Notes on advanced field theory

Matteo Giordano

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Contents

Paragraphs marked with an asterisk ($*$) were not covered and can be skipped.

Notation and conventions

Covariant vectors V with components V^μ, $\mu = 0,1,2,3$, are also denoted as $V = (V^0, \vec{V})$, $\vec{V} = (V^1, V^2, V^3)$. The Minkowski metric tensor is

$$\eta_{\mu\nu} = \mathrm{diag}(1,-1,-1,-1)\,.$$

Indices are raised and lowered by $\eta_{\mu\nu}$ and $\eta^{\mu\nu}$, $V_\mu = \eta_{\mu\nu}V^\nu$, $V^\mu = \eta^{\mu\nu}V_\nu$. The inverse of the Minkowski tensor is defined by $\eta^{\mu\rho}\eta_{\rho\nu} = \delta^\mu{}_\nu$ with $\delta^\mu{}_\nu = (1,1,1,1)$, and reads $\eta^{\mu\nu} = \mathrm{diag}(1,-1,-1,-1)$. The Minkoskian scalar product and (pseudo)norm squared are denoted by

$$A\cdot B = A^\mu B_\mu\,, \qquad A^2 = A^\mu A_\mu\,.$$

A dagger, †, denotes the adjoint of an operator, or the Hermitian conjugate of a matrix. Unitary operators corresponding to a translation by a and to a Lorentz transformation Λ are denoted by $U(a) = e^{-iP_\mu\cdot a^\mu}$ and $U(\Lambda) = e^{i\frac{1}{2}\omega_{\rho\sigma}J^{(\rho\sigma)}}$, respectively, where P_μ and $J^{(\rho\sigma)}$ are the corresponding generators, and act on covariant fields as

$$U(a)^\dagger\phi_i(x)U(a) = \phi_i(x+a)\,, \qquad U(\Lambda)^\dagger\phi_i(x)U(\Lambda) = S_{ij}(\Lambda)\phi_j(\Lambda^{-1}x)\,.$$

The invariant phase-space integration measure $d\Omega_p$ reads

$$d\Omega_p = \frac{d^3p}{(2\pi)^3 2p^0}\,, \qquad p^0 = \sqrt{\vec{p}^2+m^2}\,.$$

The strong limit of operator sequences is defined as

$$\mathrm{s}-\lim_{t\to t_0} O(t) = O_0 \quad \text{if} \quad \lim_{t\to t_0}\|(O(t)-O_0)\Psi\| = 0\,,$$

with $\|\Psi\|$ the norm induced by the scalar product in the Hilbert space.

$$f(x)\overset{\leftrightarrow}{\partial}_0 g(x) \equiv f(x)[\partial_0 g(x)] - [\partial_0 f(x)]g(x)$$

1 Review of perturbative quantisation

Why quantum field theory? The development of quantum field theory originates in the attempt to bring together quantum mechanics (QM) and special relativity (SR) to describe microscopic processes at high energies. In doing so one needs to comply with the requirements of both theories, mainly Poincaré invariance and locality from SR, and the superposition principle and the uncertainty principle from QM. The requirements from SR are most easily satisfied if one works with *fields* $\phi(x)$, i.e., objects associated with the points x of spacetime. These allow to build quite straightforwardly Poincaré-invariant theories, and to implement the locality and Poincaré-invariance of interactions, if such fields are endowed with simple symmetry transformation properties. In order to comply with QM, these objects have to be promoted to generally non-commuting linear operators acting on some Hilbert space representing the states of the system.[1]

Scattering processes The main type of high-energy processes where the use of quantum field theory is required are scattering processes, where particles are set up to collide and the products of the collision are studied. Free particles are localised objects that travel undisturbed on straighline trajectories. It is an experimental fact that systems of this type exist, and can be prepared in a laboratory. In a scattering experiment, beams of practically free particles are accelerated to the desired energy and thrown against each other, or against some fixed target. Under suitable conditions on the density of beams and targets, the typical outcome of the procedure is the interaction of one particle from a beam with one particle in the other, or with one particle in the target, when these get sufficiently close, resulting in the change of the particles' energies or momenta, or the creation of other particles. After a sufficiently long (but practically very short) time, a set of free particles is again observed, and measurements of their quantum numbers are carried out. The most important measurement is that of the *total cross section* of the process, defined operatively for a fixed target experiment as

$$\sigma = \frac{N_{\text{events}}}{N_t \frac{N_b}{A_b}} = \frac{\dot{N}_{\text{events}}}{N_t \Phi_b}\,, \tag{1.1}$$

where N_{events} is the number of scattering events (basically defined as "something happens" rather than the beam particle going on undisturbed), N_b is the number of particles in the beam and A_b its cross-sectional area, and N_t is the number of particles in the full depth of the target lying within the beam cross-section; and where $\dot{N}_{\text{events}}$ is the event rate (number of events per unit time) and Φ_b is the beam flux (number of particles crossing perpendicularly the target surface per unit surface per unit time). *Differential cross sections* are defined by the same formula Eq. (1.1) but counting only events that satisfy prescribed criteria (e.g., number, type, energy and momenta, and spin polarisation of the final particles).

Scattering states For practical purposes, the initial and final states of the system, corresponding to its preparation and to the measurement procedures, can be thought of as taking place at times $t = -\infty$ and $t = +\infty$, respectively. The statement that these states behave like

[1] More precisely, quantum fields are operator-valued *distributions*.

free particle states is expressed mathematically as[2]

$$e^{-iHt}|\Psi\rangle \underset{t\to-\infty}{\to} e^{-iH_0t}|\varphi_i\rangle\,, \qquad e^{-iHt}|\Psi\rangle \underset{t\to+\infty}{\to} e^{-iH_0t}|\varphi_f\rangle\,, \tag{1.2}$$

where the convergence is in norm. Given the exact state vector $|\Psi\rangle$ at $t=0$, its exact evolution, governed by the full Hamiltonian H, at early or late times is practically indistinguishable from the free evolution with free Hamiltonian H_0 of state vectors equal to $|\varphi_{i,f}\rangle$ at $t=0$. Equation (1.2) allows one to relate the exact state vector $|\Psi\rangle$ and the *asymptotic* state vectors $|\varphi_{i,f}\rangle$ as

$$|\Psi_+\rangle \equiv \lim_{t\to-\infty} e^{iHt}e^{-iH_0t}|\varphi_i\rangle\,, \qquad |\Psi_-\rangle \equiv \lim_{t\to+\infty} e^{iHt}e^{-iH_0t}|\varphi_f\rangle\,. \tag{1.3}$$

The states $\Psi_\pm$ are the *in* and *out* states of the system, i.e., the exact state vectors corresponding to the initial and final free states, either prepared or observed, of the system. Equation (1.2) defines the *Møller operators*[3]

$$\Omega_\pm \equiv \lim_{t\to\mp\infty} e^{iHt}e^{-iH_0t}\,. \tag{1.4}$$

These are isometric operators, $\Omega_\pm^\dagger\Omega_\pm = \mathbf{1}$. The transition amplitude of the process reads

$$S_{fi} \equiv \langle\Psi_-|\Psi_+\rangle = \langle\varphi_f|\Omega_-^\dagger\Omega_+|\varphi_i\rangle = \langle\varphi_f|S|\varphi_i\rangle\,, \tag{1.5}$$

where

$$S \equiv \Omega_-^\dagger\Omega_+\,. \tag{1.6}$$

The matrix elements of S constitute the *S-matrix*. Under the assumption that the spaces of in and out states coincide, $\Omega_\pm\Omega_\pm^\dagger = \Pi_{\rm scat}$, the S operator is unitary,

$$\begin{aligned} S^\dagger S &= \Omega_-^\dagger\Omega_+\Omega_+^\dagger\Omega_- = \Omega_-^\dagger\Pi_{\rm scat}\Omega_- = \Omega_-^\dagger\Omega_- = \mathbf{1} \\ SS^\dagger &= \Omega_+^\dagger\Omega_-\Omega_-^\dagger\Omega_+ = \Omega_+^\dagger\Pi_{\rm scat}\Omega_+ = \Omega_+^\dagger\Omega_+ = \mathbf{1}\,. \end{aligned} \tag{1.7}$$

Here it was used the fact that the projector $\Pi_{\rm scat}$ leaves an in or out state invariant, $\Pi_{\rm scat}\Omega_\pm = \Omega_\pm$. Knowledge of S allows to compute scattering cross sections from the theory.

As we will see, the formalism discussed above is not entirely adequate in quantum field theory, as it basically requires the existence of the interaction picture, which is problematic when dealing with infinitely many degrees of freedom. We will also see how one can avoid it.

Canonical quantisation The construction of a suitable Hamiltonian H that satisfies the requirements of SR is simpler if one uses quantum fields as one's basic objects. A convenient procedure is *canonical quantisation*. One start from a classical, Lorentz-invariant Lagrangian density; solves the corresponding Euler-Lagrange equations of motion; identifies the canonical momenta conjugate to the fields, treated as canonical coordinates; and imposes canonical (anti)commutation relations. By a Legendre transform one then obtains the Hamiltonian, that generates the temporal evolution of the system.

