Quantum Field Theory

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Contents

Literature

M. Srednicki, Peskin–Schröder, Weinberg, Itzykson–Zuber

1 Introduction

1.1 Beyond QM

Quantum Mechanics cannot be the ultimate theory of *subatomic particle interactions* for several reasons:

– QM is a non-relativistic theory (the Schrödinger equation is a transcription of the NR law $E_{\rm kin} = p^2/2m$ plus the deBroglie relations)

– QM assumes a fixed number of particles

– QM cannot treat particle production processes (which occur in accelerator experiments)

– QM cannot, in particular, properly treat light (a) which is necessarily relativistic and (b) with photons continuously being produced and annihilated (radiation of matter, thermodynamics with $N(T) \sim U(T)/\bar{E} \sim T^4/T = T^3$.

– QM started from the observation that light and matter have the same corpuscular *and* wave features. However, the wave function is a *probability amplitude* which is conceptually very different from the electromagnetic *field amplitude*: the former is part of the description of a *state*, while the latter is an observable on the same footing as observables like momentum = *operators* in Schrödinger QM.

– QM should be a relativistically invariant theory which treats radiation ("light") and matter ("particles") in the same way.

1.2 How to quantize fields?

Ignore relativistic invariance for the moment. A prototype of a nonrelativistic classical field is sound (the amplitude of displacement of gas molecules) or any other amplitude

$$\varphi(x)$$

that is defined at every point in space. As a dynamical quantity, it will vary with time:

$$\varphi_t(x) = \varphi(x,t).$$

We regard this temporarily as a limit of finitely many amplitudes φ_i in a discrete space, ie, we assume a discrete set of points x_i where the amplitude is

$$\varphi_i(t) = \varphi(x_i,t),$$

and have in mind a continuum limit. The variable x is therefore just a *label* for infinitely many "field amplitudes" $\varphi(x)$, rather than a dynamical variable like the position of a point particle in QM. The dynamical variables are the field amplitudes φ_i or $\varphi(x)$.

Regarding a classical field as the continuum limit of a system of many amplitudes (generalized degrees of freedom) attached to points x, we should treat a quantum field like the continuum limit of many quantum degrees of freedom.

Finitely many degrees of freedom are quantized by the canonical commutation relations for the canonical variables and momenta:

$$[X_i, P_j] = i\hbar\delta_{ij}$$

which can be cast into the equivalent form in terms of creation and annihilation operators which are suitable linear combinations of X_i and P_i, $A_i = \mu_i X_i + i\lambda_i P_i$ where $\lambda_i\mu_i = 1/2\hbar$:

$$[A_i, A_j^*] = \delta_{ij}.$$

A "field" is now a continuous system of degrees of freedom, labelled by the position x. It is quantized according to

$$[\varphi(x), \pi(y)] = i\hbar\delta(x-y)$$

or respectively in terms of a continuum of creation and annihilation operators

$$[A(x), A(y)^*] = \delta(x-y).$$

Several questions arise:

– what is the dynamics (field equation) of a quantum field, ie, the time evolution $\varphi(x) \to \varphi_t(x)$ such that $\dot\varphi = i[H,\varphi]/\hbar$?

– what are the continuum analogs $\pi(x)$ of the canonical momenta P_i?

– how can one realize the commutation relations by operators on a Hilbert space?

In addition, one should keep in mind that we are ultimately interested in a relativistic version of the problem.

1.3 Towards QFT

Our approach to QFT is (1) to look at the Lagrangean treatment of classical field theory. This tells us in particular what $\pi(x)$ is. Then (2) we shall construct a Hilbert space representation of a continuous system of oscillators. This leads us to the notion of Fock space: a Hilbert space containing states with any particle number, which is the obvious arena for dynamical processes with particle creation and annihilation. It also familiarizes us with the idea that one should no longer of states as being represented by wave functions, but develop a more abstract understanding.

In case of free fields (no interaction), the Fock space approach is most approriate for this purpose, and allows to explicitly construct the quantum fields.

Only after these preliminary steps we shall turn (3) to more realistic problems concerning relativistic invariance, the electromagnetic field, spinor fields, and their couplings. All of these present us with some new complications, which have to be controlled all at the same time (but we shall address them one-by-one). In particular, the Lagrangean approach will in retrospect not always be satisfactory.

The historical road to QFT was different. Actually, it consisted of many complementary and highly entangled roads. Some textbooks follow a different line of argument which takes the Schrödinger equation as the point of departure and tries to find relativistic versions of it. This is how the Dirac equation was discovered, along with its theoretical explanation of the spin. These equations bring along interpretational difficulties (unwanted "negative energy solutions"), which were first pragmatically resolved by the idea of the "Dirac sea", and later by a conceptional re-interpretation called "second quantization" (bringing along the notion of an "anti-particle"): The wave function $\Psi(x)$ is no longer a probability amplitude but an obervable = operator on a Hilbert space of abstract (Fock space) state vectors. The description of a relativistic particle by a quantum field is therefore forced upon us by the resolution of these difficulties.

At this point, the two roads eventually merge. Both approaches have their advantages and disadvantages, and neither can be fully appreciated without the other.

2 Classical field theory

We want to adapt classical Lagrangean mechanics to a field φ. We call a function

$$\varphi : x \mapsto \varphi(x)$$

(subject to a suitable boundary condition) a "(field) configuration", and a family

$$t \mapsto \varphi_t$$

of configurations a "trajectory" (in the infinite-dimensional configuration space).

Lagrangean density

The Lagrangean will be a functional of the configuration and its time derivative ("generalized velocity")

$$L[\varphi_t, \dot\varphi_t].$$

A discrete system of amplitudes $\varphi(x_i)$ will in general possess neighbour interactions involving $\varphi(x_i) - \varphi(x_{i+1})$. In the continuum limit, this becomes the spatial derivative $\partial_x\varphi$ (which is part of the configuration!). At the same time, the Lagrange function which is a sum over the degrees of freedom at the points x_i, will turn into an integral over the points x. One shall therefore expect a Lagrangean of the form

$$L[\varphi] = \int dx\, \mathcal{L}(\varphi(x), \vec\nabla\varphi(x), \dot\varphi(x)).$$

In a nonrelativistic system, it could actually look much more complicated, eg the integrand could also involve higher than first x-derivatives. Because the kinetic energy is always given by first-order derivatives wrt time, in a relativistic system we

also expect only first-order derivatives wrt space. Moreover, L could be a multiple integral whose integrand depends on the field value and its derivatives at different points. In this case, one would have nonlocal interactions. Such interactions would violate the causality principle of a relativistic theory. Therefore, we restrict the subsequent discussion to *local first-order Lagrangean densities* as displayed.

As a class of instructive examples, we choose

$$\mathcal{L} = \frac{1}{2}\dot\varphi(x)^2 - \frac{c^2}{2}(\nabla\varphi)^2 - V(\varphi)$$

where $V(\varphi)$ is an amplitude-dependent "potential energy density".

Equation of motion

As in Lagrangean mechanics with a finite number of degrees of freedom, the dynamics of the field, ie the *actual* trajectory of field configurations is determined by Hamilton's principle that the action functional

$$S = \int_{t_1}^{t_2} dt\, L[\varphi_t]$$

is extremal among *all* trajectories φ_t with fixed initial and final configurations $\varphi_{t_1}(x)$ and $\varphi_{t_2}(x)$. This condition is evaluated by comparing the actual solution with all infinitesimally neighbouring trajectories

$$\varphi_t^\varepsilon(x) = \varphi_t(x) + \varepsilon\cdot\eta_t(x)$$

such that $\eta_{t_1} = \eta_{t_2} = 0$ but otherwise arbitrary, and requiring

$$\partial_\varepsilon S[\varphi^\varepsilon]|_{\varepsilon=0} \stackrel{!}{=} 0.$$

This leads after partial integrations wrt t and x to

$$\int dt\,dx\,\left(\left(\frac{\partial\mathcal{L}}{\partial\varphi}\right) - \partial_t\left(\frac{\partial\mathcal{L}}{\partial\dot\varphi}\right) - \sum_i \partial_i\left(\frac{\partial\mathcal{L}}{\partial(\partial_i\varphi)}\right)\right)\eta_t(x) = 0,$$

and hence, because $\eta_t(x)$ is arbitrary, to the Euler-Lagrange equation

$$\partial_t\left(\frac{\partial\mathcal{L}}{\partial\dot\varphi}\right) + \sum_i \partial_i\left(\frac{\partial\mathcal{L}}{\partial(\partial_i\varphi)}\right) \equiv \partial_\mu\left(\frac{\partial\mathcal{L}}{\partial(\partial_\mu\varphi)}\right) = \frac{\partial\mathcal{L}}{\partial\varphi}.$$

This is the dynamical equation of motion. In our examples, it gives

$$\ddot\varphi_t(x) - c^2\,\nabla(\nabla\varphi_t(x)) = -V'(\varphi_t(x)).$$

For $V = 0$, it is just the wave equation with wave velocity c. The potential in $\mathcal{L}$ disturbs the wave dynamics by the "force" term $-V' = -\partial V/\partial\varphi$.

We notice that for c the velocity of light, both the Lagrangean density

$$\mathcal{L} = \frac{c^2}{2}\,\partial_\mu\varphi\,\partial^\mu\varphi - V(\varphi)$$

and the field equation

$$\partial_\mu\partial^\mu\varphi(t,x) = -V'\big(\varphi(t,x)\big)/c^2$$

are relativistically invariant equations if φ is a scalar field.

Another relativistic example is the Lagrangean for a Lorentz vector field $A_\mu = (A^\mu) = (\phi/c, A)$

$$\mathcal{L}(A,\partial A,x) = -\frac{1}{4\mu_0}F_{\mu\nu}F^{\mu\nu} - j_\mu(x)A^\mu,$$

Here $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$, hence $E_i = c\,F_{0i}$ and $B_i = -\frac{1}{2}\varepsilon_{ijk}F_{jk}$, and

$$-\frac{1}{4\mu_0}F_{\mu\nu}F^{\mu\nu} = \frac{\varepsilon_0}{2}E^2 - \frac{1}{2\mu_0}B^2 = \frac{\varepsilon_0}{2}(-\nabla\phi - \partial_t A)^2 - \frac{1}{2\mu_0}(\nabla\times A)^2,$$

and $(j^\mu) = (c\rho, j)$, hence

$$j_\mu(x)A^\mu(x) = \rho(x)\phi(x) - \vec{j}(x)\vec{A}(x).$$

This gives, by the same rules, the Maxwell equations

$$\partial_\mu F^{\mu\nu} = \mu_0\; j^\nu$$

for the electromagnetic field in the presence of a current.

Noether's Theorem

Continuous symmetries of the Lagrangean give rise to conservation laws. Consider a symmetry $\varphi(x) \to \varphi(x) + \varepsilon\delta\varphi(x)$: If $\mathcal{L}$ is invariant, then

$$0 = \delta\mathcal{L} \equiv \frac{d\,\mathcal{L}}{d\varepsilon}\Big|_{\varepsilon=0} = \left(\frac{\partial\mathcal{L}}{\partial\varphi}\right)\delta\varphi(x) + \left(\frac{\partial\mathcal{L}}{\partial\dot\varphi}\right)\partial_t\delta\varphi(x) + \left(\frac{\partial\mathcal{L}}{\partial(\nabla\varphi)}\right)\nabla\delta\varphi(x).$$

Using the equation of motion, this is

$$\partial_t\left(\frac{\partial\mathcal{L}}{\partial\dot\varphi}\,\delta\varphi\right) + \nabla\left(\frac{\partial\mathcal{L}}{\partial(\nabla\varphi)}\,\delta\varphi\right) = 0,$$

which is a continuity equation $\partial_t\rho + \nabla j = 0$, hence the quantity

$$Q = \int dx\,\left(\frac{\partial\mathcal{L}}{\partial\dot\varphi}\,\delta\varphi\right)$$

is conserved.

If $\mathcal{L}$ is not invariant, but changes only by a gradient: $\delta\mathcal{L} = \nabla\mathcal{K}$, then the total Lagrangean L is still invariant (assuming that the fields decay sufficiently fast at spatial infinity), but the continuity equation changes:

$$\partial_t\left(\frac{\partial\mathcal{L}}{\partial\dot\varphi}\,\delta\varphi\right) + \nabla\left(\frac{\partial\mathcal{L}}{\partial(\nabla\varphi)}\,\delta\varphi - \mathcal{K}\right) = 0.$$

Momentum and energy

Classical field theory defines the (physical) momentum as the conserved quantity related to the translation invariance of the Lagrangean due to Noether's Theorem. That point particles have a momentum, is clear. That fields also carry momentum is necessary because fields exert a force on particles and change their momentum at the cost of the field momentum. This universality feature of momentum to be exchangable between different constituents of matter requires its definition along the same lines as for particles, as follows. Under a translation by a distance a, the fields $\varphi(x)$ change into $\varphi_a(t,x) = \varphi(t, x-a)$, hence $\delta\varphi = -\nabla\varphi$, and $\delta\mathcal{L} = -\nabla\mathcal{L}$, thus we may apply Noether's Theorem with $\mathcal{K} = -\mathcal{L}$, giving the momentum of the field

$$P = -\int dx \left(\frac{\partial\mathcal{L}}{\partial\dot\varphi}\right)\nabla\varphi.$$

It is conserved if and only if the field Lagrangean is translation invariant. If the theory contains several fields, one has to sum over all fields, ie, the field momentum can be exchanged among the fields but the sum is conserved. If a point particle with position X is coupled to the field, eg by an interaction energy $V_{\rm int} \sim \varphi(X,t) = \int dx\,\delta(x-X(t))\varphi(x,t) = \int dx\,\rho(x,t)\varphi(x,t)$ as for a charged particle in an electric potential, then L is invariant under the combined transformation $X \to X+a$, $\varphi(x) \to \varphi(x-a)$. Physically this means that field momentum can be converted into particle momentum: the field exerts a force on the particle.

Similarly, one can define the energy as the conserved quantity associated with time translation invariance. As in classical point mechanics, one regards the amplitude as generalized coordinates and defines the generalized momenta (not to be confused with the physical momentum!)

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

and the field energy

$$H = \int dx\,\pi(x)\dot\varphi(x) - L = \int dx\,\mathcal{H}(\varphi,\dot\varphi,\nabla\varphi).$$

For the scalar field this gives simply

$$\pi = \dot\varphi.$$

(The field energy can as well be obtained by Noether's Theorem for time translation invariance, which however requires another modification of the theorem for transformations that involve the time.)

Canonical variables, Hamiltonian density

In the Hamiltonian approach, one regards the generalized momentum $\pi(x)$ together with the amplitude $\varphi(x)$ as canonical variables. Eliminating $\dot\varphi$ in favour of π (Legendre transform), the energy $H[\varphi,\dot\varphi]$ becomes the Hamiltonian

$$H[\varphi,\pi] = \int dx\, \mathcal{H}(\varphi, \nabla\varphi, \pi),$$

and the equation of motion is equivalent to the Hamiltonian equations

$$\partial_t F = \{F, H\}$$

where F is either φ or π or any function(al) thereof, provided one imposes the canonical Poisson bracket

$$\{\varphi(y), \pi(x)\} = \delta(x-y), \qquad \{\pi,\pi\} = \{\varphi,\varphi\} = 0$$

and uses the algebraic properties of the bracket as a bilinear antisymmetric derivation.

The idea of Canonical Quantization

This observation is the clue to "canonical quantization": replace Poisson brackets by commutators of non-commuting operators:

$$\{A, B\} \to \frac{1}{i\hbar}[A, B].$$

Thus, starting from the classical Lagrangean, one defines the canonical momenta and the Hamiltonian. One then imposes the canonical commutation relations

$$[\varphi(y), \pi(x)] = i\hbar\,\delta(x-y), \qquad [\pi,\pi] = [\varphi,\varphi] = 0,$$

and postulates the dynamics of the quantum field to be

$$i\hbar\partial_t X = [X, H].$$

The problem is to realize the CCR by Hilbert space operators, and to solve the dynamical equations. We shall turn to this in the next section.

By this approach, we have placed ourselves naturally into the "Heisenberg picture" where quantum operators are regarded as the dynamical objects, and not the state vectors as in the Schrödinger picture. This seems most reasonable because already the classical fields depend on (space and) time.

In the case of electromagnetism, another problem appears. One finds

$$\pi_i = \frac{\partial\mathcal{L}}{\partial\dot A^i} = -\varepsilon_0\, E_i, \quad \pi_0 = \frac{\partial\mathcal{L}}{\partial\dot A^0} = 0.$$

The latter equation is clearly inconsistent with the CCR between π_0 and A^0. Because this problem requires a very special treatment, and because similar problems arise with fields with spin, we shall postpone the treatment of spinor and vector fields to a later section (Sect. 4.6, 4.7) when the general techniques and features of QFT have been clarified.

3 Free scalar quantum fields

3.1 Canonical commutation relations and Fock space

We want to realize the canonical commutation relations (CCR)

$$i[\pi_0(\vec{x}), \varphi_0(\vec{y})] = \hbar\, \delta(\vec{x} - \vec{y}), \qquad [\pi_0, \pi_0] = [\varphi_0, \varphi_0] = 0$$

(at any given time $t = 0$) by hermitean operators on a Hilbert space. Because of the δ-function, the objects $\phi(x)$ at a point (where $\phi = \varphi$ or $= \pi$) cannot be operators themselves. But the fields ϕ are "*operator-valued distributions*", meaning that $\int dx f(x)\phi(x)$ are operators for arbitrary (Schwartz) test functions f. (Such integrations are called "smearing". If $f \geq 0$, one may regard it as an "averaging".)

We first pass to the Fourier transforms

$$\varphi_0(\vec{x}) = (2\pi)^{-3/2} \int d^3k\, \hat{\varphi}_0(\vec{k})\, e^{i\vec{k}\cdot\vec{x}}$$

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so that the desired CCR take the form

$$i[\hat{\pi}_0(\vec{k}), \hat{\varphi}_0(\vec{k}')] = \hbar\, \delta(\vec{k} + \vec{k}'), \qquad [\hat{\pi}_0, \hat{\pi}_0] = [\hat{\varphi}_0, \hat{\varphi}_0] = 0.$$

Hermiticity of the fields implies $\hat{\varphi}(\vec{k})^* = \hat{\varphi}(-\vec{k})$, and the same for $\hat{\pi}$. Next, we form combinations

$$A(\vec{k}) = \mu(\vec{k})\hat{\varphi}(\vec{k}) + i\lambda(\vec{k})\hat{\pi}(\vec{k})$$

and their conjugates

$$A^*(\vec{k}) = \mu(\vec{k})\hat{\varphi}(-\vec{k}) - i\lambda(\vec{k})\hat{\pi}(-\vec{k})$$

where μ and λ are real even functions such that $\mu(\vec{k})\lambda(\vec{k}) = 1/2\hbar$, to be specified later.

The desired CCR now take the form

$$[A(\vec{k}), A^*(\vec{k}')] = \delta(\vec{k} - \vec{k}'), \qquad [A, A] = [A^*, A^*] = 0.$$

These are the relations of the ladder operators for a continuous infinite system of oscillators.

In order to deal with the singular nature, we consider integrals with complex test functions

$$A^*(f) = \int d^3k\, f(\vec{k}) A^*(\vec{k})$$

and their conjugates

$$A(f) = \int d^3k\, \overline{f(\vec{k})} A(\vec{k}).$$

Now the CCR become

$$\boxed{[A(f), A^*(g)] = \int d^3k\, \overline{f(k)} g(k) = (f,g), \qquad [A,A] = [A^*, A^*] = 0.}$$

These relations extend to functions $f, g \in \mathcal{H}_1 = L^2(\mathbb{R}^3, d^3k)$ for which the scalar product is well-defined. In this form, they can be realized by operators on a Hilbert space $\mathcal{H} = \mathcal{F}(\mathcal{H}_1)$ (the **Fock space**), by the following standard construction for any Hilbert space $\mathcal{H}_1$.

We postulate the presence of a unit vector $\Omega \in \mathcal{H}$ which is annihilated by all $A(f)$:

$$A(f)\Omega = 0.$$

From this we can compute the scalar products between vectors $A^*(f)\Omega$:

$$(A^*(f)\Omega, A^*(g)\Omega) = (\Omega, A(f)A^*(g)\Omega) = (\Omega, [A(g), A^*(g)]\Omega) = (f,g)\cdot(\Omega,\Omega) = (f,g),$$

ie the vectors $A^*(f)\Omega$ in the physical Hilbert space have the same scalar products as the functions $f \in \mathcal{H}_1$. This gives rise to a natural unitary identification of these spaces:

$$A^*(f)\Omega \in \mathcal{H} \leftrightarrow f \in \mathcal{H}_1,$$

ie we may regard $\mathcal{H}_1$ as a subspace of $\mathcal{H}$.

We turn to higher excited vectors of the form $A^*(f_1)\cdots A^*(f_N)\Omega$. Inductively, one finds that two such vectors $A^*(f_1)\cdots A^*(f_N)\Omega$ and $A^*(g_1)\cdots A^*(g_M)\Omega$ are always orthogonal when $N \neq M$. Moreover, because $A^*(f)A^*(g) = A^*(g)A^*(f)$, they do not depend on the order of the entries $f_1, \ldots, f_N$. Finally, one verifies the scalar products

$$(A^*(f_1)\cdots A^*(f_N)\Omega, A^*(g_1)\cdots A^*(g_N)\Omega) = \sum_{\pi\in S_N} (f_1, g_{\pi 1})\cdots(f_N, g_{\pi N}).$$

This is the same as the scalar products between the symmetrized tensor products of the form $\sqrt{N!}\, S\,(f_1 \otimes \cdots \otimes f_N)$, where S is the symmetrization operator (= $1/N!$ times the sum over all permutations). We therefore have a natural unitary identification

$$A^*(f_1)\cdots A^*(f_N)\Omega \in \mathcal{H} \leftrightarrow \sqrt{N!}\, S\,(f_1 \otimes \cdots \otimes f_N) \in \mathcal{H}_N := S\mathcal{H}_1^{\otimes N}.$$

The subspaces $\mathcal{H}_N \subset \mathcal{H}$ are mutually orthogonal, and we obtain the *Fock space* (associated with the Hilbert space $\mathcal{H}_1$)

$$\mathcal{H} = \mathcal{F}(\mathcal{H}_1) = \mathbb{C}\Omega \oplus \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \cdots .$$

It is easy to see that on this Hilbert space, all operators $A(f)$ and $A^*(f)$ are represented by

$$A^*(f)S(f_1 \otimes \cdots \otimes f_N) = \sqrt{N+1}\, S(f \otimes f_1 \otimes \cdots \otimes f_N)$$

$$A(f)S(f_1\otimes\cdots\otimes f_N)=\sqrt{N}^{-1}\sum_{i=1}^{N}(f,f_i)S(f_1\otimes\cdots\not{f}_i\cdots\otimes f_N)$$

where $\not{f}_i$ means omission of this factor. One may take these relations as *definitions* of the operators, and verify that $A(f)^*=A^*(f)$ and $[A(f),A^*(g)]=(f,g)\mathbf{1}$ on the Fock space.

If $f_i\in\mathcal{H}_1$ $(i=1,\dots n)$ is an orthonormal basis, one may put $A_i^*=A^*(f_i)$, such that $[A_i,A_j^*]=(f_i,f_j)\delta_{ij}$ and $[A_i,A_j]=[A_i^*,A_j^*]=0$. $\mathcal{H}_N$ is spanned by orthonormal vectors $|N_1,N_2,\dots\rangle=(\prod N_k!)^{-\frac12}A_1^{*N_1}\cdots A_n^{*N_n}\Omega$ where N_k is the excitation number of the kth mode, and $N=N_1+\cdots+N_n$ is the total excitation number.

Eg, if $\mathcal{H}_1=\mathbb{C}$ with basis vector $f=1$, then $A=A(f)$ and its adjoint A^* satisfy the relations of a single oscillator, and the spaces $\mathcal{H}_N$ are all one-dimensional, spanned by the vectors $|N\rangle=(N!)^{-\frac12}A^{*N}\Omega$. The Fock space is thus $\mathcal{H}=\mathcal{F}(\mathbb{C})=\bigoplus_N\mathbb{C}|N\rangle=\ell^2$. On the other hand, in the Schrödinger representation the vectors $|N\rangle$ are represented by the Gaussian wave function $e^{-m\omega x^2/2\hbar}$ times Hermite polynomials, the well-known eigenstates of the harmonic oscillator Hamiltonian $H=\hbar\omega(AA^*+A^*A)$, where $A=\sqrt{m\omega/2\hbar}X+iP/\sqrt{2m\omega\hbar}$. The present Fock representation is more abstract, by just registering the excitation number N, but perfectly equivalent because all observables of interest (functions of X and P) can as well be expressed in terms of A and A^*.

For a finite number n of oscillators, $\mathcal{H}_1=\mathbb{C}^n$ and $\mathcal{H}_2=\mathbb{C}^{\frac12 n(n+1)}$ etc.

In our case, $\mathcal{H}_1=L^2(\mathbb{R}^3,d^3k)$ is itself the Hilbert space of a QM particle in three dimensions. Then $\mathcal{H}_1^{\otimes N}=L^2(\mathbb{R}^{3N},d^3k_1\dots d^3k_N)$, and $\mathcal{H}_N=S\,\mathcal{H}_1^{\otimes N}$ contains precisely the symmetric N-particle wave functions, ie it is the Hilbert space of N indistinguishable particles. The Fock space therefore is a Hilbert space which describes *all particle numbers at the same time*, in contrast to QM. The ladder operators are *creation and annihilation operators* for particles with a given wave function, and no longer operators changing the excitation of a single (or fixed number of) particle(s), as in QM. The excitation number N has become the particle number, and the ground state is a state with zero particles, called the vacuum.

The present formalism avoids to mention the wave functions altogether by just keeping track of the ladder operators needed to generate it from the ground state. This is particularly useful when one turns to continuously many degrees of freedom, which would naively require to consider wave functions in continuously many arguments.

Actually, in order to justify the interpretation as multi-particle states, we have to study energy and momentum of these states, which requires to understand their dynamics.

3.2 Free fields

From the Fock space realization of the CCR, we recover the time $t = 0$ fields φ_0 and π_0 in terms of oscillators: $\hat\varphi_0(\vec k) = (A(\vec k) + A^*(-\vec k))/2\mu(\vec k)$, $\hat\pi_0(\vec k) = (A(\vec k) - A^*(-\vec k))/2i\lambda(\vec k)$, and hence

$$\varphi_0(\vec x) = (2\pi)^{-3/2}\int \frac{d^3k}{2\mu(\vec k)}\big(A(\vec k)e^{i\vec k\cdot\vec x} + A^*(\vec k)e^{-i\vec k\cdot\vec x}\big)$$

$$\pi_0(\vec x) = (2\pi)^{-3/2}\int \frac{d^3k}{2i\lambda(\vec k)}\big(A(\vec k)e^{i\vec k\cdot\vec x} - A^*(\vec k)e^{-i\vec k\cdot\vec x}\big).$$

The dynamics is specified by the Lagrangean, or by the Hamiltonian. We choose the potential $V(\varphi)$ to be of the quadratic form

$$V(\varphi) = \frac{m^2c^4}{2\hbar^2}\varphi^2,$$

where m is a mass parameter. Then the Hamiltonian will be

$$H = \frac12\int d^3x\big(\pi(\vec x)^2 + c^2(\nabla\varphi(\vec x))^2 + (m^2c^4/\hbar^2)\varphi(\vec x)^2\big),$$

giving rise to the equations of motion

$$\dot\varphi(t,\vec x) = \pi(t,\vec x), \qquad \dot\pi(t,\vec x) = c^2\Delta\varphi(t,\vec x) - (m^2c^4/\hbar^2)\varphi(t,\vec x),$$

or

$$(\partial_t^2 - c^2\Delta)\varphi = -(m^2c^4/\hbar^2)\varphi$$

with the initial values $\varphi(0,\vec x) = \varphi_0(\vec x)$, $\pi(0,\vec x) = \pi_0(\vec x)$. This implies that the time evolution of the Fourier modes is given by the frequency

$$\omega(k) = \sqrt{c^2k^2 + m^2c^4/\hbar^2},$$

and that the coefficient functions λ, μ must satisfy the relation $1/\lambda = \omega/\mu$, which (together with $\mu\lambda = 1/2\hbar$) fixes their values. Hence

$$\boxed{\varphi(t,\vec x) = (2\pi)^{-3/2}\sqrt\hbar\int \frac{d^3k}{\sqrt{2\omega(\vec k)}}\big(A(\vec k)e^{-i(\omega(\vec k)t - \vec k\cdot\vec x)} + A^*(\vec k)e^{i(\omega(\vec k)t)-\vec k\cdot\vec x}\big)}$$

and

$$\pi(t,\vec x) = (2\pi)^{-3/2}\sqrt\hbar\int d^3k\,\sqrt{\omega(\vec k)/2}\,\big(-iA(\vec k)e^{-i(\omega(\vec k)t-\vec k\cdot\vec x)} + iA^*(\vec k)e^{i(\omega(\vec k)t-\vec k\cdot\vec x)}\big).$$

Notice that φ_t and π_t satisfy the CCR at every fixed time t.

This is the prototype of a quantum field. It is represented in terms of creation and annihilation operators (labelled by wave numbers k) on a Fock space. However, the described passage from the "time-zero" fields $\varphi(x)$, $\pi(x)$ to the dynamical field $\varphi(t,x)$ (by solving the equation of motion) works only thanks to the linear field equation. Thus, *interacting* fields will *not* be representable by creation and annihilation operators! The difficulty of QFT precisely consists in finding appropriate alternative ways to describe and compute interacting quantum fields.

Remark: The (singular) field operator $\varphi(\vec{x})$, acting on the vacuum vector, yields a one-particle state. But the particle is *not* localized at the point $\vec{x}$! Indeed, $\varphi(\vec{x}_0)\Omega = A^*(f)\Omega \equiv f \in \mathcal{H}_1 = L^2(\mathbb{R}^3, d^3k)$ with

$$f(\vec{k}) \sim \omega(\vec{k})^{-1/2}\, e^{-i\vec{k}\cdot\vec{x}_0}.$$

The corresponding x-space wave function ("Newton-Wigner wave function")

$$\psi(\vec{x}) \sim \int d^3k\, \omega(\vec{k})^{-1/2}\, e^{i(\vec{k}\cdot\vec{x}-\vec{k}\cdot\vec{x}_0)}$$

is strongly peaked around $\vec{x} \approx \vec{x}_0$ with a width of the order of the Compton wave length $\hbar/mc$ ($\approx 10^{-12}$m).[1]

3.3 Particle states

It is our intention to interpret the state Ω as the "vacuum", and states like $A^*(k)\Omega$ as quantum states containing a particle of mass m with momentum $p = \hbar k$ and energy $E = \hbar\omega(k) = \sqrt{p^2c^2 + m^2c^4}$. For this, we need to define operators on the Fock space that measure energy and momentum.

First we insert our solution for $\varphi(t,x)$ and $\pi(t,x)$ into the classical formula for the Hamiltonian. This gives the quantized Hamiltonian

$$H \stackrel{?}{=} \frac{\hbar}{2}\int dk\, \omega(k)(A^*(k)A(k) + A(k)A^*(k)).$$

From this we try to compute the energy of the state Ω and find the divergent integral

$$E_0 = (\Omega, H\Omega) = \frac{\hbar}{2}\int dk\, \omega(k)[A(k), A^*(k)] = \frac{1}{2}\int dk\, \hbar\omega(k)\cdot\delta(0).$$

This should not really be a surprise since we have a system of infinitely many oscillators, each having a zero-point energy. The problem can be circumvented by subtracting this infinite energy and redefining

$$H = \frac{\hbar}{2}\int dk\, \omega(k)\big(A^*(k)A(k)+A(k)A^*(k)-[A(k),A^*(k)]\big) = \hbar\int dk\, \omega(k)\, A^*(k)A(k).$$

[1] One might "absorb" the factor $\omega^{-1/2}$ into the momentum wave function, so as to obtain an x-space δ-function. But then the scalar product in x-space is given by some non-local kernel instead of $\int|\psi|^2$, which is at variance with the interpretation as a probability density.

The subtraction amounts to a reordering such that the annihilation operators are to the right of the creation operators. This prescription is called "*normal ordering*" or "*Wick product*" and is usually written as $:(\dots):$.

The effect of the normal ordering is that Ω is an eigenstate of energy zero:

$$H\Omega = 0.$$

Moreover, any state of the form $A^*(k)\Omega$ is also an eigenstate

$$HA^*(k)\Omega = \hbar\omega(k)\cdot A^*(k)\Omega,$$

and

$$HA^*(k_1)\cdots A^*(k_N)\Omega = (\hbar\omega(k_1)+\cdots+\hbar\omega(k_N))\cdot A^*(k_1)\cdots A^*(k_N)\Omega.$$

Likewise, we want to compute the momentum. We insert all our formulae into the classical expression

$$P = -\int dx\,(\frac{\partial\mathcal{L}}{\partial\dot\varphi})\nabla\varphi,$$

giving the quantized momentum operator

$$P \stackrel{?}{=} \frac{\hbar}{2}\int dk\,k\,(A^*(k)A(k)+A(k)A^*(k)).$$

Again, this results in divergent integrals (which formally add up to zero) already for the expectation value in the state Ω, and better has to be normal ordered, giving

$$P = \hbar\int dk\,k\,A^*(k)A(k).$$

Now we find finite eigenvalues

$$P\Omega = 0,$$

$$PA^*(k_1)\cdots A^*(k_N)\Omega = (\hbar k_1+\cdots+\hbar k_N)\cdot A^*(k_1)\cdots A^*(k_N)\Omega.$$

The interpretation imposes itself: Ω is a state without energy and momentum – therefore called the "vacuum". $A^*(k_1)\cdots A^*(k_N)\Omega$ is a state containing N particles, each with energy $E_i = \hbar\omega(k_i)$ and momentum $p_i = \hbar k_i$ such that

$$E = \sqrt{p^2c^2+m^2c^4}.$$

This is the energy relation for a relativistic particle of rest mass m.

We have found that the state space of a quantum *field* is spanned by states describing *particles*. This is the final meaning of the "particle–wave dualism", emerging naturally in quantum field theory. In the same way, the *states* of the electromagnetic field will describe photons, and the particles (electrons and positrons) will arise as states of the Dirac *field*.

The application of a field operator adds or removes particles from a state, while the energy and momentum operators, expressed as normal-ordered quadratic expressions in the fields, preserve the particle content.

We have defined energy and momentum as integrals over densities:

$$\rho_E(x) := :\dot\varphi(x)^2 - \mathcal{L}(x): = :\frac{1}{2}\big(\dot\varphi(x)^2 + c^2(\nabla\varphi(x))^2 + (m^2c^4/\hbar^2)\varphi(x)^2\big):$$

and

$$\vec\rho_P(x) := : - \big(\frac{\partial\mathcal{L}}{\partial\dot\varphi}\big)(x)\vec\nabla\varphi(x): = -:\dot\varphi(x)\vec\nabla\varphi(x):.$$

We can now compute, eg, the expectation value of the energy density in a one-particle state:

$$(A^*(f)\Omega, \rho_E(t,x)A^*(f)\Omega).$$

The computation gives an expression proportional to

$$\int dk_1\, dk_2\, e^{i(\omega_1-\omega_2)t - i(\vec k_1\cdot\vec x - \vec k_2\cdot\vec x)}\big(\omega_1\omega_2 + c^2\vec k_1\cdot\vec k_2 + (m^2c^4/\hbar^2)\big)\,\overline{f(\vec k_1)}f(\vec k_2)/\sqrt{\omega_1\omega_2}.$$

The energy is not sharply distributed. Even if f (the wave function in momentum space) were the Fourier transform of a δ-function in $\vec x$-space, the energy density is not concentrated in a point at any time. But as $|t|\to\infty$, $\langle\rho_E(t, x = vt)\rangle$ behaves like $\sim |f(k_v)|^2$ (by virtue of the stationary phase approximation), ie, if f is sharply peaked around some momentum k, then the energy density is peaked around the classical track $x = v_k\cdot t$. (The same holds for all other densities). The spread is slower than in Schrödinger QM because of the relativistic dispersion relation $\omega(k)$.

We see that the "position" of a particle is a delicate concept, even more so than in QM. Namely, field operators (corresponding to measurements) possess a localization in space and time indicating where and when the measurement is performed (eg, the energy density at a point x). The "position" of a particle is reveiled by the expectation values of density fields in the corresponding state, and describes a "track" only at asymptotic times $> \hbar/mc^2 \approx 10^{-21}$sec.

