambda)}(\underline{k})\epsilon_\nu^{*(\kappa)}(\underline{q}) \\
&\qquad\qquad + \Theta(y_0-x_0)e^{+ik\cdot x-iq\cdot y}\,\hat{a}_\kappa(\underline{q})\hat{a}_\lambda^\dagger(\underline{k})\epsilon_\mu^{*(\lambda)}(\underline{k})\epsilon_\nu^{(\kappa)}(\underline{q})\Big]\Big|0\Big\rangle \\
&= -\,i\int \frac{\mathrm{d}^3k}{(2\pi)^3 2k_0}\sum_{\lambda=0}^{3}\Big\langle 0\Big|\Big[\Theta(x_0-y_0)e^{-ik\cdot(x-y)}\,\epsilon_\mu^{(\lambda)}(\underline{k})\epsilon_\nu^{*(\lambda)}(\underline{k}) \\
&\qquad\qquad + \Theta(y_0-x_0)e^{+ik\cdot(x-y)}\,\epsilon_\mu^{*(\lambda)}(\underline{k})\epsilon_\nu^{(\lambda)}(\underline{k})\Big]\Big|0\Big\rangle
\end{aligned}$$

$$
\begin{aligned}
&= -ig_{\mu\nu} \int \frac{\mathrm{d}^3k}{(2\pi)^3 2k_0} \left[\Theta(x_0 - y_0) e^{-ik\cdot(x-y)} + \Theta(y_0 - x_0) e^{+ik\cdot(x-y)} \right] \\
&= -ig_{\mu\nu} \left[\Theta(x_0 - y_0) \Delta_+(x-y) + \Theta(y_0 - x_0) \Delta_-(x-y) \right] \\
&= -ig_{\mu\nu} \int \frac{\mathrm{d}^4k}{(2\pi)^4} \frac{e^{-ik\cdot(x-y)}}{k^2 + i\epsilon^+} \,.
\end{aligned} \tag{322}
$$

This is, of course, the Fourier transform of the propagator of Eq. (320)

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8 Interacting Fields

8.1 Perturbative Expansion: Born Series

Green's Function for Full Theory In the previous section we have analysed propagators, and identified them with the Green's functions of free theories.

We will now extend the treatment to also include potentials such that the Hamilton operator can be written as the sum of a free Hamilton operator plus some interactions,

$$\hat{H} \;=\; \hat{H}_0 + \hat{V}\,, \tag{323}$$

in the simplest case a potential.

Going back to Eq. (286), where we have defined the Green's function this means that we now have

$$\begin{aligned}&\left(i\partial_t - \hat{H}\right)G(t,\,\underline{x};\,t',\,\underline{x}')\\ &\quad= \left(i\partial_t - \hat{H}_0 - \hat{V}\right)G(t,\,\underline{x};\,t',\,\underline{x}') \;=\; \delta(t-t')\delta^3(\underline{x}-\underline{x}')\,.\end{aligned} \tag{324}$$

A formal solution can be obtained by starting with the Fourier transform of the free Green's function, signified with a ˜ symbol

$$\left(\omega - \hat{\tilde{H}}_0\right)\tilde{G}_0 \;=\; 1 \;\;\longrightarrow\;\; \tilde{G}_0 = \frac{1}{\omega - \hat{\tilde{H}}_0}\,, \tag{325}$$

where we have for the moment suppressed the iϵ prescription.

The Fourier transform of Eq. (324) can therefore be rewritten as

$$\left(\omega - \hat{\tilde{H}}\right) \tilde{G} = \left(\frac{1}{\tilde{G}_0} - \hat{\tilde{V}}\right) \tilde{G} = 1 . \tag{326}$$

This can be formally solved, and

$$\frac{1}{\tilde{G}} = \frac{1}{\tilde{G}_0} - \hat{\tilde{V}} \tag{327}$$

or

$$\tilde{G} = \frac{1}{\frac{1}{\tilde{G}_0} - \hat{\tilde{V}}} . \tag{328}$$

Born Series After Fourier back-transformation we arrive at the implicit equation

$$\begin{aligned} G(t, \underline{x}; t', \underline{x}') = {} & G_0(t, \underline{x}; t', \underline{x}') \\ & + \int \mathrm{d}\tau \mathrm{d}^3\xi G_0(t, \underline{x}; \tau, \underline{\xi}) \hat{V}(\tau, \underline{\xi}) G(\tau, \underline{\xi}; t', \underline{x}') , \end{aligned} \tag{329}$$

which can now be expanded in powers of interactions with the potential.

This is called the Born series or the perturbative expansion of the Green's function.

For it to converge we implicitly assume that interactions with the potential are sufficiently small.

Replacing explicit time and space coordinates with four-positions t, $\underline{x} \rightarrow x_i$, the Born series therefore reads

$$\begin{aligned} G(x_N;x_0) &= G_0(x_N;\,x_0) \\ &\quad + \int \mathrm{d}x_1 G_0(x_N;\,x_1)\,\hat{V}(x_1)\,G(x_1;\,x_0) \\ &\quad + \int \mathrm{d}x_1 \mathrm{d}x_2 G_0(x_N;\,x_2)\,\hat{V}(x_2)\,G(x_2;\,x_1)\,\hat{V}(x_1)\,G(x_1;\,x_0)\ldots\,, \end{aligned} \tag{330}$$

where in non-relativistic theory we assume a strict time ordering,

$$t_N \geq t_{N-1} \geq t_{N-2} \cdots \geq t_2 \geq t_1 \geq t_0\,. \tag{331}$$

Truncating this series after the first non-trivial term, i.e., after one interaction with the potential is called the Born approximation.

8.2 Interacting Field Theory: General Thoughts

Quantization and Particle Interpretation In principle we could try and quantize interacting theory as before, by promoting fields to field operators and by demanding suitable equal-time commutation relations.

However, the equations of motion for interacting fields are usually not linear any more, due to the potential terms responsible for the interactions and featuring more than two fields.

This prevents us from being able to solve them in closed form and we therefore lose the ability to expand the field operators in products of creation and annihilation operators and some wave that captures the solution of the E.o.M..

But this means that it is not entirely obvious any more how we arrive at a meaningful particle interpretation for our fields.

One way to answer this is to realize that ultimately we want to be able to compute numbers that we can compare with the experiment.