For a Hermitian scalar field ϕ, one takes the following real classical Lagrangian density,

$$\mathscr{L} = \frac{1}{2}(\partial_\mu\phi)(\partial^\mu\phi) - \frac{1}{2}m^2\phi^2 - V(\phi)\,, \tag{1.8}$$

[2]Limits are understood here as $\|\Psi - e^{iHt}e^{-iH_0t}\varphi\| \to 0$.

[3]Limits are understood as strong limits, i.e., $\|\Omega\varphi - e^{iHt}e^{-iH_0t}\varphi\| \to 0$.

and finds the following Euler-Lagrange equation,

$$\frac{\partial \mathcal{L}}{\partial \phi} = \partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \phi)} \Rightarrow (\Box + m^2)\phi = -V'(\phi)\,, \tag{1.9}$$

and the following conjugate momentum,[4]

$$\pi = \frac{\partial \mathcal{L}}{\partial(\partial_0 \phi)} = \partial_0 \phi\,. \tag{1.10}$$

The canonical commutation relations read

$$[\hat{\phi}(t,\vec{x}), \hat{\pi}(t,\vec{y})] = i\delta^{(3)}(\vec{x}-\vec{y}) \qquad [\hat{\phi}(t,\vec{x}), \hat{\phi}(t,\vec{y})] = [\hat{\pi}(t,\vec{x}), \hat{\pi}(t,\vec{y})] = 0\,, \tag{1.11}$$

where a caret denotes a field *operator*. The classical Hamiltonian is

$$\begin{aligned} H[\phi,\pi] &= \int d^3x \left(\pi(x)\partial_0\phi(x) - \mathcal{L}\big(\phi, \vec{\nabla}\phi, \partial_0\phi(\phi,\pi)\big)\right) \\ &= \int d^3x \left\{\frac{1}{2}\partial_0\phi(x)^2 + \frac{1}{2}\vec{\nabla}\phi(x)^2 + \frac{1}{2}m^2\phi(x)^2 + V(\phi)\right\}\,. \end{aligned} \tag{1.12}$$

Its promotion to an operator requires dealing with the problem of operator ordering. In the case of the free Lagrangian with $V = 0$, the solution of Eqs. (1.9) and (1.11) is

$$\hat{\phi}(x) = \int d\Omega_p \left\{a(p)e^{-ip\cdot x} + a(p)^\dagger e^{ip\cdot x}\right\}\,, \tag{1.13}$$

where $p^0 = \sqrt{\vec{p}^2 + m^2}$, the invariant phase-space integration measure $d\Omega_p$ reads

$$d\Omega_p \equiv \frac{d^3p}{(2\pi)^3 2p^0}\,, \tag{1.14}$$

and the *annihilation operators* $a(p)$ and the *creation operators* $a(p)^\dagger$ obey the commutation relations

$$[a(p), a(q)^\dagger] = 2p^0(2\pi)^3\delta^{(3)}(\vec{p}-\vec{q})\,, \qquad [a(p), a(q)] = [a(p)^\dagger, a(q)^\dagger] = 0\,. \tag{1.15}$$

A suitable ordering procedure of field products in this case is *normal ordering*, defined at the level of creation and annihilation operators by

$$:\mathrm{P}\left\{a(p_1)\ldots a(p_n)a(q_1)^\dagger\ldots a(q_n)^\dagger\right\}: \equiv a(q_1)^\dagger\ldots a(q_n)^\dagger a(p_1)\ldots a(p_n)\,, \tag{1.16}$$

where P denotes a generic permutation of the operators, and the order in which the creation and annihilation operators are separately arranged is irrelevant due to the second relation in Eq. (1.15). The quantum Hamiltonian is then defined as

$$H_0 = \int d^3x\ :\left\{\frac{1}{2}\partial_0\hat{\phi}(x)^2 + \frac{1}{2}\vec{\nabla}\hat{\phi}(x)^2 + \frac{1}{2}m^2\hat{\phi}(x)^2\right\}:\,, \tag{1.17}$$

[4]This relation is modified if V contains derivative couplings, i.e., $V = V(\phi, \partial_\mu\phi)$.

and one verifies that

$$\partial_0\hat{\phi}(x) = i[H_0, \hat{\phi}(x)]\,, \qquad \partial_0\hat{\pi}(x) = i[H_0, \hat{\pi}(x)]\,, \tag{1.18}$$

i.e., H_0 generates the free temporal evolution.

The main advantages of the canonical approach are the automatic enforcement of locality, implied by the canonical commutation relations, and the control over symmetry properties, guaranteed by Noether's theorem. In fact, the canonical commutation relations imply that observables built out of the fields and their derivatives will commute at spacelike separations. Moreover, for every continuous symmetry of $\mathscr{L}$ one has a conserved current J^μ that is a function of the fields and their derivatives, and a corresponding Hermitian conserved charge $Q = \int d^3x\, J^0$, that after quantisation generates the corresponding symmetry on the Hilbert space of the system. One can then build explicitly the unitary representation $U(\alpha) = e^{i\alpha Q}$ of the various symmetries, especially Poincaré symmetry.[5] The generators of translations, P^μ, are identified with the energy and momentum operators, and those of (proper orthocronous) Lorentz transformations with the boost operators, $\vec{K}$, and the angular momentum operators, $\vec{J}$.

Perturbation theory and the interaction picture The canonical quantisation programme is hampered by the fact that the equations of motion for realistic interacting Lagrangians are not amenable to analytic solution. This is dealt with by means of approximation methods, most notably *perturbation theory*. This is based on expanding the relevant quantities in a series in some small parameter.

The starting point is the passage to the *interaction picture*. As a first step, one splits the full interacting and time-independent Hamiltonian, $H = H[\phi, \pi]$, into a "free" and an "interaction" part,[6]

$$H[\phi(t), \pi(t)] = H[\phi(0), \pi(0)] = H_0[\phi(0), \pi(0)] + H_I[\phi(0), \pi(0)]\,, \tag{1.19}$$

with H_0 describing the free propagation of particles, typically of the form Eq. (1.17) and its analogues for other types of fields.[7] The splitting is necessarily done at some time $t = t_0$, here taken to be $t_0 = 0$, and while H is independent of t_0, H_0 and H_I are not: different choices of t_0 lead to different H_0 and H_I, providing, however, equivalent descriptions. Nonetheless, H_0 and H_I are trivially time-independent operators since they are defined in terms of the (Heisenberg) fields and momenta ϕ and π at fixed $t = t_0$. One then defines fields and momenta in the interaction picture, ϕ_0 and π_0, as

$$\begin{aligned}
\phi_0(t, \vec{x}) &\equiv e^{iH_0t}\phi(0, \vec{x})e^{-iH_0t} = e^{iH_0t}e^{-iHt}\phi(t, \vec{x})e^{iHt}e^{-iH_0t} = U(t)\phi(t, \vec{x})U(t)^\dagger\,, \\
\pi_0(t, \vec{x}) &\equiv e^{iH_0t}\pi(0, \vec{x})e^{-iH_0t} = e^{iH_0t}e^{-iHt}\pi(t, \vec{x})e^{iHt}e^{-iH_0t} = U(t)\pi(t, \vec{x})U(t)^\dagger\,,
\end{aligned} \tag{1.20}$$

where

$$U(t) \equiv e^{iH_0t}e^{-iHt}\,. \tag{1.21}$$

[5] This requires the existence and uniqueness of a vacuum state $|0\rangle$, invariant under the relevant symmetry. If such a state is not unique or does not exist, one faces the phenomena of spontaneous breaking and anomalous breaking of a symmetry.

[6] From now on the caret is removed from field operators for notational simplicity.

[7] It is implicitly assumed that the interacting theory describes particles, and that when adding interactions to a Hamiltonian like Eq. (1.17) one does not radically alter the spectrum of the theory.

By construction, ϕ_0 and π_0 evolve in time with some known free field Hamiltonian H_0, and since they are unitarily related to the canonically quantised fields and momenta ϕ and π, they also obey canonical commutation relations. Clearly,

$$H_0[\phi_0(t),\pi_0(t)] = e^{iH_0[\phi_0(0),\pi_0(0)]t} H_0[\phi_0(0),\pi_0(0)] e^{-iH_0[\phi_0(0),\pi_0(0)]t} = H_0[\phi_0(0),\pi_0(0)]\,. \quad (1.22)$$

On the other hand,

$$H_I[\phi_0(t),\pi_0(t)] \equiv V_I(t)\,, \quad (1.23)$$

and H expressed in terms of ϕ_0 and π_0, are time-dependent quantities. For H purely quadratic in π, $H = \frac{1}{2}\pi^2 + \ldots$, if H_I is a function of fields only then

$$\dot{\phi}_0(t,\vec{x}) = \frac{\delta H_0[\phi_0(t),\pi_0(t)]}{\delta \pi_0(t,\vec{x})} = \frac{\delta H[\phi_0(t),\pi_0(t)]}{\delta \pi_0(t,\vec{x})} = \pi_0(t,\vec{x})\,, \quad (1.24)$$

and so ϕ_0 is just a free field in the sense of Eqs. (1.13) and (1.15), and so exlicitly known. This makes also $V_I(t)$ explicitly known in terms of creation and annihilation operators.