3.4 Fluctuations and correlations

By construction, the VEV of a field operator vanishes:

$$(\Omega, \varphi(x)\Omega) = 0.$$

How about the fluctuations (ie the width of the statistical distribution of individual field strength measurements)? We need to compute the VEV of the square:

$$(\Omega, \varphi(x)^2\Omega) = \hbar(2\pi)^{-3}\int\frac{d^3k}{2\omega(k)}.$$

This integral diverges: a field operator $\varphi(x)$ has infinite fluctuations around its expectation value zero (due to the contribution of infinitely many oscillators). This singular behaviour corresponds to φ being an op-valued distribution rather than a function. We compute instead the correlation between fields at different points:

$$(\Omega, \varphi(t,\vec{x})\varphi(t',\vec{x}')\Omega) = \hbar(2\pi)^{-3}\int \frac{d^3k}{2\omega(k)} e^{-i(\omega(k)(t-t')-\vec{k}\cdot(\vec{x}-\vec{x}'))} =: \Delta_m(t-t',\vec{x}-\vec{x}').$$

This is a distribution in the variables $(t,\vec{x})$ and (t',x'). It gives rise to finite fluctuations of "smeared" field operators $\varphi(F) = \int dtd^3x F(t,x)\varphi(t,\vec{x})$:

$$(\Omega, \varphi(F)^2\Omega) = \hbar\int \frac{d^3k}{2\omega(k)} |\hat{F}(\omega(k),\vec{k})|^2.$$

This quantity gives the size of the quantum fluctuations of the operator $\varphi(F)$. It is $< \infty$ since $\hat{F}$ has rapid decay $\Leftrightarrow$ the smearing function F is smooth.

We shall also need higher-order correlations (N-point functions).They are comparably simple for free fields. In principle, one only has to "commute all annihilation operators to the right, and collect the commutators". Because one has to perform this step again and again, a more efficient approach is desired.

Weyl's formula and Wick's Theorem

We start from a simple form of the Baker-Campbell-Hausdorff formula:

$$e^X Y e^{-X} = Y + [X,Y] \quad \Leftrightarrow \quad [e^X, Y] = [X,Y]e^X,$$

whenever $[X,Y]$ commutes with X. From this, we derive **Weyl's formula**

$$\boxed{e^X e^Y = e^{\frac{1}{2}[X,Y]} e^{X+Y},}$$

whenever $[X,Y]$ commutes with X and with Y, as follows:

Consider $f_1(t) = e^{tX}e^{tY}$ and $f_2(t) = e^{\frac{1}{2}t^2[X,Y]}e^{t(X+Y)}$. We have to show that $f_1(t) = f_2(t)$ for all t. Using $\partial_t e^{tX} = Xe^{tX}$, both functions satisfy

$$\partial_t f(t) = (X + Y + t[X,Y])f(t),$$

where in the case of f_1, we have used $e^{tX}Y = (Y + t[X,Y])e^{tX}$ by the BCH formula. Since the differential equation is first-order, its solution is uniquely determined by the initial value at $t = 0$. Clearly, $f_1(0) = f_2(0) = \mathbf{1}$, hence $f_1(t) = f_2(t)$. QED

Now we consider one or more operators of the form $Z = A^- + A^+$ where A^- and A^+ are any linear combinations of annihilation and creation operators, respectively, eg $Z = X$ and $Z = P$ in QM, or field operators $Z = \varphi(x)$. This implies

$$(\Omega, Z_i Z_j \Omega) = (\Omega, (A_i^- + A_i^+)(A_j^- + A_j^+)\Omega) = (\Omega, A_i^- A_j^+ \Omega) = (\Omega, [A_i^-, A_j^+]\Omega) = [A_i^-, A_j^+].$$

The Weyl formula gives

$$\boxed{:e^Z: = e^{A^+}e^{A^-} = e^{-\frac{1}{2}[A^-,A^+]}e^{A^+ + A^-} = e^{-\frac{1}{2}(\Omega,Z^2\Omega)}e^Z.}$$

We compute

$$:e^{Z_1}:\cdots:e^{Z_N}: = \prod_i e^{-\frac{1}{2}(\Omega,Z_i^2\Omega)}\cdot e^{Z_1}\cdots e^{Z_N},$$

$$e^{Z_1}\cdots e^{Z_N} = \prod_{i<j} e^{\frac{1}{2}[Z_i,Z_j]}\cdot e^{Z_1+\cdots+Z_N}$$

(by induction in N), and

$$e^{Z_1+\cdots+Z_N} = e^{\frac{1}{2}(\Omega,(Z_1+\cdots+Z_N)^2\Omega)}\cdot :e^{Z_1+\cdots+Z_N}:.$$

Collecting the numerical prefactors, we get **Wick's Theorem (raw version)**

$$\boxed{:e^{Z_1}:\cdots:e^{Z_N}: = \prod_{i<j} e^{(\Omega,Z_iZ_j\Omega)}\cdot :e^{Z_1+\cdots+Z_N}:.} \qquad (*)$$

An immediate consequence is the

Corollary:

$$(\Omega, Z_1\cdots Z_N\Omega) = \sum_{\text{partitions, } i_k<j_k} \prod_{k=1}^{N/2} (\Omega, Z_{i_k}Z_{j_k}\Omega)$$

if $N=2n$ is even, and $=0$ otherwise. Here, a *partition* of the set $\{1,\dots,2n\}$ is a decomposition into n disjoint subsets $\{i_k,j_k\}$ with two elements each.

(Several further consequences will be derived later (cf Sect. 5.6).)

Proof: Replace Z_i by t_iZ_i in $(*)$ and take vacuum expectation values:

$$(\Omega, :e^{t_1Z_1}:\cdots:e^{t_NZ_N}:\Omega) = \prod_{i<j} e^{t_it_j(\Omega,Z_iZ_j\Omega)},$$

then expand both sides in power series in t_i and compare coefficients of the term $t_1\cdots t_N$.

Conversely, the formula in the corollary implies that the commutator is a multiple of $\mathbf{1}$:

$$[Z_i,Z_j] = \big((\Omega,Z_iZ_j\Omega)-(\Omega,Z_jZ_i\Omega)\big)\cdot\mathbf{1}.$$

For N-point functions of free fields, this yields the factorization into 2-point functions:

$$\boxed{(\Omega,\varphi(x_1)\cdots\varphi(x_N)\Omega) = \sum_{\text{partitions, } i_k<j_k} \prod_{k=1}^{N/2} (\Omega,\varphi(x_{i_k})\varphi(x_{j_k})\Omega)}$$

if N is even, and $=0$ otherwise (**Wick's Theorem for free fields**). In particular, knowing the 2-point function of a free field, one knows *all its correlations*.

One also gets

$$(\Omega, e^{i\varphi(F)}\Omega) = e^{-\frac{1}{2}\omega(F,F)}$$

where $\varphi(F) = \int dtdx\, F(t,x)\varphi(x)$ and $\omega(F,G)$ is the smeared 2-point correlation $\omega(F,G) = \int dtdx\, F(t,x)\ dt'dx'\, G(t',x')\ \Delta_m(t-t',x-x')$ (hence $\omega(F,F)$ is the vacuum fluctuation as above).

3.5 Charged fields

Consider a classical field theory with two real free fields φ_1 and φ_2 of the same mass, ie the Lagrangean is

$$\mathcal{L} = \frac{1}{2}(\dot\varphi_1(x)^2 + \dot\varphi_2(x)^2) - \frac{c^2}{2}((\nabla\varphi_1)^2 + (\nabla\varphi_2)^2) - \frac{m^2c^4}{2\hbar^2}(\varphi_1(x)^2 + \varphi_2(x)^2).$$

This Lagrangean density possesses an *inner symmetry*

$$\begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} \to \begin{pmatrix} \varphi_1^{(\alpha)} \\ \varphi_2^{(\alpha)} \end{pmatrix} = \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix} \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix}.$$

Associated with this symmetry is again a Noether conserved charge[2] which is an integral over a charge density:

$$\partial_t \sum_i \left(\frac{\partial\mathcal{L}}{\partial\dot\varphi_i}\right)\delta\varphi_i + \nabla\sum_i \left(\frac{\partial\mathcal{L}}{\partial\nabla\varphi_i}\right)\delta\varphi_i = \partial_t\rho(t,x) + \nabla j(t,x) = 0,$$

where $\delta\varphi_i$ is the infinitesimal change under the symmetry. Thus, the charge density is

$$\rho(t,x) = \sum_i \dot\varphi_i\delta\varphi_i = \dot\varphi_2\varphi_1 - \dot\varphi_1\varphi_2$$

and the current density is

$$j(t,x) = -c^2\sum_i \nabla\varphi_i\delta\varphi_i = -c^2(\nabla\varphi_2\varphi_1 - \nabla\varphi_1\varphi_2) \equiv c^2\varphi_2\overset{\leftrightarrow}{\nabla}\varphi_1.$$

Consequently, the total charge

$$Q = \int dx\ \rho(t,x)$$

is a conserved quantity.

It is more convenient to work with complex fields

$$\phi = (\varphi_1 + i\varphi_2)/\sqrt{2}, \quad \phi^* = (\varphi_1 - i\varphi_2)/\sqrt{2},$$

so that the symmetry becomes a complex phase:

$$\phi \to \phi^{(\alpha)} = e^{i\alpha}\,\phi.$$

Then

$$\rho = i(\dot\phi^*\phi - \phi^*\dot\phi), \quad j = ic^2\phi^*\overset{\leftrightarrow}{\nabla}\phi.$$

[2]The term "charge" is here just a name for the conserved quantity. Its interpretation as an *electric* charge requires that it couples to the electromagnetic field, see below.

We want to translate these classical statements into QFT. The quantization proceeds as before with the help of annihilation operators $A_1(k)$ and $A_2(k)$ and their conjugates. $A_1^{(*)}$ commute with $A_2^{(*)}$. This yields two commuting quantum fields φ_1 and φ_2. Taking complex combinations, we find

$$\phi(t,x) = (2\pi)^{-3/2}\sqrt{\hbar}\int \frac{d^3k}{\sqrt{2\omega(\vec{k})}}\left(C(\vec{k})e^{-i(\omega(\vec{k})t-\vec{k}\cdot\vec{x})} + B^*(\vec{k})e^{i(\omega(\vec{k})t)-\vec{k}\cdot\vec{x}}\right)$$

$$\phi^*(t,x) = (2\pi)^{-3/2}\sqrt{\hbar}\int \frac{d^3k}{\sqrt{2\omega(\vec{k})}}\left(B(\vec{k})e^{-i(\omega(\vec{k})t-\vec{k}\cdot\vec{x})} + C^*(\vec{k})e^{i(\omega(\vec{k})t)-\vec{k}\cdot\vec{x}}\right)$$

where $B(k) = (A_1(k) - iA_2(k))/\sqrt{2}$, $C(k) = (A_1(k) + iA_2(k))/\sqrt{2}$ satisfy the CCR

$$[B(k), B^*(k')] = [C(k), C^*(k')] = \delta(k-k'),$$

while all other commutators vanish. To quantize the charge and density operators, one has again to use normal ordering, in particular

$$Q = \int d^3x :\rho(t,x): = \int d^3k \,\left(B(k)^*B(k) - C(k)^*C(k)\right).$$

From this we see, that

$$[Q,C] = +C, \quad [Q,C^*] = -C^*, \quad [Q,B] = -B, \quad [Q,B^*] = +B^*,$$

hence ϕ and ϕ^* are ladder operators for the charge operator: $[Q,\phi(x)] = \phi(x)$, $[Q,\phi^*(x)] = -\phi^*(x)$, changing the eigenvalue of Q by ± 1 unit: B^* creates particles of charge $+1$, while C^* creates particles of charge -1. The complex field ϕ creates a positive or annihilates a negative particle, so it always changes the charge by $+1$.

The commutation relations imply that Q is the "generator of the symmetry", namely

$$e^{i\alpha Q}\phi e^{-i\alpha Q} = \phi^{(\alpha)} = e^{i\alpha}\,\phi.$$

One also has

$$Q\Omega = 0 \qquad \Leftrightarrow \qquad e^{i\alpha Q}\Omega = \Omega.$$

It follows that the vacuum expectation values $(\Omega, \phi\phi\Omega)$ and $(\Omega, \phi^*\phi^*\Omega)$ must vanish (by the standard invariance argument $(\Omega,\phi\phi\Omega) = (e^{i\alpha Q}\Omega, \phi\phi e^{i\alpha Q}\Omega) = e^{-2i\alpha}\cdot(\Omega,\phi\phi\Omega)$), while only the "neutral ones" are non-zero:

$$(\Omega, \phi^*(x)\phi(y)\Omega) = (\Omega,\phi(x)\phi^*(y)\Omega) = \Delta_m(x-y).$$

The factorization of higher correlation functions holds as for neutral free fields (Wick's Theorem still applies), but only the neutral pairings are non-zero, thus the sum extends only over "neutral partitions". In particular, all correlations of different numbers of fields ϕ and ϕ^* must vanish ("charge conservation").

Notice that the invariance argument applies, whenever there is an operator Q such that $[Q,\phi(x)] = \phi(x)$, $[Q,\phi^*(x)] = -\phi^*(x)$ and $Q\Omega = 0$, hence only neutral correlation functions can be non-zero. This may be the case even when the fields are not free fields and their VEV do not factorize.

4 Relativistic QFT

Here and from now on, $x^\mu = (ct, \vec{x})$ is a four-vector.

The Poincaré group are all transformations $\mathbb{R}^4 \ni x \mapsto \Lambda x + a$ which leave $dx_\mu dx^\mu$ invariant. It is generated by the translations $x \mapsto x + a$ and the Lorentz transformations $x^\mu \mapsto (\Lambda x)^\mu = \Lambda^\mu{}_\nu x^\nu$. In terms of the metric $\eta = diag(+---)$, the condition is

$$\eta_{\mu\kappa}\Lambda^\mu{}_\nu\Lambda^\kappa{}_\lambda = \eta_{\nu\lambda}.$$

This implies $|\det\Lambda| = 1$ and $|\Lambda^0{}_0| \geq 1$.

The Lorentz group is generated by the rotations $R_i(\alpha)$ of $\vec{x}$ (with matrix $\Lambda = \begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix}$ in the j-k plane), the boosts $B_i(\theta)$ ($\Lambda = \begin{pmatrix} \cosh\theta & \sinh\theta \\ \sinh\theta & \cosh\theta \end{pmatrix}$ in the 0-i plane), and the space and time inversions $P : \vec{x} \mapsto -\vec{x}$ and $T : x^0 \mapsto -x^0$. (Here, ijk is a cyclic permutation of 123. The boost velocity is $v = c\tanh\theta$.) The boosts and rotations have $\det\Lambda = +1$, the inversions have $\det\Lambda = -1$. Only LT involving a time inversion have $\Lambda^0{}_0 \leq -1$. Those LT with $\Lambda^0{}_0 \geq +1$ form the orthochronous subgroup.

4.1 Relativistic Invariance

Classical relativistic invariance (for a scalar field) means that along with $\varphi(x)$, also

$$\varphi_{\Lambda,a}(x) = \varphi(\Lambda x + a)$$

satisfies the respective equation of motion.

Classical relativistic invariance is an automatic consequence of Lorentz invariance of the Lagrangean density and absence of explicit x-dependence, ie Lorentz and translation invariance of the action

$$S = c^{-1}\int d^4x\mathcal{L}(\varphi, \partial\varphi).$$

Therefore, it holds for every Lagrangean of the form

$$\mathcal{L} = \frac{c^2}{2}\,\partial_\mu\varphi\,\partial^\mu\varphi - V(\varphi)$$

with equation of motion

$$\partial_\mu\partial^\mu\varphi = -V'(\varphi)/c^2.$$

While we have started from a relativistically invariant classical field theory, it is not obvious that the resulting quantum field theory preserves this invariance: the new elements are the vacuum vector and the canonical commutation relations holding at any fixed time: therefore the step of "quantization" might break the invariance.

Covariance

Quantum relativistic invariance is a much stronger property than an invariant equation of motion. It requires a unitary representation

$$(a,\Lambda)\mapsto U(a,\Lambda)$$

of the orthochronous Poincaré group, satisfying the composition law

$$U(a_2,\Lambda_2)U(a_1,\Lambda_1)=U(a_2+\Lambda_2 a_1,\Lambda_2\Lambda_1),$$

which leaves the vacuum state invariant and implements the transformation of the fields

$$U(a,\Lambda)\Omega=\Omega\quad\text{and}\quad U(a,\Lambda)\varphi(x)U(a,\Lambda)^*=\varphi(\Lambda x+a).$$

This clearly implies that all vacuum expectation values are invariant.

For free fields, $U(a,\Lambda)$ is defined by its action on the Fock space: $U(a,\Lambda)=U(a)U(\Lambda)$ with

$$U(a)A^*(\vec{k}_1)\cdots A^*(\vec{k}_N)\Omega:=e^{i\sum_n k_{n\mu}a^\mu}A^*(\vec{k}_1)\cdots A^*(\vec{k}_N)\Omega,$$

where always $k^0=\omega(\vec{k})/c$, and

$$U(\Lambda)A^*(\vec{k}_1)\cdots A^*(\vec{k}_N)\Omega:=\prod\nolimits_n\sqrt{(\Lambda k_n)^0/k_n^0}\;A^*((\Lambda k_1)^\rightarrow)\cdots A^*((\Lambda k_1)^\rightarrow)\Omega.$$

The square root factors are necessary to make U unitary (it must preserve the inner products $\sim\delta(\vec{k}-\vec{k}')$), because the Jacobi determinant is $|\det(\partial(\Lambda k)^i/\partial k^j)|=\sqrt{(\Lambda k)^0/k^0}$. This formula suggests to re-define

$$a(k)=\sqrt{(2\pi)^3 2\omega(\vec{k})}\cdot A(\vec{k})$$

so that the LT transformation law simplifies to

$$U(\Lambda)a^*(k_1)\cdots a^*(k_N)\Omega=a^*(\Lambda k_1)\cdots a^*(\Lambda k_1)\Omega.$$

Here $k^\mu=(\omega(\vec{k})/c,\vec{k})$ lies on the Lorentz invariant mass hyperboloid

$$H_m=\{k\in\mathbb{R}^4:\ k_\mu k^\mu=m^2c^2/\hbar^2,\ k^0>0\}.$$

It follows

$$U(a)a(k)U(a)^*=e^{-ika}a(k),\qquad U(\Lambda)a(k)U(\Lambda)^*=a(\Lambda k).$$

In terms of these relativistic creation and annihilation operators, the field is

$$\varphi(x)=\sqrt{\hbar/c}\int_{H_m}\widetilde{dk}\,\big(a(k)e^{-ik_\mu x^\mu}+a^*(k)e^{ik_\mu x^\mu}\big)$$

where $\widetilde{dk}$ is the Lorentz invariant measure on the mass hyperboloid

$$\widetilde{dk}=\frac{d^3k}{(2\pi)^3 2k^0}\Big|_{ck^0=\omega(\vec{k})},$$

such that

$$\int_{H_m}\widetilde{dk}\,f(k)=(2\pi)^{-3}\int_{\mathbb{R}^4}d^4k\,\delta(k_\mu k^\mu-m^2c^2/\hbar^2)\theta(k^0)\,f(k).$$

The commutation relations now read

$$[a(k), a^*(k')] = (2\pi)^3 2k^0\, \delta(\vec{k} - \vec{k}'),$$

or, putting $a^*(f) = \int_{H_m} \widetilde{dk}\, f(k) a^*(k)$,

$$[a(f), a(g)^*] = (f,g)_{\mathcal{H}_1} = \int_{H_m} \widetilde{dk}\, \overline{f(k)} g(k).$$

These formulae manifestly express the Lorentz covariance $U(a,\Lambda)\varphi(x)U(a,\Lambda)^* = \varphi(\Lambda x + a)$ of the free field. Moreover, the 2-pt fn can be written as

$$\Delta_m(x-y) = (\Omega, \varphi(x)\varphi(x')\Omega) = \hbar c^{-1}(2\pi)^{-3} \int d^4k\, \delta(k_\mu k^\mu - m^2c^2/\hbar^2)\theta(k^0)\, e^{-ik_\mu(x-x')^\mu}.$$

(Performing the k^0-integral with the help of the δ-function fixes $k^0 = \omega(\vec{k})/c$ and reproduces the factor $1/2k^0 = c/2\omega(\vec{k})$.) In this integral representation, everything is invariant: the integration measure, the arguments of the δ- and exponential functions, and the *sign* of the zero component four-vector k^μ – provided Λ is orthochronous. For a time reflection, one finds $\Delta_m(Tx - Ty) = \overline{\Delta_m(x-y)}$.

In the general case, there will not be an explicit construction of the field. However, when one can construct the correlation functions, then one can obtain the unitary representation by

$$U(a,\Lambda)\varphi(x_1)\cdots\varphi(x_N)\Omega := \varphi(\Lambda x_1 + a)\cdots\varphi(\Lambda x_N + a)\Omega$$

(for all N), which is unitary iff the correlation functions are invariant. Namely, the inner products between such vectors are the correlation functions! For the time reflection, the operator $U(T)$ defined by the same formula with $\Lambda = T$, $a = 0$ turns out to be anti-unitary iff the correlation functions go into their complex conjugates under $x \to Tx$ (as they do for the free field).

Generators

We now want to study the generators of infinitesimal transformations: If $s \mapsto g_s$ is a one-parameter subgroup, then $U(g_s) = e^{iXs/\hbar}$ where X is the generator. Taking the derivative of the covariance law $U(g_s)\varphi(x)U(g_s)^* = \varphi(g_s x)$ wrt s at $s = 0$, we have

$$i[X, \varphi(x)] = \hbar\, \partial_s \varphi(g_s(x))|_{s=0}.$$

For the translations this gives

$$i[P_0, \varphi(x)] = \hbar\partial_0\varphi(x), \qquad i[P_i, \varphi(x)] = \hbar\partial_i\varphi(x).$$

These generators are the energy and momentum operators:

$$P^\mu = (H/c, \vec{P}).$$

We write their representations as integrals over densities in a covariant way: The *stress-energy tensor* is

$$T^\mu{}_\nu := :\frac{\partial\mathcal{L}}{\partial(\partial_\mu\varphi)}\,\partial_\nu\varphi - \delta^\mu{}_\nu\mathcal{L}:.$$

Then, $T^{00} = \rho_E$ is precisely the energy density, while $T^{0i}/c = \rho_{P^i}$ is the momentum density (see Sect. 3.3). The remaining components can be interpreted as densities for the flows of energy and momentum: one has the conservation laws

$$\partial_\mu T^{\mu\nu} = 0$$

as a consequence of the equation of motion. The associated conserved quantities are

$$P^\nu = c^{-1} \int d^3x\, T^{0\nu}(x).$$

Their commutation relations with the field follow from $H = \int \frac{1}{2}\pi^2 + \dots$ and $\vec{P} = -\int \pi\nabla\varphi$ along with the CCR.

For the generators of the rotations about the i-axis and boosts in the i-direction, we find the infinitesimal transformation laws

$$i[L_i, \varphi(x)] = \hbar(x^j\partial_k - x^k\partial_i)\varphi(x), \qquad i[K_i, \varphi(x)] = \hbar(x^0\partial_i + x^i\partial_0)\varphi(x),$$

or

$$i[M_{\mu\nu}, \varphi(x)] = \hbar(x_\mu\partial_\nu - x_\nu\partial_\mu)\varphi(x).$$

with $L_i = M_{jk} = -M_{kj}$ (angular momentum), and $K_i = M_{0i} = -M_{i0}$.

Also the generators $M_{\mu\nu}$ of rotations and boosts are integrals over densities. Namely, there holds also the conservation law

$$\partial_\mu(x_\kappa T^\mu{}_\nu - x_\nu T^\mu{}_\kappa) = (x_\kappa\partial_\mu T^\mu{}_\nu + \eta_{\mu\kappa}T^\mu{}_\nu) - (\nu \leftrightarrow \kappa) = T_{\kappa\nu} - T_{\nu\kappa} = 0,$$

whenever the conserved stress-energy tensor is symmetric. This is obviously the case for our model Lagrangeans $\frac{c^2}{2}\partial_\mu\varphi\partial^\mu\varphi - V(\varphi)$, and one can show that one can always redefine a general relativistic invariant Lagrangean by adding a term that does not affect the equations of motion, so that the modified SET is symmetric. The associated conserved quantities are

$$M_{\mu\nu} = c^{-1} \int d^3x (x_\mu T^0{}_\nu - x_\nu T^0{}_\mu).$$

The required commutators of $M_{\mu\nu}$ with the field again follow from the CCR.

For the free field, all generators can be expressed in terms of a, a^*:

$$P_\mu = \hbar \int \widetilde{dk}\, a^*(k)k_\mu a(k), \quad M_{\mu\nu} = i\hbar \int \widetilde{dk}\, a^*(k)(k_\mu\partial_{k^\nu} - k_\nu\partial_{k^\mu})a(k).$$

The CR among the generators (the Poincaré Lie algebra) can be directly verified

$$[P_\mu, P_\nu] = 0, \quad [M_{\mu\nu}, P_\kappa] = i\hbar(\eta_{\nu\kappa}P_\mu - \eta_{\mu\kappa}P_\nu), \quad [M_{\mu\nu}, M_{\kappa\lambda}] = i\hbar(\eta_{\nu\kappa}M_{\mu\lambda} \pm \dots),$$

as well as their action on one-particle states $|f\rangle \equiv \int \widetilde{dk}\, f(k)a^*(k)\Omega$:

$$P_\mu|f\rangle = |p_\mu f\rangle, \quad M_{\mu\nu}|f\rangle = |m_{\mu\nu}f\rangle,$$

where $(p_\mu f)(k) = \hbar k_\mu f(k)$, $(m_{\mu\nu}f)(k) = i\hbar(k_\mu\partial_\nu - k_\nu\partial_\mu)f(k)$. The action of each generator X on multi-particle states is the sum over the actions on each one-particle state:

$$X|f_1, \dots, f_N\rangle = \sum\nolimits_{k=1}^{N} |f_1, \dots, Xf_k, \dots f_N\rangle.$$

4.2 Causality

Apart from relativistic transformation laws, Relativity demands that no signal can travel faster than light, and in particular, no events can influence each other if they are at spacelike distance. In QT, an observable represents a measurement, which changes the state ("collapse of the state"). Absence of causal influence between two measurements is then equivalent to commutativity of the corresponding operators.

We shall now see, that (free scalar) quantum fields commute at spacelike distance. This justifies the interpretation of $\varphi(x)$ as an observable that can be measured at the spacetime point x.

The Principle of Locality (or Causality) therefore asserts that all observable quantum fields should have this property

$$[\phi_1(x), \phi_2(y)] = 0 \qquad \text{whenever} \quad (x-y)^2 < 0.$$

To verify this for free fields, whose commutator is in any case a multiple of the unit operator, it is sufficient to show that the vacuum expectation value of the commutator vanishes at spacelike distance. This is equivalent to showing that the 2-point function $\Delta_m(x-y) = (\Omega, \varphi(x)\varphi(y)\Omega)$ is symmetric under $x \leftrightarrow y$ if $x-y$ is spacelike. For $x^0 = y^0$ (equal time), this property is obvious by inspection of the Fourier representation of the two-point function, since $\vec{x} \leftrightarrow \vec{y}$ can be absorbed into the change of integration variables $\vec{k} \leftrightarrow -\vec{k}$. The argument fails at different times; but then one can exploit relativistic invariance: if $x-y$ is spacelike, there is a Lorentz transformation such that $(\Lambda x)^0 = (\Lambda y)^0$, hence

$$\Delta_m(x-y) = \Delta_m(\Lambda x - \Lambda y) = \Delta_m(\Lambda y - \Lambda x) = \Delta_m(y-x).$$

4.3 $\hbar = c = 1$

It is convenient to suppress all factors of $\hbar$ and of c; eg putting $c = 1$ amounts to measuring "time" in terms of distance covered by a light ray ("light year"), and putting $\hbar = 1$ amounts to measuring energy in terms of the corresponding deBroglie frequency. It is custumary to express all dimensions as "powers of mass", eg, energy, momentum, frequency, derivatives all have dimension +1. The true constants can always be restored by remembering Einstein's and deBroglie's formula by which

$$[\text{mass} \cdot c^2] = [\text{momentum} \cdot c] = [\text{energy}] = [\hbar/\text{time}] = [\hbar c/\text{length}].$$

The physical dimension of fields is determined by the requirement that the Lagrangean action $S = c^{-1} \int d^4x \, \mathcal{L}[\phi]$ has the dimension of an action, ie $S/\hbar$ is dimensionless, and $\mathcal{L}$ is energy per volume.

Lateron, for the electromagnetic interaction, we shall also put $\varepsilon_0 = 1$ (hence $\mu_0 = 1$), thus measuring electric charges in dimensionless units (Coulomb's law $E = e^2/4\pi\varepsilon_0 r$ where E and $1/r$ already have the same dimension by $\hbar = c = 1$.) The elementary charge (of the electron) has then the magnitude $e^2 = 4\pi\alpha$, where the fine structure constant α is (in true units) $\alpha = e^2/4\pi\varepsilon_0\hbar c \approx 1/137$.)

4.4 Wigner analysis

Most realistic particles carry some spin. We shall see that the spin is a relativistic property of the one-particle space. The Wigner analysis provides a classification of all one-particle spaces with relativistic invariance and positive energy.

Wigner's Theorem states that every symmetry $\Psi \to \Psi'$ which preserves transition probabilities:

$$|(\Psi'_1, \Psi'_2)|^2 = |(\Psi_1, \Psi_2)|^2$$

is realized either by a unitary or by an anti-unitary operator

$$\Psi' = U\Psi,$$

which is unique up to a phase. A symmetry group G must then be realized by a unitary *ray* representation of the group, ie $U(g)$ satisfy the group composition law up to a phase:

$$U(g)U(h) = e^{ic(g,h)}U(gh).$$

One cannot always fix the phases of $U(g)$ in a continuous way such that all $c(g,h) = 1$. But it is always possible to get a true representation of the covering group $\widetilde{G}$.

The covering group $\widetilde{G}$ of a connected group G is the (unique) simply connected group that has "locally" the same group law as G. This means, there is a group homomorphism $\pi : \widetilde{G} \to G$ which is bijective on a neighbourhood of the identity. If G is not itself simply connected (in which case $\widetilde{G} = G$), then π is not globally injective, ie, it takes several elements of $\widetilde{G}$ to the same element of G. $\widetilde{G}$ can be defined as the group of homotopy classes of curves within the original group.

A familiar example is $SU(2)$ as the (twofold) covering of $SO(3)$. Every matrix $g \in SU(2)$ can be written as $g = e^{i\alpha\vec{n}\cdot\vec{\sigma}/2} = \cos\frac{1}{2}\alpha\,\mathbf{1}_2 + i\sin\frac{1}{2}\alpha\,\vec{n}\cdot\vec{\sigma}$ where σ_i are the Pauli matrices and $\vec{n}$ is a unit vector. Then $\pi(g) \in SO(3)$ is the rotation by the angle α around the axis $\vec{n}$. In particular $\pi(-g) = \pi(g)$ and $\pi(+\mathbf{1}_2) = \pi(-\mathbf{1}_2) = \mathbf{1}_3$. The representations of the angular momentum algebra $[J_i, J_j] = i\varepsilon_{ijk}J_k$ with halfinteger spin j are in fact representations of $SU(2)$: the rotations by the angle α around the axis $\vec{n}$ are represented by $e^{i\alpha\vec{n}\cdot\vec{J}}$ where J_k have half-integer eigenvalues, hence the full rotations about an angle 2π (given by $\mathbf{1}_3 \in SO(3)$ but $-\mathbf{1}_2 \in SU(2)$) are represented by $-\mathbf{1}_{2j+1}$.

The covering group of the connected (=proper) Lorentz group $\mathcal{L}^\uparrow_+$ is $SL(2,\mathbb{C})$. The covering projection can be described as follows. With any four vector $v = (v^0, \vec{v})$ we bijectively associate the hermitean matrix

$$M_v = v^0\mathbf{1}_2 + \vec{v}\cdot\vec{\sigma} = \begin{pmatrix} v^0 + v^3 & v^1 - iv^2 \\ v^1 + iv^2 & v^0 - v^3 \end{pmatrix}.$$

Then $det(M_v) = v_\mu v^\mu$. Since the map $M \mapsto AMA^*$ for $A \in SL(2,\mathbb{C})$ preserves hermiticity and the value of the determinant, we can define $\pi(A) = \Lambda_A$ by

$$AM_vA^* = M_{\Lambda_A v}$$

where Λ_A is a Lorentz transformation, $\Lambda_{A_1}\Lambda_{A_2} = \Lambda_{A_1A_2}$, and $\Lambda_{-A} = \Lambda_{+A}$.

In particular, the subgroup $SU(2)$ (which preserves also the trace, hence v^0) projects to the rotations as above, and the hermitean elements $\cosh\frac{1}{2}\theta\,\mathbf{1}_2+\sinh\frac{1}{2}\theta\,\vec{n}\cdot\vec{\sigma}$ of $SL(2,\mathbb{C})$ project to the boosts by the rapidity θ in the direction $\vec{n}$.

Since a particle is a particle in every Lorentz frame, the one-particle subspace should carry a unitary representation of the twofold covering of the Poincaré group.

The Wigner classification of unitary irreducible representations (UIRs) proceeds by the following steps.

1. Let P_μ be the generators of the commutative translation subgroup, $U(a) = e^{iP_\mu a^\mu}$. Since P_μ commute, they can be simultaneously diagonalized. Their joint spectrum consists of four-vectors k_μ (the momenta of the particles).

2. We have $U(A)U(a)U(A)^* = U(\Lambda_A a)$, implying $U(A)P_\mu U(A)^* = (\Lambda_A^{-1}P)_\mu$. Hence, the operator $M^2 = P_\mu P^\mu$ commutes with $U(a,A) = U(a)U(A)$. By Schur's Lemma, it must be a multiple of $\mathbf{1}$ in an irreducible representation. Let $M^2 = m^2\cdot\mathbf{1}$, then all particle momenta satisfy $k_\mu k^\mu = m^2$, hence m^2 must be nonnegative and m is the mass of the particles. Then $k \in H_m$ (the mass hyperboloid).

3. $P_\mu|k\rangle = k_\mu|k\rangle$ implies $P_\mu U(A)|k\rangle = (\Lambda_A k)_\mu U(A)|k\rangle$, hence $U(A)|k\rangle$ has eigenvalue $\Lambda_A k$. Hence if any $k \in H_m$ occurs in the spectrum, then every $k \in H_m$ occurs. For $m = 0$, the eigenvalue $k = 0$ cannot be transformed into $k \neq 0$. Thus, $H_{m=0}$ = the future null vectors without 0 and $\{0\}$ correspond to different UIRs. We discard $k = 0$ because it describes particles with zero energy and momentum.

Since the spectrum is continuous, the eigenvectors cannot be proper vectors in the Hilbert space. Normalizable Hilbert space vectors are rather of the form

$$|f\rangle = \int \widetilde{dk} \sum\nolimits_i f_i(k)|k\rangle_i.$$

4. An eigenvalue k may be degenerate. Then every other eigenvalue has the same degeneracy because eigenvectors of different k are related by the unitary operator $U(A)$, as in 3. We may choose bases $|k\rangle_i$ of the (improper) eigenspaces $\mathcal{H}_k$ with eigenvalue k, normalized such that

$${}_j\langle k'|k\rangle_i = (2\pi)^3 2k^0\delta(\vec{k}-\vec{k}')\delta_{ij}.$$

Let $k_0 \in H_m$ be some reference vector, eg $k_0 = (m,\vec{0})$ if $m \neq 0$. For every $k \in H_m$ one may choose a LT $B_k \in SL(2,\mathbb{C})$ such that $\Lambda_{B_k}k_0 = k$, eg the pure boost

$$B_k = (M_k/m)^{1/2} = \big((k^0+m)\,\mathbf{1} + \vec{k}\cdot\vec{\sigma}\big)/\sqrt{2m(k^0+m)}.$$

Then we may relate the bases in *different* eigenspaces by putting

$$|k\rangle_i := U(B_k)|k_0\rangle_i.$$

5. $U(A)$ maps the eigenspace $\mathcal{H}_k$ onto itself iff Λ_A preserves an eigenvalue: $\Lambda_A k = k$. The LTs A for which Λ_A fixes the reference eigenvalue k_0, are called the "little group". If $m > 0$ and $k_0 = (m,\vec{0})$, hence $M_{k_0} = m\mathbf{1}_2$, the little group is $SU(2) \subset SL(2,\mathbb{C})$, the covering group of the rotations. (The case $m = 0$ will be treated below.)

The little group $SU(2)$ preserves the eigenspace $\mathcal{H}_{k_0}$, ie the latter carries a UIR of $SU(2)$. But the UIRs u of $SU(2)$ are well-known: they are given by the integer- or halfinteger-spin s representations of the angular momentum algebra.