In particle physics, we usually have two colliding particles, which produce more particles in their interaction.

This means that we are mainly interested in being able to calculate cross sections.

Transition Amplitudes between Asymptotic States The cross section for a process is proportional for this process to occur.

In quantum mechanics this probability is given by the absolute square of the amplitude $\mathcal{M}_{f\leftarrow i}$, $|\mathcal{M}_{f\leftarrow i}|^2$, for the transition of an initial state $|i\rangle$ to a final state $|f\rangle$,

$$\mathcal{M}_{f\leftarrow i} = \langle f|i\rangle \,. \tag{332}$$

The definition of these states is subject on how they are being prepared (for this initial state) or measure (the final state).

For perturbation theory to work, this means that they must be prepared or measured infinitely far away, both in space and time, from the point where they collider – this assumes, of course, that the interaction between the states vanishes with increasing distance.

This assumption of *asymptotic states* is crucial for us to be able to calculate in a quantum field theory.

This is because the interacting fields are not identical to the free fields: the vacuum of interacting and free theories is potentially different, and we only know how to quantize the latter.

This implies immediately that the states $|i\rangle$ and $|f\rangle$ are eigenstates of the free field theory but usually not eigenstates of the interacting field theory.

Their interactions with a cloud of virtual particles around them, from the surrounding interacting vacuum, will ultimately force us to renormalize the external field, a topic well beyond this class.

The S matrix There is yet another problem, while the states $|IS\rangle$spanning the possible initial states of our collision are eigenstates in the initial-state Fock space of the theory, the corresponding final states $|FS\rangle$ live in the final-state Fock space.

These two sets of states are related to each other through the $\hat{S}$-matrix such that $|FS\rangle = \hat{S}\, |IS\rangle$.

Therefore the transition amplitude within the same Fock space is given by

$$\mathcal{M}_{f\leftarrow i} = \langle f|\, \hat{S}\, |i\rangle\ . \tag{333}$$

In this chapter we will discuss first steps on how to calculate the S-matrix elements, i.e.

$$\hat{S}_{fi} = \mathcal{M}_{f\leftarrow i} = \langle f|\, \hat{S}\, |i\rangle \ . \tag{334}$$

Operators and Pictures From Quantum Mechanics we know that there is a dichotomy between fields and operators and how they evolve over time, and it has become customary to distinguish between three pictures:

1. in the *Schrödinger picture*, the operators $\hat{O}^{(S)}(\underline{x})$ are time-independent, and it is the states that carry the time-dependence,

$$|\psi(t)\rangle = \exp\left[-i\hat{H}(t-t_0)\right] |\psi(t_0)\rangle \ ; \tag{335}$$

2. in the *Heisenberg picture*, the states that carry the time-independent and the operators $\hat{O}^{(H)}(\underline{x}, t)$ are time-independent,

$$\hat{O}^{(H)}(t,\, \underline{x}) = \exp\left[i\hat{H}(t-t_0)\right] \hat{O}^{(H)}(t_0,\, \underline{x}) \exp\left[-i\hat{H}(t-t_0)\right] \ ; \tag{336}$$

3. in the *interaction picture*, the Hamiltonian is split into a “free” part, $\hat{H}_0$, and an “interaction” part, $\hat{H}_{\text{int}}$ such that

$$\hat{O}^{(I)}(t,\, \underline{x}) = \exp\left[i\hat{H}_o(t-t_0)\right] \hat{O}^{(I)}(t_0,\, \underline{x}) \exp\left[-i\hat{H}_0(t-t_0)\right] \ , \tag{337}$$

and the time evolution is distributed over both operators and states.

The exponential terms $\exp[-i\, \hat{H}\, (t-t_0)]$ are known as the time evolution operator,

$$\hat{U}(t,\, t_0) \ = \ \exp[-i\hat{H}(t-t_0)]\, . \tag{338}$$

Time Evolution and Perturbation Theory Let us now take a closer look at the field operators in both the Heisenberg and the interaction picture.

It is important to stress that in the following we will only sketch the logic of how, starting from the interaction picture, we arrive at an expression that can be perturbatively evaluated.

Assuming an explicitly time-independent Hamiltonian, and identifying the operators at time $t = t_0$ with the Schrodinger-picture operators, $\hat{\phi}^{(S)}$, their relationship is given by

$$\begin{aligned} \hat{\phi}^{(H)}(t, \underline{x}) &= e^{i\hat{H}(t-t_0)}\hat{\phi}^{(S)}(\underline{x})e^{-i\hat{H}(t-t_0)} \\ &= e^{i\hat{H}(t-t_0)}e^{-i\hat{H}_0(t-t_0)}\hat{\phi}^{(I)}(t_0, \underline{x})e^{i\hat{H}_0(t-t_0)}e^{-i\hat{H}(t-t_0)} \, . \end{aligned} \tag{339}$$

Similar equations naturally also hold true for other operators in the interaction picture.

We now redefine the time-evolution operator in the interaction picture such that the "free" time-evolution is factored out:

$$\hat{U}^{(I)}(t, t_0) = \exp[i\hat{H}_0(t-t_0)]\exp[-i\hat{H}(t-t_0)] \, . \tag{340}$$

Although it looks as if the two exponentials could be directly multiplied, to result in an exponential of the interaction Hamiltonian alone, this deceptively simple picture is misleading and hold true only, if $\hat{H}_0$ and $\hat{H}_{\text{int}}$ commute.

This, however, is usually not the case and one would have to resort to the Baker-Hausdorff formula to directly calculate this operator.

Instead, let us construct a differential equation to determine $\hat{U}^{(I)}$.