At this stage one has only recast the original problem in a different formalism, but if V_I is small in some sense, one can solve the theory iteratively by expanding in powers of V_I. For example, if one is interested in the spectrum of the theory one needs to solve the eigenvalue equation

$$H\Psi = E\Psi\,. \quad (1.25)$$

Setting formally

$$\Psi = \sum_{i=0} \Psi_i\,, \qquad E = \sum_{i=0} E_i\,, \quad (1.26)$$

where each value of i corresponds to a given order in the expansion parameter, one writes

$$(H_0 + V_I)(\Psi_0 + \Psi_1 + \ldots) = (E_0 + E_1 + \ldots)(\Psi_0 + \Psi_1 + \ldots)\,, \quad (1.27)$$

and then solves iteratively the equations found at each order,

$$H_0\Psi_0 = E_0\Psi_0\,, \qquad V_I\Psi_0 + H_0\Psi_1 = E_1\Psi_0 + E_0\Psi_1\,, \qquad \ldots\,, \quad (1.28)$$

where the solutions to the first equation are known exactly, and so on.

A similar approach is employed for the S-matrix. Since [see Eq. (1.4)]

$$\Omega_\pm = \lim_{t\to\mp\infty} (e^{iH_0 t} e^{-iHt})^\dagger = \lim_{t\to\mp\infty} U(t)^\dagger\,, \quad (1.29)$$

it suffices to find an explicit form for $U(t)$. This is obtained in a more general form by solving the differential equations obeyed by $\mathcal{U}(t_2,t_1) \equiv U(t_2)U(t_1)^\dagger$,

$$\begin{aligned} \frac{\partial}{\partial t_2}\mathcal{U}(t_2,t_1) &= -ie^{iH_0 t_2}(H - H_0)e^{-iH_0 t_2}\mathcal{U}(t_2,t_1) = -iV_I(t_2)\mathcal{U}(t_2,t_1)\,, \\ \frac{\partial}{\partial t_1}\mathcal{U}(t_2,t_1) &= \quad i\mathcal{U}(t_2,t_1)e^{iH_0 t_1}(H - H_0)e^{-iH_0 t_1} = \quad \mathcal{U}(t_2,t_1)iV_I(t_1)\,. \end{aligned} \quad (1.30)$$

with the obvious initial condition $\mathcal{U}(t,t) = \mathbf{1}$. One clearly has $U(t) = \mathcal{U}(t,0)$ and $U(t)^\dagger = \mathcal{U}(0,t)$. One can directly verify that the solution is

$$\mathcal{U}(t_2,t_1) = \mathrm{Texp}\left\{-i\int_{t_1}^{t_2} dt\, V_I(t)\right\}\,, \quad (1.31)$$

where

$$\mathrm{Texp}\left\{-i\int_{t_1}^{t_2} dt\, V_I(t)\right\} = 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_{t_1}^{t_2} d\tau_1 \ldots \int_{t_1}^{t_2} d\tau_n\, \mathrm{T}\left\{V_I(\tau_1)\ldots V_I(\tau_n)\right\}\,, \tag{1.32}$$

and T denotes time ordering of the operators,

$$\mathrm{T}\left(V_I(t_1)\ldots V_I(t_n)\right) = \theta(t_1-t_2)\ldots\theta(t_{n-1}-t_n)V_I(t_1)\ldots V_I(t_n) + \text{permutations}\,. \tag{1.33}$$

The semigroup property

$$\mathcal{U}(t_2,t_0)\mathcal{U}(t_0,t_1) = \mathcal{U}(t_2,t_1) \tag{1.34}$$

follows from

$$\frac{\partial}{\partial t_0}\mathcal{U}(t_2,t_0)\mathcal{U}(t_0,t_1) = \mathcal{U}(t_2,t_0)\left[iV_I(t_0) - iV_I(t_0)\right]\mathcal{U}(t_0,t_1) = 0\,, \tag{1.35}$$

that implies $\mathcal{U}(t_2,t_0)\mathcal{U}(t_0,t_1) = \mathcal{U}(t_2,0)\mathcal{U}(0,t_1) = \mathcal{U}(t_2,t_1)$. One finally concludes

$$S = \Omega_-^\dagger\Omega_+ = \lim_{\substack{t_2\to+\infty\\ t_1\to-\infty}} U(t_2)U(t_1)^\dagger = \lim_{\substack{t_2\to+\infty\\ t_1\to-\infty}} \mathcal{U}(t_2,t_1) = \mathrm{Texp}\left\{-i\int_{-\infty}^{+\infty} dt\, V_I(t)\right\}\,, \tag{1.36}$$

known as *Dyson's formula*.

In the limit of particle states with definite momenta, from Eq. (1.5) one obtains

$$\begin{aligned} S_{fi} &= {}_0\langle p'_1,\ldots,p'_{N'}|\ \mathrm{Texp}\left\{-i\int_{-\infty}^{+\infty} dt\, V_I(t)\right\}|p_1,\ldots,p_N\rangle_0 \\ &= {}_0\langle p'_1,\ldots,p'_{N'}|1 + \sum_{n=1}^{\infty}\frac{-i}{n!}\int_{-\infty}^{+\infty} dt_1\ldots\int_{-\infty}^{+\infty} dt_n\,\mathrm{T}\left\{V_I(t_1)\ldots V_I(t_n)\right\}|p_1,\ldots,p_N\rangle_0 \\ &= \delta_{fi} + i(2\pi)^4\delta^{(4)}\left(P_f - P_i\right)\mathcal{M}_{fi}(p,p')\,, \end{aligned} \tag{1.37}$$

where $|p_1,\ldots,p_N\rangle_0$ are N-particle eigenstates of H_0 and of the free spatial-momentum operators $\vec{P}_0$, created out of the free vacuum state $|0\rangle_0$ by the action of the creation operators corresponding to the free interaction-picture fields ϕ_0, Eqs. (1.13) and (1.15). Moreover, $P_i = \sum_{j=1}^{n} p_j$ and $P_f = \sum_{j=1}^{n'} p'_j$ are the initial and final total four-momentum, whose conservation follows from translation invariance; and δ_{fi} is

$$\delta_{fi} = \delta_{N'N}\sum_{\mathrm{P}}\prod_{j=1}^{N} 2p_j^0(2\pi)^3\delta^{(3)}(\vec{p}_{\mathrm{P}(j')} - \vec{p}_j)\,, \tag{1.38}$$

where the sum is over permutations P of $1,\ldots,N$. Expanding in powers of V_I, S_{fi} can be computed at the desired level of approximation[8] since the action on the asymptotic states of V_I, which is a function of ϕ_0, is explicitly known. The calculation is made efficient by exploiting Wick's theorem to write the time-ordered products as linear combinations of normal-order products, whose matrix elements are evaluated straightforwardly. Bookkeeping is further simplified

[8]The possible level of accuracy is restricted by the fact that the perturbative series is actually not convergent but only asymptotic.

by the use of Feynman diagrams, providing a graphical representation for each contribution, which is then evaluated using the Feynman rules to associate a mathematical expression to each element of the diagram. The discussion of this topic is standard and can be found in any introductory textbook on quantum field theory. As an example, in the $\lambda\phi^4$ defined by the Lagrangian

$$\mathscr{L} = \frac{1}{2}(\partial_\mu\phi)(\partial^\mu\phi) - \frac{1}{2}m^2\phi^2 + \frac{\lambda}{4!}\phi^4\,, \tag{1.39}$$

for a process with N_i incoming and N_f outgoing particles, at order n in λ one proceeds as follows:

- draw all the graphs of distinct topology with n 4-line vertices and $N_i + N_f$ external lines, i.e., terminating in a "1-line" vertex, uniquely associated with the external particles and identified by their momenta, p_j;
- count in how many equivalent ways each graph can be built by contracting the lines coming out of the 4-line vertices with each other and with the external 1-line vertices;
- to each vertex, associate a factor $i\frac{\lambda}{4!}$;
- to each internal line, associate a four-momentum q_j (having assigned an arbitrary direction for its flow along the line) and a *propagator* $\tilde{D}(q_j)$,

$$\tilde{D}(q) = \frac{i}{q^2 - m^2 + i\epsilon}\,; \tag{1.40}$$

- to the external line identified by momentum p_j, associate a factor $u(p_j) = 1$;
- impose momentum conservation at each vertex by including factors – this results in conservation of the total momentum between the initial and the final state;
- to obtain $i\mathcal{M}_{fi}$ write down all the factors above and integrate over the internal momenta not fixed by momentum conservation at the vertices.

These rules can be extended to describe also, e.g., non-Hermitian scalar fields, fermionic spin-$\frac{1}{2}$ fields, or bosonic spin-1 (vector) fields.