6. Once we specify the mass and representation u of the little group on $\mathcal{H}_{k_0}$, the representation $U(a,A) = U(a)U(A)$ of the Poincaré group on the one-particle space $\mathcal{H}$ is fixed: we have $U(a)|k\rangle_i = e^{ika}|k\rangle_i$ and the action of $U(A)$ as follows: For $k \in H_m$ let B_k be the boost that maps k_0 to k. Then for any LT $A \in SL(2,\mathbb{C})$, $g_{A,k} := B^{-1}_{\Lambda_A k} A B_k$ maps k_0 to k_0, hence it belongs to the little group (it is called the "Wigner rotation"), and $U(g)|k_0\rangle_i = |k_0\rangle_j u_{ji}(g)$. Therefore

$$U(A)|k\rangle_i = U(B_{\Lambda_A k})U(g_{A,k})U(B_k)^*|k\rangle_i = U(B_{\Lambda_A k})U(g_{A,k})|k_0\rangle_i = \\ = U(B_{\Lambda_A k}) \textstyle\sum_j |k_0\rangle_j u_{ji}(g_{A,k}) = \sum_j |\Lambda_A k\rangle_j u_{ji}(g_{A,k}).$$

7. We conclude that the massive representations on the one-particle space are completely determined by the mass $m > 0$ and the spin s. If $s = 0$, the representation of the little group is trivial: $u(g) = 1$, and the induced representation of the Poincaré group is precisely the one we know from the scalar free field:

$$U(a,\Lambda)|k\rangle = U(a)U(\Lambda)|k\rangle = e^{ia\Lambda k}|\Lambda k\rangle.$$

If s is integer, it is a true representation ($U(\Lambda_A) = U(-A) = U(A)$), if s is halfinteger, it is a representation of the covering group ($U(-A) = -U(A)$).

8. In the massless case $k_\mu k^\mu = 0$, we cannot choose the reference eigenvalue $k_0 = (m = 0, \vec{0})$. One may choose any null vector, say $k_0 = (\frac{1}{2}, 0, 0, \frac{1}{2})$. The little group preserving this vector contains the rotations $SO(2) \subset SO(3)$ in the 1-2 plane (or rather the diagonal subgroup of $SU(2)$ in the covering group) and a two-parameter abelian subgroup T of combined rotations around the 1- and 2-axis and boosts in the 1- and 2-directions with generators $M_{0i} - M_{3i}$ ($i = 1, 2$). The unitary representations of this little group fall into two classes: Those where T is nontrivially represented, are infinite-dimensional, and those where T is trivially represented are one-dimensional: the rotations by the angle α are represented by the complex phase $e^{i\alpha h}$. Because the representation should extend to a true representation of the two-fold covering $SU(2)$ of $SO(3)$, the "helicity" h must be an integer or halfinteger number (positive or negative).

The infinite-dimensional representations seem not to be realized in nature (they cannot be associated with local free fields; yet there are recent speculations about a possible role in the dark matter problem). There remain the massless helicity representations, which are uniquely determined by the value $h \in \frac{1}{2}\mathbb{Z}$. The method is the same as above, but one has to choose other LTs B_k. One may choose $B_k = (k^0 - k^3)^{-1/2} \begin{pmatrix} k^0 - k^3 & 0 \\ k^1 + ik^2 & 1 \end{pmatrix}$, which transforms $M_{k_0} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$ to M_k. Then

$$U(A)|k\rangle = u_h(g_{A,k})|\Lambda_A k\rangle = e^{ih\alpha(A,k)}|\Lambda_A k\rangle$$

with the "Wigner phase" $\alpha(A,k)$ given by the angle of the Wigner rotation (ie the $SO(2)$ part of $g_{A,k} = B^{-1}_{\Lambda_A k} A B_k$ in the little group).

4.5 Free scalar field from the Wigner representation

After the classification of possible particle types by the Wigner analysis, we want to construct local fields that create such particles from the vacuum. The easiest case is the scalar field, which is just another way of writing our previous construction in Chap. 3.2. The cases of massless spin-1 particles (photons) and massive or massless spin-$\frac{1}{2}$ particles (electrons, neutrinos) will be treated separately.

Let $\mathcal{H}_1$ be the Hilbert space of the scalar representations with mass m of the Poincaré group. Its vectors are of the form $|f\rangle = \int \widetilde{dk}\, f(k)|k\rangle \equiv \int \frac{d^3k}{(2\pi)^3 2k^0} f(k^0,\vec{k})|k\rangle$ with norm $\langle f|f\rangle^2 = \int \frac{d^3k}{(2\pi)^3 2k^0}|f(k^0,\vec{k})|^2$. Let $\mathcal{H}$ be the associated symmetric Fock space, spanned by vectors $|f\rangle_n = \int \widetilde{dk}_1 \cdots \widetilde{dk}_n f_n(k_1,\cdots,k_n)|k_1\rangle\otimes\cdots\otimes|k_n\rangle \in \mathcal{H}_n$ where f_n are symmetric momentum space wave functions, $n\in\mathbb{N}_0$, with $\langle f_n|f_n\rangle = \int \widetilde{dk}_1\cdots\widetilde{dk}_n|f_n(k_1,\cdots,k_n)|^2$. The scalar Wigner representation canonically extends to tensor products, and hence to the Fock space.

Define the creation operators by

$$a^*(f)|f_n\rangle := \frac{1}{(n+1)!}|(f\otimes f_n)_S\rangle \in \mathcal{H}_{n+1},$$

where $(f\otimes f_n)(k,k_1,\cdots,k_n) = f(k)f_n(k_1,\cdots,k_n)$, and $(\cdot)_S$ means the sum over all permutations. Define $a(f)$ to be the adjoint of $a^*(\overline{f})$, which turns out to be

$$a(f)|f_n\rangle = |f_{n-1}\rangle \in \mathcal{H}_{n-1}$$

with $f_{n-1}(k_1,\ldots,k_{n-1}) = \int \widetilde{dk}\, f(k)f_n(k,k_1,\cdots k_{n-1})$. Since both a and a^* are linear in f, one may formally write $a^*(f) = \int \widetilde{dk}\, a^*(k)$, $a(f) = \int \widetilde{dk}\, a(k)$, thus defining $a^*(k)$ and $a(k)$ as operator-valued distributions, satisfying the same commutation relations as in Sect. 4.1. From the Wigner representation it follows that

$$U(a)a^*(k)U(a)^* = e^{ika}a^*(k) \quad \text{and} \quad U(\Lambda)a^*(k)U(\Lambda)^* = a^*(\Lambda k).$$

The scalar free field is now constructed as

$$\varphi(x) = \int \widetilde{dk}\,\big[a^*(k)e^{ikx} + a(k)e^{-ikx}\big].$$

The transformation laws of the creation and annihilation operators imply that

$$U(a)\varphi(x)U(a)^* = \int \widetilde{dk}\,\big[e^{ika}a^*(k)e^{ikx} + e^{-ika}a(k)e^{-ikx}\big] = \varphi(x+a),$$
$$U(\Lambda)\varphi(x)U(\Lambda)^* = \int \widetilde{dk}\,\big[a^*(\Lambda k)e^{ikx} + h.c.\big] = \int \widetilde{dk}\,\big[a^*(k)e^{ik\Lambda x} + h.c.\big] = \varphi(\Lambda x),$$

where the Lorentz invariance of the measure $\widetilde{dk}$ was essential.

We have thus constructed a covariant quantum field out of the Wigner representation, and the result is exactly the same as in Sect. 4.1. Its correlation functions are expressed by Wick's theorem in terms of 2-point functions, and locality follows as in Sect. 4.1 by inspection of the 2-point function. We anticipate that, trying the same construction with non-scalar representations, the presence of a Wigner rotation or Wigner phase would spoil the argument for the Lorentz covariance.

4.6 Free Maxwell field **(some details may be skipped)**

The canonical quantization of a classical pair of conjugate Hamiltonian variables turns out to be problematic in the case of gauge fields. We shall briefly sketch this approach, which can be found in most textbooks, and then present an alternative approach which starts from the Wigner analysis: The Hilbert space is the Fock space over the Wigner one-particle space, and the local fields are suitable combinations of the creation and annihilation operators, which must be found in such a way as to guarantee covariance and local commutativity.

We have already noted that the Maxwell Lagrangean $-\frac{1}{4}F_{\mu\nu}F^{\mu\nu}$ does not produce a conjugate momentum to the variable A^0. From the classical gauge invariance $A_\mu \to A_\mu + \partial_\mu\Gamma$ of electrodynamics we know that one may impose a gauge condition to eliminate (part of) this ambiguity. A relativistically invariant condition is the Lorentz gauge condition $\partial_\mu A^\mu = 0$: The idea is to add a term $\mathcal{L}_{\rm gauge} = -\frac{1}{2}\lambda(\partial_\mu A^\mu)^2$ and impose the Lorentz gauge later (making this change ineffective). [Modified EOM

$$\Box A_\mu = (1-\lambda)\partial_\mu(\partial A),$$

propagator $\sim \eta^{\mu\nu} + \frac{1-\lambda}{\lambda}\frac{k^\mu k^\nu}{k^2}$, Feynman gauge $\lambda = 1$, Landau gauge $\lambda \to \infty$.]

Adding the gauge term now produces a nontrivial conjugate momentum $\pi_0 = -\lambda\partial_\mu A^\mu$, so it makes sense to impose the covariant equal time CCR

$$[A^\mu(\vec{x}), \pi^\nu(\vec{y})] = -i\eta^{\mu\nu}\delta(\vec{x}-\vec{y}).$$

These can be realized by C & A operators a^μ and $a^{*\mu}$ satisfying CR

$$[a^\mu(k), a^{*\nu}(k')] = -2k^0\delta(\vec{k}-\vec{k}')\cdot\eta^{\mu\nu},$$

and allows to construct fields with local commutation relations in space and time.

The problem are the opposite signs of η, giving rise to states $a^{*0}(k)\Omega$ of negative norm square! (Choosing η instead of $-\eta$ clearly doesn't help.) The Fock space has indefinite scalar product and is not a Hilbert space, which spoils any probabilistic interpretation.

One overcomes this problem by imposing the gauge condition. One could try to look for a subspace of vectors with $(\partial_\mu A^\mu)\Psi = 0$. Unfortunately such vectors do not exist. Instead one imposes on "admissible" states the Gupta-Bleuler condition $(\partial_\mu A^\mu)_-\Psi = 0$ where $(\partial_\mu A^\mu)_-$ is only the annihilation part of $\partial_\mu A^\mu$. Then the full gauge condition is satisfied in the sense that $(\Psi', (\partial_\mu A^\mu)\Psi) = 0$ between any pair of physical vectors. It turns out that admissible one-particle vectors are of the form $|n\rangle = n_\mu a^{*\mu}(k)\Omega$ where $n_\mu k^\mu = 0$, ie there are only three linearly independent ones for every given $k \in H_0$. If n is parallel to k, then $|n\rangle$ has norm zero, all others have positive norm square. Indeed, it turns out that the entire admissible subspace has positive semi-definite scalar product. One then passes to a quotient space by identifying all null vectors with 0. This gives a true "physical" Hilbert space, whose

one-particle subspace contains only two "transversal" states for each k. These two states correspond to the two polarizations of classical electromagnetic waves.

Only those operators on the original space are well-defined on the quotient space, which take null vectors into null vectors. It turns out that precisely the gauge invariant operators $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ have this property. Moreover, the correlation functions $F_{\mu\nu}$ turn out to be independent of the auxiliary parameter λ in $\mathcal{L}_{\rm gauge}$. The gauge potentials are ill-defined on the physical Hilbert space.

We shall now present an alternative approach, based on the Wigner construction, which leads to the same results, but avoids intermediate indefinite spaces.

We start with the Wigner representations $m = 0$, $h = \pm 1$. Let ε be the sign of h. The Fock space is given by the symmetrized tensor products of the one-particle space. The latter is spanned by vectors

$$|f\rangle = \int \widetilde{dk} \sum\nolimits_{\varepsilon=+,-} f_\varepsilon(k)|k\rangle_\varepsilon$$

with the scalar product

$$\langle f|g\rangle = \int \widetilde{dk} \left(\overline{f_+(k)}g_+(k) + \overline{f_-(k)}g_-(k)\right).$$

We define C & A operators as in Sect. 4.5 by their action on the Fock space, in particular

$$|k\rangle_\varepsilon = a^*_\varepsilon(k)\Omega$$

with CR

$$[a_\varepsilon(k), a^*_{\varepsilon'}(k')] = {}_\varepsilon\langle k|k'\rangle_{\varepsilon'} = (2\pi)^3 2k^0\delta(\vec{k}-\vec{k}')\delta_{\varepsilon\varepsilon'}.$$

The specified representation implies

$$U(a)a^*_\varepsilon(k)U(a)^* = e^{ika}a^*_\varepsilon(k) \quad \text{and} \quad U(\Lambda)a^*_\varepsilon(k)U(\Lambda)^* = e^{i\varepsilon\alpha(\Lambda,k)}a^*_\varepsilon(\Lambda k).$$

The presence of the Wigner phase in the latter prevents us to write the same formula for two fields φ_ε as for the scalar fields, because they would not satisfy the proper Lorentz transformation law.

In order to "absorb" the undesired Wigner phase, one needs a trick to "intertwine" it into the desired transformation matrix (the tensor product $\Lambda \otimes \Lambda$) of the tensor field $F_{\mu\nu}$. We choose two four vectors

$$e^\mu_\pm = (0, 1, \pm i, 0)/\sqrt{2}$$

(amplitudes for circular polarized plane waves with wave vector $k_0 = (\frac{1}{2}, 0, 0, \frac{1}{2})$). They are eigenvectors of the Wigner rotations in the little group = rotations in the 1-2 plane: $R(\alpha)e_\varepsilon = e^{i\varepsilon\alpha}e_\varepsilon$, but the abelian part T of the little group maps e_ε to multiples of k_0. This behaviour reflects the ambiguity of the transversality condition $e_\mu k_0^\mu = 0$. We put

$$e_\varepsilon(k) := B_k e_\varepsilon.$$

Here, for simplicity, B_k stands for the true LT Λ_{B_k}. Then one has $\Lambda e_\varepsilon(k) = B_{\Lambda k}(B_{\Lambda k}^{-1}\Lambda B_k)e_\varepsilon$. Here $B_{\Lambda k}^{-1}\Lambda B_k$ is the element of the little group as in the Wigner analysis, ie it consists of the Wigner rotation $R(\alpha(\Lambda,k))$ in the 1-2 plane and some part in the abelian part T of the little group. The rotation acting on e_ε produces the Wigner phase $e^{i\varepsilon\alpha(\Lambda,k)}$ (helicities $\varepsilon = \pm 1$), while the abelian part produces a multiple of k_0, hence we get an inhomogeneous transformation law of the form

$$\Lambda e_\varepsilon(k) = e^{i\varepsilon\alpha(\Lambda,k)}(e(\Lambda k) + \gamma\,\Lambda k),$$

where the precise form of the function $\gamma \in \mathbb{C}$ doesn't matter. Then the fields

$$A_\varepsilon^\mu(x) = \int \widetilde{dk}\,\big(e_\varepsilon^\mu(k)a_\varepsilon(k)e^{-ikx} + \overline{e_\varepsilon^\mu(k)}a_\varepsilon^*(k)e^{ikx}\big)$$

transform "almost" covariantly as follows. We have

$$e_\varepsilon^\mu(k)\;U(\Lambda)a_\varepsilon(k)U(\Lambda)^* = e_\varepsilon^\mu(k)\;e^{-i\varepsilon\alpha(\Lambda,k)}a_\varepsilon(\Lambda k) = (\Lambda^{-1}e(\Lambda k) - \gamma\,k)^\mu\;a_\varepsilon(\Lambda k).$$

The Wigner phase has been absorbed in favour of a factor Λ^{-1}, and an inhomogeneous term proportional to k. We insert this into $U(\Lambda)A^\mu(x)U(\Lambda)^*$ and change the integration variable k to $\Lambda^{-1}k$. Then

$$U(\Lambda)A_\varepsilon^\mu(x)U(\Lambda)^* = \int \widetilde{dk}\,\big((\Lambda^{-1}e_\varepsilon(k))^\mu a(k)e^{-i(\Lambda^{-1}k)x} + cc.\big) + \int \widetilde{dk}\,k^\mu\,(\tilde\Gamma e^{-ikx} + cc.)$$

We have found a simultaneous transformation of the argument and of the four vector A^μ:

$$U(\Lambda)A_\varepsilon^\mu(x)U(\Lambda)^* = (\Lambda^{-1})^\mu{}_\nu A_\varepsilon^\nu(\Lambda x) + \partial^\mu\Gamma$$

along with a gauge transformation where the precise form of Γ does not matter. (The correct translation behaviour $U(a)A_\varepsilon^\mu(x)U(a)^* = A_\varepsilon^\mu(x+a)$ is obvious.) Moreover, because all momenta lie in $H_{m=0}$, one obviously has the equation of motion

$$\Box A_\varepsilon = 0.$$

Because of the Γ-term, the correlation functions are not Lorentz invariant. We can kill this term by passing to the fields

$$F_\varepsilon^{\mu\nu}(x) = \partial^\mu A_\varepsilon^\nu - \partial^\nu A_\varepsilon^\mu$$

which transform homogeneously like Lorentz tensors:

$$U(\Lambda)F_\varepsilon^{\mu\nu}(x)U(\Lambda)^* = (\Lambda^{-1})^\mu{}_\kappa(\Lambda^{-1})^\nu{}_\lambda F_\varepsilon^{\kappa\lambda}(\Lambda x).$$

But this is not sufficient for a relativistic QFT: The fields A_ε^μ and $F_\varepsilon^{\mu\nu}$ are neither hermitean, nor do they satisfy local commutativity, ie they violate the relativistic principle of causality. We can compute the two-point function:

$$(\Omega, A_\varepsilon^\mu(x)A_\varepsilon^\kappa(y)\Omega) = 4\pi\int \widetilde{dk}\,e_\varepsilon^\mu(k)\overline{e_\varepsilon^\kappa(k)}\,e^{-ik(x-y)}.$$

It fails to be local because the polarization vectors spoil the argument which showed commutativity at spacelike distance for the scalar 2-point function $\Delta_m(x-y)$.

This failure cannot be cured for the vector potentials. But for the Maxwell fields one can restore local commutativity by summing over both helicities:

$$F_{\mu\nu}(x) := F_{+\mu\nu}(x) + F_{-\mu\nu}(x).$$

Indeed, the identity

$$\sum\nolimits_{\varepsilon}(k^\mu e^\nu_\varepsilon(k) - k^\nu e^\mu_\varepsilon(k))\overline{(k^\kappa e^\lambda_\varepsilon(k) - k^\lambda e^\kappa_\varepsilon(k))} = k^{[\mu}\eta^{\nu][\kappa}k^{\lambda]}$$

(with the obvious anti-symmetries) allows to write the two-point function

$$(\Omega, F_{\mu\nu}(x)F_{\kappa\lambda}(y)\Omega) = 4\pi\ \partial_{[\mu}\eta_{\nu][\kappa}\partial_{\lambda]}\, D(x-y)$$

where the distribution $D(x) = \Delta_{m=0}(x)$ is the massless scalar two-point function (cf Sect. 5.7), which is local; hence the 2-point function of the electromagnetic field is also local. One also sees that $F^{\mu\nu}$ solves all the classical sourcefree Maxwell equations

$$\partial_\kappa F_{\mu\nu} + (\text{cyclic}) = 0, \quad \partial_\mu F^{\mu\nu} = 0.$$

Comparing the two approaches, we learn several things. The demands of relativistic covariance, locality, and Hilbert space positivity are quite nontrivial. For the vector potential, it is impossible to satisfy them simultaneously. In the canonical approach, positivity fails, while the first two fail in the Wigner approach. For the gauge invariant fields, the obstruction disappears. We should keep this in mind when we shall later quantize full electrodynamics with interaction $j_\mu A^\mu$ – a term that cannot be separately defined.

Second, we have seen that we need both helicities combined in the local electromagnetic fields $F^{\mu\nu}$. This is an instance of a more general theorem that in a covariant and local QFT with positive energy, every particle must have an anti-particle: helicity + and − photons are each other's anti-particles.

4.7 Free massive Dirac field (some details may be skipped)

We want to construct quantum fields for particles of mass m and spin $\frac{1}{2}$, again by combining the creation and annihilation operators of a Fock space to form covariant and local fields. The creation operators defined by

$$a^*_i(k)\Omega = |k\rangle_i$$

satisfy the transformation law

$$U(A)a^*_i(k)U(A)^* = a^*_j(\Lambda_A k)u(g_{A,k})_{ji}, \quad U(A)a_i(k)U(A)^* = a_j(\Lambda_A k)\overline{u(g_{A,k})_{ji}}.$$

Here, $g_{A,k} = B^{-1}_{\Lambda_A k}AB_k \in SU(2)$ is the Wigner rotation as before, and its spin-$\frac{1}{2}$ representation is given by $u(g) = g \in SU(2)$ (so that $|k\rangle_i$ are eigenvectors of L_3 in the particle's rest frame). Considering (a^*_i) as a column two-vector, we write $U(A)a^*(k)U(A)^* = g^T_{A,k}a^*(\Lambda_A k) = B^T_k A^T B^T_{\Lambda_A k}{}^{-1}a^*(\Lambda_A k)$.

We can get rid of the k-dependent rotation matrix by writing a covariant "creation part"

$$\varphi(x)_+ = \sqrt{m}\int \widetilde{dk}\, B_k^{T-1} a^*(k) e^{ikx}$$

where $mB_k^{-2} = (M_k)^{-1} = (k^0\mathbf{1}_2 - \vec{k}\cdot\vec{\sigma}) = k_\mu\sigma^\mu$ (with $\sigma^\mu = (\mathbf{1}_2, \vec{\sigma})$), such that

$$U(A)\varphi(x)_+U(A)^* = A^T\varphi(\Lambda_A x)_+.$$

The hermitean conjugate of φ_+ satisfies a different transformation with the matrix $\overline{A^T}$ instead of A^T. Hence, $\varphi(x)_+ + h.c.$ would not define a covariant quantum field. But there is a second option to get rid of the Wigner rotation: Because g is unitary, we have $g^T = \overline{g^{-1}} = \overline{B_k^{-1}}\,\overline{A^{-1}}\,\overline{B_{\Lambda_A k}}$. Therefore, $\overline{B_k}a^*(k)$ transforms into $\overline{A^{-1}}(\overline{B_{\Lambda_A k}}a^*(\Lambda_A k))$, and $B_k a(k)$ transforms into $A^{-1}(B_{\Lambda_A k}a(\Lambda_A k))$. Moreover, the (real) matrix

$$\mathcal{E} = i\sigma^2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \qquad \Rightarrow \quad \sigma^{iT}\mathcal{E} = -\mathcal{E}\sigma^i$$

has the property that $A^T\mathcal{E} = \mathcal{E}A^{-1}$ for all $A \in SL(2,\mathbb{C})$. From this, we see that

$$\varphi(x)_- = \sqrt{m}\int \widetilde{dk}\, \mathcal{E}B_k a(k) e^{-ikx}$$

transforms in the same way (with A^T) as $\varphi(x)_+$. Therefore

$$\varphi(x) = \sqrt{m}\int \widetilde{dk}\, \big(\mathcal{E}B_k a(k)e^{-ikx} + B_k^{T-1}a^*(k)e^{ikx}\big)$$

is a two-component ("spinor") field that transforms covariantly as

$$U(A)\varphi(x)U(A)^* = A^T\varphi(\Lambda_A x).$$

The hermitean conjugate field is (using that B_k are hermitean, hence $\overline{B_k} = B_k^T$)

$$\varphi^*(x) = \sqrt{m}\int \widetilde{dk}\, \big(B_k^{-1}a(k)e^{-ikx} + \mathcal{E}B_k^T a^*(k)e^{ikx}\big).$$

It transforms as

$$U(A)\varphi^*(x)U(A)^* = \overline{A^T}\varphi^*(\Lambda_A x).$$

In order to emphasize the different transformation laws, it is common usage to denote the components of the spinor field φ by φ_α, and those of the conjugate spinor by $\varphi^*_{\dot\alpha}$, eg $U(A)\varphi^*_{\dot\alpha}(x)U(A)^* = \varphi^*(\Lambda_A x)_{\dot\beta}\overline{A_{\dot\beta\dot\alpha}}$.

Let us now compute 2-point functions. We find

$$(\Omega, \varphi^*_{\dot\alpha}(x)\varphi_\alpha(y)\Omega) = m\int \widetilde{dk}\, (B_k^{-2})_{\dot\alpha\alpha} e^{-ik(x-y)}.$$

Here, B_k^{-2} is a positive matrix, as it should by Hilbert space positivity.

Using $mB_k^{-2} = (M_k)^{-1} = k_\mu\sigma^\mu$ (see above), we can also write this as

$$(\Omega, \varphi^*_{\dot\alpha}(x)\varphi_\alpha(y)\Omega) = i\,(\sigma^\mu)_{\dot\alpha\alpha}\partial_\mu \int \widetilde{dk}\, e^{-ik(x-y)} = i\,(\sigma^\mu)_{\dot\alpha\alpha}\partial_\mu \Delta_m(x-y).$$

Similarly, with $\mathcal{E}^T = \mathcal{E}^{-1}$ and $\mathcal{E}B_k^2\mathcal{E}^{-1} = (B^{-2})^T$

$$(\Omega, \varphi_\alpha(y)\varphi^*_{\dot\alpha}(x)\Omega) = m\int \widetilde{dk}\,(\mathcal{E}B_k^2\mathcal{E}^T)_{\alpha\dot\alpha}e^{-ik(y-x)} = i\,(\sigma^\mu)_{\dot\alpha\alpha}\partial_\mu\Delta_m(y-x).$$

This is also positive definite, as it should. But there is a conflict with local commutativity: for x spacelike, $\Delta_m(x) = -\Delta_m(x)$ is an even function, hence $\partial_\mu\Delta(x)$ is an odd function! Hence for spinor fields at spacelike distance, we *find*

$$(\Omega, \varphi_\alpha(y)\varphi^*_{\dot\alpha}(x)\Omega) = -(\Omega, \varphi^*_{\dot\alpha}(x)\varphi_\alpha(y)\Omega),$$

ie they **anti-commute** rather than commute. This is inevitable for fields of half-integer spin. Indeed, for spin-s fields, the representation $u(g)$ is the symmetric part of $g^{\otimes 2s}$, hence one has essentially to replace the elements of $SL(2,\mathbb{C})$ everywhere in the above by their $2s$-fold tensor products. In the last step, also the operator $i\sigma^\mu\partial_\mu$ has to be replaced by its $2s$-fold tensor product, producing a sign $(-1)^{2s}$ which equals $+1$ for integer spin, and -1 for half-integer spin.

This general feature, known as the **Spin-Statistics Theorem**, is a necessary consequence of covariance and Hilbert space positivity. It implies that the creation and annihilation operators have to satisfy **canonical anti-commutation relations**

$$\{a, a\} = \{a^*, a^*\} = 0, \qquad \{a(k), a^*(k')\} = (2\pi)^3 2k^0\delta(\vec k - \vec k').$$

Consequently, multi-particle states $a^*(k_1)\dots a^*(k_N)\Omega$ are anti-symmetric rather than symmetric under permutations. The Fock space is

$$\mathcal{H} = \bigoplus\nolimits_N P_N^- \mathcal{H}_1^{\otimes N}$$

where P_N^- is the projection on the completely anti-symmetric vectors. This is the explanation for the antisymmetry of many-electron states, and hence the Pauli principle, which had to be imposed adhoc in QM. On the other hand, Fermi fields clearly violate the Principle of Causality (Sect. 4.2). This implies that Fermi fields cannot themselves be observables, but only even products of them (such as currents or the stress-energy tensor, see below).

Both φ and φ^* solve the Klein-Gordon equation

$$(\Box + m^2)\varphi^{(*)} = 0.$$

They are also not independent of each other: The operator $-i\sigma^\mu\partial_\mu$ produces a factor $\pm mB^2$ on $e^{\pm ikx}$. Hence (using $\mathcal{E}^2 = -1$ and $B_k^{-2}\mathcal{E} = \mathcal{E}B_k^{T2}$)

$$-im^{-1}(\sigma^\mu\partial_\mu)\mathcal{E}\varphi(x) = \sqrt{m}\int \widetilde{dk}\,\big(-B_k^{-2}\mathcal{E}^2B_k a(k)e^{-ikx} + B_k^{-2}\mathcal{E}B_k^{T-1}a^*(k)e^{ikx}\big) = \varphi^*(x).$$

This relation is called the **Majorana equation** (and φ a **Majorana field**). It expresses the feature that the fields φ and φ^* create the same particle states. It can be solved for φ by using the Klein-Gordon equation: Namely, one has $\mathcal{E}\sigma^\mu\mathcal{E} = (-\mathbf{1}_2, \overline{\vec\sigma})$, so that $(\overline{\sigma^\mu}\partial_\mu)\mathcal{E}\circ(\sigma^\nu\partial_\nu)\mathcal{E} = -\eta^{\mu\nu}\partial_\mu\partial_\nu$, hence

$$\varphi = im^{-1}(\overline{\sigma^\mu}\partial_\mu)\mathcal{E}\varphi^*.$$

This feature cannot be expected in the case of charged particles, ie the Majorana spinors are no good candidates for a field describing electrons. If the eigenvalue of a charge operator Q is raised by one unit by the creation operators, then it is lowered by the annihilation operator, and consequently a linear combination of the former and the latter cannot transform into itself under the symmetry $U(\alpha) = e^{i\alpha Q}$. One has, therefore, to postulate a second set of creation operators, with the same Poincaré transformation laws but carrying the opposite charge, ie creating the corresponding **anti-particles** of charge -1, as in Sect. 3.5. One denotes these operators by $b^*(k)$ and $c^*(k)$, such that

$$Q = \int \widetilde{dk} \sum\nolimits_i \big(b_i^*(k)b_i(k) - c_i^*(k)c_i(k)\big),$$

ie b^* create particles of charge $+1$, c^* those of charge -1. (The necessity to introduce anti-particles is another inevitable consequence of QFT. It is known (in a stronger version) as the **PCT Theorem.**)

Then we may construct

$$\varphi(x) = \sqrt{m} \int \widetilde{dk} \left(\mathcal{E} B_k b(k) e^{-ikx} + B_k^{T-1} c^*(k) e^{ikx}\right),$$

and $\chi(x)$ the same expression with b and c interchanged, such that

$$U(\alpha)\varphi(x)U(\alpha)^* = e^{-i\alpha}\varphi(x), \qquad U(\alpha)\chi(x)U(\alpha)^* = e^{+i\alpha}\chi(x),$$

ie, χ and φ are oppositely charged.

Instead of the Majorana equation relating φ^* with φ, one now has

$$\chi^*(x) = -im^{-1}(\sigma^\mu\partial_\mu)\mathcal{E}\varphi(x), \qquad \varphi = im^{-1}(\overline{\sigma^\mu}\partial_\mu)\mathcal{E}\chi^*.$$

The **Dirac field** is formed by combining the pair of equally charged two-spinors φ and χ^* into a four-spinor (and redefining $c_i^*(k) = \mathcal{E}_{ij}d_j^*(k)$)

$$\psi(x) = \begin{pmatrix}\varphi(x)\\ \chi^*(x)\end{pmatrix} = \sqrt{m}\int \widetilde{dk}\left[\begin{pmatrix}\mathcal{E}B_k\\ B_k^{-1}\end{pmatrix} b(k)e^{-ikx} + \begin{pmatrix}\mathcal{E}B_k\\ -B_k^{-1}\end{pmatrix} d^*(k)e^{ikx}\right].$$

It transforms under Lorentz transformations in a reducible representation

$$U(A)\psi_a(x)U(A)^* = \psi_b(\Lambda_A x)S(A)_{ba}, \qquad \text{where} \quad S(A) = \begin{pmatrix} A & 0\\ 0 & \overline{A}\end{pmatrix}.$$

The above relations between φ and χ^* translate into the equation of motion $i\begin{pmatrix}0 & (\overline{\sigma^\mu}\partial_\mu)\mathcal{E}\\ -(\sigma^\mu\partial_\mu)\mathcal{E} & 0\end{pmatrix}\psi = m\psi$. This can also be written as

$$\boxed{(i\gamma^\mu\partial_\mu - m)\psi = 0 \qquad \textbf{Dirac equation}}$$

where the Dirac matrices $\gamma^0 = \begin{pmatrix} 0 & \mathcal{E} \\ -\mathcal{E} & 0 \end{pmatrix}$ and $\gamma^i = \begin{pmatrix} 0 & \overline{\sigma^i}\mathcal{E} \\ -\sigma^i\mathcal{E} & 0 \end{pmatrix} = \begin{pmatrix} 0 & -\mathcal{E}\sigma^i \\ -\sigma^i\mathcal{E} & 0 \end{pmatrix}$ satisfy the relations

$$\boxed{\gamma^\mu\gamma^\nu + \gamma^\mu\gamma^\nu = 2\eta^{\mu\nu} \qquad \text{and} \qquad \gamma^0\gamma^\mu\gamma^0 = \gamma_\mu = \gamma^{\mu *}.}$$

By applying $(i\gamma^\mu\partial_\mu + m)$, the Klein-Gordon equation follows.

The subsidiary **Majorana condition** $\psi^* = (\sigma^1 \otimes \mathbf{1}_2)\psi \Leftrightarrow \chi = \varphi$ would give back the Majorana field.

For many purposes, it is useful to change $\psi \to V\psi$ with a constant unitary matrix V. This changes the explicit forms of $S(A) \to V^{T*}S(A)V^T$ and $\gamma^\mu \to V\gamma^\mu V^*$, but preserves all their algebraic relations. Common are the "chiral representation":

$$V = \begin{pmatrix} \mathcal{E} & 0 \\ 0 & \mathbf{1} \end{pmatrix} \quad \Rightarrow \quad \boxed{\gamma^0 = -\sigma^1 \otimes \mathbf{1}, \quad \gamma^i = \mathcal{E} \otimes \sigma^i,}$$

or the Dirac repn (in which S is no longer block diagonal, ie the "upper" and "lower" two-spinors mix under boosts):

$$V = \begin{pmatrix} -\mathcal{E} & \mathbf{1} \\ -\mathcal{E} & -\mathbf{1} \end{pmatrix}/\sqrt{2} \quad \Rightarrow \quad \boxed{\gamma^0 = \sigma^3 \otimes \mathbf{1}, \quad \gamma^i = \mathcal{E} \otimes \sigma^i.}$$

The infinitesimal Lorentz transformation law can now be written as

$$i[M_{\mu\nu}, \psi(x)] = \big(x_\mu\partial_\nu - x_\nu\partial_\mu + \frac{1}{4}[\gamma_\mu, \gamma_\nu]\big)\psi(x).$$

The matrix contribution $\frac{1}{4}[\gamma_\mu, \gamma_\nu]$ describes the spin of the Dirac field. Eg for the rotations, $-\frac{i}{4}[\gamma_i, \gamma_j] = -\frac{1}{2}\varepsilon_{ijk}\mathbf{1} \otimes \sigma^k$ in both rep'ns (Dirac and chiral), so that the 1- (resp. 2-) components of both two-spinor fields lower (resp. raise) the spin by $\frac{1}{2}$.

The standard (textbook) way of writing the Dirac field is

$$\boxed{\psi(x) = \sqrt{2m}\int \widetilde{dk} \sum\nolimits_{i=1,2} \Big[u_i(k)e^{-ikx}b_i(k) + v_i(k)e^{ikx}d_i^*(k)\Big]}$$

where the four-spinors u_i and v_i are the columns of the resulting two 4×2 coefficient matrices, eg, $u(k) = \begin{pmatrix} (k^0+m)\mathbf{1} \\ \vec{k}\cdot\vec{\sigma} \end{pmatrix}/\sqrt{2m(k^0+m)}$ and $v(k) = \begin{pmatrix} \vec{k}\cdot\vec{\sigma} \\ (k^0+m)\mathbf{1} \end{pmatrix}/\sqrt{2m(k^0+m)}$ in the Dirac representation. Putting $k = k_0$, one concludes that the rest-frame operators $d_1^*(k_0)$ and $b_1(k_0)$ (resp. $d_2^*(k_0)$ and $b_2(k_0)$) lower (resp. raise) the spin by $\frac{1}{2}$, and hence b_1^* and d_2^* (resp. d_1^* and b_2^*) create particles of spin up (resp. down).

It is conventional to introduce the notation

$$\overline{\psi} := \psi^\dagger\gamma^0$$

where the symbol † means hermitean conjugation (as operators on $\mathcal{H}$) as well as transposition (as a column four-spinor).