Differentiation with respect to time yields

$$
\begin{aligned}
& i\frac{\partial \hat{U}^{(I)}(t,\, t_0)}{\partial t} = e^{i\hat{H}_0(t-t_0)}\hat{H}_0(t_0)e^{-i\hat{H}(t-t_0)} - e^{i\hat{H}_0(t-t_0)}\hat{H}(t_0)e^{-i\hat{H}(t-t_0)} \\
&= -e^{i\hat{H}_0(t-t_0)}\left[\hat{H}(t_0) - \hat{H}_0(t_0)\right]e^{-i\hat{H}(t-t_0)} = -e^{i\hat{H}_0(t-t_0)}\hat{H}_{\text{int}}(t_0)e^{-i\hat{H}(t-t_0)} \\
&= -e^{i\hat{H}_0(t-t_0)}\hat{H}_{\text{int}}(t_0)e^{i\hat{H}_0(t-t_0)}e^{i\hat{H}_0(t-t_0)}e^{-i\hat{H}(t-t_0)} \\
&= \hat{H}^{(I)}_{\text{int}}(t)\hat{U}^{(I)}(t,\, t_0) \qquad (341)
\end{aligned}
$$

the formal solution to this differential equation is given by

$$
\begin{aligned}
& \hat{U}^{(I)}(t,\, t_0) \\
&= \int_{t_0}^{t} \mathrm{d}t_1 \sum_{n=0}^{\infty}\left[(-i)^n \int_{t_0}^{t}\mathrm{d}t_1 \int_{t_0}^{t_1}\mathrm{d}t_2 \ldots \int_{t_0}^{t_{n-1}}\mathrm{d}t_n\, \hat{H}^{(I)}_{\text{int}}(t_1)\hat{H}^{(I)}_{\text{int}}(t_2)\ldots\hat{H}^{(I)}_{\text{int}}(t_n)\right] \qquad (342) \\
&= T\left[\exp\left(-i\int_{t_0}^{t}\mathrm{d}t'\,\hat{H}^{(I)}_{\text{int}}(t')\right)\right],
\end{aligned}
$$

where we have used the time-ordering symbol T, that we already encountered when we constructed propagators for the fields.

Connection to the S-Matrix Recalling that the S-matrix describes the transition from the initial to the final state, with the former in the infinite past and the latter in the infinite future, we can connect it to the interaction Hamiltonian and write

$$\hat{S} = \lim_{t_\pm \to \pm\infty} \hat{U}^{(I)}(t_+, t_-) = T\left[\exp\left(-i \int_{-\infty}^{+\infty} \mathrm{d}t\, \hat{H}_{\text{int}}^{(I)}(t)\right)\right]. \tag{343}$$

To evaluate it we will usually go back and expand the exponential to arrive at an expression like the first line of Eq. (342), and we would truncate this series after the first few terms.

This is well justified if there is a small parameter – usually a coupling constant – in the relevant parts of interaction Hamiltonian that steer its size.

8.3 Interacting Field Theory: $\lambda\phi^4$

Lagrangian & S-Matrix We will now specify the results of the previous chapter to a Klein-Gordon field with quartic interactions.

This theory, specified by its Lagrangian

$$\mathcal{L} = \frac{1}{2}(\partial_\mu \phi)(\partial^\mu \phi) - \frac{m^2}{2}\phi^2 - \frac{\lambda}{4!}\phi^4\,, \tag{344}$$

is probably the most used example on how to construct and evaluate interacting field theories.

The Taylor expansion of its S-matrix elements is thus given by

$$\begin{aligned}\langle f|\hat{S}|i\rangle &= \langle f|\hat{1}|i\rangle + \left(\frac{-i\lambda}{4!}\right)\int \mathrm{d}^4x \left\langle f\left|T\left[\hat{\phi}^4(x)\right]\right|i\right\rangle \\ &+ \left(\frac{-i\lambda}{4!}\right)^2 \int \mathrm{d}^4x\mathrm{d}^4y \left\langle f\left|T\left[\hat{\phi}^4(x)\hat{\phi}^4(y)\right]\right|i\right\rangle + \dots .\end{aligned} \tag{345}$$

This perturbative expansion will succeed, if λ is sufficiently small.

It is worth noting that the first term, $\langle f|\hat{1}|i\rangle$, reduces to a δ in initial and final states.

S-Matrix vs. Creation and Annihilation Operators Let us now see, how we can evaluate this expression.

We will discuss a $2 \to 2$ scattering process, where two ϕ-particles with momenta p_1 and p_2 scatter to become two ϕ-particles with momenta q_1 and q_2 , $p_1 + p_2 \to q_1 + q_2$.

This means we will have to manipulate expressions like $\langle \underline{q}_1\underline{q}_2;\mathrm{out}|\underline{p}_1\underline{p}_2;\mathrm{in}\rangle$ between the in-space and the out-space.

For the sake of clarity we will keep a notation, where we make it explicit to which space the states and operators belong.

Let us start by using creation and annihilation operators to move one of the in-particles, $\underline{p}_1$, from the state-ket into operators:

$$
\begin{aligned}
\left\langle \underline{q}_1 \underline{q}_2; \text{out} \,\middle|\, \underline{p}_1 \underline{p}_2; \text{in} \right\rangle &= \left\langle \underline{q}_1 \underline{q}_2; \text{out} \left| \hat{a}^\dagger(\underline{p}_1; \text{in}) \right| \underline{p}_2; \text{in} \right\rangle \\
&= \left\langle \underline{q}_1 \underline{q}_2; \text{out} \left| \hat{a}^\dagger(\underline{p}_1; \text{out}) \right| \underline{p}_2; \text{in} \right\rangle \\
&\quad + \left\langle \underline{q}_1 \underline{q}_2; \text{out} \left| \left(\hat{a}^\dagger(\underline{p}_1; \text{in}) - \hat{a}^\dagger(\underline{p}_1; \text{out}) \right) \right| \underline{p}_2; \text{in} \right\rangle .
\end{aligned} \tag{346}
$$

The first term vanishes, unless one of the two momenta $\underline{q}_{1,2} = \underline{p}_1$.

But this would mean that one particle would not really participate in the scattering, something that is usually called a “disconnected diagram”.

In such cases we wouldn’t calculate an amplitude that contributes to a scattering cross section, and we ignore contributions like this.

This leaves us with the second term.

Here, it is important to realize that the in-operator lives at times $t = -\infty$, while the out-operator is positioned at time $t = +\infty$.

This will help us when we re-express the creation and annihilation operators $\hat{a}^\dagger$ and $\hat{a}$ with the field operators $\hat{\phi}$.