Ultraviolet divergences A major practical complication in the development of the perturbative approach to canonical quantisation is the appearance of divergences in the matrix elements of Eq. (1.37). These are related to the singular nature of products of quantum fields at identical spacetime points, leading to short distance singularities in the vacuum expectation values of fields at different points. The matrix elements of Eq. (1.37) can be obtained from the n-point Green's functions of the fully interacting field,

$$G_n(x_1, \ldots, x_n) \equiv \langle 0|\, \mathrm{T}\{\phi(x_1)\ldots\phi(x_n)\}\, |0\rangle\,, \tag{1.41}$$

by means of suitable reduction formulas. It is practically more convenient to use their momentum space version ($p_{\rm tot} = \sum_{j=1}^n p_j$),

$$(2\pi)^4\delta^{(4)}\,(p_{\rm tot})\,\tilde{G}_n(p_1, \ldots, p_n) \equiv \int d^4x_1\, e^{ip_1\cdot x_1} \ldots \int d^4x_n\, e^{ip_n\cdot x_n}\, G_n(x_1, \ldots, x_n)\,, \tag{1.42}$$

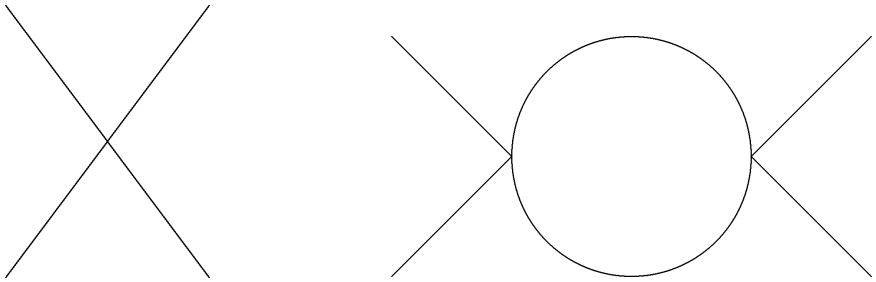

Figure 1: Lowest-order perturbative contributions to the four-point function in scalar ϕ^4 theory.

where the Dirac delta originates in the translation invariance of the theory. The $\tilde{G}_n$ can be computed systematically by means of Feynman diagrams. Beyond lowest order, these are plagued by divergences originating from the large-momentum behaviour of the momentum integrals corresponding to internal loops. In scalar $\lambda\phi^4$ theory, one finds for the four-point function to lowest orders $\tilde{G}_4 = \tilde{G}_4^{\text{0-loop}} + \tilde{G}_4^{\text{1-loop}}$, with (see Fig. 1)

$$\begin{aligned} &\tilde{G}^{\text{0-loop}} = i\lambda\,, \\ &\tilde{G}^{\text{1-loop}} \propto \lambda^2 \int^{\Lambda} \frac{d^4q}{(2\pi)^4} \frac{1}{q^2+m^2-i\epsilon} \frac{1}{(p-q)^2+m^2-i\epsilon} = \lambda^2 A \log\frac{\Lambda}{\mu} + \dots\,, \end{aligned} \tag{1.43}$$

where a UV cutoff Λ has been introduced in the integral for regularisation purposes, and μ is an arbitrary scale used to make the logarithm meaningful. As the cutoff is removed by sending $\Lambda \to \infty$, $\tilde{G}^{\text{1-loop}}$ blows up logarithmically fast, while the omitted terms remain finite. Divergences are similarly found in other Green's functions. The way this is dealt with is by defining renormalised field, $\phi = Z_\phi \phi_R$, mass, $m = Z_m m_R$, and coupling, $\lambda = Z_\lambda \lambda_R$, and adjusting the renormalisation constants $Z_{\phi,m,\lambda}$ in order to reabsorb the divergences. This procedure is known as *renormalisation*. In the present example, one sets

$$\lambda = Z_\lambda \lambda_R = \lambda_R + i\lambda_R^2 A \log\frac{\Lambda}{\mu}\,, \tag{1.44}$$

so that to order λ_R^2 in the renormalised coupling one finds

$$\tilde{G}_4 = i\lambda + \lambda^2 A \log\frac{\Lambda}{\mu} = i\left(\lambda_R + i\lambda_R^2 A \log\frac{\Lambda}{\mu}\right) + \lambda_R^2 A \log\frac{\Lambda}{\mu} = i\lambda_R\,. \tag{1.45}$$

Since after all the actual value of the coupling should be determined by comparison with experiments, it is the finite quantity λ_R that is experimentally determined, while the bare quantity λ is only a parameter used in the construction of the theory, with no direct physical meaning.

Renormalisation: general remarks The renormalisation procedure outlined above raises several questions, some of somewhat philosophical nature, and some much more practical. The main philosophical question is: is the renormalisation procedure justified? As a matter of fact, it tampers with the elegant canonical quantisation procedure, and one may feel that it spoils it. Redefining the parameters of the theory by an infinite amount and hiding this behind the unobservability of the bare parameters sounds dodgy. These concerns are, however, not justified.

First of all, the canonical procedure is not written in stone, and if one has to supplement it with renormalisation, so be it. Insofar as the main features of canonical quantisation, namely the manifest locality and Poincaré symmetry of the resulting theory, are not spoiled by the procedure, one can be happy with the result. Our real purpose was never really to successfully implement the canonical procedure, but rather to obtain finite Green's functions with suitable locality and symmetry properties and build the S-matrix from them: how that is achieved in inconsequential, since after all one still needs to check against experiments if the theoretical description correctly matches Nature.

Moreover, while the redefinition of the bare parameters at first looks like nothing more than a sleight of hand, a closer look shows that is actually a constructive procedure to define the theory in a mathematically sound way, by dealing with well-defined objects at every step. The bare parameters have indeed no physical meaning, being merely quantities that appear in the intermediate, regularised step of the construction, and whose tuning to remove the ultraviolet divergences of loop diagrams reduces the sensitivity to the regulator (i.e., the UV cutoff Λ) to an acceptable $O(1/\Lambda)$ behaviour, that entirely disappears as the cutoff is removed. We return on this point in the next paragraph.

From a more practical point of view, one wonders what happens to locality and symmetries. Since locality is preserved in the intermediate, regularised step, it survives the renormalisation procedure; using suitable regularisation procedures that do not break Lorentz and translation invariance, one can show that Poincaré symmetry is enforced in the final result. On the other hand, we have provided no argument to show that the renormalisation procedure will work at every perturbative order, leading to a complete removal of divergences and to a mathematically meaningful theory. As a matter of fact, this is not always possible; we will discuss below under what conditions it is. It turns out that renormalisation properly works in the physically relevant cases.

Another aspect of renormalisation that is worth mentioning is that it is actually not a bug but a feature of the perturbative quantisation approach descibed above. In fact, Haag's theorem tells us that the interaction picture, in the terms in which we described it above, does not exists: if a field is unitarily related to a free field, then it must be a free field as well. This originates in the infinite number of degrees of freedom that appear in a quantum field theory defined in continuum Minkowski space. On the other hand, in a fully regularised setting where both a UV cutoff (e.g., in the form of a momentum cutoff) and an IR cutoff (e.g., in the form of a finite volume) are imposed, the number of degrees of freedom is large but finite and so one is basically studying quantum mechanics, where the interaction picture can be rigorously shown to exist. Problems show up when the regularisation is removed, and if that could be done smoothly then Haag's theorem tells us that we would end up with a free field theory, despite our attempts at describing interactions. The appearance of divergences requires that we suitably redefine our bare fields and parameters to obtain a finite result; the interacting field with finite Green's functions is the renormalised field ϕ_R, which is *not* unitarily related to the free field ϕ_0 used in perturbative calculations.

Renormalisation as a constructive procedure We now discuss how renormalisation is conceptually independent of the presence of divergences, and how it provides a constructive way to relate the parameters that one has to *input* in their theoretical setup, e.g., in the Lagrangian defining their theory, to the parameters describing the *output* of calculations.

For definiteness, consider a canonically quantised theory characterised by a single mass

parameter m and a single coupling parameter g, e.g., the $\lambda\phi^4$ theory of Eq. (1.39). After UV regularisation, e.g., by a momentum cutoff Λ, the coordiante and momentum space Green's functions of the regularised theory have generally the following functional dependence,

$$G = G(x; m, g; \Lambda)\,, \qquad \tilde{G} = \tilde{G}(p; m, g; \Lambda)\,, \tag{1.46}$$

where x and p denote collectively the various coordinates and momenta. At low energies ($|\vec{p}| \ll \Lambda$), $\tilde{G}$ displays Lorentz invariance to a good approximation; correspondingly, G displays Lorentz invariance except at very short distances $|\Delta\vec{x}| \ll 1/\Lambda$. At large negative or positive times, the coordinate space Green's functions should be well approximated by free Green's functions,[9] describing the propagation of free particle. In particular, for the two-point function one expects

$$G_2(x_1, x_2; m, g; \Lambda) \underset{x^0_{1,2}\to\mp\infty}{\to} Z_\phi D_{\rm free}(x_1 - x_2; m_{\rm phys}, g_{\rm phys})\,, \tag{1.47}$$

with $D_{\rm free}$ the usual free (and cutoff-independent) propagator, with Fourier transform

$$\tilde{D}_{\rm free}(p; m_{\rm phys}, g_{\rm phys}) = \frac{i}{p^2 - m^2_{\rm phys} + i\epsilon}\,. \tag{1.48}$$

Here $m_{\rm phys}$ denotes the physical mass of the particles that the theory describes, and $g_{\rm phys}$ the physical value of the coupling obtained from the theory; both should eventually be matched with their experimental values (see below for $g_{\rm phys}$). A factor Z_ϕ has been included to account for the fact that the interacting field, when acting on the vacuum, can generate more than simply one-particle states, differently from a free field.