The Dirac equation can also be derived from a Lagrangean density

$$\boxed{\mathcal{L}[\psi] = \overline{\psi}(i\gamma^\mu\partial_\mu - m)\psi.}$$

Here, the problems with canonical quantization are even worse than in the Maxwell case. First, the conjugate momenta are just functions of the canonical variables. This can be dealt with by "Dirac's formalism". Second, there is no classical justification of demanding CAR rather than CCR. But fortunately the canonical formalism is not essential to construct Majorana and Dirac fields.

The Lagrangean formalism yields a canonical stress-energy tensor, which is not symmetric, but can be made symmetric. The quantum SET is then

$$T^{\mu\nu}(x) = \frac{i}{2}:\big(\bar\psi\gamma^\mu\overset{\leftrightarrow}{\partial^\nu}\psi + (\mu\leftrightarrow\nu)\big):$$

where normal ordering of fermionic creation and annihilation operators takes into account the anticommutativity:

$$:A^*A: = A^*A, \qquad :AA^*: = -A^*A, \qquad \text{etc} \quad (A = b, d).$$

The invariance of $\mathcal{L}$ under $\psi \to e^{i\alpha}\psi$ gives rise to a conserved Noether current

$$j^\mu_{\rm Dirac} = :\bar\psi\gamma^\mu\psi:.$$

The conserved charge $Q_{\rm Dirac} = \int d^3x\, j^0_{\rm Dirac}(t,\vec x)$ coincides with the above charge operator $Q = \int(b^*b - c^*c) = \int(b^*b - d^*d)$. Thus, if we identify the particle created by b^* with the electron of charge $-e$, the electromagnetic current is $j^\mu_{\rm elm} = -e\, j_{\rm Dirac}$.

The problem of QED is to formulate an interaction between the Maxwell field and the Dirac current.

4.8 P, T, and C

(**P**) Let $Px = P(t,\vec x) = (t,-\vec x)$ the total space reflection. Then the operator $\mathbf{P}\prod_i a^*(k_i)\Omega = \prod_i a^*(Pk_i)\Omega$ is unitary, satisfies $\mathbf{P}^2 = 1$, and

$$\mathbf{P}\varphi(x)\mathbf{P} = \varphi(Px).$$

This operator is called **parity operator**.

(**T**) Let $Tx = T(t,\vec x) = (-t,\vec x)$ the time reflection (actually, $T = -P$). There cannot be a unitary operator preserving the vacuum, such that $\mathbf{T}\Omega = \Omega$ and

$$\mathbf{T}\varphi(t,x)\mathbf{T} = \varphi(-t,x).$$

Namely, as t varies, the complex phases of $\varphi(t,x)\Omega$ run "forwards" like $e^{i\omega t}$, while those of $\varphi(-t,x)\Omega$ run "backwards" like $e^{-i\omega t}$. However, if $\mathbf{T}$ is allowed to be *anti-linear*, then it is in fact *anti-unitary* (and $\mathbf{T}^2 = 1$), because the 2-point function satisfies $\Delta_m(Tx) = \overline{\Delta_m(x)}$. In terms of creation operators, this relation means

$$\mathbf{T}a^*(k)\Omega = a^*(Pk)\Omega,$$

(the same as for **P**!). But because the anti-linearity takes $e^{\pm ikx}$ to $e^{\mp ikx}$, we have $e^{\mp i(Pk)x} = e^{\pm i(Tk)x} = e^{\pm ik(Tx)}$, as desired. $\mathbf{T}$ is called **time reversal operator**.

(**C**) Consider the model with two real scalar fields φ_1, φ_2. It has a symmetry transformation $\varphi_2 \to -\varphi_2$. In QFT, the corresponds the unitary operator $\mathbf{C}$ acting on the one-particle space by $\mathbf{C}a_1^*(k)\Omega = a_1^*(k)\Omega$, $\mathbf{C}a_2^*(k)\Omega = -a_2^*(k)\Omega$, extending to the Fock space in the obvious way. Then clearly $\mathbf{C}^2 = 1$, and

$$\mathbf{C}\varphi_1(x)\mathbf{C} = \varphi_1(x), \qquad \mathbf{C}\varphi_2(x)\mathbf{C} = -\varphi_2(x),$$

or equivalently,

$$\mathbf{C}\phi(x)\mathbf{C} = \phi^*(x).$$

The current and charge operators change sign:

$$\mathbf{C}j(x)\mathbf{C} = -j(x), \qquad \mathbf{C}Q\mathbf{C} = -Q.$$

For this reason, $\mathbf{C}$ is called the **charge conjugation operator**. In the case of the single (neutral) scalar field, $\mathbf{C}$ may be chosen to act trivially: $\mathbf{C}\varphi\mathbf{C} = \varphi$.

The three operators are separately "conserved" in the sense that

$$[H, \mathbf{P}] = [H, \mathbf{T}] = [H, \mathbf{C}] = 0.$$

One can define $\mathbf{P}$, $\mathbf{T}$, $\mathbf{C}$ also for the Maxwell field and for the Dirac field. For the Maxwell field, the definitions are very similar as for the scalar field, but $\mathbf{P}$ and $\mathbf{T}$ also invert the spatial components of the vector potential, hence $\mathbf{P}$ preserves the magnetic and inverts the electric field strengths, while the opposite holds for $\mathbf{T}$, and the field changes sign under $\mathbf{C}$:

$$\mathbf{P}A^\mu(x)\mathbf{P} = (PA)^\mu(Px), \quad \mathbf{T}A^\mu(x)\mathbf{T} = -(TA)^\mu(Tx), \quad \mathbf{C}A^\mu(x)\mathbf{C} = -A^\mu(x).$$

The first two imply $U(\Lambda)A^\mu(x)U(\Lambda)^* = \mathrm{sign}\,(\Lambda_0^0)(\Lambda^{-1}A)^\mu(\Lambda x)$ for general LTs.

For the Dirac field, the situation is more complicated. In order to assure the desired symmetries, one may define on the Wigner one-particle space: $\mathbf{P}b_i^*(k)\Omega = b_i^*(Pk)\Omega$, $\mathbf{P}d_i^*(k)\Omega = -d_i^*(Pk)\Omega$, $\mathbf{T}a_i^*(k)\Omega = \mathcal{E}_{ij}a_j^*(Pk)\Omega$ for both $a = b$ or d, and $\mathbf{C}b_i^*(k)\Omega = \mathcal{E}_{ij}d_j^*(k)\Omega$, $\mathbf{C}d_i^*(k)\Omega = -\mathcal{E}_{ij}b_j^*(k)\Omega$, hence $\mathbf{P}^2 = 1$, $\mathbf{T}^2 = -1$, $\mathbf{C}^2 = 1$. This leads to the transformation laws

$$\mathbf{P}\psi(x)\mathbf{P} = \gamma^0 \cdot \psi(Px), \quad \mathbf{T}\psi(x)\mathbf{T}^* = \gamma^1\gamma^3 \cdot \psi(Tx), \quad \mathbf{C}\psi(x)\mathbf{C} = i\gamma^2 \cdot \psi^*(x)$$

where (in the chiral representation)

$$\gamma^0 = \begin{pmatrix} 0 & \mathcal{E} \\ -\mathcal{E} & 0 \end{pmatrix}, \quad \gamma^1\gamma^3 = \begin{pmatrix} \mathcal{E} & 0 \\ 0 & \mathcal{E} \end{pmatrix}, \quad i\gamma^2 = \begin{pmatrix} 0 & \mathbf{1}_2 \\ \mathbf{1}_2 & 0 \end{pmatrix}.$$

The Majorana condition $\chi = \varphi$ reads $\mathbf{C}\psi\mathbf{C} = \psi$. From these, one can verify that

$$\mathbf{P}j^\mu(x)\mathbf{P} = (Pj)^\mu(Px), \quad \mathbf{T}j^\mu(x)\mathbf{T}^* = -(Tj)^\mu(Tx), \quad \mathbf{C}j^\mu(x)\mathbf{C} = -j^\mu(x).$$

All these transformation laws of scalar, Maxwell and Dirac fields are in accord with the symmetries of classical theory, as implied by the view of currents as charges in motion, where the velocity is reversed both under space and time reversal.

There are in fact many different choices of the operations **P**, **T**, and **C**, giving rise to different transformation laws. Eg, the actions of **P** or **C** on the one-particle space (and hence their commutation relations with the fields) may involve extra $-$ signs ("intrinsic parity" resp. "charge parity"; eg the Maxwell vector potential has deliberately been assigned charge parity -1 above), while **T** may be modified by an overall phase.

Whenever the Hamiltonian is invariant under one of the discrete symmetries, there is an associated conservation law, ie eigenvalues are preserved in scattering processes. Notice that eigenvalues of **P** in multi-particle states are not just the product of intrinsic parities but, due to the action on the arguments, also get a contribution from the angular momentum ("orbital parity"). Notice also that preservation of charge parity is not to be confused with charge conservation!

One can prove that in a general QFT satisfying the principles of locality, covariance, positive energy and positive-definite Hilbert space, there is always an anti-unitary operator Θ commuting with H and preserving the vacuum, which has the joint features of **PCT**, ie it implements the total spacetime reflection $x \to -x$ and inverts all charges of the QFT; in general, however, **P**, **T**, **C** might not be defined separately. This fact is known as the **PCT Theorem**. Experimentally, we know that **P** and **CP** (hence also **T**) are broken symmetries in high-energy physics.

A simpler form of the statement is that $\mathbf{P}, \mathbf{T}, \mathbf{C}$ can always be chosen for the free fields of a QFT in such a way that the interaction Lagrangean density is invariant under the product **PCT**, provided it is a local Lorentz invariant hermitean quantity. As a consequence, also the Hamiltonian commutes with **PCT**.

With the above choices, the QED Lagrangean density $j_\mu A^\mu$ is separately invariant under all three symmetries. Likewise, the neutral scalar field $j(x) = :\bar\psi\psi:(x)$ transforms like

$$\mathbf{P}j(x)\mathbf{P} = j(Px), \quad \mathbf{T}j(x)\mathbf{T} = j(Tx), \quad \mathbf{C}j(x)\mathbf{C} = j(x)$$

hence the Dirac mass term is separately invariant, and so is the Yukawa coupling $\varphi\cdot :\bar\psi\psi:$ provided the intrinsic parities of the neutral scalar field are assigned properly. On the other hand, let $\gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3$ ($(\gamma^5)^2 = \mathbf{1}$, in the chiral representation $\gamma^5 = Diag(+\mathbf{1}_2, -\mathbf{1}_2)$). The hermitean pseudoscalar field $j^5 = i:\bar\psi\gamma^5\psi:$ transforms as

$$\mathbf{P}j^5(x)\mathbf{P} = -j^5(Px), \quad \mathbf{T}j^5(x)\mathbf{T} = -j^5(Tx), \quad \mathbf{C}j^5(x)\mathbf{C} = j^5(x).$$

Separate $\mathbf{C}, \mathbf{P}, \mathbf{T}$ invariance of the hermitean coupling $\varphi\cdot i:\bar\psi\gamma^5\psi:$ therefore would require a different assignment of intrinsic parities of the scalar field. If both couplings are present, **P** and **T** cannot be separately preserved ("parity is not conserved"), but **CPT** is. The axial vector field $j^{\mu 5} = :\bar\psi\gamma^\mu\gamma^5\psi:$ transforms as

$$\mathbf{P}j^{\mu 5}(x)\mathbf{P} = -(Pj)^{\mu 5}(Px), \quad \mathbf{T}j^{\mu 5}(x)\mathbf{T}^* = -(Tj)^{\mu 5}(Tx), \quad \mathbf{C}j^{\mu 5}(x)\mathbf{C} = j^{\mu 5}(x)$$

(differing from j^μ in **P** and **C**); therefore the vector and axial vector couplings $A_\mu \cdot j^\mu$ (Maxwell) and $A_\mu \cdot j^{\mu 5}$ cannot be simultaneously parity preserving: if they are both present, parity symmetry is broken.

5 Interaction with classical fields

The coupling of the Maxwell field to its sources is given by the "interaction term"

$$\mathcal{L}_{\rm int} = -j^\mu_{\rm elm}(x)A_\mu(x) = -\rho(x)\phi(x) + \vec{j}(x)\vec{A}(x).$$

We want to simplify matters by regarding an analogous coupling

$$\mathcal{L}_{\rm int} = j(x)\varphi(x)$$

of a scalar quantum field φ to a source $j(x)$, treated as a classical (numerical, ie commuting with everything) field. Adding this term to the Lagrangean, changes the equation of motion:

$$(\Box + m^2)\varphi(x) = j(x),$$

while the formula for the conjugate momenta $\pi = \dot\varphi$ and hence the equal-time commutators of φ and $\dot\varphi$ (CCR) are unchanged.

5.1 The scattering matrix

Let us assume that the source is nonzero only within a finite time interval, say $[t_0, t_1]$. At $t < t_0$, we have the free field equations, and we quantize the field as before, that is, the interacting field $\varphi_{\rm int}$ coincides at $t < t_0$ with the free field on the Fock space (satisfying the free field equations at all times), which one traditionally calls $\varphi_{\rm in}$. At time $t > t_1$, we have again the free field equations and the CCR, hence $\varphi_{\rm int}$ coincides at $t > T$ with another free field, called $\varphi_{\rm out}$. The latter satisfies the same algebraic relations and the same equation of motion. This could be realized by any unitary operator S (called "scattering matrix") such that

$$\varphi_{\rm out} = S^*\varphi_{\rm in}S.$$

We shall see below that, for the interaction with a classical field, such an operator S exists on the Fock space of the ingoing free field and can be explicitly computed.

It follows that the creation and annihilation operators of the outgoing free field differ from the ingoing ones:

$$a^*(k)_{\rm out} = S^*a^*(k)_{\rm in}S, \qquad a(k)_{\rm out} = S^*a(k)_{\rm in}S,$$

and hence also its vacuum state is different: $a_{\rm out}$ annihilate the vector

$$\Omega_{\rm out} = S^*\,\Omega_{\rm in}.$$

Notice that measurements of energy and momentum are performed with the density operators which are constructed from the field at the respective time. Since with a time dependent source, energy and momentum are not conserved during the interaction, the total energy and momentum operators are not expected to be

the same before and after the interaction. This explains why the in- and outgoing vacuum states differ from each other (and likewise for N-particle states): the interpretation of a given Hilbert space vector as an N-particle state is linked to the respective density operators, and these will change during the interaction.

External fields may dynamically create and annihilate particles.

Consider a state $|k_1,\dots,k_N\rangle_{\rm in} = a^*_{\rm in}\dots a^*_{\rm in}\Omega_{\rm in}$. This state can be decomposed into a superposition of outgoing states (with a sum over all N' and suitable integration measures)

$$|k_1,\dots,k_N\rangle_{\rm in} = \sum\!\!\!\!\!\!\int |k'_1,\dots,k'_{N'}\rangle_{\rm out}\cdot {}_{\rm out}\langle k'_1,\dots,k'_{N'}|k_1,\dots,k_N\rangle_{\rm in}.$$

Because

$$|k_1,\dots,k_N\rangle_{\rm in} = S|k_1,\dots,k_N\rangle_{\rm out},$$

we have

$${}_{\rm out}\langle k'_1,\dots,k'_{N'}|k_1,\dots,k_N\rangle_{\rm in} = {}_{\rm out}\langle k'_1,\dots,k'_{N'}|S|k_1,\dots,k_N\rangle_{\rm out},$$

ie, the expansion coefficients are the "matrix elements" of the scattering matrix. The probability density that the given N-particle state before the interaction looks like the specified N'-particle state after the interaction, is

$$p = |{}_{\rm out}\langle k'_1,\dots,k'_{N'}|S|k_1,\dots,k_N\rangle_{\rm out}|^2 = |{}_{\rm in}\langle k'_1,\dots,k'_{N'}|S|k_1,\dots,k_N\rangle_{\rm in}|^2.$$

We shall now proceed to compute the scattering matrix in terms of free fields, so that these probabilities can be computed in terms of free field theory.

5.2 Scalar quantum field coupled to a classical source

Let $G(x)$ be a Green function for the Klein-Gordon operator:

$$(\Box + m^2)G(x) = \delta^4(x).$$

If φ solves the EOM $(\Box+m^2)\varphi = j(x)$, then $\varphi_{\rm free} = \varphi - \int d^4y\, G(x-y)j(y)$ solves the free EOM. $\varphi_{\rm free}$ and $\pi_{\rm free} = \dot\varphi_{\rm free}$ also satisfy the CCR, because the addition of the numerical term $\int Gj$ does not change commutators. Hence $\varphi_{\rm free}$ is a free field.

$\varphi_{\rm free}$ depends on the choice of the Green function. The retarded GF is $G_{\rm ret}(x-y) = i\theta(x^0-y^0)(\Delta_m(x-y)-\Delta_m(y-x))$ (see Sect. 5.7 for a compilation of the relevant functions) with the property that $G_{\rm ret}(x-y)\neq 0$ only when x is in the future of y. If the source is turned on at time t_0, it follows $\int G_{\rm ret}j = 0$ at times $t<t_0$, hence $\varphi_{\rm free} = \varphi = \varphi_{\rm in}$. Hence $\varphi_{\rm free} = \varphi_{\rm in}$ at all times. Similarly, when we choose the advanced Green function $G_{\rm adv}$ with the property that $G_{\rm adv}(x-y)\neq 0$ only when x is in the past of y, we conclude that $\varphi_{\rm free} = \varphi_{\rm out}$. This implies

$$\varphi_{\rm out}(x) - \varphi_{\rm in}(x) = \int d^4y (G_{\rm ret}-G_{\rm adv})(x-y)j(y).$$

But $(G_{\rm ret} - G_{\rm adv})(x) = i(\Delta_m(x) - \Delta_m(-x)) = i[\varphi_{\rm as}(x_1), \varphi_{\rm as}(x_2)]$ for $x = x_1 - x_2$ (see Sect. 5.7). ("as" means either "in" or "out".) This gives

$$\varphi_{\rm out}(x) = \varphi_{\rm in}(x) + [\varphi_{\rm in}(x), i\int d^4y\, \varphi_{\rm in}(y) j(y)].$$

Using the BCH formula, we find the explicit formula for the scattering matrix

$$\boxed{\varphi_{\rm out} = S^*\varphi_{\rm in} S \qquad \text{with} \quad S = e^{i\int d^4y\, \varphi_{\rm in}(y) j(y)} = e^{i\int \mathcal{L}_{\rm int}[\varphi_{\rm in}]} = e^{i\int \mathcal{L}_{\rm int}[\varphi_{\rm out}]}.}$$

We can now compute scattering amplitudes. Let $j(y) = (2\pi)^{-4}\int d^4k\, e^{-ikx}\,\hat j(k)$, and hence $\varphi_{\rm as}(j) \equiv \int d^4y\, \varphi_{\rm as}(y) j(y) = a_{\rm as}(\hat j) + a^*_{\rm as}(\hat j)$. By Weyl's formula,

$$S = e^{-\frac12\omega(j,j)} {:}e^{i\int d^4y\, \varphi(y) j(y)}{:} = e^{-\frac12\omega(j,j)} e^{ia^*_{\rm as}(\hat j)} e^{ia_{\rm as}(\hat j)},$$

where $\omega(j_1, j_2) = (\Omega, \varphi_{\rm as}(j_1)\varphi_{\rm as}(j_2)\Omega) = \int\int j_1(x) j_2(y) \Delta_m(x-y)$. Hence,

$${}_{\rm out}\langle K'|K\rangle_{\rm in} = e^{-\frac12\omega(j,j)}\ {}_{\rm as}\langle K'|e^{ia^*_{\rm as}(\hat j)} e^{ia_{\rm as}(\hat j)}|K\rangle_{\rm as}.$$

Eg, the probability amplitude for the transition $\Omega_{\rm in} \to \Omega_{\rm out}$ is just given by ${}_{\rm out}\langle 0|0\rangle_{\rm in} = e^{-\frac12\omega(j,j)}$. Notice that the exponent is negative, hence the probability is < 1, because $\omega(j,j) = \|\varphi_{\rm as}(j)\Omega\|^2 = \int \widetilde{dk} |\hat j(k)|^2 \geq 0$. Hilbert space positivity is therefore essential to have the desired probabilistic interpretation.

Other probability amplitudes can be computed using the identity $e^{ia(\hat j)} a^*(k) = (a^*(k) + i\overline{\hat j(k)}) e^{ia(\hat j)}$ (from BCH) which gives the expression in terms of free fields

$$\boxed{\langle k'_1 \cdots k'_M|S|k_i \cdots k_N\rangle = e^{-\frac12\omega(j,j)}\Big(\prod (a^*(k'_i) + i\overline{\hat j(k'_i)})\Omega, \prod (a^*(k_i) + i\overline{\hat j(k_i)})\Omega\Big).}$$

(Graphical representation: pairings between in- and outgoing particles; non-paired particles are attached to a source factor $\hat j$: induced emission and absorption.)

5.3 The infrared problem

One may expect that the same formula holds true when the source is not exactly zero before t_0 and after t_1, but tends to zero asymptotically. A problem arises in the massless case, when $\widetilde{dk} \sim d^3k/2|\vec k|$. The integral $\omega(j,j) = \int \widetilde{dk} |\hat j(k)|^2$ may diverge at small $\vec k$ when $\hat j(k)$ grows too fast near $\vec k = 0$ (long wave lengths: hence "IR"). In particular, j cannot be chosen time-independent because $\hat j(\vec k, \omega_k) = f(\vec k)\delta(\omega_k)$ is too singular at $\omega_k = |\vec k| = 0$. In this case, $e^{-\frac12\omega(j,j)} = 0$, and consequently *all scattering amplitudes vanish!* All in-states are orthogonal to all out-states. In fact, the average total number of out-particles in the in-vacuum state can be shown to be $\bar n_{\rm out} = \omega(j,j)$, so when, eg, a strict time cutoff is gradually relaxed, this number grows to infinity. Likewise, the state $\Omega_{\rm in}$ will have divergent "out-energy". This energy is produced by the interaction with the IR modes of the external field.

The mathematical side of the problem is that states with infinite particle number are not in the Fock space, and the unitary equivalence by an operator S on the same Hilbert space fails. This is an instance where the ingoing and outgoing free fields are realized by creation and annihilation operators in *inequivalent representations* of the CCR. The physical interpretation is that the total interaction, integrated over all times (and space), changes the dynamical fields in a more substantial way than can be afforded on the same Fock space.

The IR problem will reappear in various versions again and again, when the source decreases too slowly with time (or with $\vec{x}$).

5.4 Maxwell field coupled to classical sources

In the case of the electromagnetic field, the source is a four-vector j_μ. Classically, the expression $\int A_\mu j^\mu$ is gauge invariant, because the contribution from a gauge transformation $\int \partial_\mu \Gamma \cdot j^\mu = -\int \Gamma \cdot \partial_\mu j^\mu$ vanishes provided the current j is conserved and goes sufficiently fast to zero at infinity.

For the quantum field, one has to quantize A_μ on the indefinite Fock space, where $\int A_\mu j^\mu$ can be defined. If $j^\mu(x)$ is conserved, we have $k_\mu \hat{j}^\mu(k) = 0$. One can write

$$\hat{j}^\mu(k) = k^\mu J_{\rm long}(k) + J_1(k) e_1^\mu(k) + J_2(k) e_2^\mu(k)$$

where $e_i = (0, \vec{e}_i)$ are two transversal vectors, $\vec{e}_i \cdot \vec{k} = 0$, $\vec{e}_i \cdot \vec{e}_j = \delta_{ij}$. Proceeding as in Sect. 5.2, the exponenent $-\frac{1}{2}\omega(j,j) = -\frac{1}{2}\int \widetilde{dk}\, |\hat{j}(k)|^2$ is replaced by

$$+\eta_{\mu\nu}\frac{1}{2}\int \widetilde{dk}\, \overline{\hat{j}^\mu(k)} j^\nu(k) = -\frac{1}{2}\int \widetilde{dk}\, (|J_1(k)|^2 + |J_2(k)|^2).$$

This result is independent of the gauge parameter λ, and ≤ 0, as it should be; the longitudinal component of the field does not contribute.

In this case, the IR problem ($e^{-\frac{1}{2}\int \widetilde{dk}\,(|J_1(k)|^2+|J_2(k)|^2)} = 0$) arises not due to a deliberate choice of a slowly decaying external field, but by necessity because a conserved current of nonzero total charge cannot decay rapidly. In physical terms, the IR divergence reflects the fact that charged sources may and will create an infinite number of "soft" (low energy) photons.

5.5 The interaction picture

We want to generalize the formula for the S-matrix, when the interaction is not linear in the fields, eg,

$$\mathcal{L}_{\rm int}(\bar\psi, \psi; x) = -A_\mu(x) j^\mu \qquad \text{or} \qquad \mathcal{L}_{\rm int}(\varphi; x) = -V(\varphi; x) = -\frac{1}{4} g(x) \varphi^4,$$

where $j^\mu = -e{:}\overline{\psi}\gamma^\mu\psi{:} = -e j^\mu_{\rm Dirac}$ is the electromagnetic current and A_μ a classical background field ("source"); in the second, self-interacting case, the strength of the coupling is admtted to be space-time dependent and plays the role of the source.

We want to solve the Hamiltonian equation of motion

$$\partial_t \varphi(t) = i[H(t), \varphi(t)],$$

where summarily φ stands for all fields and conjugate momenta. $H(t)$ is required to be unitary, but not necessarily constant. The time evolution is then given by

$$\varphi(t) = U(t,s)\varphi(s)U(t,s)^*$$

where $U(t,s)$ is unitary, $U(s,s) = 1$, satisfies $U(t,r)U(r,s) = U(t,s)$, and solves the equation

$$\partial_t U(t,s) = iH(t)U(t,s).$$

If H is constant, $U(t,s) = e^{i(t-s)H}$. Otherwise, the solution can be obtained as a limit

$$\lim_{N\to\infty} e^{i\Delta\tau_N H(\tau_N)} \cdot \ldots \cdot e^{i\Delta\tau_1 H(\tau_1)}$$

where the time interval (s,t) has been split into a large number of small intervals $\Delta\tau_i$ around $\tau_1 < \cdots < \tau_N$ during which $H(t) = H(\tau_i)$ are constant. One writes

$$U(t,s) = Te^{i\int_s^t d\tau H(\tau)},$$

where the symbol T stands for "time ordering": all products of time-dependent operators involved in the exponential are ordered according to the rule "later left":

$$T\big[H(\tau_1)H(\tau_2)\big] = \theta(\tau_1-\tau_2)\cdot H(\tau_1)H(\tau_2) + \theta(\tau_2-\tau_1)\cdot H(\tau_2)H(\tau_1).$$

Then the time-ordered exponential can also be thought of as a power series expansion where each term is separately time-ordered.

Let the Hamiltonian be a "function" of φ, that can be decomposed as

$$H(t) = H_0(\varphi(t)) + h(\varphi(t), t),$$

where H_0 is the Hamiltonian of a free QFT and h is the interaction term $h(\varphi(t),t) = -\int d^3x \mathcal{L}_{\rm int}(\varphi(t,x),t,x)$.

We assume now that at times $t < t_0$ the interaction is absent, eg because the source vanishes. This assumption cannot always be physically justified, and will be discussed later.

At times $s < t_0$, the field coincides with a free field: $\varphi(s) = \varphi_{\rm in}(s)$, that evolves according to $\varphi_{\rm in}(t) = U_0(t,s)\varphi_{\rm in}(s)U_0(t,s)^*$. At later times $t > t_0$, we have

$$\varphi(t) = U(t,s)\varphi_{\rm in}(s)U(t,s)^* = V(t)^*\varphi_{\rm in}(t)V(t)$$

where $V(t) = U_0(t,s)U(t,s)^*$ describes the deviation from the free evolution.

We now heuristically use the "conjugation rule"

$$V^*F(A)V = F(V^*AV)$$

which holds for quite arbitrary functions of a self-adjoint operator, but may be problematic for functions of operator-valued distributions, involving Wick products (normal ordering). It implies

$$\partial_t V(t) = iH_0(\varphi_{\rm in}(t))V(t) - iV(t)H(\varphi(t),t) = i\big(H_0(\varphi_{\rm in}(t)) - H(\varphi_{\rm in}(t),t)\big)V(t).$$

At least formally, we arrive at the evolution equation

$$\partial_t V(t) = -ih(\varphi_{\rm in}(t), t) \cdot V(t).$$

This equation involves only the interaction part of the Hamiltonian. Therefore, $V(t)$ is called the time evolution in the *interaction picture*.

For $t < t_0$ we have the initial condition $V(t) = 1$, hence

$$V(t) = Te^{-i\int_{t_0}^t d\tau h(\varphi_{\rm in}(\tau),\tau)} = Te^{i\int_{t_0}^t d\tau d^3x \mathcal{L}_{\rm int}(\varphi_{\rm in}(\tau),\tau)}.$$

When the interaction is turned off at $t > t_1$, the field is again a free field, but it differs from the incoming field by the unitary operator $V(t_1)$. (Note that $V(t)$ is constant at $t > t_1$.) Hence $V(t_1)$ is the S-matrix implementing the relation

$$\varphi_{\rm out} = S^* \varphi_{\rm in} S.$$

Finally, because $\mathcal{L}_{\rm int}(t) = 0$ when $t < t_0$ or $t > t_1$, we find

$$\boxed{S = Te^{i\int d^4x\, \mathcal{L}_{\rm int}(\varphi_{\rm in})} = Te^{i\int d^4x\, \mathcal{L}_{\rm int}(\varphi_{\rm out})}.}$$

(The second equality follows from $S = S^*SS$, by applying the conjugation rule again.) If $\mathcal{L}_{\rm int}$ is linear in the field, eg $= j\varphi$ as in Sect. 5.2, the Weyl formula gives

$$e^{-i\Delta\tau_{n+1}h(\tau_{n+1})}e^{-i\Delta\tau_n h(\tau_n)} = e^{-\frac{1}{2}\Delta\tau_{n+1}\Delta\tau_n[h(\tau_{n+1}),h(\tau_n)]} \cdot e^{-i\Delta\tau_{n+1}h(\tau_{n+1})-i\Delta\tau_{n+1}h(\tau_{n+1})},$$

from which

$$Te^{i\int d^4x\, j(x)\varphi_{\rm in}(x)} = e^{i\alpha} \cdot e^{i\int d^4x\, j(x)\varphi_{\rm in}(x)}$$

where $\alpha = \frac{i}{2}\int d^4x\, d^4y\, \theta(x^0 - y^0)[\varphi_{\rm in}(x), \varphi_{\rm in}(y)]j(x)j(y) = \frac{1}{2}G_{\rm ret}(j,j)$ is real, ie the general formula reproduces the previous one up to an irrelevant complex phase.

The advantage is that the scattering matrix S is expressed in terms of free fields only. Via Wick's Theorem (Sect. 5.6), the computation of amplitudes is reduced to free-field time-ordered 2-point functions ("propagators"), which are well-known (Sect. 5.7). The drawback is that the formula relies on quite formal manipulations. This will be punished by divergent expressions when we compute scattering processes, thus necessitating renormalization to get finite numbers.

5.6 Wick's Theorem

Recall the general formula $(*)$ in the raw version of **Wick's Theorem** (cf Sect. 3.4). Replacing Z_i by $t_i Z_i$ and comparing the factors multiplying any given monomial $\prod_i t_i^{n_i}$ on both sides, one obtains

$$:\varphi(x_1)^{n_1}: \ldots :\varphi(x_N)^{n_N}: = \sum_{\substack{\text{restricted}\\ \text{partial pairings}}} \prod_{\substack{\text{pairs}\\ i_k<j_k}} (\Omega, \varphi(x_{i_k})\varphi(x_{j_k})\Omega) \cdot : \prod_{\substack{\text{remaining}\\ \text{factors}}} \varphi(x_i)^{m_i}:.$$

"Restricted" means that two operators within any Wick power on the lhs must not be paired. "Partial" means that not all operators need to be paired.

This formula expands products of Wick products of free fields into Wick products times products of vacuum expectation values. It remains true when the Wick powers $:\varphi(x_i)^{n_i}:$ are replaced by Wick products such as $:\prod_{\alpha=1}^{n_i}\varphi_{i\alpha}(x_{i\alpha}):$, eg

$$:\varphi_1\varphi_2::\varphi_3\varphi_4: = :\varphi_1\varphi_2\varphi_3\varphi_4: + (23):\varphi_1\varphi_4: + (24):\varphi_1\varphi_3: + \cdots + (13)(24) + (14)(23)$$

where (ij) is the VEV and ... stand for two more terms, but *not*, eg, the term $(12):\varphi_3\varphi_4:$ which would be singular if $x_1 = x_2$. In particular, Wick products are regular at coinciding points.

For time-ordered products of Wick products (eg, in the expansion of the S-matrix, Sect. 5.5), the same expansion holds (**Wick's Theorem** (time-ordered version)), except that the VEV have to be replaced by the time-ordered VEV (Feynman propagators)

$$(\Omega, T[\varphi(x)\varphi(y)]\Omega) = -iG_F(x-y).$$

For Fermi fields, the same expansions hold again, but each term is multiplied by the sign $(-1)^\pi$ of the permutation from the order of operators on the lhs to that on the rhs (**Wick's Theorem** (fermionic versions)), eg

$$T[:\psi_1\psi_2:\overline{\psi}_3] = (2\bar{3})_T\psi_1 - (1\bar{3})_T\psi_2$$

where $(i\bar{j})_T$ stands for the time-ordered VEV.

5.7 2-point functions and Green functions

2-point function

Definition:

$$\Delta_m(x-y) = (\Omega, \varphi(x)\varphi(y)\Omega).$$

Properties: $(\Box + m^2)\Delta_m(x) = 0$. Local, ie $\Delta_m(x) = \Delta_m(-x)$ when x spacelike. Fourier representation:

$$\Delta_m(x) = \int \frac{d^4k}{(2\pi)^3}\,\delta(k^2-m^2)\theta(k^0)e^{-ikx} \equiv \int \widetilde{dk}\,e^{-ikx}.$$

(In x-space, it can be expressed in terms of a modified Bessel function $K_1(\sqrt{-m^2x^2})$.)

Commutator function

Definition:

$$i\Delta_-(x-y) = (\Omega, [\varphi(x), \varphi(y)]\Omega) = [\varphi(x), \varphi(y)] = \Delta_m(x-y) - \Delta_m(y-x).$$

Properties: $(\Box + m^2)\Delta_m(x) = 0$. Real-valued. Antisymmetric. Causal, ie $\Delta_-(x) = 0$ when x spacelike. At equal time:

$$\Delta_-(x)|_{x^0=0} = 0, \qquad \partial_0\Delta_-(x)|_{x^0=0} = -\delta(\vec{x}).$$

Fourier representation:

$$\Delta_-(x) = -i\int \frac{d^4k}{(2\pi)^3}\,\delta(k^2-m^2)\mathrm{sign}\,(k^0)e^{-ikx} \equiv -2\int \widetilde{dk}\,\sin(kx).$$

Retarded Green function

Definition:

$$G_{\rm ret}(x-y) = -\theta(x^0-y^0)\Delta_-(x-y).$$

Properties: $(\Box + m^2)G_{\rm ret}(x) = \delta^4(x)$. Real-valued. Retarded, ie $G_{\rm ret}(x) = 0$ when $x^0 < 0$ or x spacelike.

Fourier representation:

$$G_{\rm ret}(x) = \lim_{\varepsilon\downarrow 0}\int \frac{d^4k}{(2\pi)^4}\,\frac{e^{-ikx}}{m^2-k^2-i\varepsilon k^0}.$$

Advanced Green function

Definition:

$$G_{\rm adv}(x-y) = +\theta(y^0-x^0)\Delta_-(x-y).$$

Properties: $(\Box + m^2)G_{\rm adv}(x) = \delta^4(x)$. Real-valued. Advanced, ie $G_{\rm adv}(x) = 0$ when $x^0 > 0$ or x spacelike. $G_{\rm adv}(x) = G_{\rm ret}(-x)$, $G_{\rm ret}(x) - G_{\rm adv}(x) = -\Delta_-(x)$.

Fourier representation:

$$G_{\rm adv}(x) = \lim_{\varepsilon\downarrow 0}\int \frac{d^4k}{(2\pi)^4}\,\frac{e^{-ikx}}{m^2-k^2+i\varepsilon k^0}.$$

Time-ordered 2-point function = Feynman propagator

Definition:

$$G_F(x-y) = i(\Omega, T[\varphi(x)\varphi(y)]\Omega) = i\big(\theta(x^0-y^0)\Delta_m(x-y) + \theta(y^0-x^0)\Delta_m(y-x)\big).$$

Properties: $(\Box + m^2)G_F(x) = \delta^4(x)$. Symmetric. $G_F(x) = G_{\rm adv}(x) + i\Delta_m(x) = G_{\rm ret}(x) + i\Delta_m(-x)$. $G_F(x) = i\Delta_m(\pm x)$ when $\pm x^0 > 0$ or x spacelike.