External Particles through Field Operators Starting from Eq. (145) to write the creation operator as

$$
\begin{aligned}
\hat{a}(\underline{k}) &= \int \mathrm{d}^3x\, e^{ik\cdot x} \left[k_0\, \hat{\phi}(t,\, \underline{x}) + i\hat{\pi}(t,\, \underline{x})\right] \\
&= \int \mathrm{d}^3x \left[\left(\frac{-i\partial}{\partial t} e^{ik\cdot x}\right) \hat{\phi}(t,\, \underline{x}) + e^{ik\cdot x} \frac{i\partial}{\partial t} \hat{\pi}(t,\, \underline{x})\right] \\
&= i \int \mathrm{d}^3x \left[e^{ik\cdot x} \overleftrightarrow{\partial_t}\, \phi(t,\, \underline{x})\right] \\
\hat{a}^\dagger(\underline{k}) &= -i \int \mathrm{d}^3x \left[e^{-ik\cdot x} \overleftrightarrow{\partial_t}\, \phi(t,\, \underline{x})\right] ,
\end{aligned}
\tag{347}
$$

where we have redefined, for this chapter,

$$
a \overleftrightarrow{\partial} b = a(\partial b) - (\partial a) b\,. \tag{348}
$$

This allows us to replace the in-space and out-space creation operators in Eq. (346) with expressions for the field operators from Eq. (347).

Using that

$$
\int \mathrm{d}^3x\, f(t,\, \underline{x}) = \int \mathrm{d}t \partial_t \int \mathrm{d}^3x\, f(t,\, \underline{x}) = \int \mathrm{d}^4x \partial_t f(t,\, \underline{x}) \tag{349}
$$

allows us to replace the in-space and out-space field operator $\hat{\phi}_{\text{in}}$ and $\hat{\phi}_{rmout}$ with the field operators in the limits t $\to -\infty$ and t $\to +\infty$ resulting ultimately in

$$
\begin{aligned}
\left\langle \underline{q}_1\underline{q}_2;\text{out}\,\middle|\, \underline{p}_1\underline{p}_2;\text{in}\right\rangle &= \left\langle \underline{q}_1\underline{q}_2;\text{out}\,\middle|\left(\hat{a}^\dagger(\underline{p}_1;\text{in}) - \hat{a}^\dagger(\underline{p}_1;\text{out})\right)\middle|\, \underline{p}_2;\text{in}\right\rangle \\
&= -i \lim_{\substack{t_i\to-\infty\\ t_f\to+\infty}} \int \mathrm{d}^3x \left\{ e^{-ip_1\cdot x} \overleftrightarrow{\partial} \left\langle \underline{q}_1\underline{q}_2;\text{out}\,\middle|\left[\hat{\phi}(t_f,\,\underline{x};\text{out})\right.\right.\right. \\
&\qquad\qquad\qquad\qquad\qquad\qquad \left.\left.\left. -\hat{\phi}(t_i,\,\underline{x};\text{in})\right]\middle|\,\underline{p}_2;\text{in}\right\rangle\right\} \\
&= -i \lim_{\substack{t_i\to-\infty\\ t_f\to+\infty}} \int_{t_i}^{t_f} \mathrm{d}t \int \mathrm{d}^3x \frac{\partial}{\partial t}\left[e^{-ip_1\cdot x} \overleftrightarrow{\partial} \left\langle \underline{q}_1\underline{q}_2;\text{out}\,\middle|\hat{\phi}(t,\,\underline{x})\middle|\,\underline{p}_2;\text{in}\right\rangle\right] \\
&= -i \int \mathrm{d}^4x \left[E_1^2 e^{-ip_1\cdot x} \left\langle \underline{q}_1\underline{q}_2;\text{out}\,\middle|\hat{\phi}(t,\,\underline{x})\middle|\,\underline{p}_2;\text{in}\right\rangle \right. \\
&\qquad\qquad \left. + e^{-ip_1\cdot x}\partial_t^2 \left\langle \underline{q}_1\underline{q}_2;\text{out}\,\middle|\hat{\phi}(t,\,\underline{x})\middle|\,\underline{p}_2;\text{in}\right\rangle\right] \\
&= -i \int \mathrm{d}^4x \left[\left(\underline{\nabla}^2 + m^2\right) e^{-ip_1\cdot x} \left\langle \underline{q}_1\underline{q}_2;\text{out}\,\middle|\hat{\phi}(t,\,\underline{x})\middle|\,\underline{p}_2;\text{in}\right\rangle \right. \\
&\qquad\qquad \left. + e^{-ip_1\cdot x}\partial_t^2 \left\langle \underline{q}_1\underline{q}_2;\text{out}\,\middle|\hat{\phi}(t,\,\underline{x})\middle|\,\underline{p}_2;\text{in}\right\rangle\right] \\
&= -i \int \mathrm{d}^4x\, e^{-ip_1\cdot x} \left(\Box_x + m^2\right) \left\langle \underline{q}_1\underline{q}_2;\text{out}\,\middle|\hat{\phi}(x)\middle|\,\underline{p}_2;\text{in}\right\rangle . \qquad (350)
\end{aligned}
$$

In going from the third to the fourth line we have used that $e^{-ip_1\cdot x}$ is a solution for the Klein-Gordon equation, which allowed us to replace the energy square E_1^2 with $(\underline{p}_1^2 + m^2)$, , and in going from the fourth to the fifth line we have integrated by parts, which shifts the $\underline{\nabla}^2$ from the plane wave to the field operator.

This step is possibly only because the interaction is localized, $\phi^4(x)$ and we assume that the fields vanish fast enough for $x \to \infty$ such that the surface terms equal zero.

In a similar way, we can "pull" a state from the final-state bra through annihilation operators into a field operator, and we arrive at

$$\begin{aligned}
&\left\langle \underline{q}_1 \underline{q}_2; \mathrm{out} \middle| \hat{\phi}(x) \middle| \underline{p}_2; \mathrm{in} \right\rangle \\
&= -i \lim_{\substack{t_i \to -\infty \\ t_f \to +\infty}} \int \mathrm{d}^3 y \left\{ e^{-iq_1 \cdot y} \overleftrightarrow{\partial} \left\langle \underline{q}_2; \mathrm{out} \middle| \left[\hat{\phi}_{\mathrm{out}}(t_f, \underline{y}; \mathrm{out}) \hat{\phi}(x) \right.\right.\right. \\
&\qquad\qquad \left.\left.\left. - \hat{\phi}(x) \hat{\phi}(t_i, \underline{y}; \mathrm{in}) \right] \middle| \underline{p}_2; \mathrm{in} \right\rangle \right\} \\
&= -i \int \mathrm{d}^4 y \, e^{-iq_1 \cdot y} \left(\Box_y + m^2 \right) \left\langle \underline{q}_2; \mathrm{out} \middle| T \left[\hat{\phi}(y) \hat{\phi}(x) \right] \middle| \underline{p}_2; \mathrm{in} \right\rangle , \qquad (351)
\end{aligned}$$

where the time-ordering results from the limits for the temporal integration.