In general, there is no reason why the input parameters m and g should equal the output quantities $m_{\rm phys}$ and $g_{\rm phys}$: what is the mass of the particles described by the theory at asymptotic times is for the theory to decide, after all interactions are taken into account; the same applies to the strength of the interactions as can be inferred from, e.g., scattering cross sections. In fact, one can (arbitrarily, but reasonably) define $g_{\rm phys}$ from the low-energy limit of the $2 \to 2$ elastic scattering amplitude $\mathcal{M}_{2\to2}$ as $g_{\rm phys} = \mathcal{M}_{2\to2}(\vec{p}_i = 0)$, which in turn is related to the low-energy limit of the four-point Green's function G_4 via a reduction formula,

$$\begin{aligned}
&i\mathcal{M}_{2\to2}(p'_1, p'_2, p_1, p_2) \\
&= \frac{1}{Z^4_\phi} \int d^4x_1\, e^{ip'_1\cdot x_1}(\Box_{x_1} + m^2_{\rm phys}) \int d^4x_2\, e^{ip'_2\cdot x_2}(\Box_{x_2} + m^2_{\rm phys}) \\
&\quad \times \int d^4x_3\, e^{-ip_1\cdot x_3}(\Box_{x_3} + m^2_{\rm phys}) \int d^4x_4\, e^{-ip_2\cdot x_4}(\Box_{x_4} + m^2_{\rm phys}) G_4(x_1, x_2, x_3, x_4) \\
&= \lim_{\substack{p_i^2\to m^2_{\rm phys} \\ p_i'^2\to m^2_{\rm phys}}} \frac{1}{Z^4_\phi}(p'^2_1 - m^2_{\rm phys})(p'^2_2 - m^2_{\rm phys})(p^2_1 - m^2_{\rm phys})(p^2_2 - m^2_{\rm phys})\tilde{G}_4(p_1, p_2, p_3, p_4)
\end{aligned} \tag{1.49}$$

Generally, with this definition of physical coupling one has $g_{\rm phys} = g$ to lowest perturbative order, but things change at higher order.

In conclusion, one generally finds $m \neq m_{\rm phys}$ and $g \neq g_{\rm phys}$. The parameters m and g then have to be tuned in order for the physical mass and coupling to take the desired value,

[9] One should suitably smear G in space before the large time limit, corresponding to the description of localised wave packets.

i.e., one needs to invert the relations that determine $m_{\rm phys}$ and $g_{\rm phys}$ as functions of m and g, and choose their values get physical parameter matching the experimental values. This has nothing to do with divergences, and should be done even if all Green's functions were finite. What divergences do is to complicate the procedure from the technical point of view, without changing its conceptual aspect. In the regularised theory one finds

$$\begin{cases} m_{\rm phys} = f_m(m, g; \Lambda)\,, \\ g_{\rm phys} = f_g(m, g; \Lambda)\,, \end{cases} \tag{1.50}$$

but the limits $\Lambda \to \infty$ do not exist. Nonetheless, if the theory is renormalisable one can tune the mass parameter $m = m(\Lambda) = Z_m(\Lambda) m_R$, and the coupling parameter $g = g(\Lambda) = Z_g(\Lambda) g_R$, where m_R and g_R are finite and cutoff-independent, so that the limits

$$\begin{cases} m_{\rm phys} = f_m(Z_m(\Lambda)m_R, Z_g(\Lambda)g_R; \Lambda) \underset{\Lambda\to\infty}{\to} f_m^{(R)}(m_R, g_R)\,, \\ g_{\rm phys} = f_g(Z_m(\Lambda)m_R, Z_g(\Lambda)g_R; \Lambda) \underset{\Lambda\to\infty}{\to} f_g^{(R)}(m_R, g_R)\,, \end{cases} \tag{1.51}$$

are finite. Equation (1.51) can be inverted to give the renormalised parameters as a function of the physical ones,

$$\begin{cases} m_R = F_m^{(R)}(m_{\rm phys}, g_{\rm phys})\,, \\ g_R = F_g^{(R)}(m_{\rm phys}, g_{\rm phys})\,, \end{cases} \tag{1.52}$$

and so in order to obtain a finite theory with prescribed physical mass and coupling one needs to tune the mass and coupling parameters of the theory through

$$\begin{cases} m = m(\Lambda) = Z_m(\Lambda) F_m^{(R)}(m_{\rm phys}, g_{\rm phys})\,, \\ g = g(\Lambda) = Z_g(\Lambda) F_g^{(R)}(m_{\rm phys}, g_{\rm phys})\,. \end{cases} \tag{1.53}$$

The choice of m_R and g_R is arbitrary, since one could always include a further finite factor in the $Z_{m,g}(\Lambda)$ that does not alter the fact that they remove the UV divergences of the regulated Green's functions. One can set $m_R = m_{\rm phys}$ and $g_R = g_{\rm phys}$, but this is neither mandatory, nor always the most convenient choice. The arbitrariness in the choice of the renormalised parameters can in fact be turned to one's advantage: for example, it allows one to improve the accuracy of the perturbative series, and to study the behaviour of the momentum-space Green's functions under a common scaling of the momenta.

As a concrete example, one can write the full propagator of the interacting theory, i.e., $\tilde{G}_2$, as

$$\tilde{G}_2(p) = \frac{i}{p^2 - m^2 - \Sigma(p^2) + i\epsilon}\,, \tag{1.54}$$

where $\Sigma(p^2)$ denotes the sum of all the one-particle irreducible diagrams with two external lines, with the external lines removed ("amputated"). For p^2 close to $m^2_{\rm phys}$, Eq. (1.48) tells us that we must find a pole,

$$\tilde{G}_2(p) \underset{p^2\to m^2_{\rm phys}}{\to} \frac{iZ_\phi}{p^2 - m^2_{\rm phys} + i\epsilon}\,, \tag{1.55}$$

for some residue Z_ϕ. This depends on the normalisation of the field [see Eq. (1.47)], can be changed by rescaling the field,[10] and is any case removed in S-matrix elements [see (1.49)], so it does not affect physical predictions. The general properties of a renormalisable theory tell us (see below) that divergences must be polynomial in momenta and masses, and polynomial or logarithmic in the cutoff. It follows that the denominator in Eq. (1.54) must take the form

$$p^2 - m^2 - \Sigma(p^2) = (d_1 - D_1)\left\{p^2 - [(d_2 - D_2)m^2 - D_3 - d_3] - F_R(p^2)\right\}\,, \tag{1.56}$$

where $D_{1,2}$ are divergent functions of $\log\Lambda$, D_3 diverges proportionally to Λ^2, and $d_{1,2,3}$ and F are finite quantities. Clearly, one can change the values of $d_{1,2,3}$ compensating it with a change in F_R. This depends on the actual renormalisation scheme employed to take care of divergences. One then sets

$$p^2 - m^2 - \Sigma(p^2) = Z_1^{-1}[(p^2 - m_R^2) - F_R(p^2)]\,, \tag{1.57}$$

where

$$Z_1^{-1} = (d_1 - D_1)\,, \qquad m_R^2 = \{(d_2 - D_2)m^2 - D_3 - d_3\}\,, \tag{1.58}$$

to find

$$\tilde{G}_2(p) = \frac{iZ_1}{p^2 - m_R^2 - F(p^2) + i\epsilon}\,. \tag{1.59}$$

Comparison with Eq. (1.55) shows that

$$m^2_{\rm phys} - m_R^2 - F_R(m^2_{\rm phys}) = 0\,, \qquad -\frac{d}{dp^2}F_R(p^2)\Big|_{p^2=m^2_{\rm phys}} = Z_1 Z_\phi^{-1}\,. \tag{1.60}$$

For the "physical" renormalisation choice, $m_R = m_{\rm phys}$ and $Z_\phi = Z_1$, one finds

$$F_R^{\rm phys}(m^2_{\rm phys}) = 0\,, \qquad -\frac{d}{dp^2}F_R^{\rm phys}(p^2)\Big|_{p^2=m^2_{\rm phys}} = 1\,. \tag{1.61}$$

In general, setting $m_R^2 = z_m m^2_{\rm phys}$ and $z_1 = Z_1 Z_\phi^{-1}$, renormalisation schemes are parameterised by the values of

$$1 - \frac{F_R(m^2_{\rm phys})}{m^2_{\rm phys}} = z_m\,, \qquad -\frac{d}{dp^2}F_R(p^2)\Big|_{p^2=m^2_{\rm phys}} = z_1\,. \tag{1.62}$$

In practice, it is more convenient to prescribe the values of $F_R(p^2)$ and $F_R'(p^2)$, i.e., the renormalisation *scheme*, at an arbitrarily chosen mass scale μ, i.e., the renormalisation *scale*. A similar procedure is carried out for the coupling constant renormalisation by studying the four-point function. Varying the scale for a fixed renormalisation scheme one obtains *running* mass and coupling constants, with μ dependence determined in an essential way by the structure of the theory, and by the choice of renormalisation scheme for the finer details.