Fourier representation:

$$G_F(x) = \lim_{\varepsilon\downarrow 0}\int \frac{d^4k}{(2\pi)^4}\,\frac{e^{-ikx}}{m^2-k^2-i\varepsilon}.$$

Proof by closing the k^0-integration path in the upper (if $x^0 < 0$) or lower (if $x^0 > 0$) complex half-plane and applying the residue formula. For $G_{\rm ret}$, $G_{\rm adv}$, G_F the poles lie at $k^0 = \pm\omega - i\varepsilon$, $k^0 = \pm\omega + i\varepsilon$, $k^0 = \pm(\omega - i\varepsilon)$, respectively.

Massless case

The massless 2-point function $D(x) = \Delta_{m=0}(x)$ is an elementary function:

$$D(x) = \lim_{\varepsilon\downarrow 0}\frac{1}{(2\pi)^2}\frac{-1}{(x^0-i\varepsilon)^2-\vec{x}^2} \equiv \lim_{\varepsilon\downarrow 0}\frac{1}{(2\pi)^2}\frac{-1}{x^2-i\varepsilon x^0}.$$

The commutator function (Pauli-Jordan function) is

$$iD_-(x) = D(x) - D(-x) = \frac{-i}{2\pi}\,\mathrm{sign}\,(x^0)\delta(x^2),$$

and the Feynman propagator

$$G_F(x) = i\big(\theta(x^0)D(x) + \theta(-x^0)D(-x)\big) = \lim_{\varepsilon\downarrow 0}\frac{1}{(2\pi)^2}\frac{-i}{x^2-i\varepsilon}.$$

Dirac case

The 2-point function is

$$(\Omega, \psi_a(x)\overline{\psi}_b(y)\Omega) =: S_{ab}(x-y) = (m\mathbf{1} + i\gamma^\mu\partial_\mu)_{ab}\Delta_m(x-y)$$

$\Rightarrow (m\mathbf{1} - i\gamma^\mu\partial_\mu)S = 0$, and $(\Omega, \overline{\psi}_b(x)\psi_a(y)\Omega) = -(m\mathbf{1} - i\gamma^\mu\partial_\mu)_{ab}\Delta_m(x-y)$. Similar for Green functions and Feynman propagator: $S_{F,ab}(x-y) := i(\Omega, T\psi_a(x)\overline{\psi}_b(y)\Omega)$, where fermionic time-ordering involves a $-$ sign if $x^0 < y^0$. Then,

$$S_F(x) = (m\mathbf{1} + i\gamma^\mu\partial_\mu)G_F(x) = \lim_{\varepsilon\downarrow 0}\int \frac{d^4k}{(2\pi)^4}\,\frac{m\mathbf{1} + \gamma^\mu k_\mu}{m^2 - k^2 - i\varepsilon}e^{-ikx}$$

and $(m\mathbf{1} - i\gamma^\mu\partial_\mu)S_F(x) = \delta^4(x)$.

Maxwell case

The functions for the vector potential (in the Gupta-Bleuler approach, cf Sect. 4.6) depend on the arbitrary "gauge parameter" λ, but the λ-dependence drops out for $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$. The 2-point function equals

$$(\Omega, F_{\mu\nu}(x)F_{\kappa\lambda}(y)\Omega) = \partial_{[\mu}\eta_{\nu][\kappa}\partial_{\lambda]}\,D(x-y)$$

and accordingly the commutator function. The Feynman propagator is

$$G_F^{\mu\nu}(x-y) = i(\Omega, T[A^\mu(x)A^\nu(y)]\Omega) = \lim_{\varepsilon\downarrow 0}\int \frac{d^4k}{(2\pi)^4}\,\big(\eta^{\mu\nu} - (1-\lambda^{-1})\frac{k^\mu k^\nu}{k^2 + i\varepsilon}\big)\frac{e^{-ik(x-y)}}{k^2 + i\varepsilon}.$$

In the "Feynman gauge" $\lambda = 1$, it simplifies to $-\eta^{\mu\nu}G_F^{(m=0)}(x-y)$.

5.8 Dirac field in a classical elm background

As an example where the interaction is quadratic in the field, we consider the S-matrix for the quantized Dirac field interacting with a classical electromagnetic (elm) field

$$S = Te^{-i\int d^4x\, A_\mu(x)j^\mu_{\rm elm}(x)} = Te^{ie\int d^4x\, A_\mu(x)j^\mu_{\rm Dirac}(x)}.$$

Here we have introduced the *positive* elementary charge unit e, so that the elm current is $j^\mu_{\rm elm} = -e\,j^\mu_{\rm Dirac} = -e\,{:}\overline{\psi}\gamma^\mu\psi{:}$, hence $Q_{\rm elm} = -e\int \widetilde{dk}\, b_i^*(k)b_i(k) + e\int \widetilde{dk}\, d_i^*(k)d_i(k)$ (because $\psi \sim \int(b + d^*)$). This means that $b_i^*(k)\Omega$ are interpreted as one-electron states, and $d_i^*(k)\Omega$ are one-positron states.

Without computation, conservation laws give us some a priori information. Eg, because j^μ is neutral, it commutes with the charge operator Q, hence S commutes with Q, and the in- and out-states must have the same charge. Thus, particles and anti-particles can only be produced in pairs. Also, because j^μ is quadratic in the Dirac field, the particle number can change only by multiples of two.

${}_{\rm out}\langle 0|0\rangle_{\rm in} = (\Omega_{\rm in}, S\,\Omega_{\rm in})$ is the probability amplitude that the background field does not produce any particles. The absolute squares of the amplitudes

$$\begin{aligned}(a)\quad & {}_{\rm out}\langle k'|k\rangle_{\rm in} = (b^*_{\rm in}(k')\Omega_{\rm in}, S\; b^*_{\rm in}(k)\Omega_{\rm in}),\\ (b)\quad & {}_{\rm out}\langle k_1k_2|0\rangle_{\rm in} = (b^*_{\rm in}(k_1)d^*_{\rm in}(k_2)\Omega_{\rm in}, S\;\Omega_{\rm in}),\end{aligned}$$

are the probability densities that (a) an electron with momentum k is deflected to momentum k', or that (b) the elm field produces one electron-positron pair.

To compute such matrix elements, one has to (i) expand S = time-ordered exponential as a power series, then (ii) expand the resulting time-ordered products of Wick products into Wick products (by Wick's Theorem), and finally (iii) evaluate the matrix elements by applying Wick's Theorem to the creation and annihilation operators for the in- and outgoing particles.

Expanding the exponential gives a power series in the electric charge. Since $e^2 = \alpha = 1/137$ is rather small, one may be confident that the overall behaviour is captured by the first few nontrivial terms. The actual computations are rather straightforward, but require quite some book-keeping for all the contributing terms.

Let us evaluate in n-th order

$$\frac{(ie)^n}{n!}\int\prod_m dx_m \langle K'|T\prod_m :\overline{\psi}\gamma^{\mu_m}\psi(x_m):|K\rangle\prod_m A_{\mu_m}(x_m)$$

where $|K\rangle = \prod b^*(k_i)d^*(k_j)\Omega$ is a state describing several incoming electrons and positrons, and similarly $\langle K'| = (\Omega, \prod b(k'_i)d(k'_j)$ for the outgoing particles. Recall

$$\psi(x)\sim\int\widetilde{dk}\,\textstyle\sum_i\big[u_ie^{-ikx}b_i + v_ie^{ikx}d_i^*\big],\quad \overline{\psi}(x)\sim\int\widetilde{dk}\,\textstyle\sum_i\big[\overline{v}_ie^{-ikx}d_i + \overline{u}_ie^{ikx}b_i^*\big].$$

Apart from direct contractions between in- and outgoing creation and annihilation operators (which describe contributions where some particles just go unscattered), each incoming electron (b^*) or positron (d^*) must be contracted with one of the field operators $\psi(x)$ or $\overline{\psi}(x)$, giving factors depending on the incoming momenta

$$(\Omega,\psi_a(x)b_i^*(k)\Omega) = \sqrt{2m}\,u_{ai}(k)e^{-ikx},\qquad (\Omega,\overline{\psi}_a(x)d_i^*(k)\Omega) = \sqrt{2m}\,\overline{v}_{ai}(k)e^{-ikx}.$$

Likewise, outgoing electrons (b) or positrons (d) must be contracted via

$$(\Omega,b_i(k')\overline{\psi}_a(x)\Omega) = \sqrt{2m}\,\overline{u}_{ai}(k')e^{ik'x},\qquad (\Omega,d_i(k')\psi_a(x)\Omega) = \sqrt{2m}\,v_{ai}(k')e^{ik'x}.$$

The remaining field operators must be contracted among each other according to

$$(\Omega,T\big[\psi_a(x)\overline{\psi}_b(y)\big]\Omega) = -iS_F(x-y)_{ab},\ (\Omega,T\big[\overline{\psi}_b(x)\psi_a(y)\big]\Omega) = iS_F(y-x)_{ab}.$$

The summations over the spinor indices a, b give rise to matrix multiplications, involving alternating products of γ-matrices and propagators. There arise three types of structures: matrix elements $\overline{u}\gamma S_F\ldots\gamma u$, $\overline{v}\gamma S_F\ldots\gamma v$, or traces $\mathrm{tr}\,(\gamma S_F\ldots\gamma S_F)$.

One visualizes these structures by diagrams: each γ^{μ_m} (arising from an interaction term at the point x_m) is represented by a vertex labelled x_m, each propagator $S_F(x_m - x_n)$ by an oriented line from x_n to x_m. An incoming electron and an outgoing positron are depicted as a line pointing into the respective contraction vertex, while an incoming positron and an outgoing electron are depicted as a line pointing out of the contraction vertex. The orientation corresponds to the product order of spinor matrices. In this way, the first two types of contraction schemes gives rise to a continuous oriented "lepton line" passing through several vertices, while the last type gives a loop with several vertices. Every fully contracted contribution may consist of several subdiagrams of all three types.

Each diagram has to be multiplied by $\prod_m A_{\mu_m}(x_m)$ and integrated over all x_m. Collecting also the numerical coefficients, one finds an overall factor e^n, and a factor $\mp i$ for each $e^\pm$ line, and a factor -1 for each loop. The $1/n!$ is cancelled by $n!$ permutations of the interaction points x_m, which all give rise to the same diagram and hence to the same analytical expression.

Next, we insert the Fourier representation of the propagator

$$S_F(x-y) = \lim_{\varepsilon\downarrow 0} \int \frac{d^4q}{(2\pi)^4} \, \frac{m\mathbf{1} + \gamma^\lambda q_\lambda}{m^2 - q^2 - i\varepsilon} \, e^{-iq(x-y)},$$

and perform the x_m-integrations. This gives rise to the following rules: The momenta k (or k') are assigned to the external lines for incoming (or outgoing) particles, flowing into (or out of) the diagram. This means that external electron (positron) momenta flow in the same (opposite) direction as the orientation of the lines. An internal momentum q is assigned to each internal line, flowing in the direction of the orientation of the line. As a result, the γ^μ matrices at each vertex go contracted with the numerical factor $\hat{A}_\mu(p)$ where p is the sum of the momenta flowing out of the vertex along the lepton lines. One should think of p as an energy-momentum transfer from the electromagnetic field into the quantum system, either changing the momentum of a particle or producing a particle-antiparticle pair.

In particular, in the above cases (a) and (b), we observe that in first order, the momentum p of the elm field must be $k - k'$ or $k + k'$, resp. But k and k' both lie on the mass hyperboloid, hence p cannot be null. Thus, if the elm field is a solution of the Maxwell equations, the 1st order contribution vanishes.

To evaluate the diagrams further, one has to compute the matrix elements or traces over several γ matrices, coming both from the vertices and from the propagators. The traces can be derived directly from the defining properties, eg $\operatorname{tr}\gamma^\mu = 0$, $\operatorname{tr}\gamma^\mu\gamma^\nu = 4\eta^{\mu\nu}$, $\operatorname{tr}\gamma^\mu\gamma^\nu\gamma^\kappa = 0$, $\operatorname{tr}\gamma^\mu\gamma^\nu\gamma^\kappa\gamma^\lambda = 4(\eta^{\mu\nu}\eta^{\kappa\lambda} + \eta^{\nu\kappa}\eta^{\lambda\mu} - \eta^{\mu\kappa}\eta^{\nu\lambda})$; while the matrix elements are more complicated.

The result is a polynomial in external and internal momenta, multiplying the denominators $\prod_l (m^2 + q_l^2 - i\varepsilon)^{-1}$ and the Fourier amplitudes $\prod_m \hat{A}(p_m)$ of the external field at $p_m =$ sums or differences of external and internal momenta. The integration over the internal momenta amount to integrations over the p_m, with one additional integration in the case of loops.

6 Interaction among quantum fields

6.1 IR and UV divergences

Quantum Electrodynamics has the interaction Lagrangean density

$$\mathcal{L}_{\rm int} = -j^\mu_{\rm elm} A_\mu = e\, j^\mu A_\mu$$

where j^μ is the quantized Dirac current and A_μ is the quantized Maxwell field. The two fields can be simultaneously quantized on a Fock space which is the tensor product of two Fock spaces (one of them indefinite), ie the product should be read as $j^\mu \otimes A_\mu$. This is meaningful since in the S-matrix

$$S = Te^{ie\int d^4x\, j^\mu A_\mu}$$

the fields are free ("in") fields. However, the argument for the derivation of this formula assumed that the interaction can be turned on and off. This is, of course, physically meaningless in QED. The best one can try to do is to "mentally" regard the charge (coupling constant) e as a function of time (and space), define the S-matrix for a coupling constant that vanishes at $t \to \pm\infty$ as in Sect. 5.5, and "in the end" take a limit $e \to const.$ This limit will in fact produce another instance of the infrared problem: namely $e(x)$ plays a similar role as the classical current $j(x)$ in Sect. 5.1, or the classical vector potential $A_\mu(x)$ in Sect. 5.8, whose Fourier transform cannot be put to a δ function. This problem requires a more flexible setup (see below).

In order to disentangle the complicated kinematics of Fermi and Maxwell fields, as well as the Hilbert space positivity problem going along with the quantized vector potential, from the new features associated with the translation invariant interaction between quantum fields, we return to our simple model with a single scalar field with self-interaction $V(\varphi)$, eg $\frac{1}{4}g\varphi^4$, where the salient features become visible as well. Our formal derivation of the S-matrix as in the previous section leads to

$$S = Te^{-i\int d^4x\, g(x)/4:\varphi_{\rm in}(x)^4:}.$$

The power series expansion gives

$$S = 1 + \frac{i}{4}\int d^4x\, g(x):\varphi_{\rm in}(x)^4: - \frac{1}{2\cdot 4^2}\int d^4x d^4y\, g(x)g(y)\, T\big[:\varphi_{\rm in}(x)^4::\varphi_{\rm in}(y)^4:\big] + \dots$$

(graphical representation by Wick's Theorem: x-space Feynman diagrams.) This formula has several problems. Eg, let us look at the second-order term. By Wick's Theorem, it contains the term with four contractions:

$$-X_2 = -\frac{24}{2\cdot 4^2}\int d^4x d^4y\, g(x)g(y)\, G_F(x-y)^4.$$

Clearly, it is impossible to put $g(x)$ to a constant, because then the integrand depends only on $x-y$, so that X_2 diverges $\sim \int d^4x$. This is the return of the

IR problem of Sect. 5.3. Similar IR divergent numerical terms X_n occur in any order $n \geq 2$, and they contribute to every amplitude. All these terms sum up to $\prod_{n\geq 2} e^{-X_n} = 0$. In particular, the vacuum-to-vacuum amplitude would vanish. But this time, this fact cannot be ascribed to a violation of energy conservation (cf Sect. 5.1), because the limit theory with $g = const$ is time-independent. It is therefore an unacceptable feature: instead, if S commutes with the Hamiltonian, and the vacuum is the unique state with energy 0, then we *must* have $S\Omega = \Omega$ (up to a phase), and hence $|_{\rm out}(\Omega, \Omega)_{\rm in}|^2 = |(\Omega, S\Omega)|^2 = 1$.

This IR problem due to the unphysical assumption that the coupling could be switched off can be eliminated with a better definition of the S-matrix, cf Sect. 6.4, at the expense of abandoning the CCR for the interacting field.

The terms with three and two contractions are

$$-\frac{4^2 \cdot 6}{2 \cdot 4^2} \int d^4x d^4y \, g(x)g(y) \, G_F(x-y)^3 {:}\varphi(x)\varphi(y){:}$$

and

$$-\frac{12^2 \cdot 2}{2 \cdot 4^2} \int d^4x d^4y \, g(x)g(y) \, G_F(x-y)^2 {:}\varphi(x)^2\varphi(y)^2{:}.$$

They contribute to processes involving two or more external particles, eg we have a contribution

$${}_{\rm out}\langle p'|p\rangle_{\rm in} = \cdots - 3 \int d^4x d^4y \, g(x)g(y) \, G_F(x-y)^3 (e^{-ipx+ip'y} + e^{-ipy+ip'x}) + \ldots$$

Here, putting $g = const$ is no problem, and we get in momentum space

$$\sim -g^2 \delta(p'-p) \int \frac{d^4k_1}{k_1^2 - m^2 + i\varepsilon} \frac{d^4k_2}{k_2^2 - m^2 + i\varepsilon} \frac{d^4k_3}{k_3^2 - m^2 + i\varepsilon} \delta(k_1 + k_2 + k_3 - p).$$

Similarly, there is a contribution to the scattering amplitude ${}_{\rm out}\langle p_1' p_2'|p_1 p_2\rangle_{\rm in}$

$$\sim -g^2 \delta(p_1' + p_2' - p_1 - p_2) \int \frac{d^4k_1}{k_1^2 - m^2 + i\varepsilon} \frac{d^4k_2}{k_2^2 - m^2 + i\varepsilon} \delta(k_1 + k_2 - p_1 - p_2).$$

The δ-function prefactors represent the overall energy-momentum conservation under a space-time independent interaction. But the integrals are divergent at large k (UV-divergent).

These UV-problems (due to the very-high frequency fluctuations of quantum fields) are omnipresent in QFT and require a more subtle treatment: renormalization, postponed to Chap. 7.

6.2 A priori considerations

A translation invariant interaction Lagrangean can contain only the quantum fields, but no classical functions (sources, or time dependent coupling "constants"). In particular, the formula $S = Te^{i\int \mathcal{L}_{\rm int} dx}$ for the scattering matrix is bound to fail via the IR problem, which makes ${}_{\rm out}\langle 0|0\rangle_{\rm in} = 0$, whereas in a translation invariant theory the S matrix should commute with the Hamiltonian, implying $|0\rangle_{\rm out} = |0\rangle_{\rm in}$.

In Sect. 6.4, another formula for the scattering matrix is given in terms of (time-ordered) correlation functions of the interacting field, without any reference to a Lagrangean. This approach assumes that an interacting quantum field can be constructed in some way – no matter how. In order that this method works, certain properties of the interacting fields must be required. (Most of) these properties can be formulated in a model-independent way and are of rather fundamental nature, in the sense that they should hold in every local relativistic quantum field theory.

Axiomatic approaches (there are several versions) consist in formulating these fundamental requirements, and extracting general physical insight only from the mathematical interplay of these axioms. This will only be sketched here.

The basic version (Wightman axioms) requires that

• Fields are operator-valued distributions on a Hilbert space (defined along with their adjoints on a common stable dense domain).
• The Hilbert space carries a unitary representation U of the proper orthochronous Poincaré group, and the fields transform in a covariant way under the adjoint action: $\phi(x) \to U(a,A)\phi(x)U(a,A)^* = S(A)^T\phi(\Lambda_A x + a)$.
• The spectrum of the four-momentum P^μ is contained in the (closed) forward light-cone, and there is a unique ground state (the vacuum) with eigenvalue $P^\mu = 0$.
• The fields are local: commutators vanish at spacelike distance.

From these axioms, one infers far-reaching analytic properties of the correlation distributions $(\Omega, \phi_1(x_1)\dots\phi_N(x_N)\Omega)$. The "reconstruction theorem" states that knowledge of all correlation functions (satisfying these properties) uniquely determines the quantum field(s). Thus, the axioms can be formulated directly in terms of correlations functions.

One consequence of these properties is that one has the equality

$$(\Omega, \phi_1(x_1)\dots\phi_N(x_N)\Omega) = (\Omega, \phi_N(-x_N)\dots\phi_1(-x_1)\Omega) \quad \big(\equiv \overline{(\Omega, \phi_1^*(-x_1)\dots\phi_N^*(-x_N)\Omega)}\big),$$

from which the PCT theorem (Sect. 4.8) follows. If one admits also anti-commutativity instead of locality, then the Spin-Statistics theorem (fields with half-integer spin must anti-commute, cf Sect. 4.7) can be proven. The LSZ formula (Sect. 6.4) is a consequence of the axioms with a sharpened version of the spectral axiom.

The problem of the actual construction of interacting quantum fields remains. Several methods exist, using some further input so as to specify the interaction. The hard part is to verify all axioms from the construction. Often, Lorentz invariance has to be broken (or other essential features have to be abandoned) at intermediate steps, and one has to show that they can be recovered in appropriate limits.

6.3 Nonlinear field equations (optional)

We present an rather naive, and not very successful, idea to construct an interacting quantum field by solving a nonlinear equation of motion, like

$$(\Box + m^2)\varphi(x) = -g\varphi^2(x).$$

Notice that the rhs is not even defined, because products of quantum fields at a point are singular, and Wick products can be defined only for free fields. So the task also consists in giving a meaning to the rhs along the way. We admit $g = g(x)$ to be a function of x, to be put constant at some later stage ("adiabatic limit").

Let G be a Green function for the KG operator. Then defining φ_0 by

$$\varphi_0(x) := \varphi(x) + \int dy\, G(x-y)\cdot g(y)\varphi(y)^2,$$

φ_0 solves the free KG equation. If we choose the retarded GF (cf Sect. 5.7)

$$G_{\rm ret}(x-y) = \theta(x^0-y^0)(\Delta_m(y-x)-\Delta_m(x-y)),$$

then the integrand vanishes at $y^0 > x^0$. If the coupling $g(y)$ is switched on at a time t_0, then the integral vanishes for $x^0 < t_0$, and the field φ_0 coincides with the field φ before t_0. Thus, φ_0 is the "incoming" free field.

We therefore arrive at the integral equation

$$\varphi(x) = \varphi_{\rm in}(x) - \int dy\, G_{\rm ret}(x-y)\cdot g(y)\varphi(y)^2.$$

Here, we "insert the lhs into the rhs", getting

$$\varphi(x) = \varphi_{\rm in}(x) - \int dy\, G_{\rm ret}(x-y)\cdot g(y) \prod\nolimits_1^2 \Big(\varphi_{\rm in}(y) - \int dz_i\, G_{\rm ret}(y-z_i)\cdot g(z_i)\varphi(z_i)^2\Big).$$

In the leading term of the product we have free fields, so we may define the product as the Wick product. For the remaining terms, we iterate the procedure by again replacing φ by its integral representation, thus shifting the ill-defined products to higher and higher orders of the coupling. In the end, one obtains an expansion of the interacting field as an infinite power series of nested integrals over Wick products of free fields at earlier times. A typical term of this series is

$$\int dy\, G_{\rm ret}(x-y)\, g(y) \int dz\, G_{\rm ret}(y-z)\, g(z) {:}\big[\varphi_{\rm in}(y){:}\varphi_{\rm in}(z)^2{:} + {:}\varphi_0(z)^2{:}\varphi_{\rm in}(y)\big]{:}.$$

Working out the square bracket by Wick's Theorem produces terms involving

$$G_{\rm ret}(y-z)\big(\Delta_m(y-z)+\Delta_m(z-y)\big)\varphi_{\rm in}(z) = \theta(y^0-z^0)\big(\Delta_m(z-y)^2-\Delta_m(y-z)^2\big)\varphi_{\rm in}(z).$$

The first problem here is to deal with such products of distributions which have divergent Fourier representations. The question whether they can be defined at all, and if so, to identify possible ambiguities, is another formulation of the renormalization program. The second problem is the IR problem in the adiabatic limit $g \to const.$ The hardest problem is the convergence of the resulting power series. (There are good arguments that perturbative series never converge.)

Up to these problems, one arrives at a perturbative scheme to express the interacting field in terms of free fields, allowing to compute all its correlation functions as power series of integrals over free correlation functions. However, in practice a different route is taken, cf Sect. 6.8 ff.

6.4 LSZ formula

Lehmann, Symanzik and Zimmermann gave a formula for the S-matrix, which is entirely intrinsic in terms of the correlation functions of the interacting quantum field. Instead of "switching off" the interaction, the theory is assumed to be Poincaré invariant, in particular time-translation invariant, with a unique vacuum vector $P^\mu\Omega = 0$, and a one-particle subspace $\mathcal{H}_1$ according to some representation of the Poincaré group of mass $m > 0$ (Sect. 4.4). One also assumes that the spectrum of the mass operator $P_\mu P^\mu$ on the subspace $\mathcal{H}^\perp$ orthogonal to Ω and $\mathcal{H}_1$ starts at some value $m'^2 > m^2$ ("mass gap").

For simplicity, we work with a hermitean scalar field. An interacting quantum field cannot be represented in terms of creation and annihilation operators. Instead, the strategy will be to "extract" approximate such operators from the field.

Translation invariance of Ω implies that $(\Omega, \varphi(x)\Omega)$ cannot depend on x, hence it is some constant v. We replace $\varphi(x)$ by $\varphi(x) - v$, so that WLOG $(\Omega, \varphi(x)\Omega) = 0$.

Let $\Psi_k = |k\rangle \in \mathcal{H}_1$ be a one-particle eigenvector with the standard normalization. Translation covariance implies that

$$(\Psi_k, \varphi(x)\Omega) = e^{ikx} f(k).$$

Lorentz invariance implies that $f(k) = f(\Lambda k)$, hence $f(k)$ is some constant $Z^{1/2}$ along H_m. For a free field, we would have $Z = 1$. We only assume $Z \neq 0$, and can then enforce $f(k) = 1$ by a re-scaling of the field φ by the factor $Z^{-1/2}$.

One now *defines* at any fixed time t quantities

$$a^*(k)_t = -i \int_{x^0=t} d^3x e^{-ikx} \overset{\leftrightarrow}{\partial_0} \varphi(x),$$

where φ is the re-scaled field. For a free field, this would in fact not depend on t, and coincide with the creation operator $a^*_{\text{free}}(k)$. By inserting into the above, we find $(\Omega, a^*(k)_t\Omega) = 0$, and for $\Psi_{k'} \in \mathcal{H}_1$,

$$(\Psi_{k'}, a^*(k)_t\Omega) = (2\pi)^3 2k^0 \delta(\vec{k} - \vec{k}').$$

This means that

$$a^*(k)_t \Omega\Psi_k \in \mathcal{H}^\perp,$$

ie the would-be creation operators indeed create *time-independent* one-particle states plus some unknown time-dependent excited states in $\mathcal{H}^\perp$. The crucial point is that the latter part becomes small as $t \to \pm\infty$ in the following weak sense.

Let Ψ_p be a vector in $\mathcal{H}^\perp$ with four momentum eigenvalues p^μ, $p^2 \geq m'^2 > m^2$. By covariance, we have the x-dependence

$$(\Psi_p, \varphi(x)\Omega) = e^{ipx} F(p)$$

with some function $F(p)$, which implies

$$(\Psi_p, a^*(k)_t\Omega) = -i \int_{x^0=t} d^3x\, e^{-ikx} \overset{\leftrightarrow}{\partial_t} e^{ipx} F(p) = \int_{x^0=t} d^3x\, (p^0 + k^0) e^{i(p-k)x} F(p).$$

The $\vec{x}$-integration gives $\delta(\vec{k}-\vec{p})$, hence

$$(\Psi_p, a^*(k)_t\Omega) \sim (p^0+k^0)F(p^0,\vec{k})e^{it(p^0-k^0)},$$

where $p^0 \geq \sqrt{\vec{k}^2+m'^2} > \sqrt{\vec{k}^2+m^2} = k^0$. Smearing with a test function $f(\vec{k})$, we get an integral of the form

$$\int d^3k\; G(\vec{k})\; e^{it\,g(\vec{k})}$$

where $g(\vec{k}) \neq 0$ thanks to the mass gap. Such integrals vanish $\sim |t|^{-\frac{3}{2}}$ by the Riemann-Lebesgue lemma as $t \to \pm\infty$, due to the rapidly oscillating exponential.

By similar methods, Haag and Ruelle (and Hepp) have shown that the would-be creation operators and their conjugates behave asymptotically like their free-field counterparts, in particular they satisfy CCR in the limit $|t| \to \infty$. The physical mechanism underlying the proof is that wave packets with disjoint momentum support separate more and more with time, so that the interaction is suppressed.

We define the asymptotic multi-particle states

$$|k_1 \dots k_N\rangle_{\rm as} = \lim_{t\to\pm\infty} a^*(k_1)_t \dots a^*(k_N)_t\Omega$$

as limits $t \to -\infty$ ("in-states") or $t \to +\infty$ ("out-states"). We want to compute scattering matrix elements

$${}_{\rm out}\langle k'_1 \dots k'_{N'}|k_1 \dots k_N\rangle_{\rm in} = (a^*(k'_1)_{+\infty} \dots \Omega, a^*(k_1)_{-\infty} \dots \Omega).$$

Let $|K\rangle_{\rm in}$ and $|K'\rangle_{\rm out}$ be multi-particle scattering states. We compute the following integrals over matrix elements of time-ordered products of field operators:

$$I^\pm := i\int d^4x\, e^{\pm ikx}(\Box_x + m^2)\,{}_{\rm out}\langle K'|T[\varphi(x_1)\dots\varphi(x_{n-1})\varphi(x)]|K\rangle_{\rm in},$$

where $k \in H_m$. Integrating by parts, the spatial Laplacian $-\vec{\nabla}^2$ is moved to $e^{\pm ikx}$, where it equals $-m^2-\partial_t^2$, hence we may replace $\Box+m^2$ by $\overrightarrow{\partial_t^2} - \overleftarrow{\partial_t^2}$:

$$I^\pm = {}_{\rm out}\langle K'|i\int d^4x\,\partial_t\Big(e^{\pm ikx}\overset{\leftrightarrow}{\partial_t}T[\varphi(x_1)\dots\varphi(x_{n-1})\varphi(x)]\Big)|K\rangle_{\rm in}.$$

Here, the t-integration just yields the limiting values as $t \to \pm\infty$. For e^{-ikx} resp. e^{+ikx}, the x-integration then gives the asymptotic would-be creation resp. annihilation operators $a^{(*)}_{\pm\infty}(k)$, which are inserted to the left ($t=+\infty$) or right ($t=-\infty$) of the time-ordered product. If k is different from all momenta in the scattering states, then $a_{-\infty}(k)|K\rangle_{\rm in} = 0$ and ${}_{\rm out}\langle K'|a^*_{+\infty}(k) = 0$. Hence the above integrals $I^\pm$ are reduced to matrix elements of the time-ordered product with one field operator less, but with one additional ingoing or outgoing particle:

$$I^+ = {}_{\rm out}\langle K',k|\,T[\varphi(x_1)\dots\varphi(x_{n-1})]\,|K\rangle_{\rm in}, \qquad I^- = {}_{\rm out}\langle K'|\,T[\varphi(x_1)\dots\varphi(x_{n-1})]\,|k,K\rangle_{\rm in}.$$

Reversing and iterating the argument, one finds the **LSZ formula**

$$\begin{aligned}{}_{\rm out}\langle k'_1\dots k'_{N'}|k_1\dots k_N\rangle_{\rm in} &= i^{N+N'}\int d^4x_1\, e^{-ik_1x_1}\dots\int d^4x'_1\, e^{+ik'_1x'_1}\dots\\ &(\Box_1+m^2)\dots(\Box'_1+m^2)\dots(\Omega,T[\varphi(x_1)\dots\varphi(x'_1)\dots]\Omega) \quad +\delta\text{-terms.}\end{aligned}$$

The δ-terms arise when the momenta are not disjoint. They are of the general form $\delta(\vec{k}'_i-\vec{k}_j)$ times similar integrals with less entries. They correspond to processes where some particles pass unscattered.

The LSZ formula expresses scattering amplitudes in terms of **time-ordered correlation functions**, also called **(generalized) Green functions**

$$\tau_N(x_1,\dots x_N)\equiv(\Omega,T\big[\varphi(x_1)\dots\varphi(x_N)\big]\Omega)$$

of the interacting field (after a suitable shift and multiplicative re-normalization). Knowing the latter, fixes the scattering matrix.

Sect. 6.9 will give a perturbative formula for the interacting Green functions.

Notice that even if the original interacting field φ satisfied the CCR, the need for a re-scaling by $Z^{-1/2}$ would destroy the CCR. Indeed, **Haag's Theorem** asserts that in a Lorentz invariant interacting QFT it is impossible to maintain CCR.

In terms of the Fourier transforms of the GFs, the LSZ formula reads

$${}_{\rm out}\langle K'|K\rangle_{\rm in} = i^{N+N'}(m^2-k_1^2)\dots(m^2-k_1'^2)\dots\widehat{\tau}(-k'_1,\dots,+k_1,\dots) \quad +\delta\text{-terms.}$$

Therefore, in order to get a non-vanishing S-matrix, the Green functions must have poles at $k^2=m^2$ in momentum space, such that the amplitude is essentially the residue.

The position of the poles (and hence the masses of the interacting particles!) will be influenced by the dynamics, and cannot be imposed apriori.

The LSZ formula generalizes to the Dirac and Maxwell fields. One has to replace the operators $\int d^4x\, e^{\pm ikx}(\Box+m^2)$ acting on $(\Omega,T[\dots\varphi(x)\dots]\Omega)$ by

$$\bar v_s(k)\int d^4x\, e^{-ikx}(m\mathbf{1}-i\gamma^\lambda\partial_\lambda) \qquad \text{resp.} \qquad \bar u_s(k)\int d^4x\, e^{+ikx}(m\mathbf{1}-i\gamma^\lambda\partial_\lambda)$$

acting on $(\Omega,T[\dots\psi(x)\dots]\Omega)$ for an incoming positron resp. outgoing electron,

$$\int d^4x\, e^{-ikx}(m\mathbf{1}+i\gamma^\lambda\partial_\lambda)u_s(k) \qquad \text{resp.} \qquad \int d^4x\, e^{+ikx}(m\mathbf{1}+i\gamma^\lambda\partial_\lambda)v_s(k)$$

acting on $(\Omega,T[\dots\overline{\psi}(x)\dots]\Omega)$ for an incoming electron resp. outgoing positron (where the matrices multiply from the right); and by

$$e^\mu_\varepsilon(k)\int d^4x\, e^{-ikx}(-\eta_{\mu\nu}+(1-\lambda)\partial_\mu\partial_\nu) \quad \text{resp.} \quad \overline{e^\mu_\varepsilon(k)}\int d^4x\, e^{+ikx}(-\eta_{\mu\nu}+(1-\lambda)\partial_\mu\partial_\nu)$$

acting on $(\Omega,T[\dots A^\nu(x)\dots]\Omega)$ for an incoming resp. outgoing photon.

6.5 Cross sections

We wish to convert probability amplitudes into scattering cross sections. We assume that a beam of incoming particles (the projectile) hits a particle at rest (the target). This is called the fixed targed (FT) frame, as opposed to the center-of-mass (CM) frame. The differential cross section is the probability that the outgoing particles have momenta within some given (infinitesimal) range (ie the expectation value of the corresponding projection operator), relative to the time-integrated flux of incident particles:

$$d\sigma = \frac{{}_{\rm in}\langle K|d\Pi_{\rm out}|K\rangle_{\rm in}}{{}_{\rm in}\langle K|K\rangle_{\rm in}\cdot\text{flux per particle}\cdot\text{time}} \qquad d\Pi_{\rm out} = \prod \widetilde{dk}'_i\ |K'\rangle_{\rm out\ out}\langle K'|.$$

For n identical outgoing particles, $\Pi_{\rm out}$ has a correction factor $1/n!$.

For two outgoing particles, energy and momentum conservation plus the on-shell conditions leave only two parameters of the outgoing momenta undetermined, which are usually taken as a scattering solid angle (ϑ,φ) (deflection of the projectile). For scalar particles, rotation invariance implies that ${}_{\rm out}\langle K'|K\rangle_{\rm in}$ and hence the cross section depends only on ϑ. (Conversely, for spinor and vector fields, there will be a correlation between the spin and the direction of scattering. This anisotropy is in fact used to determine the spin of an unknown particle.)