Lehmann-Symanzik-Zimmermann Pulling all particles from the bras and kets into the fields we arrive at the Lehmann-Symanzik-Zimmermann (LSZ) formula; for our case of four particles it reads

$$\begin{aligned}
\left\langle \underline{q}_1 \underline{q}_2 \middle| \underline{p}_1 \underline{p}_2 \right\rangle &= (-i)^2 (i)^2 \int \mathrm{d}^4 x_1 \mathrm{d}^4 x_2 \mathrm{d}^4 y_1 \mathrm{d}^4 y_2 \left\{ e^{-i(p_1 \cdot x_1 + p_2 \cdot x_2 - q_1 \cdot y_1 - q_2 \cdot y_2)} \right. \\
&\quad \times \left(\Box_{x_1} + m^2 \right) \left(\Box_{x_2} + m^2 \right) \left(\Box_{y_1} + m^2 \right) \left(\Box_{y_2} + m^2 \right) \\
&\quad \times \left. \left\langle 0 \middle| T \left[\hat{\phi}(y_1) \hat{\phi}(y_2) \hat{\phi}(x_1) \hat{\phi}(x_2) \right] \middle| 0 \right\rangle \right\} \qquad (352)
\end{aligned}$$

The pattern is clear: each external particle with momentum k results in an integral over all space, d^4x, and obtains a plane-wave factor $\exp(\pm ik\cdot x)$, an inverse propagator term, and is represented by a corresponding field operator in the vacuum expectation value of a time-ordered product of such operators.

The inverse propagator terms ultimately reduce the S-matrix to the normalized residue of this vacuum expectation value by, pictorially speaking, "truncating" (cutting off) the effect of the external particles propagating to the interaction zone.

Wick's Theorem To evaluate the perturbative series encoded in the LSZ formula, Eq. (352) we will use Wick's theorem.

It connects time-ordered products of field operators with their normal ordered products and products of Feynman propagators.

Without any attempt at proving it we will just state it for some examples below.

1. For two field operators we have

$$T\left[\hat{\phi}(x)\hat{\phi}(y)\right] = :\hat{\phi}(x)\hat{\phi}(y): + \Delta_F(x-y)\,, \tag{353}$$

2. and for four field operators it reads

$$\begin{aligned} T\left[\hat{\phi}(x_1)\hat{\phi}(x_2)\hat{\phi}(x_3)\hat{\phi}(x_4)\right] = \; & :\hat{\phi}(x_1)\hat{\phi}(x_2)\hat{\phi}(x_3)\hat{\phi}(x_4): \\ & + \sum_{i<j;k<l} :\hat{\phi}(x_i)\hat{\phi}(x_j):\; \Delta_F(x_k - x_l) \\ & + \sum_{i<j;i<k;k<l} \Delta_F(x_i - x_j)\Delta_F(x_k - x_l) \end{aligned} \tag{354}$$

By using that the vacuum expectation value of any normal-ordered product vanishes when sandwiched between vacua,

$$\left\langle 0 \left| :\hat{\phi}(x_1)\hat{\phi}(x_2)\ldots\hat{\phi}(x_n): \right| 0 \right\rangle = 0\,, \tag{355}$$

and by realizing that the Feynman propagators are just numbers, for example Eq. (301), and that therefore the vacuum expectation number of any product of them just equals their product,

$$\langle 0\,|\Delta_F(x_1 - x_2)\Delta_F(x_3 - x_4)\ldots|\,0\rangle = \Delta_F(x_1 - x_2)\Delta_F(x_3 - x_4)\ldots \tag{356}$$

we see that the vacuum expectation value of the time-ordered product of fields reduces to a product of Feynman propagators and, possibly, “vertex factors” related to interaction points, where three or more of these fields interact.

0th-**Order** Let us now see how this plays out for the 0th-order term, where we merely have the four field operators.

This is equivalent to the term $\langle f|\hat{1}|i\rangle$, the first term in the perturbative expansion of Eq. (345).

Going back to Eq. (352) we therefore end up with

$$
\begin{aligned}
&\left\langle \underline{q}_1 \underline{q}_2 \middle| \hat{1} \middle| \underline{p}_1 \underline{p}_2 \right\rangle \\
&\qquad = \int \mathrm{d}^4x_1 \mathrm{d}^4x_2 \mathrm{d}^4y_1 \mathrm{d}^4y_2 \Big\{ e^{-i(p_1\cdot x_1 + p_2\cdot x_2 - q_1\cdot y_1 - q_2\cdot y_2)} \\
&\qquad\qquad \times \left(\Box_{x_1} + m^2\right)\left(\Box_{x_2} + m^2\right)\left(\Box_{y_1} + m^2\right)\left(\Box_{y_2} + m^2\right) \\
&\qquad\qquad \times \Big[\Delta_F(x_1 - x_2)\Delta_F(y_1 - y_2) \\
&\qquad\qquad\quad + \Delta_F(x_1 - y_1)\Delta_F(x_2 - y_2) \\
&\qquad\qquad\quad + \Delta_F(x_1 - y_2)\Delta_F(x_2 - y_1) \Big] \Big\} \\
&\qquad = \int \mathrm{d}^4x_1 \mathrm{d}^4x_2 \mathrm{d}^4y_1 \mathrm{d}^4y_2 \Big\{ e^{-i(p_1\cdot x_1 + p_2\cdot x_2 - q_1\cdot y_1 - q_2\cdot y_2)} \\
&\qquad\qquad \times \left(\Box_{x_1} + m^2\right)\left(\Box_{x_2} + m^2\right)\left(\Box_{y_1} + m^2\right)\left(\Box_{y_2} + m^2\right) \\
&\qquad\qquad \times \Big[\int \frac{\mathrm{d}^4k_1}{(2\pi)^4} \frac{\mathrm{d}^4k_2}{(2\pi)^4} \frac{e^{-ik_1(x_1 - x_2)}}{k_1^2 - m^2 - i\epsilon^+} \frac{e^{-ik_2(y_1 - y_2)}}{k_2^2 - m^2 - i\epsilon^+} \\
&\qquad\qquad\quad + \int \frac{\mathrm{d}^4k_1}{(2\pi)^4} \frac{\mathrm{d}^4k_2}{(2\pi)^4} \frac{e^{-ik_1(x_1 - y_1)}}{k_1^2 - m^2 - i\epsilon^+} \frac{e^{-ik_2(x_2 - y_2)}}{k_2^2 - m^2 - i\epsilon^+} \\
&\qquad\qquad\quad + \int \frac{\mathrm{d}^4k_1}{(2\pi)^4} \frac{\mathrm{d}^4k_2}{(2\pi)^4} \frac{e^{-ik_1(x_1 - y_2)}}{k_1^2 - m^2 - i\epsilon^+} \frac{e^{-ik_2(x_2 - y_1)}}{k_2^2 - m^2 - i\epsilon^+} \Big] \Big\}
\end{aligned}
$$