[10] We are implicitly considering a Lagrangian with a redundant coupling that can be reabsorbed in a redefinition of the field and other couplings. For the $\lambda\phi^4$ theory, one has in general

$$\mathscr{L} = \frac{Z}{2}(\partial_\mu\phi')(\partial^\mu\phi') - \frac{1}{2}m'^2\phi'^2 + \frac{\lambda'}{4!}\phi'^4\,,$$

that can be put in the form Eq. (1.39) by reabsorbing Z in a redefinition of the field, $\phi = Z^{\frac{1}{2}}\phi'$, and setting $m^2 = Z^{-1}m'^2$ and $\lambda = Z^{-2}\lambda'$. This allows for an arbitrary choice of normalisation of the field for what concerns the one-particle matrix elements $\langle 0|\phi(0)|p\rangle$.

Renormalisation and symmetries The need for a regulator in order to quantised a classical theory in a mathematically meaningful way leads to break one or more of the symmetries of the classical Lagrangian. For example, a momentum cutoff breaks Lorentz symmetry, as well as local, gauge symmetries. Replacing continuum Minkowski space with a discrete lattice breaks both Lorentz and translation symmetry, but gauge symmetries can be preserved, together with discrete subgroups of the Poincaré group. Making sure that the desired symmetries spoiled by regulator are recovered after renormalisation is a hard task, so it is better not to spoil them in the first place, as much as possible. Still, it may be impossible to find a regulator that does not break all the symmetries that one wants: in this case one has to check the effects of one's renormalisation procedure on the symmetries of interest, and it can happen that some of these symmetries are not recovered in the end. In this case one speaks of an *anomalously broken symmetry*.

Dimensional regularisation and minimal subtraction For a perturbative approach, the most convenient regularisation is dimensional regularisation, that basically amounts to changing the dimension of spacetime form 4 to d. This preserves Poincaré symmetry and gauge symmetries (but spoils the internal chiral symmetry of massless fermions). The cutoff in this approach is the dimensionless parameter $\varepsilon = 4 - d$, measuring the deviation from the physical case of 4 dimensions. Divergences in the perturbative series show up as poles in ε, corresponding to the logarithmic divergences of more physical regularisation schemes; power divergences are absent. Moreover, divergences are independent of the mass parameters of the theory. Dimensional regularisation is often paired with the minimal subtraction scheme (MS), where only the poles in ε are included in the renormalisation constants, or with the modified minimal subtraction scheme ($\bar{\text{MS}}$) where a recurringly appearing constant is also subtracted. Renormalisation of coupling and mass then takes the general form

$$g = \mu^{c\varepsilon} Z_g(g_R, \varepsilon) g_R \qquad m = Z_m(g_R, \varepsilon) m_R \tag{1.63}$$

where μ is an arbitrary mass scale. Its appearance is due to the fact that if the mass dimension of the coupling is $[g] = 0$ in $d = 4$, then it must be of the form $[g] = c\varepsilon$ in dimension d near 4, with c depending on the details of the theory; μ is then required to restore the correct mass dimension. At fixed values of the physical coupling and masses g_{phys}, m_{phys}, the bare parameters g, m depend on ε but not on μ,

$$g = g(\varepsilon; g_{\text{phys}}, m_{\text{phys}}) \qquad m = m(\varepsilon; g_{\text{phys}}, m_{\text{phys}})\,. \tag{1.64}$$

It follows that g_R and m_R must depend on μ, $g_R(\mu)$, $m_R(\mu)$, with μ dependence determined by the renormalisation group equations

$$\mu \frac{dg}{d\mu} = 0 \qquad \mu \frac{dm}{d\mu} = 0\,. \tag{1.65}$$

Path integral quantisation An alternative quantisation procedure, in most cases perturbatively equivalent to canonical quantisation, is path integral quantisation. This is based on the (formally defined) integration over the space of field configurations. The following generating functional,

$$Z[J] = \int \mathrm{D}\phi\, e^{i\int d^4x(\mathcal{L}[\phi] + J\phi)} = \int \mathrm{D}\phi\, e^{iS[\phi] + iJ\cdot\phi}\,, \qquad \mathrm{D}\phi = \prod_x d\phi(x)\,, \tag{1.66}$$

allows one to obtain the Green's functions of the theory by functional differentiation, e.g.,

$$\begin{aligned} -i\frac{\delta \log Z[J]}{\delta J(x)}\bigg|_{J=0} &= \langle\phi(x)\rangle = \langle 0|\hat{\phi}(x)|0\rangle\,, \\ (-i)^2\frac{\delta^2 \log Z[J]}{\delta J(x)\delta J(y)}\bigg|_{J=0} &= \langle\phi(x)\phi(y)\rangle - \langle\phi(x)\rangle\langle\phi(y)\rangle \\ &= \langle 0|T\big\{\hat{\phi}(x)\hat{\phi}(y)\big\}|0\rangle - \langle 0|\hat{\phi}(x)|0\rangle\langle 0|\hat{\phi}(y)|0\rangle\,, \end{aligned} \tag{1.67}$$

where a caret is used again to distinguish field operators and c-number integration variables. Path integrals are ill-defined objects, and the measure $\mathrm{D}\phi$ needs to be regularised. Except for Gaussian integrals and other simple cases, path integrals cannot be computed in closed form. A perturbative approach, on the other hand, can be set up straighforwardly, and even more simply than for canonical quantisation; of course, it still needs regularisation and renormalisation, as in canonical procedure. The main advantages of path-integral quantisation are that it is more intuitive to deal with, and that allows for non-perturbative approaches based on its discretisation on a spacetime lattice, which (in the Euclidean formulation of quantum field theory) is amenable to direct numerical simulations.

Renormalisation to all orders We now discuss under how renormalisation generally proceeds to all orders in perturbation theory. To this end, consider the most general theory of a real scalar field, defined by a Lagrangian

$$\mathscr{L}(\phi; m; g) = \frac{1}{2}(\partial_\mu\phi)(\partial^\mu\phi) - \frac{1}{2}m^2\phi^2 + \sum_i g_i V_i(\phi, \partial\phi)\,, \tag{1.68}$$

with vertices V_i of schematic form $V_i = \partial_\mu^{k_i}\phi^{n_i}$, i.e., involving n_i fields and k_i derivatives, and associated coupling constant g_i. Using path-integral quantisation and a perturbative approach, one first defines the renormalised quantities

$$\phi = Z_\phi^{\frac{1}{2}}\phi_R\,, \qquad m^2 = Z_m m_R^2\,, \qquad g_i = Z_{g_i} g_{iR}\,, \tag{1.69}$$

and splits the Lagrangian into two parts,

$$\begin{aligned} \mathscr{L}(\phi; m; g) &= \mathscr{L}(\phi_R; m_R; g_R) + \delta\mathscr{L}(\phi_R; m_R; g_R)\,, \\ \delta\mathscr{L}(\phi_R; m_R; g_R) &= (Z_\phi - 1)\frac{1}{2}(\partial_\mu\phi_R)(\partial^\mu\phi_R) - (Z_\phi Z_m - 1)\frac{1}{2}m_R^2\phi_R^2 \\ &\quad + \sum_i \left(Z_{g_i} Z_\phi^{\frac{n_i}{2}} - 1\right) g_{iR} V_i(\phi_R, \partial\phi_R)\,. \end{aligned} \tag{1.70}$$

The quantity $\delta\mathscr{L}$ is called the counterterm Lagrangian. It is a general property of perturbatively quantised local quantum field theories that the new divergences that appear in Feynman diagrams at a given perturbative order must be polynomial in m and in the external momenta q. This basically follows from the fact that taking derivatives with respect to m or q one increases the power of loop momenta appearing in the denominator of the diagrams. An example is provided by the following 1-loop integral,

$$\begin{aligned} I &= \int \frac{d^4p}{(2\pi)^4}\frac{1}{(p+q)^2 - m^2 + i\epsilon}\frac{1}{p^2 - m^2 + i\epsilon} \sim \log\Lambda \\ \frac{dI}{dq_\mu} &= \int \frac{d^4p}{(2\pi)^4}\frac{-2(p+q)_\mu}{[(p+q)^2 - m^2 + i\epsilon]^2}\frac{1}{p^2 - m^2 + i\epsilon} = \text{finite}\,. \end{aligned} \tag{1.71}$$

This implies that UV divergences have the same structure as the contribution of the local vertices $V_i(\phi_R, \partial\phi_R)$, or of the kinetic terms $(\partial\phi_R)^2$ and $m_R^2\phi_R^2$, but with divergent coefficients δZ_i, or δZ_ϕ, or δZ_m. This means that by choosing

$$Z_\phi - 1 = \delta Z_\phi \,, \qquad Z_\phi Z_m - 1 = \delta Z_m \,, \qquad Z_{g_i} Z_\phi^{\frac{n_i}{2}} - 1 = \delta Z_i \,, \tag{1.72}$$

one cancels the divergences entirely. Clearly, if the local vertex corresponding to a divergence was not originally present in the Lagrangian, it must be added.