Because all τ-functions are translation invariant, all S-matrix elements involve a factor for the total energy-momentum conservation, hence we may write

$${}_{\rm out}\langle K'|K\rangle_{\rm in} = (2\pi)^4\delta\big(\sum k_i - \sum k'_j\big)\ iT(K';K)$$

where $T(K;K)$ is a reduced scattering amplitude. For the probability, we need the absolute square of ${}_{\rm out}\langle K'|K\rangle_{\rm in}$. This is of course problematic because of the δ-function; but this is to be expected because we work in scattering theory with unnormalizable states (constant flux of incoming particles of sharp momenta). One should work with smearing functions

$$|K\rangle_{\rm in} = \int \widetilde{dk}_1\widetilde{dk}_2 f(k_1)f(k_2)|k_1,k_2\rangle_{\rm in}$$

and take a limit of $f(k_1)$ approaching δ-functions. It is, however, legitimate to ignore this complication provided one replaces expressions like $(2\pi)^3\delta(\vec{0})$ by a volume V, and $(2\pi)^4\delta(0)$ by VT where $V\to\infty$ corresponds to a wave function which is constant within V and zero outside, and T is the time duration of the experiment. Thus, for one-particle states

$$\langle k|k\rangle = (2\pi)^3 2k^0\delta(\vec{0}) = 2k^0\,V,$$

and $[(2\pi)^4\delta(\sum k_i - \sum k'_j)]^2$ may be replaced by $(2\pi)^4\delta(\sum k_i - \sum k'_j)$ times

$$(2\pi)^4\delta\big(\sum k_i - \sum k'_j\big) = (2\pi)^4\delta(0) = V\Delta T.$$

With these approximations, and using the flux of the projectile flux $= v/V = |\vec{k}_1|/k_1^0 V$, all factors V and ΔT cancel out (as they should), and we get the following expression (for two particles in the in-state, in the FT frame: $k_2^0 = m_2$)

$$d\sigma = \frac{|T|^2}{4|\vec{k}_{1\mathrm{FT}}|m_2}(2\pi)^4\delta\big(k_1+k_2-\sum k_j'\big)\prod \widetilde{dk}_i'.$$

This formula can be made Lorentz invariant by introducing the relativistic invariant

$$s := (k_1+k_2)^2.$$

In the FT frame, we have $s = m_1^2+m_2^2+2m_2E_{1\mathrm{FT}} = m_1^2+m_2^2+2m_2\sqrt{m_1^2+|\vec{k}_1^2|_{\mathrm{FT}}}$, and in the CM frame $s = (k_1^0+k_2^0)_{\mathrm{CM}} = (E_1+E_2)^2_{\mathrm{CM}}$. Therefore, in the denominator

$$2|\vec{k}_1|_{\mathrm{FT}}m_2 = \sqrt{(s-m_1^2-m_2^2)^2-4m_1^2m_2^2} = 2|\vec{k}_1|_{\mathrm{CM}}\sqrt{s}.$$

Let us concentrate on the case of two outgoing particles (masses m_1', m_2'). In the CM frame, s determines $|\vec{k}_1| = |\vec{k}_2|$ and $|\vec{k}_1'| = |\vec{k}_2'|$, and hence all the energies, while the scattering angle ϑ is an independent kinematical variable; in contrast in the FT frame, only $E_{1\mathrm{FT}}$ is determined by s, while the two final energies and the scattering angle are related by two relations $E_1'+E_2' = m_2+E_1$ and

$$m_2'^2 = (k_1+k_2-k_1')^2 = m_1^2+m_1'^2+m_2^2+2m_2(E_1-E_1')_{\mathrm{FT}}-2(E_1E_1'-|\vec{k}_1||\vec{k}_1'|\cos\vartheta)_{\mathrm{FT}}.$$

It is convenient to define the second invariant (the squared energy-momentum transfer)

$$t := (k_1-k_1')^2 = m_1^2+m_1'^2-2(E_1E_1'-|\vec{k}_1||\vec{k}_1'|\cos\vartheta),$$

which is sensitive to the scattering angle. At fixed s, one has

$$dt = \big(2|\vec{k}_1||\vec{k}_1'|\,d\cos\vartheta\big)_{\mathrm{CM}} = \Big(\frac{2m_2|\vec{k}_1||\vec{k}_1'|^2}{m_2|\vec{k}_1'|+|\vec{k}_1'|E_1-|\vec{k}_1|E_1'\cos\vartheta}\,d\cos\vartheta\Big)_{\mathrm{FT}}.$$

The invariant relation between the outgoing measure and the solid angle $d\Omega = 2\pi\,d\cos\vartheta$ is obtained by integrating over all other kinematic parameters except t, at fixed s: one finds (eg, by computation in the CM frame)

$$\int(2\pi)^4\delta\big(k_1+k_2-k_1'-k_2'\big)\,\widetilde{dk}_1'\widetilde{dk}_2' = \frac{dt}{8\pi\sqrt{(s-m_1^2-m_2^2)^2-4m_1^2m_2^2}},$$

and therefore the frame-independent formula

$$d\sigma = \frac{|T(s,t)|^2\,dt}{16\pi((s-m_1^2-m_2^2)^2-4m_1^2m_2^2)}$$

with the previous frame-dependent relations between dt and $d\cos\vartheta$.

For more than two particles, one needs more variables to specify the out-state, and for particles with spin or helicity, the cross section will also depend on the azimuthal angle φ. Accordingly, one has to modify the measures $\widetilde{dk}'$ and refer the infinitesimal cross section $d\sigma$ to more refined kinematical regions.

6.6 Generating functional and Gaussian integrals

We want to find a prescription how to compute the time-ordered correlation functions $\tau(x_1, \dots x_N)$ in an interacting QFT (again, for simplicity for a scalar field φ). It is convenient to think in terms of a **generating functional** given by

$$T[J] = (\Omega, Te^{i\int d^4x\,\varphi(x)J(x)}\Omega) \equiv \sum\nolimits_N \frac{i^N}{N!}\int \Big(\prod\nolimits_i d^4x_i\; J(x_i)\Big)\; \tau_N(x_1, \dots x_N)$$

where J is an arbitrary auxiliary function whose only purpose is to allow to recover the actual Green functions by functional derivatives:

$$\boxed{\tau_N(x_1, \dots x_N) = \big(-i\frac{\delta}{\delta J(x_1)}\big)\dots\big(-i\frac{\delta}{\delta J(x_N)}\big)\; T[J]\Big|_{J=0}.}$$

In the free field case, the generating functional is given by Wick's Theorem (cf Sect. 5.6)

$$\boxed{T[J]_{\rm free} = e^{-\frac{1}{2}\tau_{2\rm free}(J,J)}},$$

where $\tau_{2\rm free}(J,J) = \int d^4x d^4y\, J(x)J(y)\;\; \tau_{2\rm free}(x,y) = \lim_{\varepsilon\downarrow 0} i\int d^4k \frac{|\hat J(k)|^2}{k^2-m^2+i\varepsilon}$, from which we read off, in the same way as in Sect. 3.4, the time-ordered free correlation functions = sums over products of $\tau_{2\rm free}(x_i,x_j)$ if N is even, and $=0$ otherwise.

In order to prepare the construction of a formula for $T[J]$ also in the interacting case, we rewrite the above free formula. First, we regard $-\Box - m^2$ as an operator acting on functions $J(x)$, and write

$$\tau_{2\rm free}(J,J) = i(J, (-\Box - m^2 + i\varepsilon\mathbf{1})^{-1}J).$$

With this, $T[J]_{\rm free}$ can be rewritten as the result of an infinite-dimensional integration ("path integral").

Gaussian integrals ("completing the square")

For a positive number a or a strictly positive symmetric real matrix A one has

$$\int dx\; e^{-\frac{1}{2}ax^2} = \sqrt{\frac{2\pi}{a}} \quad\Rightarrow\quad \int dx\; e^{-\frac{1}{2}ax^2}e^{ibx} = \sqrt{\frac{2\pi}{a}}\cdot e^{-\frac{1}{2}b^2/a}.$$

$$\int d^Nx\; e^{-\frac{1}{2}(x,Ax)} = \sqrt{\frac{(2\pi)^N}{\det A}} \quad\Rightarrow\quad \int d^Nx\; e^{-\frac{1}{2}(x,Ax)}e^{i(b,x)} = \sqrt{\frac{(2\pi)^N}{\det A}}\cdot e^{-\frac{1}{2}(b,A^{-1}b)}.$$

The same holds if A is complex as long as its real part has strictly positive eigenvalues, hence (replacing A by $-i(A+i\varepsilon\mathbf{1})$), one gets for arbitrary real A and $\varepsilon > 0$

$$\int d^Nx\; e^{\frac{i}{2}(x,(A+i\varepsilon\mathbf{1})x)}e^{i(b,x)} = \sqrt{\frac{\pi}{\det(-iA+\varepsilon\mathbf{1})}}\cdot e^{-\frac{i}{2}(b,(A+i\varepsilon\mathbf{1})^{-1}b)}.$$

Generalizing this to infinite dimensions, one can write formally

$$\boxed{T[J]_{\text{free}} = \int D\phi\; e^{\frac{i}{2}(\phi,(-\Box-m^2+i\varepsilon)\phi)} e^{i(\phi,J)} \equiv \int D\phi\; e^{i\int d^4x(\frac{1}{2}\partial_\mu\phi\partial^\mu\phi-\frac{1}{2}m^2\phi(x)^2+J(x)\phi(x))},}$$

where ϕ is an "infinite-dimensional integration variable", ie the integration "extends over all real functions" $\phi : \mathbb{R}^4 \to \mathbb{R}$ (field trajectories). All the constant factors have been included into the normalization of the formal integration measure $D\phi$ such that $T[0] = 1$. The exponent is the classical Lagrangean action as if the free scalar field were coupled to an external source J, with the only proviso that m^2 should be given a small imaginary part $-i\varepsilon$, and the limit $\varepsilon \downarrow 0$ is understood.

Remarkably, the same $i\varepsilon$ that originally appeared in the Fourier transform of the Feynman propagator to produce the time-ordering, now is responsible for the (formal) convergence of the Gaussian integral.

By taking variational derivatives wrt J it follows that

$$\tau_{N\,\text{free}}(x_1,\dots x_N) = \int D\phi\; \phi(x_1)\cdots\phi(x_N)\; e^{i\int d^4x\,\mathcal{L}_{\text{free}}[\phi(x)]}.$$

(Actually, an infinite-dimensional Lebesgue measure $D\phi$ does not exist mathematically, but the Gaussian measure $D\mu(\phi)$ formally behaving like

$$D\mu(\phi) = e^{\frac{i}{2}\int d^4x\left(\frac{1}{2}\partial_\mu\phi\partial^\mu\phi-\frac{1}{2}m^2\phi(x)^2\right)}\; D\phi$$

can be rigorously defined, so that the integrals over polynomials like $\phi(x_1)\cdots\phi(x_N)$ exist and the above formula holds.)

6.7 Path integral in QM

We have (by now only for the free field) expressed the generating functional for the time-ordered correlation functions as an integral over all field trajectories, with an oscillating phase given by the classical action. This formula, obtained just by comparison of the explicit expressions, is not accidental. In QM, one can actually prove it also for non-trivial interaction potentials, as follows.

We assume a QM system with a finite number of degrees of freedom, summarily called $\underline{Q}$ and their canonical momenta $\underline{P}$, quantized with CCR, and with time-independent Hamiltonian $H = T + V$. For simplicity, we assume that $T > 0$ is quadratic in $\underline{P}$, and V depends only on $\underline{Q}$. We also assume that the system has a unique ground state $|0\rangle$ with energy 0, and we introduce complete systems of generalized eigenstates of $\underline{Q}$ and $\underline{P}$ (separately) such that

$$\underline{Q}|\underline{q}\rangle = \underline{q}|\underline{q}\rangle, \qquad \underline{P}|\underline{p}\rangle = \underline{p}|\underline{p}\rangle, \qquad \langle\underline{q}|\underline{p}\rangle = (2\pi)^{-1}e^{i\underline{q}\cdot\underline{p}}.$$

In general, $|0\rangle$ will be eigenstate neither of $\underline{Q}$ nor of $\underline{P}$. We use the Heisenberg picture, ie $\underline{Q}$ and $\underline{P}$ are functions of time:

$$\underline{Q}(t) = e^{iHt}\underline{Q}e^{-iHt}, \qquad \underline{P}(t) = e^{iHt}\underline{P}e^{-iHt},$$

hence their eigenstates also evolve according to

$$|\underline{q}\rangle_t = e^{iHt}|\underline{q}\rangle, \qquad |\underline{p}\rangle_t = e^{iHt}|\underline{p}\rangle,$$

while the eigenvalues are constant, eg $\underline{Q}(t)|\underline{q}\rangle_t = \underline{q}|\underline{q}\rangle_t$. We want to compute transition amplitudes

$${}_{t_f}\langle \underline{q}_f|\underline{q}_i\rangle_{t_i} = \langle \underline{q}_f|e^{-iH(t_f-t_i)}|\underline{q}_i\rangle.$$

We split the time interval into many small intervals δt, and insert complete $\underline{Q}$-bases several times:

$$= \int d\underline{q}_K \dots d\underline{q}_1 \; \langle \underline{q}_f|e^{-iH\delta t}|\underline{q}_K\rangle\langle \underline{q}_K|e^{-iH\delta t}\dots e^{-iH\delta t}|\underline{q}_1\rangle\langle \underline{q}_1|e^{-iH\delta t}|\underline{q}_i\rangle.$$

By the Baker-Campbell-Hausdorff formula

$$e^{A+B} = e^A\, e^B\, e^{-\frac{1}{2}[A,B]+\text{higher commutators}},$$

we write $e^{-iH\delta t} = e^{-iT\delta t}\; e^{-iV\delta t}\; e^{O(\delta t^2)}$. In the limit $K\to\infty$, we may ignore the terms $O(\delta t^2)$. Inserting a complete $\underline{P}$-basis, we have

$$\langle \underline{q}_{k+1}|e^{-iH\delta t}|\underline{q}_k\rangle = \int d\underline{p}_k \langle \underline{q}_{k+1}|e^{-iT\delta t}|\underline{p}_k\rangle\langle \underline{p}_k|e^{-iV\delta t}|\underline{q}_k\rangle = \int \frac{d\underline{p}_k}{2\pi} e^{-iH(\underline{p}_k,\underline{q}_k)\delta t} e^{i\underline{p}_k\cdot(\underline{q}_{k+1}-\underline{q}_k)}.$$

We insert this for each factor in our formula for ${}_{t_f}\langle \underline{q}_f|\underline{q}_i\rangle_{t_i}$, and obtain

$$= \int \prod_k d\underline{q}_k d\underline{p}_k \; \prod_k e^{-i(H(\underline{p}_k,\underline{q}_k)-\underline{p}_k\cdot\dot{\underline{q}}_k)\delta t} = \int DqDp\; e^{-i\int_{t_i}^{t_f} dt\,(H(\underline{p},\underline{q})-\underline{p}\cdot\dot{\underline{q}})}.$$

The integration extends over all paths in phase space $(\underline{q}(t),\underline{p}(t))$ starting at $\underline{q}(t_i) = \underline{q}_i$ and ending at $\underline{q}(t_f) = \underline{q}_f$. In this expression, there are no operators anymore. Since $T(\underline{p})$ is quadratic in $\underline{p}$, we can perform the quadratic (Gaussian) $\underline{p}$-integration by completing the square for the $\underline{p}\cdot\dot{\underline{q}}$-term. Let $T = \frac{1}{2}(\underline{p}, M^{-1}\underline{p})$, then

$$\int d\underline{p}\; e^{-\frac{i}{2}(\underline{p},M^{-1}\underline{p})+i(\underline{p},\underline{q})} = const\cdot e^{\frac{i}{2}(\dot{\underline{q}},M\dot{\underline{q}})},$$

provided one understands M equipped with a small positive imaginary part (ie, H is equipped with a small negative imaginary part). But this has precisely the same effect as solving $\dot{\underline{q}} = \partial H/\partial\underline{p}$ for $\underline{p}$ and eliminating $\underline{p}$:

$$\dot{\underline{q}} = M^{-1}\underline{p} \quad\Rightarrow\quad T - \underline{p}\cdot\dot{\underline{q}} = \frac{1}{2}(\dot{\underline{q}}, M\dot{\underline{q}}).$$

Hence we arrive at the path integral representation of the transition amplitude

$${}_{t_f}\langle \underline{q}_f|\underline{q}_i\rangle_{t_i} = const\cdot\int Dq\; e^{i\int_{t_i}^{t_f} dt\, L(\underline{q},\dot{\underline{q}})},$$

where the integration extends over all paths $\underline{q}(t)$ from $\underline{q}(t_i)$ to $\underline{q}(t_f)$.

Now, it is important that the Hamiltonian is positive. Let $|\underline{q}\rangle = \sum_n c_n(\underline{q})\,|n\rangle$ be the decomposition into eigenstates of H. Then subtracting a small imaginary part as above is equivalent to multiplying H by $(1-i\varepsilon)$

$$|\underline{q}\rangle_t = \sum\nolimits_n e^{i(1-i\varepsilon)E_n t}\, c_n(\underline{q})\;|n\rangle, \qquad {}_t\langle\underline{q}| = \sum\nolimits_n e^{-i(1-i\varepsilon)E_n t}\,\overline{c_n(\underline{q})}\;|\bar{n}\rangle.$$

Then, $|\underline{q}\rangle_t$ and ${}_t\langle\underline{q}|$ are dominated by the ground state contributions as $t\to-\infty$ and as $t\to-\infty$, respectively. Thus, we will have

$$Z^{-1}\cdot\int Dq\; e^{i\int_{-\infty}^{\infty} dt\, L(\underline{q},\dot{\underline{q}})} = \langle 0|0\rangle = 1$$

with some constant Z. Hence Z equals the (divergent in the limit) integral.

Consider now more general path integrals with insertions of the form

$$\int Dq\;\underline{q}(t_1)\dots\underline{q}(t_N)\; e^{i\int_{-\infty}^{\infty} dt\, L(\underline{q},\dot{\underline{q}})}.$$

Since the integral is symmetric under permutation of the times t_n, we may assume that $t_1\geq\cdots\geq t_N$. Following the previous computation backwards, one sees that the additional factors $\underline{q}(t)$ are produced if, upon splitting the time evolution operator $e^{-iH(t_f-t_i)}$ into interval propagators $e^{-iH(t_{k+1}-t_k)}$, the factor $\langle\underline{p}_k|e^{-iV\delta t}|\underline{q}_k\rangle$ is replaced by $\langle\underline{p}_k|e^{-iV\delta t}Q|\underline{q}_k\rangle$ where $\underline{q}_k$ corresponds to the intermediate time $t_k = t$. Likewise, several insertions $\underline{q}(t_n)$ amount to inserting operators $Q(t_n)$ at the appropriate places. This yields the **Feynman-Kac formula**,

$$\boxed{\langle 0|T[\underline{Q}(t_1)\dots\underline{Q}(t_N)]|0\rangle = Z^{-1}\cdot\int Dq\;\underline{q}(t_1)\dots\underline{q}(t_N)\; e^{i\int_{-\infty}^{\infty} dt\, L(\underline{q},\dot{\underline{q}})}.}$$

When $t_1\geq\cdots\geq t_N$, the time-ordering operation does nothing. But in this form, the formula holds indeed for *any* ordering of the times t_n, because both expressions are symmetric under permutations.

The path-integral with insertions produces quantum-mechanical time-ordered vacuum expectation values.

We can now identify the generating functional for the time-ordered vacuum expectation values with the normalized path integral with a source term:

$$T(\underline{f}) \equiv \sum_N \frac{i^N}{N!}\int dt_1\dots dt_N\,\underline{f}(t_1)\dots\underline{f}(t_N)\cdot\langle 0|T[\underline{Q}(t_1)\dots\underline{Q}(t_N)]|0\rangle = \frac{Z(\underline{f})}{Z(\underline{0})},$$

where

$$\boxed{Z(\underline{f}) = \int Dq\; e^{i\int_{-\infty}^{\infty} dt\,\left(L(\underline{q},\dot{\underline{q}})+\underline{f}(t)\cdot\underline{q}(t)\right)}.}$$

It can be shown that the division by $Z(\underline{0})$ makes this divergent expression well-defined (for a class of sufficiently regular Lagrangeans). In the analogous QFT case, it will assure (Sect. 6.9 (A)) the systematic cancellation of all contributions which exhibit the IR divergence ($\sim d^4x$ by translation invariance) as in Sect. 6.1.

6.8 The path integral in QFT

The path-integral definition of an interacting QFT relies on the idea that the QM formula for the generating functional of time-ordered VEVs holds (or at least can be given sense) also in QFT: the only difference being that QFT is "QM with infinitely many degrees of freedom" $\varphi(\vec{x})$ instead of $\underline{Q}$. The auxiliary function $\underline{f}(t)$ has to be replaced by a "source" $J(x)$. Hence *by definition*

$$\boxed{T[J] := \frac{Z[J]}{Z[0]}} \quad \text{where} \quad \boxed{Z[J] := \int D\phi \; e^{i\int d^4x(\mathcal{L}[\phi(x)]+J(x)\phi(x))}.}$$

The real task, however, is to define the path integral beyond the previous formal heuristics (see below). If one then can compute the path integral, one gets the Green functions

$$\big(\Omega, T\big[\varphi(x_1)\dots\varphi(x_2)\big]\Omega\big) = Z[0]^{-1}\cdot\big(-i\frac{\delta}{\delta J(x_1)}\big)\dots\big(-i\frac{\delta}{\delta J(x_N)}\big)\,Z[J]\Big|_{J=0},$$

from which one computes the S-matrix by the LSZ formula. We have seen above, that this formal recipe indeed gives the correct result in the free field case.

In the case of Fermi fields quantized by canonical *anti*-CR, one has to use "Grassmann path integrals", ie the field integration variables are "anticommuting numbers", with certain modifications of the rules for integration.

Comments

The interacting path integral is not a priori defined. As said before, the integration measure $D\phi$ does not exist, but $D\mu(\phi) = D\phi\, e^{i\int \mathcal{L}_{\rm free}}$ can be defined on $e^{i\int J\phi}$ and on polynomial functionals of ϕ. The basic question is therefore, whether the additional term $e^{i\int \mathcal{L}_{\rm int}}$ is integrable with the measure $D\mu(\phi)$. In perturbation theory, one circumvents this question, by expanding $e^{i\int \mathcal{L}_{\rm int}}$ as a power series, but still the Gaussian integral has to be defined on pointwise products like $\varphi^n(x)$. Alternative definitions of the path integral proceed by lattice approximations in the limit of small lattice spacing (cf Sect. 8.7).

Because the PI with the Gaussian measure generates free time-ordered correlations functions, one can write

$$Z[J] = \int D\phi\; e^{i\int d^4x\,\mathcal{L}_{\rm free}[\phi]}\; e^{i\int d^4x(\mathcal{L}_{\rm int}(\phi)+J\phi)} = (\Omega, Te^{i\int d^4x(\mathcal{L}_{\rm int}(\varphi_{\rm free})+J\varphi_{\rm free})}\Omega)_{\rm free}.$$

The operator on the rhs looks very similar to the "old" formula for the S-matrix as in Sect. 5.5, but the meaning is very different. First, the function $J(x)$ is not a physical external field, but just an auxiliary "source term" to generate insertions by variational derivatives. The value at $J = 0$ is just the normalization factor necessary to make the vacuum-to-vacuum amplitude = 1, as it should be in a time-translation invariant theory. Finally, the resulting generating functional is not yet the S-matrix, but the latter has to be computed by the LSZ formula.

The last remark has an important consequence: In the derivation of the PI, it was assumed that equal-time CCR hold as in QM. But in the derivation of the LSZ formula, we had to shift and renormalize the field to get vanishing VEV and the proper scalar product with the one-particle states. To generate the properly normalized Green functions (ie, the time-ordered correlation functions of $Z_\phi^{-1/2}(\varphi(x)-v)$), the source term should rather be $\int J(x)Z_\phi^{-1/2}(\phi(x)-v)$. One may then make a change of the PI integration variable by renaming $Z_\phi^{-1/2}(\phi(x)-v)$ to ϕ. This changes the form of the Lagrangean, eg the kinetic term will become $Z_\phi\,\partial_\mu\phi\partial^\mu\phi$. Also, there is no a priori reason that the path integral produces Green functions with poles at $k^2 = m^2 =$ the mass appearing in the Lagrangean. The physical mass, determined by the poles of the Green function, may be different. Finally, also the physical coupling constant, defined by the value of some reference amplitude (eg, the two-to-two-particles scattering amplitude), need not coincide with the Lagrangean parameter g. Therefore, the Lagrangean appearing in the PI should rather be parametrized as

$$\mathcal{L}[\phi] = \frac{1}{2}Z_\phi\,\partial_\mu\phi\partial^\mu\phi - \frac{1}{2}Z_m\,m^2\,\phi^2 - \frac{1}{24}Z_g\,g\,\phi^4 - Y_3\,\phi^3 - Y_1\,\phi.$$

The constants are yet unknown and must be determined so as to satisfy the LSZ normalization conditions, and to produce Green functions with the physical mass and coupling constants. This will be the issue of renormalization theory.

6.9 Feynman rules

The perturbative expansion of the formula

$$Z[J] = (\Omega, Te^{i\int d^4x(\mathcal{L}_{\rm int}(\varphi_{\rm free})+J\varphi_{\rm free})}\Omega)_{\rm free}$$

yields the **Gell-Mann–Low formula** (which can actually also derived without the PI, using the interaction picture)

$$(\Omega, T[\varphi(x_1)\dots\varphi(x_N)]\Omega) = \frac{\sum\frac{i^n}{n!}(\Omega, T\big[\varphi_{\rm free}(x_1)\dots\varphi_{\rm free}(x_N)\big(\int\mathcal{L}_{\rm int}(\varphi_{\rm free}(y))dy\big)^n\big]\Omega)_{\rm free}}{\sum\frac{i^n}{n!}(\Omega, T\big(\int\mathcal{L}_{\rm int}(\varphi_{\rm free}(y))dy\big)^n\Omega)_{\rm free}}.$$

Notice that the right-hand-side is entirely in terms of free fields, and can be computed term by term. (Notice also that it does not involve any path integral.)

The term-by-term evaluation uses Wick's Theorem. The following graphical rules emerge (for the numerator) in the case of an interaction $\mathcal{L}_{\rm int} = -\frac{1}{\nu!}g:\varphi^\nu:$.

1. Draw N external vertices, labelled by the points $x_1,\dots x_N$.

2. Draw n interaction vertices.

3. Draw lines between internal and external vertices in all possible ways such that each external vertex has one line attached, and each interaction vertex has ν lines attached.

The result is a **Feynman diagram** G. Each of these diagrams represents one contribution according to Wick's Theorem. The corresponding analytical expression is given by the following rules:

4. Each interaction vertex is assigned a coordinate y_j.

5. The diagram corresponds to the **Feynman integral**

$$I(G) = \big(\frac{-ig}{\nu!}\big)^n \int dy_1 \dots dy_n \prod_{\text{lines}} (-iG_F),$$

where the arguments of the Feynman propagators are the endpoints of the lines.

6. Each diagram arises with a coefficient $1/n!$ times a "counting factor" $C(G)$ (the number of pairings that give rise to the same diagram, where diagrams with different numberings of interaction vertices are identified). The counting factor $C(G)$ can also be expressed through a "symmetry factor" $S(G)$ = number of permutations of interaction vertices and their "slots" where the internal lines are attached, that do not change the diagram. One has then $C(G)/(\nu!)^n n! = 1/S(G)$.

Hence

$$\text{Numerator} = \sum_n \frac{1}{n!(\nu!)^n} \sum_G C(G) \cdot I(G)$$

where for each n the sum extends over all diagrams with the given number of N external vertices and n interaction vertices. For the denominator, one only sums over diagrams with no external vertices.

For several interaction terms $(g_\nu/\nu!){:}\varphi^\nu{:}$, one would have to replace $(g/\nu!)^n/n!$ by $\prod_\nu (g_\nu/\nu!)^{n_\nu}/n_\nu!$ for a graph containing n_ν vertices of order ν.

Before we turn to the evaluation of the integrals $I(G)$, we notice some systematic facts. Each diagram can be decomposed into **connected diagrams**, and the corresponding Feynman integral is the product of the connected integrals. In fact, these integrals are of the same type as those considered in Sect. 6.1, and tend to have IR and UV divergences, that have to be dealt with.

A: (**Vacuum diagrams**) A vacuum diagram is a connected diagram without external lines. Because the integrand of a vacuum diagram depends only on the *differences* $y_i - y_j$, the integral will always involve the IR divergent factor $\int dy$. Recall that this led to $\langle 0|S|0\rangle = 0$ in the "old" S-matrix formula, which was the reason why we had to reject it! But with the GML formula, all vacuum diagrams exactly cancel. To see this, consider the schematic structure of the numerator

$$= \sum_n \frac{1}{n!} \sum_G (\text{vac}) \cdot (\text{non-vac}) = \sum_n \frac{1}{n!} \sum_p \frac{n!}{p!(n-p)!} (\text{vac})_p \cdot (\text{non-vac})_{n-p}$$

where eg $(\text{vac})_p$ is the sum of all products of vacuum diagrams with a total of p vertices. The combinatorial factor reflects the number of possibilities to choose p out of n interaction vertices. Rewriting the sum

$$= \sum_{p,q} \frac{1}{p!q!} (\text{vac})_p \cdot (\text{non-vac})_q = \big(\sum_p \frac{1}{p!} (\text{vac})_p\big) \cdot \big(\sum_q \frac{1}{q!} (\text{non-vac})_q\big)$$

we see that the first factor equals $Z[0]$ and is cancelled by the denominator. Hence

$$\tau_N(x_1,\dots,x_N) = \sum_n \frac{1}{n!} \sum_{\substack{G \text{ without} \\ \text{vacuum subdiagrams}}} C(G)\cdot I(G).$$

The denominator $Z[0]$ systematically cancels the obvious IR divergent vacuum diagrams.

B: (**Connected diagrams**) It is sufficient to compute connected diagrams, because a disconnected diagram is the product of the connected parts. One can show ("Linked Cluster Theorem") that the generating functional $T[J] = Z[J]/Z[0]$ equals

$$T[J] = e^{T^{\rm conn}[J]}$$

where $T^{\rm conn}[J]$ is the sum over all connected diagrams only. Schematically, if $\tau_N^{\rm conn}$ represent all connected graphs with N external lines (and assuming $\tau_1^{\rm conn}=0$):

$$\begin{aligned} 1 + (\tfrac{1}{2}J^2\tau_2^{\rm conn} + \tfrac{1}{6}J^3\tau_3^{\rm conn} + \tfrac{1}{24}J^4\tau_4^{\rm conn} + \dots) + \tfrac{1}{2}(\tfrac{1}{2}J^2\tau_2^{\rm conn} + \dots)^2 + \dots \\ = 1 + \tfrac{1}{2}J^2(\tau_2^{\rm conn}) + \tfrac{1}{6}J^3(\tau_3^{\rm conn} + \tfrac{1}{24}J^4(\tau_4^{\rm conn} + 3\tau_2^{\rm conn2}) + \dots . \end{aligned}$$

Eg, the combinatorial factor 3 in the disconnected 4-point function properly reproduces the three possible possible products of two connected 2-point functions.

C: (**Momentum conservation**) The Fourier transform $\hat\tau_N(k_1,\dots,k_N) = \int\prod d^4x_i\, e^{ik_ix_i}\tau_N(x_1,\dots,x_N)$ is a sum over the FT $\hat I(G)$ of the Feynman integrals $I(G)$. We insert for each propagator its Fourier representation. The x and y-integrations produce V δ-functions for all momenta flowing in or out of each vertex (convention: external momenta k flow out of the diagram). The n δ-fns for L momentum integrals produce a factor $\delta(\sum_{i=1}^N k_i)$ for the conservation of the total four-momentum and otherwise reduce the L momentum integrations by $n-1$. Moreover, the integrand of the external lines is fixed to be $\frac{-i}{m^2-k_i^2}$, hence the integral has the form

$$\hat I(G) = \prod_{i=1}^N \frac{-i}{m^2-k_i^2}(2\pi)^4\delta(k_1+\dots k_N)\cdot i\Gamma(G)$$

with functions $i\Gamma(G)$ to be further specified below.

D: (**Loops**) Let N be the number of external vertices of a connected diagram, L the total number of lines, hence $L-N$ internal lines, and $V\equiv n$ the number of interaction vertices. Then we are left with

$$l := L - N - (V-1)$$

independent internal momentum integrations. It turns out that l is exactly the number of independent loops of the diagram: For *tree diagrams* (no loops), this is evident because in order to connect V interaction vertices one needs $V-1$ internal

lines, hence $L = N + (V-1)$, $l = 0$. Each additionial line connecting two vertices will produce a loop. This step increases L by 1 without changing N and V.

For vertices of order $\nu \geq 3$, one also has $N + \nu V = 2L$, hence $(\nu-2)V = 2l + N - 2$. This means, that for fixed N (a fixed process of interest), the order of perturbation theory counted by the number V of vertices, increases proportional to the number l of loops. This is why PT is also called "loop expansion". The lowest order is given by the tree diagrams, $l = 0 \Rightarrow V = (N-2)/(\nu-2)$.

After these preparations, the Feynman rules are as follows. The Fourier transform of the connected time-ordered correlation function is of the form

$$\boxed{\hat\tau_N^{\rm conn}(k_1,\dots,k_N) = \prod_{i=1}^N \frac{-i}{m^2-k_i^2}(2\pi)^4\delta(k_1+\dots k_N)\cdot i\Gamma_N(k_1,\dots,k_N).}$$

When inserted into the LSZ formula, the factors $\frac{-i}{m^2-k_i^2}$ will completely cancel out (also after the necessary renormalization, see Chap. 7). Notice that the external momenta k here are not assumed to be "on-shell" ($k \in H_m$ for outgoing or $-k \in H_m$ for incoming particles), hence once some $\Gamma(G)$ has been computed, it can also be used for a subgraph of some other graph. Only when one uses the final expression for the τ-functions in the LSZ formula, one has to put k on-shell.

Here, $i\Gamma_N$ is a sum over "amputated" (external propagators removed) connected momentum space Feynman integrals

$$i\Gamma_N(k_1,\dots,k_N) = \sum_{\substack{G\text{ connected}\\ \text{without vacuum subdiagrams}}} \frac{C(G)}{\prod_\nu V_\nu(G)!}\cdot i\Gamma(G),$$

where

$$\boxed{i\Gamma(G) = i\prod_\nu\Big(\frac{-g_\nu}{\nu!}\Big)^{V_\nu}\int \frac{\prod_{\rm loops}(-i)\,d^4q_i/(2\pi)^4}{\prod_{\substack{\rm internal\\ \rm lines}}(m^2-p_j^2)}.}$$

In the denominator, p_j are linear combinations of the external momenta k_i (flowing out of the graph) and the independent loop momenta q_i in the numerator, as dictated by momentum conservation at each vertex. The only exception is the single line graph which has two external momenta attached to the same line, and no vertex. For this graph, $i\Gamma(\text{line}) = i(m^2-k^2)$ is the inverse of the propagator, because it has to be multiplied with the square of the external propagator.

The $i\varepsilon$ subtractions are understood everywhere. We shall see later that Γ_N are real functions.

Finally, the full τ-functions are obtained, in a symbolic notation (X = set of arguments), by

$$\tau_N(X) = \sum_{\substack{\rm partitions\\ X=\dot\cup X_i}}\prod \tau_{N_i}^{\rm conn}(X_i).$$

E: (**Daisies and tadpoles**) Internal lines cannot connect with both ends to the same vertex ("daisy diagrams"), because by Wick's Theorem there are no internal pairings. In the PI formulation (where "normal ordering" is meaningless) one must argue differently. Each daisy leaf at a vertex of order ν would contribute a (divergent) integral $C = \int d^4p/(m^2 - p^2)$, which has the same effect in the Feynman integral as an interaction vertex of order $\nu-2$ with coupling Cg_ν. One can systematically cancel these terms by adding "counterterms" of the form $-Cg_\nu\varphi^{\nu-2}$ to $\mathcal{L}_{\rm int}$. This is just a **renormalization** of the coupling constant $g_{\nu-2}$. Assuming WLOG that this step has already been taken, one may just drop all daisy diagrams.