$$
\begin{aligned}
&= \int \mathrm{d}^4x_1 \mathrm{d}^4x_2 \mathrm{d}^4y_1 \mathrm{d}^4y_2 \left\{ e^{-i(p_1\cdot x_1 + p_2\cdot x_2 - q_1\cdot y_1 - q_2\cdot y_2)} \right. \\
&\quad \times \int \frac{\mathrm{d}^4k_1}{(2\pi)^4}\frac{\mathrm{d}^4k_2}{(2\pi)^4} \left(k_1^2 - m^2\right)^2 \left(k_2^2 - m^2\right)^2 \\
&\quad \times \left[\frac{e^{-ik_1(x_1-x_2)}}{k_1^2 - m^2 - i\epsilon^+} \frac{e^{-ik_2(y_1-y_2)}}{k_2^2 - m^2 - i\epsilon^+} \right. \\
&\qquad + \frac{e^{-ik_1(y_1-x1)}}{k_1^2 - m^2 - i\epsilon^+} \frac{e^{-ik_2(y_2-x2)}}{k_2^2 - m^2 - i\epsilon^+} \\
&\qquad \left. \left. + \frac{e^{-ik_1(y_2-x_1)}}{k_1^2 - m^2 - i\epsilon^+} \frac{e^{-ik_2(y_1-x_2)}}{k_2^2 - m^2 - i\epsilon^+} \right] \right\} \\
&= \int \frac{\mathrm{d}^4k_1}{(2\pi)^4}\frac{\mathrm{d}^4k_2}{(2\pi)^4} \left(k_1^2 - m^2\right) \left(k_2^2 - m^2\right) \\
&\quad \times \left[\quad \delta^4(k_1+p_1)\delta^4(k_1-p_2)\delta^4(k_2+q_1)\delta^4(k_2-q_2) \right. \\
&\qquad + \delta^4(k_1+p_1)\delta^4(k_1+q_1)\delta^4(k_2+p_2)\delta^4(k_2+q_2) \\
&\qquad \left. + \delta^4(k_1+p_1)\delta^4(k_1+q_2)\delta^4(k_2+p_1)\delta^4(k_2+q_1) \right] \\
&= \left[\quad \delta^4(p_1-p_2)\delta^4(q_1-q_2) \left(p_1^2 - m^2\right) \left(q_1^2 - m^2\right) \right. \\
&\quad + \delta^4(p_1-q_1)\delta^4(p_2-q_2) \left(p_1^2 - m^2\right) \left(p_2^2 - m^2\right) \\
&\quad \left. + \delta^4(p_1-q_1)\delta^4(p_2-q_2) \left(p_1^2 - m^2\right) \left(p_2^2 - m^2\right) \right] .
\end{aligned}
\tag{357}
$$

Looking at this, we realize that the first term will vanish if all external particles have positive energies - which they should as we want to calculate a physical cross section.

This leaves us the last two terms where particle $p_{1,2}$ transit directly, without interaction, into particles $q_{1,2}$ or vice versa.

The absence of an interaction should not come as a surprise: as a starting point we have only sandwiched the free theory between initial and final state.

1st-**Order** This however changes, when we go to the first order of perturbation theory, or the first term with an interaction Hamiltonian sandwiched between $\langle f |$ and $| i \rangle$, i.e., the second term on the right-hand side of Eq. (345).

In this case, and in order to arrive at connected diagram, i.e. those where all external lines are connected through propagators, we will have to connect the four outgoing particles with the interaction vertex.

Integrating over all possible permutations of possible connections and over all space for the vertex position we arrive at

$$\int \mathrm{d}^4 z \left\langle \underline{q}_1 \underline{q}_2 \right| \; : -\frac{i\lambda}{4!}\hat{\phi}^4(z) : \; \left| \underline{p}_1 \underline{p}_2 \right\rangle$$

$$= -\frac{i\lambda}{4!} \sum_{\{x_1,x_2,y_1,y_2\}} \int \mathrm{d}^4x_1 \mathrm{d}^4x_2 \mathrm{d}^4y_1 \mathrm{d}^4y_2 \mathrm{d}^4z \left\{ e^{-i(p_1\cdot x_1 + p_2\cdot x_2 - q_1\cdot y_1 - q_2\cdot y_2)} \right.$$

$$\times \; \left(\Box_{x_1} + m^2\right)\left(\Box_{x_2} + m^2\right)\left(\Box_{y_1} + m^2\right)\left(\Box_{y_2} + m^2\right)$$

$$\left. \times \; \left[\Delta_F(x_1 - z)\Delta_F(x_2 - z)\Delta_F(z - y_1)\Delta_F(z - y_2)\right] \right\}$$

$$= -i\lambda \int \mathrm{d}^4x_1 \mathrm{d}^4x_2 \mathrm{d}^4y_1 \mathrm{d}^4y_2 \mathrm{d}^4z \left\{ e^{-i(p_1\cdot x_1 + p_2\cdot x_2 - q_1\cdot y_1 - q_2\cdot y_2)} \right.$$

$$\times \; \int \frac{\mathrm{d}^4k_1}{(2\pi)^4} \frac{\mathrm{d}^4k_3}{(2\pi)^4} \frac{\mathrm{d}^4k_3}{(2\pi)^4} \frac{\mathrm{d}^4k_4}{(2\pi)^4}$$

$$\times \; \left(\Box_{x_1} + m^2\right)\left(\Box_{x_2} + m^2\right)\left(\Box_{y_1} + m^2\right)\left(\Box_{y_2} + m^2\right)$$

$$\times \; \left[\; \frac{e^{-ik_1\cdot(z-x1)}}{k_1^2 - m^2 + i\epsilon^+} \frac{e^{-ik_2\cdot(z-x2)}}{k_2^2 - m^2 + i\epsilon^+} \right.$$

$$\left. \left. \times \; \frac{e^{-ik_3\cdot(y1-z)}}{k_3^2 - m^2 + i\epsilon^+} \frac{e^{-ik_4\cdot(y2-z)}}{k_4^2 - m^2 + i\epsilon^+} \right] \right\}$$