It should be specified more clearly what is meant above by "new divergences" at a given perturbative order. In general, divergences appear in a Feynman diagram when the corresponding integral over the momenta of internal lines is not convergent at large momenta. Divergences are of two general types:

- an *overall divergence* is present in a diagram if the integral is not covergent in the momentum region corresponding to scaling all internal momenta as $p_i \to \kappa p_i$ and sending $\kappa \to \infty$;
- a *subdivergence* is present if the integral is not convergent in the momentum region corresponding to again scaling $p_i \to \kappa p_i$ and sending $\kappa \to \infty$, but keeping certain linear combination Δp of momenta fixed.

Other possible large-momentum limits (e.g., rescaling $p_i \to \kappa_i p_i$ with different κ_i) can be reduced to the two cases above. A diagram may have an overall divergence with one or more subdivergences, or without any; or one or more subdivergences, but no overall divergence. When increasing the perturbative order (at fixed number of external lines), the overall divergences one may find are certainly new, given the larger number of internal momenta over which one integrates. For an overall divergence, since no combination Δp is kept fixed, one always makes the integrand better behaved at large momenta by taking derivatives with respect to masses and/or external momenta. The general form of the integrand is in fact

$$\mathcal{I}(p) = P(p) \prod_i \frac{1}{(p_i + q_i)^2 - m^2 + i\epsilon} \prod_j \frac{1}{(p_j + \Delta q_j)^2 - m^2 + i\epsilon} \,, \tag{1.73}$$

where Δq_j are linear combinations of the external momenta q_j and $P(p)$ is some polynomial of the internal momenta (the dependence on external momenta q is irrelevant here). Taking derivatives one finds qualitatively

$$\frac{\partial \mathcal{I}(p)}{\partial q_\mu} \sim \frac{p_\mu \mathcal{I}(p)}{p^2} \,, \qquad \frac{\partial \mathcal{I}(p)}{\partial m} \sim \frac{m \mathcal{I}(p)}{p^2} \,, \tag{1.74}$$

and so an improved convergence rate. This may not be the case when certain combinations Δp of internal momenta are kept fixed, since an extra power of Δp in the denominator does nothing for the convergence rate. The consequence is that taking sufficient many derivatives the integral is made convergent, implying that the overall divergence is *local*, i.e., polynomial in q_μ (or equivalently in ∂_μ in coordinate space) and in m. This implies that these divergent contributions have the same mass and momentum dependence as contribution originating from the insertion of a vertex corresponding to a local operator, and so can be cancelled by subtracting the divergent prefactor from the coefficient of this operator in the counterterm Lagrangian. This is done order

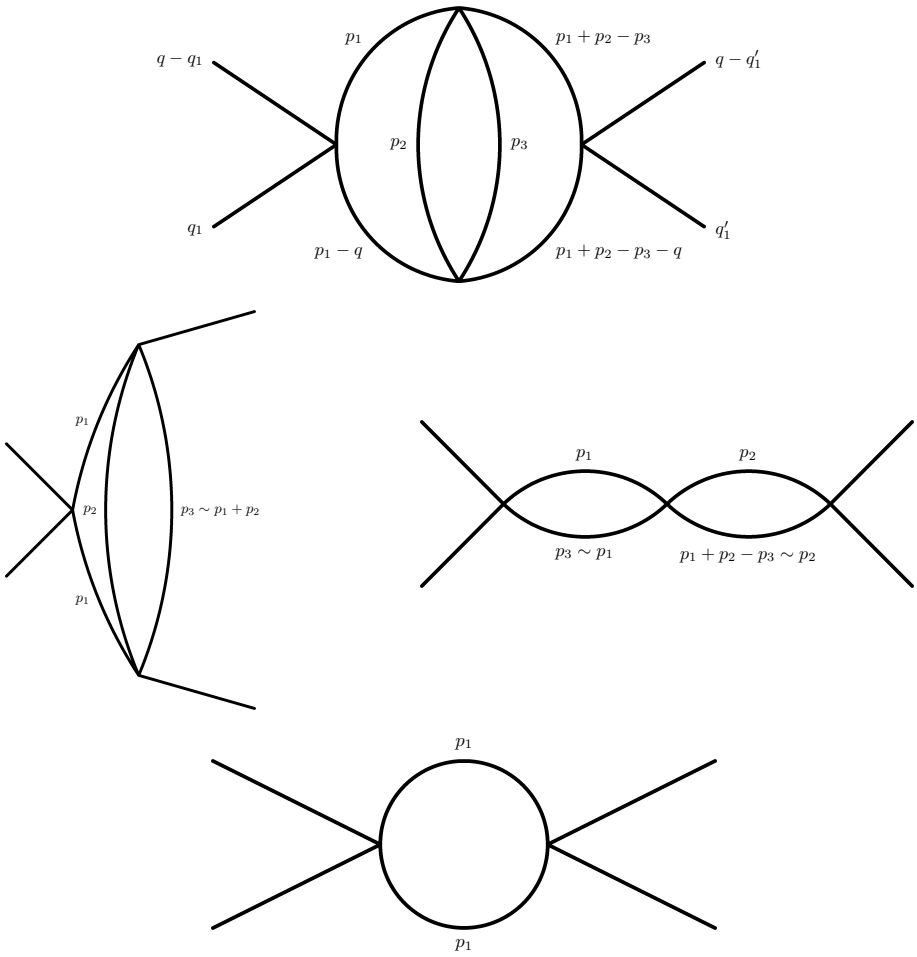

Figure 2: A three-loop diagram in scalar $\lambda\phi^4$ theory, and the two-loop and one-loop diagrams corresponding to its subdivergences.

by order in perturbation theory, so that at the next order the divergence subtracted here will appear contribute to the prefactor of the corresponding vertex in the counterterm Lagrangian.

An example from scalar $\lambda\phi^4$ theory is shown in Fig. 2. When the internal momenta $p_{1,2,3}$ all become large without any combination kept fixed, one studies the overall divergence of the diagram. When the combination $p_1 + p_2 - p_3$ is kept fixed, one finds the same divergence as in the 2-loop diagram at the centre left: one has $p_3 \sim p_1 + p_2$, while the lines with momentum $p_1 + p_2 - p_3$ and $p_1 + p_2 - p_3 - q$ do not affect the convergence rate. If instead $p_1 - p_3$ is kept fixed, then the divergence is the same as that of the diagram at the centre right; the same holds if $p_2 - p_3$ is kept fixed, up to relabelling $p_1 \leftrightarrow p_2$. If besides $p_1 + p_2 - p_3$ also the combination $p_1 + p_2$ is kept fixed, then one finds the same divergence as in the 1-loop diagram at the bottom, since $p_3 \sim 0$ and $p_1 \sim -p_2$.

It is a matter of combinatorics to show that at each perturbative order, subdivergences are

fully removed by the counterterms, as determined by the subtractions performed up to the previous perturbative order. As pointed out above, new divergences are necessarily local, and so can be cured by a suitable redefinition of the coupling constant of a local term in the counterterm Lagrangian. The renormalised value of the couplings are kept finite, and can in principle be fixed by matching with experimental results. What could possibly go wrong is that the number of terms in $\delta\mathscr{L}$ increases indefinitely as the perturbative order increases, so that an infinite amount of experiments is required to fully determine the theory, which is then never fully predictive.[11]

Renormalisability of a theory We now briefly discuss under what conditions is the renormalisation procedure going to succeed to all orders in perturbation theory, by redefining a *finite* number of bare coouplings. There is a simple power counting criterion for this, based on the mass dimension of the couplings in the Lagrangian. Given a diagram G, its mass dimension is determined as follows. Each internal bosonic or fermionic line contributes a factor of order $p^{-d_{B,F}}$ from the corresponding propagator, and an integration measure d^4p. Usually $d_B = 2$ and $d_F = 1$, but there are exceptions. Each vertex contributes a momentum-conserving delta function; one of these is factored out to enforce overall momentum conservation of the diagram, and does not effectively enter the counting. Moreover, the i-th type of vertex, of schematic form $\mathcal{V}_i = \partial_\mu^{k_i}\phi^{n_{Bi}}\bar{\psi}^{\bar{o}_{Fi}}\psi^{n_{Fi}-\bar{o}_{Fi}}$, contributes a further factor p^{k_i}. All in all, the mass dimension D_G of the diagram is

$$D_G = (4-d_B)I_B + (4-d_F)I_F + 4 - 4\sum_i V_i + \sum_i V_i k_i \,. \tag{1.75}$$