Similarly, we consider "tadpole diagrams", ie subdiagrams without external vertices, which are connected to the rest of a diagram by one internal line only. (Tadpoles can occur only if there are interaction vertices of odd order.) Nonzero tadpoles give rise to nonzero 1-point functions. But we have seen earlier that a nonzero VEV of the field can be removed by a shift of the field by a constant, which gives rise (among other things) to a linear term in the Lagrangean. Indeed, the momentum conservation implies that the momentum flowing across the "tail" of the tadpole is zero. Hence the integral representing the "head" of the tadpole is just some constant Y. If one adds to the interaction Lagrangean a counterterm $-Y\varphi$, this corresponds to a new vertex of order 1 with coupling constant $g_1 = -Y$. The additional tadpoles ending on this new vertex will precisely cancel the old tadpoles. One may therefore also ignore all tadpole diagrams (both the original ones and the ones coming from the counterterm).

Summary: The Fourier transforms of time-ordered correlation functions are given by sums of products of connected diagrams, representing an integral. Each connected Feynman integral is a function of the external momenta, given by a δ-function for the total energy-momentum conservation, times a loop integral over the propagators. There are no vacuum diagrams, no daisies and no tadpoles.

For the tree diagram ($l = 0$) with a single vertex ($V = 1$) of order ν (hence $N = \nu$ and $C(G) = \nu!$), we find the leading connected contribution

$$\Gamma_N^{(0)} = -g_\nu,$$

ie precisely the coupling constant for the interaction term φ^ν. By the LSZ formula, this is the leading term for the amplitude of processes where 2 particles are scattered into $\nu - 2$ particles. The higher order (loop) corrections to Γ_N will modify the strength of the interaction.

In the case of Dirac or vector fields with the QED interaction $ej^\mu A_\mu$, the Feynman rules have to be modified. Each time-ordered VEV

$$(\Omega, T\big[\psi_{a_1}(x_1)\overline{\psi}_{b_1}(x_2)\dots\psi_{a_N}(x_{2N-1})\overline{\psi}_{b_N}(x_{2N})A^{\mu_1}(x_{2N+1})\dots A^{\mu_M}(x_{2N+M})\big]\Omega)$$

is represented by a sum over diagrams with diagram $2N$ external Dirac lines and M external photon lines. In each vertex, one photon line is attached to a pair of

directed Dirac lines. In particular, Dirac lines form chains that "never end": either they connect a pair of external Dirac lines, or they form a closed loop. In the Feynman integral, each vertex contributes a factor $e\gamma^\mu$, and each line a corresponding Dirac or Maxwell propagator, in such a way that Lorentz indices are contracted and Dirac matrices are multiplied according to the structure of the diagram. In particular, each open chain of Dirac lines produces a Dirac matrix (alternating product of propagator matrices and γ-matrices from the vertices), while each closed Dirac loop produces a trace over Dirac matrices. Similarly, external photon lines carry an uncontracted Lorentz index.

Due to the anti-commutativity, there arise certain relative signs, where the overall sign is irrelevant. Take any reference diagram and label the external Dirac lines $1, 2 \dots 2N$ such that the directed lines run from $2i-1$ to $2i$. For any other diagram, the same prescription would yield a different labelling. For tree diagrams, the relative sign is the sign of this permutation, while there is an additional $-$ sign for each closed Dirac loop.

Otherwise, the rules are the same, eg the omission of daisies, tadpoles, and vacuum diagrams, and the factorization into products of connected functions (with permutation signs). Clearly, τ-functions with a different number of ψ and $\overline{\psi}$ fields vanish due to charge conservation.

In order to extract S-matrix elements from the τ-functions by the LSZ method, one has to contract the Lorentz indices of the vector potentials with the polarization vectors $e^\mu_\pm(-k)$ (incoming) or $\overline{e^\mu_\pm(k)}$ (outgoing) of the desired photon states, and the Dirac indices of the Dirac fields with the u- and v-spinors and their conjugates for the desired spin states of the electrons and positrons, according to the same rules as in the previously discussed interaction with an external field.

6.10 Example: Compton scattering

As an example, we want to compute the Compton scattering amplitude at tree level (no integrations). For the same reason as with the classical elm field (energy-momentum conservation, cf Sect. 5.8), every diagram with one incoming and one outgoing electron line and only one external photon line vanishes "on-shell". The lowest order process involves two vertices and two photons, ie the photon cannot be just absorbed but has to be re-emitted.

According to the Feynman rules, we obtain

$$\langle k', s'; q', \varepsilon' | k, s; q, \varepsilon\rangle = (2\pi)^4\delta(k'+q'-k-q)\cdot iT, \quad T = \overline{e^\mu_{\varepsilon'}(q')}\overline{u}_{s'}(k')\Gamma_{\mu\nu}u_s(-k)e^\nu_\varepsilon(-q)$$

where k and q are the electron and photon momenta, s and ε the spin and helicities, and

$$\Gamma_{\mu\nu} = e^2\Big(\gamma_\mu\frac{m\mathbf{1}+\gamma^\lambda(k+q)_\lambda}{m^2-(k+q)^2}\gamma_\nu + \gamma_\nu\frac{m\mathbf{1}+\gamma^\lambda(k-q')_\lambda}{m^2-(k-q')^2}\gamma_\mu\Big)$$

has contributions from two possible diagrams. The probability density $|T|^2$ depends on the spins and helicities, but it simplifies considerably if one averages over the

incoming quantum numbers and sums over the outgoing ones (this corresponds to an experiment with instruments that are insensitive to spin and helicity): One has the identities

$$\sum\nolimits_s u_s(k)\,\overline{u}_s(k) = m\mathbf{1} + \gamma^\lambda k_\lambda$$

as well as

$$\sum\nolimits_\varepsilon \overline{e^\rho_\varepsilon(q)}\; e^\sigma_\varepsilon(q) = -\eta^{\rho\sigma} + (\text{terms } \sim q^\rho q^\sigma).$$

The latter terms will cancel out in later steps of the computation because of the conservation of the Dirac current, or – equivalently – by gauge invariance (because a gauge transformation would add arbitrary more such terms, and the result must not depend on them. With this and $\gamma^0\gamma^\mu\gamma^0 = \gamma^{\mu *}$, the averaged probability density becomes

$$\langle|T|^2\rangle = \frac{1}{4}\,\mathrm{tr}\,\big(m\mathbf{1} + \gamma^\lambda k'_\lambda)\Gamma_{\mu\nu}(m\mathbf{1} - \gamma^\kappa k_\kappa)\Gamma_{\nu\mu}\big),$$

involving products of up to 8 γ-matrices. This can be worked out, giving after a lengthy computation

$$\langle|T|^2\rangle = 2e^4\Big(\frac{m^4 + m^2(3s+u) - us}{(m^2-s)^2} + \frac{m^4 + m^2(3u+s) - us}{(m^2-u)^2} + \frac{2m^2(4m^2-t)}{(m^2-s)(m^2-u)}\Big)$$

where $s = (k+q)^2$, $t = (k-k')^2$, $u = (k-q')^2 = 2m^2 - s - t$. In the FT frame of the electron, this can be expressed in terms of the photon energies ω, ω':

$$\langle|T|^2\rangle = \frac{2e^4}{\omega^2\omega'^2}\big(\omega\omega'(\omega^2+\omega'^2) - 2m\omega\omega'(\omega-\omega') + m^2(\omega-\omega')^2\big)$$

where by energy-momentum conservation

$$\omega - \omega' = \frac{\omega\omega'(1-\cos\vartheta)}{m}.$$

This gives the differential cross section (cf Sect. 6.5)

$$\frac{d\sigma_{\mathrm{Comp}}}{d\Omega_{\mathrm{FT}}} = \frac{e^4\omega'}{32\pi^2 m^2\omega^3}\big(\omega^2+\omega'^2 - \sin^2\vartheta\cdot\omega\omega'\big) = \frac{\alpha^2}{2m^2}\frac{\omega'^2}{\omega^2}\Big(\frac{\omega}{\omega'} + \frac{\omega'}{\omega} - \sin^2\vartheta\Big).$$

This is the Klein-Nishina formula for (tree level) Compton scattering.

By the same method, one can also compute the pair annihilation process $e^-e^+ \to 2\gamma$. In the LSZ formula, one only has to exchange the outgoing electron momentum $+k'_1$ by the ingoing positron momentum $-k_2$, and similarly $-q'_1$ by $+q_2$. This amounts to replacing $s \leftrightarrow t$ and reversing the overall sign in the expression for $\langle|T|^2\rangle$. In this case, one rather works in the CM frame, giving the final result

$$\frac{d\sigma_{\mathrm{ann}}}{d\Omega_{\mathrm{CM}}} = \frac{\alpha^2}{4E^2}\,\frac{E^4 + 2\sin^2\vartheta\, m^2p^2 - \cos^4\vartheta\, p^4}{(E^2 - \cos^2\vartheta\, p^2)^2}.$$

7 Renormalization

7.1 Preparations

While tree diagrams are just products of coupling constants and propagators, loop diagrams involve integrations over four-momenta "circulating in the loops". These integrals tend to be UV divergent. Renormalization is a procedure to remove these divergences by adding suitable "counter terms" to the Lagrangean (or other, equivalent, methods). We have seen simple instances of counter terms before, when cancelling the infinities due to daisy and tadpole diagrams.

As a consequence, we shall see that the parameters m and g appearing in the classical Lagrangean have no direct physical meaning. The true masses and coupling constants are implicitly determined by the interaction itself.

Renormalization factors

As already mentioned in Sect. 6.8, the mismatch between the CCR used in the derivation of the Gell-Mann–Low formula via the formal generalization of the QM path integral, and the need of a field redefinition in the derivation of the LSZ formula requires the Lagrangean in the path integral to be rather of the form

$$\mathcal{L}[\phi] = \frac{1}{2}Z_\phi\ \partial_\mu\phi\partial^\mu\phi - \frac{1}{2}Z_m\, m^2\ \phi^2 - \frac{1}{24}Z_g\, g\ \phi^4 - Y_3\ \phi^3 - Y_1\ \phi,$$

where the factors still have to be determined. Eg, Z_ϕ must be chosen such as to produce the correct scalar product with the one-particle states. It depends on the interaction, and $Z_\phi = 1$ for free fields. We shall therefore write $Z_\phi = 1 + A(g)$ where $A(g)$ is a power series starting with order g, and regard the piece $\frac{A}{2}\partial_\mu\phi\partial^\mu\phi$ as part of $\mathcal{L}_{\rm int}$. The need to do so will become apparent soon.

Likewise, we write $Z_m = 1 + B(g)$ where $B(g)$ is at least of order g. Everything beyond the free Lagrangean belongs to

$$\mathcal{L}_{\rm int}[\phi] = \frac{1}{2}A(g)\ \partial_\mu\phi\partial^\mu\phi - \frac{1}{2}B(g)\, m^2\ \phi^2 - \frac{1}{24}Z_g(g)\, g\ \phi^4 - Y_3(g)\ \phi^3,$$

where $Z_g = 1 + O(g)$ and $Y_3 = O(g)$. (We already know that we may disregard $Y_1\,\phi$ whose sole effect is to cancel all tadpoles.)

The general structure of loop integrations

All propagators $G_F(q)$ have manifest singularities when $q^2 = m^2$. The $i\varepsilon$-prescription turns these singular functions into well-behaved distributions. When integrating over loop momenta, the q^0-integration can be deformed to pass along the imaginary axis. Then, regarding $(q^0/i, \vec{q}) \in \mathbb{R}^4$ as a Euclidean four vector, we may replace

$$(-i)d^4q \to d^4q_E, \qquad \frac{1}{m^2 - q^2 - i\varepsilon} \to \frac{1}{m^2 + q_E^2}.$$

With this substitution, the Γ_N become systematically real functions of the Euclidean momenta $(k^0/i, \vec{k})$.

Next, with the help of the identity

$$\frac{1}{A_1\cdots A_n} = (n-1)!\int_0^1 \prod du_i\, \frac{\delta(u_1+\cdots+u_n-1)}{[u_1A_1+\cdots+u_nA_n]^n}$$

and a suitable linear transformation of the Euclidean integration variables, all (scalar) amputated loop integrals with l loops and n internal propagators can be brought into the form

$$I(k) = \int_0^1 \prod du_i\, \delta(u_1+\cdots+u_n-1)\; g(u) \int \frac{d^{4l}Q_E}{(m^2+Q_E^2+F(k_E,u))^n}$$

where $F(k_E,u)$ is a $SO(4)$ invariant quadratic form in the Euclidean external momenta depending on the Feynman parameters $u_1,\dots u_n$, and the function $g(u)$ depends on the details of the diagram. Eg, for graphs with two external lines, $F(k_E,u) = f(u)k_E^2$; one loop: $g(u)=1$, $f(u)=u_1u_2$; two loops: $g(u) = 2(u_1u_2+u_1u_3+u_2u_3)^{-2}$ and $f(u) = u_1u_2u_3/(u_1u_2+u_1u_3+u_2u_3)^{-1}$ It is apparent from this form that the Q-integral will diverge at large Q whenever $4l \geq 2n$. On the other hand, taking sufficiently many derivatives wrt some of the invariants of the external momenta, the power of the denominator can be increased and the integral becomes convergent. This means that the divergent part of the loop integral is always a polynomial in these invariants. We shall make crucial use of this fact.

To get control of the divergence one can introduce a UV cutoff, eg replacing $d^{4l}q_E$ by $d^{4l}Q_E\, e^{-Q_E^2/\Lambda^2}$. Rescaling Q_E by Λ, one can conclude the degree of divergence: the integral diverges $\sim \Lambda^{4l-2n}$ if $4l > 2n$, and like $\log(\Lambda^2/m^2)$ if $4l = 2n$.

One-particle irreducible diagrams

It is evident from the Feynman rules that a diagram G which consists of two subdiagrams G_1, G_2 connected by a single internal line, factorizes in momentum space according to

$$i\Gamma(G) = i\Gamma(G_1)\cdot(-iG_F(q))\cdot i\Gamma(G_2), \qquad \text{ie} \quad \Gamma(G) = \Gamma(G_1)\cdot G_F\cdot\Gamma(G_2)$$

where the momentum q of the connecting propagator is determined by the outer momenta. In particular, there is no further integration involved in this composition.

This means that it is sufficient to compute (and renormalize) only the *one-particle irreducible diagrams*: those diagrams which cannot be split into two by removing one internal line. By definition, 1PI diagrams are amputated.

7.2 Renormalization of the propagator

Consider the propagator $G_{F\text{int}}$ of the interacting field, ie the sum over all FD with two external lines of external momentum k. It is given by the free propagator plus a sum over diagrams involving at least one interaction vertex. The latter may not be 1PI, but they are always chains of 1PI diagrams connected by free propagators:

$$G_{F\text{int}} = G_F(k) + G_F(k)\Sigma(k^2)G_F(k) + G_F(k)\Sigma(k^2)G_F(k)\Sigma(k^2)G_F(k) + \dots$$

where $i\Sigma(k^2)$ is the sum over all (amputated) 1PI diagrams with two external lines. This is a geometric series that can be summed:

$$G_{F\mathrm{int}} = G_F(k) \cdot \big(1 - \Sigma(k^2) G_F(k)\big)^{-1} = \frac{1}{m^2 - k^2 - \Sigma(k^2)}.$$

Using the Feynman parametrization, the lowest order contribution to $\Sigma(k^2)$ with two φ^4 interaction vertices is

$$g^2\Sigma^{(2)} \sim g^2 \int du_1 du_2 du_3 \; \delta(u_1+u_2+u_3-1)\; g(u) \int \frac{d^8 Q_E}{(m^2 + Q_E^2 - f(u)k^2)^3},$$

where $g(u) = 2/(u_1u_2 + u_1u_3 + u_2u_3)^2$ and $f(u) = u_1u_2u_3/(u_1u_2 + u_1u_3 + u_2u_3)$. This integral is UV divergent $\sim \Lambda^2$, its derivative wrt k^2 diverges $\sim \log(\Lambda^2/m^2)$, and all higher derivatives are finite. Hence, the Taylor expansion around $k^2 = m^2$ is

$$\Sigma^{(2)}_\Lambda = m^2 F_0(\Lambda, m^2) + F_1(\Lambda, m^2)(k^2 - m^2) + (k^2 - m^2)^2 \cdot (\text{finite})$$

where F_0 and F_1 are quadratically and logarithmically divergent.

At this point, the "counter terms" $\frac{1}{2}A(g)\,\partial_\mu\phi\partial^\mu\phi - \frac{1}{2}B(g)\,m^2\,\phi^2$ come into play: if $A(g)$ and $B(g)$ have contributions ag^2 and bg^2, they will also contribute to Σ with a term $g^2(ak^2 - bm^2)$. Therefore, one may (and has to) adjust a and b such as to cancel the divergent first two Taylor coefficients; in particular, a and b (and hence $A(g)$ and $B(g)$) will also be cutoff-dependent, and diverge as $\Lambda \to \infty$.

More precisely, because of the LSZ normalization condition, one needs the total propagator $1/D(k^2)$ to have a pole with unit residue at $k^2 = m^2$. Since the denominator with cutoff and counter terms is

$$D_\Lambda(k^2) = m^2 - k^2 - g^2\big((a+F_1)k^2 + (F_0 - F_1 - b)m^2 + (\text{finite})\cdot(k^2-m^2)^2\big) + O(g^4),$$

he LSZ condition requires to choose $a = -F_1$ and $b = F_0 - F_1$. One can then take the limit $\Lambda \to \infty$, and the result is the renormalized (to order g^2) propagator

$$G_{F\mathrm{ren}}(k) = \Big(m^2 - k^2 + g^2 \cdot (\text{finite}) \cdot (k^2 - m^2)^2 + O(g^4)\Big)^{-1}.$$

The finite terms $O((m^2 - k^2)^2)$ do not affect the residue. But they may and will have a nontrivial dependence on k^2, leading to a modification of the propagator to be inserted in higher order diagrams.

Note that it is not necessary to actually *compute* the divergent parts of $\Sigma^{(2)}$: it suffices to know the finite second derivative $\partial^2_{k^2}\Sigma^{(2)}(k^2)$ as a function of k^2, which completely determines the remaining terms.

For the same reason, it is also not necessary to specify the exact cutoff prescription – the finite result will be independent of it.

On the other hand, it is essential that this prescription has to be repeated at each order of PT, because there will be diagrams with more and more loops contributing to $\Sigma(k^2)$ at higher order in g. Moreover, at higher order the coupling constant has to be replaced by $Z_g(g)g = g + O(g^2)$, thus mixing the renormalization of the propagator with that of the vertex, to be discussed in the next subsection.

One could as well Taylor expand $\Sigma^{(2)}_\Lambda(k^2)$ around any other point $k^2 = m'^2$, with different divergent coefficients F'_0 and F'_1, and a different finite part $O((k^2 - m'^2)^2)$. One can then adjust the counter terms a and b such that the renormalized propagator has its pole with unit residue at $k^2 = m'^2$. This implies that the physical mass (fixed by the *choice* of the position of the pole) is entirely independent of the original Lagrangean mass parameter (which is modified by the counter term anyway.)

7.3 Renormalization of the interaction

We now consider 1PI diagrams with four external lines, contributing to the vertex function $i\Gamma(k_1, k_2, k_3, k_4)$. At $k_i^2 = m^2$, this quantity is the scattering amplitude for $2 \to 2$ particles. At tree level, Γ just equals the coupling constant $-g$. In the next order, there are three diagrams (counting factor 288) distinguished only by the labels of the external lines. The corresponding integrals are permutations of

$$\sim g^2 \int \frac{-i\, d^4q}{(m^2 - q^2)(m^2 - (q - k_1 - k_2)^2)} + (\text{permutations})$$

This integral diverges logarithmically, while its first derivative wrt $s = (k_1 + k_2)^2$ is finite:

$$\sim g^2\big(\log(\Lambda^2/m^2) + (\text{finite function of } (k_1 + k_2)^2 + \text{permutations})\big)$$

The divergent part does not depend on the momenta, and can therefore be cancelled by a counter term $-cg^2\phi^4/24$ in the Lagrangean (ie $Z_g(g) = 1 + cg + O(g^2)$), which is equally divergent, say $c \sim \log(\Lambda^2/m^2)$, so that

$$\Gamma(k_1, k_2, k_3, k_4) - cg = -g + g^2(\text{finite}) + O(g^3).$$

This quantity depends on the external momenta, ie the strength of the interaction becomes energy-dependent. The "physical" coupling constant g_{ren} is the value of this function at some conveniently chosen reference point $(k_1, k_2, k_3, k_4)_{\text{ref}}$. Hence, what one calls g_{ren} will depend on the choice of this "renormalization point".

We have here concentrated on the removal of divergences. Notice however, that the physics (eg the energy dependence of the coupling strength) resides in the finite parts, of which we have shown how to isolate them in principle, but which are quite involved to actually compute.

Notice also that the renormalization has to be iterated at each order of PT, where eg the lower-order corrections (here: the finite part $O((k^2 - m^2)^2)$ of $\Sigma^{(2)}$) to the propagators have to be taken into account when computing higher-order diagrams! This gives rise to a quite complicated recursive scheme.

Finally, notice that counter terms are vertices of the same order as the divergent diagrams. Therefore, if there is no vertex of odd order at tree level – as in a pure φ^4 theory – there will never be any diagrams with an odd number of external lines that could require a counter term, and therefore $Y_3(g)$ above will be zero.

7.4 Renormalizability to all orders

Renormalization is a recursive scheme: at every loop order, there arise more divergent diagrams which require more counter terms. In the best case, these CTs mean only a (cumulative) re-adjustment of the coefficients of the terms in the classical Lagrangean. Thus, the structure of the interaction is never changed, but the Lagrangean coefficients (including the CTs) are meaningless because they are power series in g, divergent at every order, recursively selected such that the resulting time-ordered correlation functions are finite. The values of these functions at special points are the physical parameters (mass, coupling constant) of the theory.

However, it is in principle possible that there arise divergent diagrams (eg, 1PI diagrams with a growing number of external lines) which require counter terms not already present in the Lagrangean. These CTs cannot be dumped into a renormalization of some Lagrangean coefficients, but rather constitute some new fundamental type of interaction. In the worst case, one would have to introduce (as the recursion proceeds) an infinite number of new interactions with adjustable physical parameters, meaning that the theory looses all its predictive power.

Whether or not this scenario arises, can be analyzed by a simple dimensional argument: what matters is the dependence of the degree of divergence of a 1PI diagram on the number of external lines and loops. We shall show that there are conditions on the type of couplings, for which all divergences can be absorbed into finitely many constants appearing in $\mathcal{L}_{\rm int}$, in such a way that all time-ordered correlation functions are finite order by order.

In scalar QFT with interaction φ^ν, we have seen that the numbers of external lines N, internal lines $L-N$, vertices V and loops l are related by

$$l = L - N - (V-1) \qquad \text{and} \qquad N + \nu V = 2L.$$

Now consider a 1PI diagram. Using the Feynman parametrization, the loop integration takes the form

$$\int \frac{d^{lD}Q_E}{(Q_E^2+X)^{L-N}},$$

where we have replaced 4 spacetime dimensions by D (in order to emphasize the systematic nature of the consideration). Clearly, this integral is divergent if

$$\omega := lD - 2(L-N) \geq 0.$$

Using the above relations, one can rewrite this expression as

$$\omega = [g_N] - V[g_\nu]$$

where $[g_\nu] = D + \nu - \nu D/2$ is the mass dimension of the coupling constant of a vertex of order ν (because a scalar field has dimension $D/2-1$ and the Lagrangean has dimension D). This can be read as follows. Suppose $[g_\nu]$ is positive ($\nu < 4$

in $D = 4$). Then, adding more vertices to a diagram with a fixed number N of external lines decreases degree of divergence ω, so that there are only finitely many divergent diagrams. Renormalization is completed in some finite order of perturbation theory. Such theories are called "super-renormalizable".

Suppose $[g_\nu]$ is zero ($\nu = 4$ in $D = 4$). Then the degree of divergence is independent of the order of perturbation theory, but goes down with N. Hence only diagrams with $N \leq \nu$ external lines need to be renormalized, but renormalization has to be iterated at each order of PT. Such theories are called "renormalizable".

Suppose $[g_\nu]$ is negative ($\nu > 4$ in $D = 4$). Then for each N, one may produce diagrams (by increasing V) for which ω is positive: hence one needs a counter term of the form $Y_N\varphi^N$, ie the renormalized theory has independent couplings of arbitrary order. But this is a theory with infinitely many parameters: such a theory is unacceptable because it has almost no "predictive power". Therefore a theory with coupling constants of negative mass dimension is rejected as "unrenormalizable".

The present "power counting" argument only assesses the maximal expected divergence. There is always the possibility that by some hidden symmetry some or all divergences cancel systematically, allowing for renormalizable theories even with couplings of negative dimension: eg, a canonical quantization of gravity is superficially non-renormalizable, while supersymmetry improves the situation drastically, although not sufficient to prove renormalizability.

We also see that models in lower dimension have weaker divergences; eg in $D = 2$ all powers φ^ν are renormalizable.

The power counting method works also for fields with spin, where massive fields of spin s have dimension (in $D = 4$) $1 + s$ (notice the numerator $m\mathbf{1} + \gamma^\mu k_\mu$ of the Feynman propagator of Dirac fields). Only interaction terms are admitted which have total dimension of the involved fields ≤ 4. Since local fields constructed from the Dirac field of the form $:\overline{\psi}\gamma \ldots \gamma\psi:$ have at least dimension 3, they can only couple to fields of dimension 1: this admits Yukawa couplings $:\overline{\psi}\psi:\varphi$ to a scalar field, as well as gauge couplings $:\overline{\psi}\gamma^\mu\psi:A_\mu$, where A_μ is a massless vector field. (A massive vector field has dimension 2, due to an additional factor $k^\mu k^\nu$ in the propagator. This is why massive vector bosons W and Z cannot be included directly into the SM, requiring instead the Higgs mechanism. On the other hand, a massless vector field has instead a factor $k^\mu k^\nu/k^2$ reducing its effective dimension to 1. However, it has other difficulties which can only be overcome by gauge invariance. Indeed, this symmetry can be made responsible for the reduction of the effective mass dimension of A_μ.) Together with the Higgs self-coupling of φ^4-type, these are all the couplings present in the Standard Model, cf Chap. 8.

It may be interesting to notice that with renormalizable interactions in 4D, the maximal degree of divergence of any diagram is $\omega = 2$ occuring in diagrams with $N = 2$. This implies that the counter terms contains at most k^2, hence are at most quadratic in the field derivatives in x-space. Is this a secret reason why all equations of motion are at most second order in time?

7.5 The effective action (optional)

A "vertex function" is the sum over all contributions from 1PI diagrams to a given time-ordered function. Eg, for $N = 3$, it is just the amputated Green function

$$i\Gamma_3^{\rm 1PI} = (\prod_1^3 \tau_2^{-1}) \cdot \tau_3^{\rm conn} = i\Gamma_3,$$

(suppressing the arguments of the respective functions in momentum space; recall that amputation means removal of the factors $\tau_2 = -iG_F = -i/(m^2 - k^2 - \Sigma(k^2))$; and for $N = 4$ one has to subtract all the one-particle reducible contributions:

$$i\Gamma_4^{\rm 1PI} = i\Gamma_4 - 3\, i\Gamma_3 \cdot \tau_2 \cdot i\Gamma_3 = (\prod_1^4 \tau_2^{-1}) \cdot (\tau_4^{\rm conn} - 3\, \tau_3^{\rm conn} \cdot \tau_2^{-1} \cdot \tau_3^{\rm conn}),$$

which is equivalent to

$$\tau_4^{\rm conn} = (\prod_1^4 \tau_2) \cdot (i\Gamma_4^{\rm 1PI} + 3\, i\Gamma_3^{\rm 1PI} \cdot \tau_2 \cdot i\Gamma_3^{\rm 1PI}).$$

(The factor 3 stands for three different assignments of the four external legs.)

This gives the expansion of all connected diagrams by connecting 1PI diagrams with intermediate propagators.

One puts by definition $i\Gamma_2^{\rm 1PI} = -\tau_2^{-1}$, and considers the generating functional

$$\Gamma^{\rm 1PI}[\varphi] = \sum\nolimits_{N\geq 2} \frac{1}{N!} \int \Big(\prod\nolimits_i d^4x_i\, \varphi(x_i) \Big)\, \Gamma_N^{\rm 1PI}(x_1, \dots x_N),$$

where φ is another auxiliary parameter function wrt which one has to vary in order to get the vertex functions

$$\Gamma_N^{\rm 1PI}(x_1, \dots x_N) = \frac{\delta}{\delta\varphi(x_1)} \cdots \frac{\delta}{\delta\varphi(x_N)}\, \Gamma^{\rm 1PI}[\varphi]|_{\varphi=0}.$$

A remarkable combinatorial formula says that $\Gamma^{\rm 1PI}[\varphi]$ is the Legendre transform of $T^{\rm conn}[J]$: If one defines

$$\varphi[J](x) := \frac{\delta T^{\rm conn}[J]}{i\delta J(x)} = \int dy\, \tau_2(x,y)\, iJ(y) + \dots$$

as a power series in J, and solves this for $J[\varphi](x)$, then one finds

$$\boxed{i\Gamma^{\rm 1PI}[\varphi] = T^{\rm conn}[J[\varphi]] - i \int dx\, \varphi(x) J[\varphi](x).}$$

Conversely,

$$\boxed{T^{\rm conn}[J] = i\Gamma^{\rm 1PI}[\varphi[J]] + i \int dx\, \varphi[J](x) J(x),}$$

where

$$J[\varphi](x) = -\frac{\delta\Gamma^{\rm 1PI}[\varphi]}{\delta\varphi(x)} = -\int dx\, \Gamma_2^{\rm 1PI}(x,y)\varphi(y) + O(g\varphi^3).$$

The linear contribution is $(\Box + m^2 + O(g^2))\varphi(x)$, (because $\Gamma_2^{\rm 1PI} = k^2 - m^2 - O(g^2)$ in momentum space).

Thus, from the knowledge of $\Gamma^{\rm 1PI}[\varphi]$, one can recover the connected functional $T^{\rm conn}[J]$ by a Legendre transformation, then the time-ordered functional $T[J]$ by exponentiation, and finally the scattering matrix by LSZ.

The last equation has the form of a classical equation of motion for a field $\varphi(x)$ with an action $\Gamma^{\rm 1PI}[\varphi]$, when an additional source term $\int dx\,\varphi(x)J(x)$ is added. For this reason, one calls $\Gamma^{\rm 1PI}[\varphi]$ the "effective action". The tree-level (no loops) contributions are just the classical action:

$$\Gamma^{\rm 1PI}[m,g,\varphi] = \int dx\Big(\frac{1}{2}\partial_\mu\varphi(x)\partial^\mu\varphi(x) - \frac{1}{2}m^2\varphi^2(x) - \frac{g}{4}\varphi^4\Big) + O(g^2).$$

The higher-order terms = quantum corrections due to 1PI loop diagrams will no longer be integrals over local densities. (No problem, as φ is not supposed to be a local field, but just an auxiliary parameter function in a generating functional!)

The loop corrections to the 1PI functions are finite when a suitable UV cutoff Λ is introduced as before, and diverge when $\Lambda\to\infty$.

Renormalization consists in Λ-dependent redefinitions (= counter terms) of the mass and coupling constant and of the field normalization, such that the generating functional

$$\Gamma^{\rm 1PI}_{\rm ren}[\varphi] := \lim_{\Lambda\to\infty} \Gamma^{\rm 1PI}_\Lambda[m(\Lambda), g(\Lambda), Z(\Lambda)^{\frac{1}{2}}\varphi]$$

generates finite 1PI vertex functions and hence full Green functions. The divergent functions $m(\Lambda), g(\Lambda), Z(\Lambda)$ must be chosen such (the hard stuff, of course, is to show that this can be done!) that $\Gamma^{\rm 1PI}_{\rm ren}$ has the form

$$\Gamma^{\rm 1PI}_{\rm ren}[\varphi] = \int dx\Big(\frac{1}{2}\partial_\mu\varphi(x)\partial^\mu\varphi(x) - \frac{1}{2}m^2_{\rm ren}\varphi^2(x) + \frac{g_{\rm ren}}{4}\varphi^4(x)\Big) + \text{finite},$$

where the renormalized mass and coupling constant are given by the values of the Fourier transform of the coefficient functions at some reference point $p^2=\mu^2$ (ie, the energy scale at which these constants are measured in terms of cross-sections derived from Green functions, cf Sect. 7.3).

At a different reference point μ, $m_{\rm ren}$ and $g_{\rm ren}$ are different but still finite. The "renormalization group equation" describes this dependence. Some theories (eg non-abelian gauge theories, cf Sect. 8.3) exhibit "asymptotic freedom": namely $g_{\rm ren}(\mu)$ becomes small with increasing μ. This is the reason why "quarks" are confined at low energies, but behave like free particles in high-energy collisions.

Nonperturbative approaches to renormalization attempt to directly define the path integral without "expanding the exponential".

This method can be made mathematically rigorous by exploiting analyticity properties of correlation functions which allow to (temporarily) "Wick rotate" (ie analytically continue) to imaginary time variables. Then, the oscillating path integral becomes an exponentially suppressed integral. The Osterwalder-Schrader axioms formulate conditions on the renormalized limit that allow to Wick rotate back to real time and obtain a local quantum field theory satisfying the Wightman axioms.

8 Elements of the Standard Model

8.1 Quantum Electrodynamics

QED is the Maxwell and Dirac fields with classical Lagrangean

$$\mathcal{L} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \overline{\psi}(i\gamma^\mu\partial_\mu - m)\psi + e\, j^\mu A_\mu.$$

(Here, we have chosen the electromagnetic units such that $\varepsilon_0 = \mu_0 = 1$, hence e^2 has the numerical value $4\pi\alpha \approx 1/10$, cf Sect. 4.3. e is the *positive* unit of charge, and $j^\mu = \overline{\psi}\gamma^\mu\psi$ is the Dirac current, so the elm current is $-ej^\mu$.)

Using the Gell-Mann–Low formula requires the free photon propagator $\langle TA_\mu A_\nu\rangle$, which is not defined on the positive-definite Wigner Fock space of the field strength $F_{\mu\nu}$. Instead, one has to quantize the vector potential itself by adding a term $-\frac{1}{2}\lambda(\partial_\mu A^\mu)^2$ as in Sect. 4.6. This gives indeed a renormalizable QFT, but on an *indefinite state space* (because the free field space is indefinite). Therefore, one must show that the observables are well-defined on a positive definite quotient space, and that their correlation functions are independent of the parameter λ.

A crucial fact for this purpose is **gauge symmetry**. Classical electrodynamics is invariant under the **gauge transformation**

$$A_\mu(x) \to A_\mu(x) - \partial_\mu\alpha(x)$$

where α is an arbitrary function of x. However, the interaction term $e\, j^\mu A_\mu \to e\, j^\mu(A_\mu - \partial_\mu\alpha(x))$ is obviously not gauge invariant.

The Dirac and interaction term are *together gauge invariant* if the Dirac field is also gauge transformed:

$$\psi(x) \to \psi(x)\, e^{-ie\,\alpha(x)}.$$

This is a "local" version of the "global" Noether symmetry $\psi(x) \to \psi(x)\, e^{-ie\,\alpha}$ ($\alpha = $ const.) associated with the Dirac current, cf Sect. 4.7.

The invariance under this huge group of symmetries can be exploited for the construction of QED. Essentially, the Gupta-Bleuler method (that worked for free Maxwell theory, Sect. 4.6) has to be generalized to the interacting theory, cf Sect. 8.4. The result is a perturbative construction of QED.

QED has been tested experimentally with huge precision. We mention three important effects: the anomalous magnetic moment of the electron, the Lamb shift, and photon-photon scattering. The magnetic moment of the electron is measured by its motion in a magnetic field, which is an instance of Compton scattering with photons. Treating the magnetic field as a classical field as in Sect. 5.8 (only diagrams without internal photon lines) produces the Landé factor $g = 2$, ie the magnetic moment is twice as big as predicted by a naive picture of a rotating charged rigid body. Quantum effects are taken into account by diagrams with internal photon lines. This gives a small correction: $g = 2(1 + \alpha/2\pi + \dots)$.

One may compute the spectrum of an electron in the Coulomb potential of the hydrogen nucleus in a similar spirit (we shall however not treat bound state problems in these lectures). The Maxwell coupling of the classical potential to the Dirac field gives several deviations from the non-relativistic Rydberg spectrum (eg, the spin-orbit coupling is a relativistic effect); but the energy levels ${}^2S_{\frac12}$ and ${}^2P_{\frac12}$ remain degenerate. QED quantum corrections produce a small energy difference between these levels: the Lamb shift.

Photon-photon scattering is allowed by virtue of the non-vanishing Feynman diagram with one Dirac loop with four external photon lines attached. (The diagram with three photon lines is zero because of charge parity conservation!)