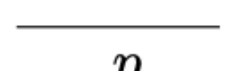
$$
\begin{aligned}
= & -i\lambda \int \mathrm{d}^4x_1 \mathrm{d}^4x_2 \mathrm{d}^4y_1 \mathrm{d}^4y_2 \mathrm{d}^4z \left\{ e^{-i(p_1\cdot x_1 + p_2\cdot x_2 - q_1\cdot y_1 - q_2\cdot y_2)} \right. \\
& \times \int \frac{\mathrm{d}^4k_1}{(2\pi)^4} \frac{\mathrm{d}^4k_3}{(2\pi)^4} \frac{\mathrm{d}^4k_3}{(2\pi)^4} \frac{\mathrm{d}^4k_4}{(2\pi)^4} \\
& \times \left(k_1^2 - m^2\right) \left(k_2^2 - m^2\right) \left(k_3^2 - m^2\right) \left(k_4^2 - m^2\right) \\
& \times \left[\quad \frac{e^{-ik_1\cdot(z-x1)}}{k_1^2 - m^2 + i\epsilon^+} \frac{e^{-ik_2\cdot(z-x2)}}{k_2^2 - m^2 + i\epsilon^+} \right. \\
& \quad \left. \left. \times \frac{e^{-ik_3\cdot(y1-z)}}{k_3^2 - m^2 + i\epsilon^+} \frac{e^{-ik_4\cdot(y2-z)}}{k_4^2 - m^2 + i\epsilon^+} \right] \right\} \\
= & -i\lambda \int \frac{\mathrm{d}^4k_1}{(2\pi)^4} \frac{\mathrm{d}^4k_3}{(2\pi)^4} \frac{\mathrm{d}^4k_3}{(2\pi)^4} \frac{\mathrm{d}^4k_4}{(2\pi)^4} \left[(2\pi)^4 \delta^4(k_1 + k_2 - k_3 - k_4) \right. \\
& \times (2\pi)^4 \delta^4(k_1 - p_1)(2\pi)^4 \delta^4(k_2 - p_2) \\
& \left. \times (2\pi)^4 \delta^4(k_3 - q_1)(2\pi)^4 \delta^4(k_4 - q_2) \right] \\
= & (2\pi)^4 \delta^4(p_1 + p_2 - q_1 - q_2) i\lambda \, .
\end{aligned}
\tag{358}
$$

We realize that, after this long calculation, the amplitude for the 2 →2 - scattering including one interaction vertex is given by the value λ of the interaction vertex, when taking into account the 4! combinations of combining the four external legs with the vertex.

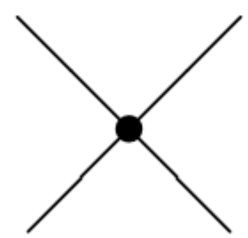
Feynman Rules This finding allows us to formulate simpler rules for the construction of amplitudes.

The LSZ formula above guarantees that we only have to take into account interaction vertices connecting the internal lines for particles, and we know that they are given by the time-ordered products – or commutators – of the fields.

This gives rise to the Feynman rules for the $\lambda\phi^4$ theory, namely



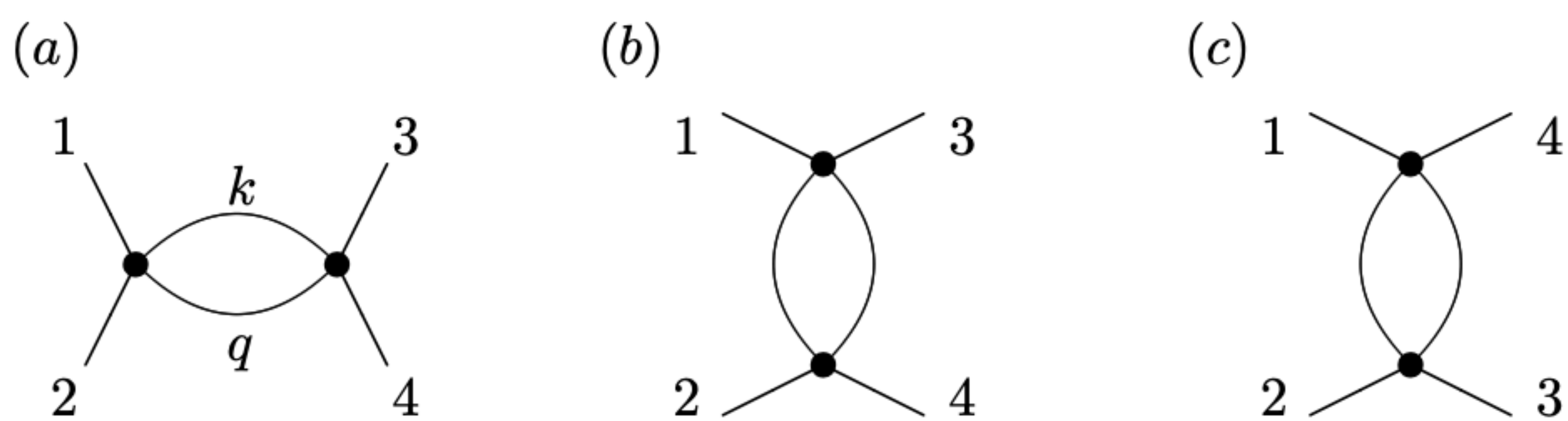
$$= \frac{-i}{p^2 - m^2 + i\epsilon^+}$$



$$= \frac{-i\lambda}{4!} \tag{359}$$

2nd-**Order Amplitude** Let us now construct a second order amplitude for the 2 →2 - scattering, using the Feynman rules from Eq. (359).

Labelling incoming particles as 1, 2 and outgoing particles as 3, 4, we find three different diagrams, namely



(360)

Let us focus now on diagram (a) and translate it into an expression for the amplitude.

We have

$$\begin{aligned}\hat{S}^{(a)} &= \left(-\frac{i\lambda}{4!}\right)^2 \int \frac{\mathrm{d}^4k}{(2\pi)^4}\frac{\mathrm{d}^4q}{(2\pi)^4}\left[\frac{-i}{k^2-m^2+i\epsilon^+}\,\frac{-i}{q^2-m^2+i\epsilon^+}\right.\\ &\quad\left.\times\,\frac{(4!)^2}{2}(2\pi)^4\delta(p_1+p_2-q-k)(2\pi)^4\delta(q+k-p_3-p_4)\right]\\ &= \frac{\lambda^2}{2!}\,(2\pi)^4\delta(p_1+p_2-p_3-p_4)\\ &\quad\times\int\frac{\mathrm{d}^4k}{(2\pi)^4}\,\frac{1}{[k^2-m^2+i\epsilon^+][(P-k)^2-m^2+i\epsilon^+]}\,, \qquad (361)\end{aligned}$$

where we have introduced $P = p_1 + p_2$.

The two factorials 4! from the interaction vertex are compensated by similar factors from attaching lines to the vertices, but modified by 1/2.

This "symmetry factor" stems from the fact that there are two internal lines connecting the two vertices at positions y_1 and y_2, taking out a combinatorial factor of 2!.

For diagrams (b) and (c) we arrive at similar expressions, where P is modified to become $P = p_1 - p_3$ and $P = p_1 - p_4$, respectively.

Closer inspection of the k-integration reveals that this diagram gives rise to a logarithmic divergence.

To see this, consider a limit where k becomes infinitely large, $k \to \infty$.

In this limit the integral assumes the asymptotic form of d^4k/k^4, and using polar coordinates in four dimensions, we can write this as $k^3 d^3\Omega dk/k^4$, where $d_3\Omega$ takes care of the finite angular integrals.

This leaves us with a final integral dk/k which diverges for $k \to \infty$.

This constitutes yet another divergence in Quantum Field Theory, and, similar to the treatment before, it is cured by subtracting suitable terms, this time directly in the Lagrangian.

These terms are constructed after “regularizing” the integrals, i.e., after quantifying the degree of their divergence and its prefactors.

The overall procedure of dealing with these ultraviolet divergences is known as “renormalization”.

Cross Section To arrive at a cross section $\sigma_{i \to f}$ for a process $i \to f$, we have to

- absolute-square the transition amplitude, $|S_{fi}|^2$
- sum or average over all outgoing or incoming unobserved internal degrees of freedom such as spins, polarisations, or colours, indicated by the symbol $\bar{\sum}$
- integrate over Lorentz invariant phase space given by the outgoing momenta, q_i
- and multiply the result with the Lorentz-invariant flux that describes the phase space density of the incoming particle beam (the term $1/(4\sqrt{\ldots})$ in front of the overall expression).

Expressed as an equation and using that $p_{1,2}^2 = m_{1,2}^2$, and making four-momentum conservation explicit this therefore reads

$$\begin{aligned}\sigma_{i\to f} &= \frac{1}{4\sqrt{(p_1\cdot p_2)^2 - p_1^2 p_2^2}} \\ &\quad \times \int \prod_{i=1}^{n} \frac{\mathrm{d}^3 q_i}{(2\pi)^3 2E_i} \bar{\sum_{d.o.f.}} |\hat{S}_{fi}|^2 (2\pi)^4 \delta^4 \left(p_1 + p_2 - \sum_{i=1}^{n} q_i\right)\end{aligned} \tag{362}$$

For the case at hand, we have the first-order amplitude from Eq. (358).

Stripping out the overall four-momentum conservation it is given by $\hat{S}_{fi} = \mathrm{i}\lambda$.

Assuming incident momenta

$$p_{1,2} = (E,\, 0,\, 0,\, \pm\sqrt{E^2 - m^2})\,, \tag{363}$$

we arrive at

$$
\begin{aligned}
\sigma_{i\to f} &= \frac{\lambda^2}{4\sqrt{(2E^2-m^2)^2-m^4}} \\
&\quad\times \int \frac{\mathrm{d}^3 q_1}{(2\pi)^3 2E_1}\frac{\mathrm{d}^3 q_2}{(2\pi)^3 2E_2}(2\pi)^4\delta^4\left(p_1+p_2-q_1-q_2\right) \\
&= \frac{\lambda^2}{8E\sqrt{E^2-m^2}}\int \frac{\mathrm{d}^3 q_1}{(2\pi)^3 4E_1E_2}(2\pi)\delta(2E-E_1-E_2)\Bigg|_{E_2=\sqrt{\underline{q}_1^2+m^2}} \\
&= \frac{\lambda^2}{32\pi^2 E\sqrt{E^2-m^2}}\int \frac{\underline{q}_1^2\mathrm{d}|\underline{q}_1|\mathrm{d}^2\Omega_1}{4(\underline{q}_1^2+m^2)}\delta(2E-2\sqrt{\underline{q}_1^2+m^2}) \\
&= \frac{\lambda^2}{32\pi E\sqrt{E^2-m^2}}\int \frac{(E_1^2-m^2)\mathrm{d}E_1}{E_1^2}\delta(2E-2E_1) \\
&= \frac{\lambda^2}{32\pi E^2}\sqrt{1-\frac{m^2}{E^2}} \qquad (364)
\end{aligned}
$$

for the cross section at the lowest order in the coupling constant, $O(\lambda^2)$ where we have used polar coordinates for the q_1-integration and realized that $\mathrm{d}|q_1| = \mathrm{d}E_1$.

The cross section has units of inverse energy squared or area and is usually given in units of “barn”, where

$$
1\,\mathrm{barn} \;=\; 1\,\mathrm{b} \;=\; 10^{-28}\mathrm{m}^2\,. \qquad (365)
$$