8.2 Weak interaction

Neutrons are slightly heavier than protons and can β-decay into a proton and an electron. The distribution of angles and energies of the decay products shows that energy is not conserved, therefore there is another invisible decay product: the neutrino. Today we know that nucleons are not elementary but composite particles, while the fundamental fields are quarks (called "up" and "down", plus some more species). β decay is actually the decay of a down quark into an up quark, an electron and a neutrino.

Thus, one needs more Dirac (or Majorana) fields ψ_X to describe all these spin-$\frac12$ particles. They have different electric charge; consequently the coupling of the corresponding Dirac currents to the vector potential is given by $-q_X j^\mu_X A_\mu$ where q_X is the charge of the particle, and the gauge transformation law is

$$\psi_X(x) \to \psi(x)\, e^{+iq_X\,\alpha(x)}.$$

By the observed conservation of the numbers of baryons (quarks) and of leptons (electrons and neutrinos) separately, the interaction must be described by terms containing hadronic and leptonic charged currents

$$j^\mu_h = \overline{\psi_u}\gamma^\mu\psi_d \qquad \text{and} \qquad j^\mu_\ell = \overline{\psi_\nu}\gamma^\mu\psi_e,$$

or similar expressions involving more γ matrices. An obvious four-fermion interaction is of the form

$$F\ (j_{h\mu})^* j^\mu_\ell.$$

It fits low-energy experiments reasonably well at tree level, with the coupling constant $F \approx 10^{-5} m_p^{-2}$. However, this coupling is non-renormalizable in higher loops! A possible way out is to regard the β decay as a second order process of an interaction with a vector boson described by a field W_μ and interactions of the form

$$g_B\ j^\mu_h W_\mu \qquad \text{and} \qquad g_\ell\ j^\mu_\ell W_\mu.$$

The leading (tree level) truncated diagram is essentially given by the propagator of the W-field. If this field were massless, then this propagator would exhibit a

strong energy dependence $1/q^2$ which is not consistent with experiment. Instead, if it is very massive, then the propagator is essentially $1/M^2$ at energies $s \ll M^2$: consequently, the amplitude is the same as with the Fermi coupling constant $F = g_B g_\ell / M^2$. Given the empirical value of F, either the couplings g_h, g_ℓ must be rather small or the new vector boson must be much heavier than the proton.

The nature of this new interaction has been resolved by scattering experiments at high energies (where s is no longer negligible against M^2). It turned out that indeed the mass is large ($\approx 75 m_p$), *and* the product of the couplings is small (weak interaction). Moreover, the observed distributions of scattering angles and their correlations with the spin of the particles imply that the couplings are not only of the vector type $j^\mu W_\mu$ but also contain axial vector couplings $j^{\mu 5} W_\mu$ with equal magnitude ("$V - A$" structure).

The $V-A$ combinations $j^\mu - j^{\mu 5} = :\bar\psi \gamma^\mu (\mathbf{1} - \gamma^5)\psi$: involve the projection matrix $P_L = \frac{1}{2}(\mathbf{1} - \gamma^5)$ (recall that $(\gamma^5)^2 = \mathbf{1}$). The components $\psi_L = P_L \psi$ of the Dirac spinor in the range of P_L are called "**left-handed Weyl spinors**" (for massless spinors, they have negative helicity $-\frac{1}{2}$; in the chiral representation, ψ_L are just the lower two components of the Dirac spinor). The $V - A$ structure of the interaction means that only the left-handed fermions participate in the weak interaction.

Because the currents j_h and j_ℓ change the electric charge, the $W_\mu = W^+_\mu$ field must also carry an electric charge, and there must also be the hermitean conjugate coupling to the field W^-_μ of opposite charge. The discovery of high-energy scattering processes that must be mediated by *neutral* currents of the form $\bar\psi_e \gamma^\mu P_L \psi_e$ etc (also right-handed) requires also the presence of a neutral massive vector boson field Z_μ.

Remarkably, all the weak interaction couplings are of the same general structure as the Maxwell coupling $j^\mu A_\mu$ of QED. There arise, however, a number of problems:

(1) Quantization of vector fields introduces negative norm states, which have to be eliminated. The only known way to achieve this, is to exploit gauge invariance. One should therefore construct a Lagrangean, including the dynamics of the vector fields, that exhibits gauge symmetry. This leads us to a non-abelian generalization of QED (cf Sect. 8.3).

(2) However, a mass term for the vector particles is not gauge-invariant, and therefore not admissible in the Lagrangean. One has to find a method to obtain massive vector fields without a mass term!

(3) The $V - A$ structure implies that left-handed Weyl fermions have different gauge transformations than right-handed ones. Therefore, also mass terms for the fermions $m\overline{\psi}\psi = m\overline{\psi}_R \psi_L + m\overline{\psi}_L \psi_R$ are not gauge-invariant, and one needs also a method to generate fermion masses without writing them into the Lagrangean.

(4) The Higgs mechanism solves both problems (2) and (3). One has to introduce a suitable multiplet of scalar fields (Higgs fields) with gauge-invariant interactions. The ground state however (which is different from a Fock vacuum!), is *not* gauge-invariant. This is called "spontaneous symmetry breaking" (cf Sect. 8.5).

(5) The effect of SSB is that the other fields coupled to the Higgs fields behave

as if they were massive. Gauge invariance fixes the masses of the vector bosons. On the other hand, the masses of the fermions (given by Yukawa type couplings, cf Sect. 8.6) are essentially undetermined by the theory.

(6) All coupling types, that are renormalizable by power-counting (Dirac/Weyl, Yukawa, and cubic and quartic interactions among scalar and massless vector fields), actually occur in this model. However, it has to be established that renormalizability is not spoiled by the spontaneous symmetry breaking.

(7) In particular, there may occur so-called "anomalies", ie violations of symmetries of the Lagrangean that cannot be preserved upon quantization. If gauge symmetries have anomalies, renormalizabaility will fail. The absence of potential gauge anomalies must be enforced by adjusting the particle content of the model. Essentially, gauge anomaly cancellation requires "full generations of particles" (a charged lepton, a neutrino and two times three quarks).

In the sequel, we shall give brief overviews over the issues (1)–(7).

8.3 Non-abelian gauge theory

Non-abelian gauge symmetry generalizes the $U(1)$ gauge symmetry of QED,

$$\psi(x) \to e^{-ie\,\alpha(x)}\,\psi(x), \qquad A_\mu(x) \to A_\mu(x) - \partial_\mu\alpha(x).$$

Let G be a compact Lie group, such as $U(1)$ or $SU(2)$. Let τ_a be infinitesimal generators of the Lie group ($\tau_0 \equiv 1$ for $U(1)$ and $\tau_a \equiv \frac{1}{2}$ times the Pauli matrices for $SU(2)$). This means that infinitesimal group elements are of the form $g = 1 + i\theta^a\tau_a$ ($\theta^a \in \mathbb{R}$ infinitesimally small). The generators form a Lie algebra

$$[\tau_a, \tau_b] = i f^c_{ab}\tau_c$$

with structure constants $f^c_{ab} \in \mathbb{R}$ ($= 0$ for $U(1)$, $= \varepsilon_{ijk}$ for $SU(2)$). Next, let $g \mapsto \pi(g)$ be a unitary representation of G by $N \times N$ matrices $\pi(g)$, eg $\pi(e^{it}) = e^{int}$ for $U(1)$, or the spin-j representation for $SU(2)$. It induces a representation of the Lie algebra such that for infinitesimal group elements $\pi(g) = \mathbf{1} + i\theta^a\pi(\tau_a)$.

Then one considers a multiplet of N Dirac fields ψ_n, and the gauge transformation law

$$\psi_n(x) \to \pi(g(x)^{-1})_{nm}\psi_m(x)$$

(summation over m understood). The Dirac kinetic term

$$i\overline{\psi}_n\gamma^\mu\partial_\mu\psi_n$$

is not gauge invariant. It can be made gauge invariant by introducing a Lie-algebra-valued gauge field $\mathcal{A}_\mu$ that transform as

$$\mathcal{A}_\mu(x) \to g(x)^{-1}\mathcal{A}_\mu(x)g(x) + ig(x)^{-1}\partial_\mu g(x).$$

Note that if τ is in the Lie algebra, then $g^{-1}\tau g$ is in the Lie algebra, and if g is a group-valued function, then $ig^{-1}\partial g$ is a LA-valued function. The actual new quantum fields are the coefficients A^a_μ of $\mathcal{A}_\mu$ in the basis τ_a, see below.

Now we replace the derivative by the **covariant derivative**

$$(D_\mu\psi)_m(x) = \big(\partial_\mu \mathbf{1}_N - i\pi(\mathcal{A}_\mu(x))\big)_{mn}\psi_n(x).$$

This ensures that

$$D_\mu\psi(x) \to \pi(g(x)^{-1})D_\mu\psi(x)$$

transforms in the same way as the field itself, and therefore

$$i\overline{\psi}\gamma^\mu D_\mu\psi = i\overline{\psi}\gamma^\mu\partial_\mu\psi + \overline{\psi}\gamma^\mu\pi(\mathcal{A}_\mu)\psi$$

is gauge invariant.

The covariant derivative can be understood geometrically: One cannot directly compare components of field multiplets $\psi(x) \in V_x$ and $\psi(y) \in V_y$ at different points, because gauge transformations act independently on V_x and V_y. The gauge potential induces a "parallel transport" $U_{y,x} : V_x \to V_y$ by the path-ordered exponential

$$U^{(C)}_{y,x} = \pi\big(P \exp i \int_C \mathcal{A}_\mu dx^\mu\big)$$

where the integral extends along a curve from x to y. Thus $U^{-1}_{y,x}\psi(y)$ and $\psi(x)$ are both $\in V_x$. Then

$$D_\mu\psi(x) = \frac{d}{ds}U^{-1}_{x+se_\mu,x}\psi(x+se_\mu)|_{s=0}$$

is the differental quotient of two vectors in the same space V_x.

We still need a Lagrangean for the gauge fields. We define the Lie-algebra-valued field strength tensor $\mathcal{F}_{\mu\nu}$ by

$$gF^a_{\mu\nu}\tau_a := \mathcal{F}_{\mu\nu} = \partial_\mu\mathcal{A}_\nu - \partial_\nu\mathcal{A}_\mu - i[\mathcal{A}_\mu, \mathcal{A}_\nu],$$

which transforms in the adjoint representation of G, ie, as

$$\mathcal{F}_{\mu\nu}(x) \to g(x)^{-1}\mathcal{F}_{\mu\nu}(x)g(x).$$

Note also that

$$[D_\mu, D_\nu]\psi(x) = -i\pi(\mathcal{F}_{\mu\nu}(x)) \cdot \psi(x),$$

(hence the field strength is mathematically a very similar object as the curvature in General Relativity). Then the **Yang-Mills-Lagrangean** is

$$\mathcal{L}_{\rm YM} = -\frac{1}{4g^2}\langle\mathcal{F}_{\mu\nu}, \mathcal{F}_{\mu\nu}\rangle$$

where $\langle\ ,\ \rangle$ is a positive definite G-invariant quadratic form on the Lie algebra, and g is a coupling constant. This can be brought into a more standard form by exhibiting the Lie algebra coefficients:

$$\mathcal{A}_\mu(x) = g \cdot A^a_\mu(x)\tau_a, \qquad \text{and} \qquad \mathcal{F}_{\mu\nu}(x) = g \cdot F^a_{\mu\nu}(x)\tau_a,$$

such that

$$F^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu - ig\ f^a_{bc}A^b_\mu A^c_\mu.$$

If one chooses the basis τ_a to be orthonormal wrt this scalar product, then

$$\mathcal{L}_{YM} = -\frac{1}{4} F^a_{\mu\nu} F^{a\mu\nu},$$

which is a sum of Maxwell-like terms for each generator a, plus cubic and quartic self-interaction terms involving the structure constants, with coupling constants g and g^2, respectively. When we insert the expansion of $\mathcal{A}$ into the covariant derivatives, the term $\overline{\psi}\gamma^\mu\pi(\mathcal{A}_\mu)\psi$ becomes

$$g\ \overline{\psi}\gamma^\mu\pi(\tau_a)\psi\ A^a_\mu \equiv g\ j^\mu_a\ A^a_\mu.$$

These **minimal couplings** of the gauge potentials A^a_μ to the currents $j^a_\mu = \overline{\psi}\gamma^\mu\pi(\tau_a)\psi$ generalize the QED coupling $ej^\mu A_\mu$.

In the case of QED, we choose $G = U(1)$ and the coupling constant $g = e$. We may write $g(x) = e^{ie\alpha(x)}$, and recover all the old formulae; in particular, the "abelian YM" Lagrangean is the Maxwell Lagrangean, and, if the representation is $\pi(e^{it}) = e^{int}$, the Dirac field describes a particle of electric charge ne. In the non-abelian case, $\mathcal{L}_{\rm YM}$ is the sum of Maxwell terms for each generator a, plus cubic and quartic self couplings due to the commutators in $\mathcal{F}_{\mu\nu}$, and the representation π generalizes the notion of "electric charge measured in units of the coupling constant".

All the above couplings (minimal and gauge self-couplings) are completely fixed, once the gauge group G and the representation π are specified. In the case of the weak interaction, because the currents connect two different fields (neutrino and electron, up and down quark), the gauge multiplets should be doublets, and the gauge group $G = U(1) \times SU(2)$. Hence we have one $U(1)$ vector potential called W^0_μ (not yet the photon field!) and three vector potentials for $SU(2)$, called W^i_μ, $i = 1, 2, 3$. There are two coupling constants, g_1 for $U(1)$ and g_2 for $SU(2)$. g_1 does not appear in $\mathcal{L}_{\rm YM}$, while the cubic and quartic self-couplings of W^i $(i = 1, 2, 3)$ are proportional to g_2 and g_2^2, resp, and involve the structure constants ε_{ijk}.

The $SU(2)$ gauge fields couple only to left-handed currents. Therefore, left-handed Weyl fields transform in the spin-$\frac{1}{2}$ representation $\pi_L(g) = g$, while right-handed fields transform in the trivial repn of $SU(2)$, $\pi_R(g) = 1$. Their transformations under $U(1)$ are specified by coefficients $y_R = \pi_R(\tau_0)$ and $y_L = \pi_L(\tau_0)$ (called "hypercharges") to be specified in Sect. 8.5. The resulting minimal couplings are

$$\mathcal{L}_{\rm min} = g_1 \left(y_R \overline{\psi}_R \gamma^\mu \psi_R + y_L \overline{\psi}_L \gamma^\mu \psi_L \right) W^0_\mu + \frac{g_2}{2}\ \overline{\psi}_L \gamma^\mu \sigma^i \psi_L\, W^i_\mu.$$

8.4 BRST

We shall be very brief about the BRST (Becchi, Rouet, Stora, Tyutin) method.

Apart from the indefinite-norm problem, there is the problem that the path integral extends over all configurations of the gauge potentials, while the integrand is constant for all gauge potentials that are gauge transforms of each other – one therefore expects a divergence proportional to the infinite "volume" of the huge group of all gauge transformations.

One should rather modify the integration so as to count only one configuration per gauge orbit, selected by a suitable gauge fixing condition $G(A,\phi)=\omega$, where ϕ stands for all other fields, and ω some function.

Faddeev and Popov proposed to insert a functional δ-function $\prod_x \delta(G(A,\phi)(x)-\omega(x))$ into the PI, which has to be corrected by a functional Jacobi determinant so that each gauge orbit is counted with the same weight. This Jacobi determinant can be represented as a path integral over additional "ghost fields", which are fermionic scalar fields, ie they violate the Spin-Statistics theorem. (Fermionic fields are represented by Grassmann path integrals, ie the field integration variables are "anticommuting numbers".) Then, the result should not depend on the function ω, and by a suitable averaging over it, one arrives at a total Lagrangean involving Dirac or Weyl, gauge, ghost and further auxiliary fields.

This Lagrangean is invariant under a new type of infinitesimal symmetries, called BRST transformations: $\delta_{\rm BRST}(\mathcal{L})=0$. The latter act on the Dirac/Weyl and gauge fields like infinitesimal gauge transformations with ghost-field-valued parameters, and on the auxiliary fields in such a way that (for all fields X)

$$\delta_{\rm BRST}(\delta_{\rm BRST}(X))=0.$$

This feature can be exploited as follows: On the resulting indefinite Fock space $\mathcal{H}'$ of all fields (represented by this path integral), there exists a fermionic operator $Q_{\rm BRST}$ with the property $Q_{\rm BRST}^2=0$, which implements

$$\delta_{\rm BRST}(X)=[Q_{\rm BRST},X]_\pm$$

with the commutator for bosonic and the anti-commutator for fermionic fields.

(i) Let $\mathcal{H}_0$ be the subspace of vectors $\psi\in\mathcal{H}'$ such that $Q_{\rm BRST}\psi=0$, and $\mathcal{H}_{00}$ the subspace of all vectors of the form $Q_{\rm BRST}\psi$. Then $\mathcal{H}_{00}\subset\mathcal{H}_0\subset\mathcal{H}'$.

(ii) Because $Q_{\rm BRST}$ is hermitean wrt to the inner product of $\mathcal{H}'$, every vector $\in\mathcal{H}_{00}$ is orthogonal to every vector $\in\mathcal{H}_0$; in particular, every vector $\in\mathcal{H}_{00}$ has zero norm, and $\|\psi+\psi_{00}\|^2=\|\psi\|^2$ for $\psi\in\mathcal{H}_0$ and $\psi_{00}\in\mathcal{H}_{00}$.

(iii) One must show that the indefinite inner product of $\mathcal{H}'$ is semi-definite on $\mathcal{H}_0$, and every vector of zero norm belongs to $\mathcal{H}_{00}$. Therefore the quotient space

$$\mathcal{H}=\mathcal{H}_0/\mathcal{H}_{00}$$

is a Hilbert space. (Elements of the quotient space are equivalence classes, where $\psi_1\sim\psi_2$ if $\psi_1-\psi_2\in\mathcal{H}_{00}$. This structure is called a "cohomology".)

(iv) The **physical Hilbert space** $\mathcal{H}$ contains the vacuum, and only two transversal (=circular) polarization states per photon, but no ghost states.

(v) Operators on $\mathcal{H}'$ that (anti-)commute with $Q_{\rm BRST}$, obviously preserve the subspaces $\mathcal{H}_0$ and $\mathcal{H}_{00}$, hence they are well-defined operators on $\mathcal{H}$. One therefore defines the **physical observables**, acting on $\mathcal{H}$, as those operators X that are BRST-invariant:

$$\delta_{\rm BRST}(X)=0.$$

(vi) Time-ordered VEV of observables computed via Gell-Mann–Low do not depend on the details of the averaging over the gauge fixing functions ω, and the same follows for S-matrix elements between physical states $\in \mathcal{H}_0$ via LSZ.

8.5 Higgs mechanism

How can one describe massive vector bosons? A mass term like $M^2 W_\mu W^\mu$ is not gauge-invariant, and would spoil BRST. Instead one introduces a complex scalar doublet ("Higgs field")

$$\Phi(x) = \begin{pmatrix} \Phi_1(x) \\ \Phi_2(x) \end{pmatrix}$$

The Higgs field has a $U(2)$ invariant potential

$$V(\Phi) = \lambda\big(\Phi^\dagger\Phi - \frac{1}{2}v^2\big)^2$$

with $\lambda > 0$ which has a degenerate classical minimum at $\Phi^\dagger\Phi = \frac{1}{2}v^2$. One may expect that in the ground state, the doublet Φ has a vacuum expectation value Φ_0 which is any one of the classical minima: while the potential is invariant under $U(2)$ transformations, the VEV is not: this is called "**spontaneous breakdown of symmetry**". WLOG we may assume $\Phi_0 = \frac{1}{\sqrt{2}}(0, v)$.

One may then parametrize Φ by four real scalar fields

$$\Phi(x) = \frac{1}{\sqrt{2}} \begin{pmatrix} \varphi(x) + i\varphi'(x) \\ v + \rho(x) + i\rho'(x) \end{pmatrix}.$$

Inserting this into the Higgs potential, one finds the only quadratic contribution to be $\lambda v^2 \rho^2$, plus cubic and quartic self-couplings, ie a Lagrangean with self-interactions among a field ρ of mass $M_H^2 = 2\lambda v^2$ and three massless fields ρ', φ, φ'. This is an instance of the **Goldstone Theorem** (obtained in axiomatic settings), which asserts that the spontaneous breakdown of a continuous symmetry is always accompanied by the emergence of massless particles (Goldstone bosons). Notice that the $U(1)$ subgroup with generator $\frac{1}{2}\mathbf{1} + \tau_3$ (complex phase transformations of the first component) preserves Φ_0, and hence remains unbroken.

Now promote the $U(2)$ symmetry to a $U(1) \times SU(2)$ gauge symmetry with local transformation law

$$\Phi \to e^{-it(x)} g^{-1}(x)\ \Phi,$$

ie in the representation given by $U(1)$ hypercharge $y_{\text{Higgs}} = 1$ and $SU(2)$-spin $\frac{1}{2}$. The covariant derivative is therefore

$$(D_\mu\Phi)_m(x) = \partial_\mu\Phi_m(x) - ig_1 W_\mu^0\ \Phi_i(x) - i\frac{g_2}{2} W_\mu^i\ (\sigma^i)_{mn}\Phi_n,$$

such that the kinetic term $(D^\mu\Phi)^\dagger D_\mu\Phi$ involves interaction terms of the form

$$-i\partial_\mu\Phi^\dagger\sigma^a\Phi\ W^{a\mu} + c.c. \qquad \text{and} \qquad \Phi^\dagger\sigma^a\sigma^b\Phi\ W^{a\mu}W_\mu^b,$$

summed over a and b with coefficients g_1 for $a, b = 0$ and $\frac{1}{2}g_2$ for $a, b = 1, 2, 3$.

Now by a local gauge transformation, one can transform Φ to take the form

$$\Phi(x) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v + \rho(x) \end{pmatrix},$$

where $\rho(x)$ is real. One may choose this form as the gauge fixing condition ("unitary gauge"). The massless Goldstone bosons ρ', φ, φ' have disappeared. Instead, inserting this form into the minimal Higgs couplings, the kinetic term $(D^\mu\Phi)^\dagger D_\mu\Phi$ now involves quadratic contributions $\frac{1}{2}v^2(\sigma^a\sigma^b)_{22}\, W^{a\mu}W^b_\mu$, summing up to

$$\frac{1}{8}v^2\Big[(2g_1W^0 - g_2W^3)^\mu(2g_1W^0 - g_2W^3)_\mu + g_2^2(W^{1\mu}W^1_\mu + W^{2\mu}W^2_\mu)\Big].$$

Together with the kinetic terms $-\frac{1}{4}(\partial^\mu W^{a\nu} - \partial^\nu W^{a\mu})(\partial_\mu W^a_\nu - \partial_\nu W^a_\mu)$, these act as mass terms for the gauge potentials: the fields W^1 and W^2 have mass $M_W^2 = \frac{1}{4}\, v^2 g_2^2$. Passing to the orthonormal combinations of the "diagonal" gauge potentials

$$A_\mu = \tfrac{1}{\sqrt{4g_1^2+g_2^2}}(g_2W^0_\mu + 2g_1W^3_\mu), \quad Z_\mu = \tfrac{1}{\sqrt{4g_1^2+g_2^2}}(2g_1W^0_\mu - g_2W^3_\mu),$$

one sees that the field Z_μ has mass $M_Z^2 = \frac{1}{4}v^2(4g_1^2 + g_2^2)$. This generation of mass for three of the four gauge bosons is the **Higgs Mechanism**. The field A_μ remains massless. It is the vector potential wrt to the unbroken $U(1)$ subgroup which leaves $\Phi_0 = \frac{1}{\sqrt{2}}(0, v)^T$ invariant. This is the QED photon field.

Expressing the minimal couplings $\mathcal{L}_{\min}$ between currents and gauge bosons in the new basis of the latter, one finds the desired weak interaction terms

$$\frac{g_2}{\sqrt{2}}(\overline{\psi}_L\sigma^+\gamma^\mu\psi_L\, W^+_\mu + \overline{\psi}_L\sigma^-\gamma^\mu\psi_L\, W^-_\mu)$$

where $W^\pm_\mu = \frac{1}{\sqrt{2}}(W^1_\mu \mp W^2_\mu)$, and $\sigma^\pm = \frac{1}{2}(\sigma^1 \pm i\sigma^2)$. In addition, Z_μ couples to the combination

$$\frac{1}{\sqrt{4g_1^2 + g_2^2}}\Big(2g_1^2\big(y_R\,\overline{\psi}_R\gamma^\mu\psi_R + y_L\,\overline{\psi}_L\gamma^\mu\psi_L\big) - \frac{1}{2}g_2^2\,\overline{\psi}_L\sigma^3\gamma^\mu\psi_L\Big),$$

and A_μ couples to the combination

$$\frac{2g_1g_2}{\sqrt{4g_1^2 + g_2^2}}\Big(\overline{\psi}_R\big(\frac{1}{2}y_R\big)\gamma^\mu\psi_R + \overline{\psi}_L\big(\frac{1}{2}y_L + \frac{1}{2}\sigma^3\big)\gamma^\mu\psi_L\Big).$$

In the last term appears the generator of the unbroken gauge group in the specified representations, given by ($\frac{1}{2}$ hypercharge + eigenvalue of $\pi(\tau_3)$):

$$Q = \frac{1}{2}Y + T_3 \quad (\equiv \pi(\frac{1}{2}\tau_0 + \tau_3))$$

(**Gell-Mann–Nishijima formula**). Therefore, the couplings of A_μ can be identified with the electromagnetic interaction, provided one identifies

$$\frac{2g_1g_2}{\sqrt{4g_1^2 + g_2^2}} = e$$

with the electric charge unit, and Qe with the electric charge q of the particles described by the various Dirac fields.

One assigns the hypercharge $y_L = -1$ to left-handed leptons, so that the upper components ($T_3 = +\frac{1}{2}$) are electrically neutral (neutrinos), while the lower components ($T_3 = -\frac{1}{2}$) describe particles of electric charge $-e$ (electrons). The right-handed components have the same electric charge provided $y_R = 0$ for the upper components and $y_R = -2$ for the lower components. Similarly, one assigns $y_L = \frac{1}{3}$ to the left-handed quarks and $y_R = (\frac{4}{3}, -\frac{2}{3})$ to the right-handed quarks, so that the upper (lower) components have electric charge $+\frac{2}{3}e$ ($-\frac{1}{3}e$).

The assignments for y_R are made such that left- and right-handed leptons carry the same electric charge, ie the electromagnetic couplings preserve parity:

$$q\,(j_L^\mu + j_R^\mu)A_\mu = q\; j^\mu A_\mu.$$

We have thus obtained massive charged and neutral vector fields $W_\mu^\pm$ and Z_μ in addition to the photon field, at least at the Lagrangean level, without violating the gauge invariance of the Lagrangean. The Lagrangean involves several non-abelian self-couplings of the gauge fields, self-couplings of the Higgs field, and minimal couplings of the gauge fields to the Higgs and Weyl fields.

Apart from the gauge group and the specified representations, the weak interaction has four fundamental numerical parameters: λ, v, g_1, and g_2; or, equivalently, the Higgs mass, the W-mass, the electric charge e and the **Weinberg angle** ϑ:

$$M_H^2 = 2\lambda v^2, \quad M_W^2 = \frac{1}{4}v^2 g_2^2, \quad e = \frac{2g_1 g_2}{\sqrt{4g_1^2 + g_2^2}}, \quad \sin\vartheta = \frac{2g_1}{\sqrt{4g_1^2 + g_2^2}}.$$

These numbers fix the Z-mass $M_Z = M_W/\cos\vartheta$, as well as the coefficients of all couplings. It follows that the coefficients of the individual coupling terms cannot be independent. To renormalize the theory, one has to introduce renormalization factors for each individual interaction term. Preservation of the gauge symmetry requires that the relations between the coefficients are preserved ("**Ward identities**"). To prove that the necessary Ward identities are indeed satisfied in every order of PT, is one of the non-trivial challenges of perturbative renormalization.

8.6 Yukawa couplings

Because $\overline{\psi}\psi = \overline{\psi}_L\psi_R + \overline{\psi}_R\psi_L$ mixes left- and right-handed Weyl fields, a mass term $m\,\overline{\psi}\psi$ as in the free Dirac Lagrangean is incompatible with the chiral gauge transformation laws. Another way to obtain massive fermions is needed.

Indeed, the assignments of hypercharges and $SU(2)$ representations are such that **Yukawa couplings** of the form

$$\Phi^\dagger(\overline{e}_R l_L), \qquad \Phi \times (\overline{\nu}_R l_L), \qquad \Phi^\dagger(\overline{d}_R q_L), \qquad \Phi \times (\overline{u}_R q_L)$$

(and their hermitean conjugates) are *electrically neutral gauge-invariant scalars.* Here, l_L and q_L are left-handed lepton and quark doublets, ν_R, e_R, u_R, and d_R are right-handed neutrino, electron, up-quark and down-quark singlets, and "$A \times B$" stands for the $SU(2)$-invariant combination $\varepsilon_{mn}A_m B_n$ of two 2-vectors.

Replacing Φ by its expansion around the VEV, one obtains gauge-invariant lepton and quark mass terms, plus further interactions between the Fermi and the Higgs field. If a Yukawa coupling comes with coefficient c, then the resulting masses are $\sim vc$, and the resulting Higgs interactions are $\sim c$. Therefore, (a) the masses of the fermions can be freely adjusted by choosing the Yukawa couplings c, and (b) the interaction strengths with the Higgs field are proportional to the masses. (Thus, the Higgs boson will preferably decay into the heaviest quark, $H \to t\bar{t}$.)

The fermions come in three "families" with the same quantum numbers. The Yukawa couplings may also mix different families, eg, the left-handed myon family with the right-handed electron in the first coupling type. Thus, not only are the masses different in different families, but there can be also mass terms non-diagonal wrt the families. Family mixing is responsible for decay of strange particles, and also for neutrino oscillations provided the neutrino masses are different. Also, with three families, the most general hermitean mass mixing matrix can exhibit a complex phase that violates **CP** symmetry. The details of the mass mixing matrices are not constrained by gauge symmetry, and are therefore responsible for most of the free adjustable parameters of the Standard Model, apart from the gauge coupling constants and the Higgs mass.

8.7 Strong interaction

The modern theory of the strong interaction is a non-abelian gauge theory with gauge group $SU(3)$, called QCD (**Quantum Chromodynamics**). Quarks arise as triplets ("color") in the vector representation of $SU(3)$, and the eight QCD gauge bosons are called "gluons". Because the coupling constant is large, the perturbative approach is very unreliable; in particular, quarks and gluons do not exist as asymptotic free particles (**confinement**). Furthermore, hadronic bound states (baryons and mesons) cannot be viewed just as bound states of three quarks or a quark and an anti-quark, but have a very complicated structure involving many "virtual" additional quarks and gluons.

At high energies, the strong interaction becomes very weak due to renormalization effects (**asymptotic freedom**): therefore, in "deep-inelastic scattering" electrons interact with only one of the three quarks making up a nucleon, which is only loosely bound to the other quarks at high energy. This can be computed perturbatively. The predictions are quantitatively well confirmed, up to certain *structure functions*, which describe the interior structure of hadrons and the formation of hadrons out of scattered quarks after the interaction. These functions cannot be computed with perturbation theory, but must be fitted from experiment.

An experimental method to "count" the number of three colors is the total hadronic production cross section in e^+e^- annihilation; namely the relevant Feynman diagrams contain a sum over all colors. An independent, purely theoretical reason is as follows: The parity-violating weak $SU(2)$ symmetry produces divergent diagrams with fermion loops with three gauge vertices, which would require

a cubic gauge field counter term involving the totally antisymmetric ε tensor, not present in the unrenormalized Lagrangean. (In the abelian case, this is known as **Adler anomaly**). This anomaly would violate gauge invariance, and hence spoil BRST. The coefficient of the anomaly turns out to be a sum over certain quantum numbers of the representations of all particles in a family (cubes of the charges in the abelian case). This sum vanishes – provided each quark is counted three times.

Because the coupling constant is not small, the perturbative approach (expansion in Feynman integrals) is not a good approximation. Instead, a non-perturbative approach to QCD is the **lattice approximation**: it consists in taking the path integral serious (ie not as a Gaussian integral with a power series expansion) and approximating it by an integral over field configurations in a discrete space-time. In order to do this, one takes advantage of the "Euclidean" reformulation of QFT, from which the true QFT in Minkowski spacetime can be recovered, and the geometric interpretation of gauge fields as a "parallel transport".

More precisely:

(a) One replaces all times by imaginary times such that $x^4 = ix^0$ is real, and writes $x_E = (x_1, \dots, x_4) \in \mathbb{R}^4$. Then the action $S = \int d^4x \mathcal{L}$ (say, for a scalar field) becomes

$$i \int d^4x_E \big(\frac{1}{2}\partial_\mu\phi\partial_\mu\phi + V(\phi)\big) = iS_E.$$

Thus the integrand e^{iS} of the path integral becomes e^{-S_E}, which is exponentially damped rather than oscillatory (and the PI has the same form as a partition function $\int e^{-\beta H}$ of a four-dimensional system in Statistical Mechanics).

One then restricts the fields to the points of a Euclidean lattice $a\mathbb{Z}^4 \subset \mathbb{R}^4$ which can be made finite by imposing, say, periodic boundary conditions $\phi(\vec{n} + N\vec{e}_\mu) = \phi(\vec{n})$ ($\vec{n} \in \mathbb{Z}^4$). Derivatives are replaced by difference quotients

$$\partial_\mu\phi(\vec{x}) = a^{-1}\big(\phi(\vec{n} + \vec{e}_\mu) - \phi(\vec{n})\big).$$

Thus, the PI consists of finitely many rapidly convergent integrals, and is mathematically well-defined.

(b) In the case of gauge theories, the parallel transport between two points is a unitary operator $U^{(C)}_{y,x} = \pi\big(P \exp ig \int_C A^a_\mu \tau_a dx^\mu\big)$. On the lattice, instead of integrating over gauge potentials, one assigns a unitary matrix $U_{\vec{n}+\vec{e}_\mu,\vec{n}}$ to each lattice edge, and replaces the covariant derivative by

$$D_\mu\phi(\vec{x}) = a^{-1}\big(\pi(U^{-1}_{\vec{n}+\vec{e}_\mu,\vec{n}})\phi(\vec{n} + \vec{e}_\mu) - \phi(\vec{n})\big).$$

From this, one also obtains a lattice version of the field strengths F^a_{mn} as the commutator of lattice covariant derivatives. One then integrates over the compact unitary group, giving rise to another finite number of convergent integrations.

The continuum limit requires to take $a \to 0$ (UV) and $N \to \infty$ (IR). Clearly, these limits are divergent and must be renormalized. For finite a and N, one can simulate the behavior of quarks by fast computers, and indeed finds the expected signals for confinement; but computer power allows only very small N.

9 Resume

The lectures should have made it clear that "writing down an interacting Lagrangean" by no means defines a QFT, but is just the seed whose specification marks the beginning of the actual work.

- Free fields are constructed with creation and annihilation operators on a Fock space. This can be generalized to all unitary positive-energy representations of the Poincaré group.
- Quantum fields can be coupled to external (classical) sources. The scattering matrix describes the integrated change of multi-particle states during the presence of the external fields. In the interaction picture, the time-ordered exponential
$$S = Te^{i\int \mathcal{L}_{\rm int}}$$
is a formal expression for the scattering matrix. An infrared divergence notoriously appears when the external fields are taken to be constant.
- The same formula for self-coupled quantum fields cannot avoid the IR problem, because interactions cannot be "switched off". Therefore it must be discarded. (In addition, UV divergences appear.)
- The LSZ formula provides a different formula for the scattering matrix in terms of time-ordered vacuum expectation values of the interacting fields.
- The Gell-Mann–Low formula expresses interacting time-ordered VEV in terms of free fields.
- Perturbative evaluation of this formula using Wick's theorem leads to Feynman diagrams, representing Feynman integrals. The previous IR problem is absent. UV divergences must be dealt with by renormalization. The combinatorics is controlled by generating functionals. Euclidean methods, like the path integral, provide helpful analytic tools.
- The standard model of elementary particles is described by a renormalizable QFT. However, the perturbative treatment requires an indefinite Hilbert space. The passage to a positive Hilbert space substantially exploits gauge invariance. But massive standard model particles are in conflict with gauge invariance. The Higgs mechanism is a way to describe massive particles without explicit mass terms in the Lagrangean.
- In spite of its success, the perturbative treatment is unsatisfactory: first, the coupling constant of the strong interaction is not small; second (and more fundamentally), the perturbative series is expected to be divergent. Better, non-perturbative methodes for the construction of QFT are required.
- Axiomatic approaches allow complementary structural insight, based on fundamental properties of QFT that are independent of a constructive scheme.