This is the superficial degree of divergence of the diagram, expected by simple power counting, and corresponding to an overall divergence. If a diagram diverges with the UV cutoff Λ as Λ^{ω_G}, we call ω_G the degree of divergence of the diagram. This may be lower than the superficial one due to cancellations, so in general $\omega_G \leq D_G$. It is worth noticing that the mass dimension of the coupling g_i, corresponding to the vertex $\mathcal{V}_i$, reads

$$d_{g_i} = 4 - k_i - n_{Bi} - \frac{3}{2}n_{Fi} < 4\,, \tag{1.76}$$

where the upper bound comes from the fact that there are no local operators of negative mass dimension in $d = 4$; and that the only operator of dimension 0 is an uninteresting numerical constant. Exploiting now the well known topological relations between the number of internal and external lines and the number of vertices,

$$E_{B,F} + 2I_{B,F} = \sum_i V_i n_{B,Fi}\,, \tag{1.77}$$

one finds that

$$\begin{aligned} D_G &= \tfrac{4-d_B}{2}\left(\textstyle\sum_i V_i n_{Bi} - E_B\right) + \tfrac{4-d_F}{2}\left(\textstyle\sum_i V_i n_{Fi} - E_F\right) + 4 - 4\textstyle\sum_i V_i + \sum_i V_i k_i \\ &= 4 - \tfrac{4-d_B}{2}E_B - \tfrac{4-d_F}{2}E_F + \textstyle\sum_i V_i\left(k_i - 4 + \tfrac{4-d_B}{2}n_{Bi} + \tfrac{4-d_F}{2}n_{Fi}\right) \\ &= f(E_B, E_F) + \sum_i V_i\left[k_i - f(n_{Bi}, n_{Fi})\right]\,, \end{aligned} \tag{1.78}$$

[11] Since operators of higher dimension are suppressed by increasing inverse powers of a mass M, the theory renormalised at a given order n will be predictive up to energies E where the order $n+1$ term, of magnitude proportional to $(E/M)^{c(n+1)}$, becomes comparable with the order n term, of magnitude $(E/M)^{cn}$.

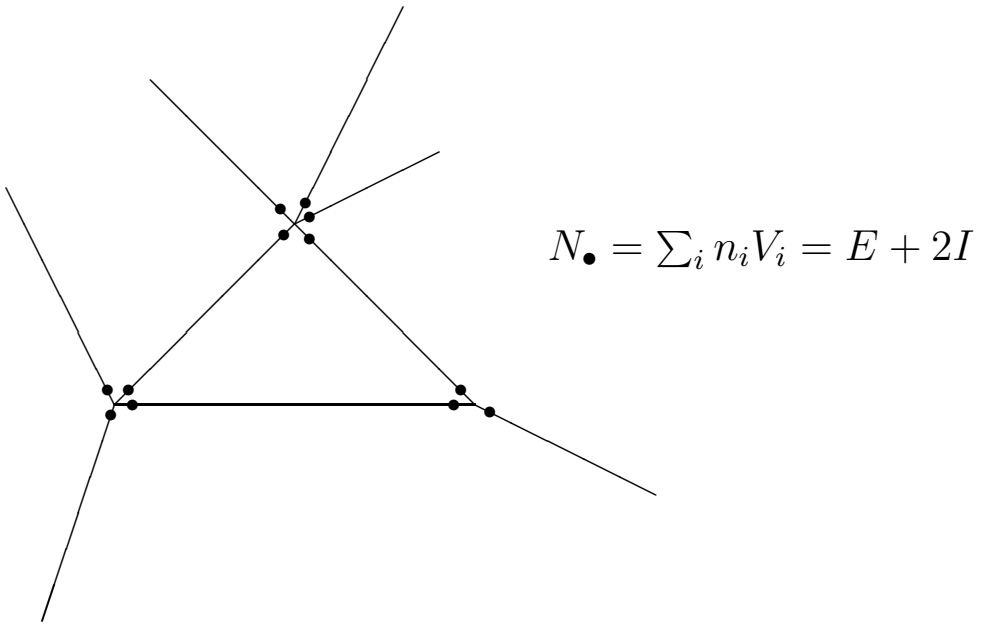

Figure 3: Derivation of the topological relations, Eq. (1.77). Dots can be counted in two ways: as a property of vertices, or as a property of internal and external lines.

where

$$f(n_B, n_F) = 4 - \frac{4 - d_B}{2} n_B - \frac{4 - d_F}{2} n_F \,, \tag{1.79}$$

which is a decreasing function of $n_{B,F}$. If every vertex in the Lagrangian satisfies

$$k_i \leq f(n_{Bi}, n_{Fi}) \,, \tag{1.80}$$

then $\omega_G \leq f(E_B, E_F)$. If *all* vertices satisfying $k_i \leq f(n_{Bi}, n_{Fi})$ have been included in $\mathscr{L}$, then the divergence in G must be of the same form of one of those vertices, and can be renormalised away by redefining the corresponding coupling. As the number of fields increases, the requirement on the number of derivatives becomes more stringent, until eventually no derivatives are allowed. For terms without derivatives $f(n_{Bi}, n_{Fi}) \geq 0$, so the possible choice of number of fields is finite. In summary, the number of possible vertices satisfying $k_i \leq f(n_{Bi}, n_{Fi})$ is finite, and if they are all included in the Lagrangian, then all divergences can be removed by renormalisation as outlined above, and the theory is said to be a *renormalisable by power counting*.

On the other hand, if for some vertex $\bar{\imath}$ one has $k_{\bar{\imath}} > f(n_{B\bar{\imath}}, n_{F\bar{\imath}})$, then increasing the number $V_{\bar{\imath}}$ of vertices of this type any ω_G becoms possible, and in general new types of vertices need to be included in the Lagrangian at each perturbative order. In this case the theory is said to be *non-renormalisable by power counting*.

Using Eq. (1.76), the inequality Eq. (1.80) can be recast as follows,

$$\frac{2 - d_B}{2} n_{Bi} + \frac{1 - d_F}{2} n_{Fi} \leq 4 - k_i - n_{Bi} - \frac{3}{2} n_{Fi} = d_{g_i} \,. \tag{1.81}$$

In the standard case $d_B = 2$, $d_F = 1$, one finds that Eq. (1.80) boils down to $d_g \geq 0$, i.e., all coupling must have non-negative mass dimension.

Examples of renormalisable and non-renormalisable theories

Scalar field For a real scalar field ϕ one can write for the most general interaction Lagrangian

$$V(\phi) = \sum g_{n,\{m_i\}} T^{\mu_{1,1}\cdots\mu_{n,m_n}} \prod_{i=1}^{n} \Big(\prod_{j=1}^{m_i} \partial_{\mu_{i,j}} \Big) \phi \,, \qquad d_{g_{n,\{m_i\}}} = 4 - \sum_{i=1}^{n} (1 + m_i) \,, \tag{1.82}$$

for some Lorentz-invariant tensor $T^{\mu_{1,1}\cdots\mu_{n,m_n}}$ (which can only be built out of the metric tensor and the Levi-Civita tensor). Positivity of the mass dimension requires no more than four fields; Lorentz invariance imposes that zero or two derivatives appear. Terms with two derivatives have at most two fields: those with two fields are identical to the derivative term in the kinetic part (up to a total derivative), and the term with one field is total derivative. The most general renormalisable Lagrangian is then of the form (up to field renormalisation)

$$\mathcal{L} = \frac{1}{2} \partial_\mu \phi \partial^\mu \phi - \frac{1}{2} m^2 \phi^2 + h\phi + \frac{c}{3!} \phi^3 + \frac{\lambda}{4!} \phi^4 \,. \tag{1.83}$$

If $h = c = 0$, the appearance of counterterms odd in ϕ is forbidden by the symmetry $\phi \to -\phi$. On the otehr hand, if $h = 0$, $c \neq 0$ (resp. $h \neq 0$, $c = 0$) a counterterm linear (resp. cubic) in ϕ can (almost certainly will) be generated by the renormalisation procedure.

Fermi theory For the most general four-fermion interaction Lagrangian,

$$\mathscr{L}_I = \sum_i G_i (\bar{\psi} \Gamma_A \psi)(\bar{\psi} \Gamma^A \psi) \,, \tag{1.84}$$

with $\{\Gamma_A\}$ a basis for 4×4 Hermitian matrices, the theory is non-renormalisable by power counting since $d_{G_i} = 4 - 4\frac{3}{2} = -2$.

Proca field The free propagator for a massive vector field (Proca field) A^μ reads

$$D^{\text{Proca}}_{\mu\nu}(p) = \frac{-i(\eta_{\mu\nu} - \frac{p_\mu p_\nu}{m^2})}{p^2 - m^2 + i\epsilon} \,, \tag{1.85}$$

so that $d_B = 0$, and the constraint for renormalisability reads $n_B \leq d_g < 4$. Renormalisable terms are:

- $n_B = 1$ terms complying with Lorentz invariance are either $\partial_\mu A^\mu$ and $\Box \partial_\mu A^\mu$, which are total derivatives (and in the second case $d_g = 0 \leq 1$ forbids it); or the coupling to a vector current, $J_\mu A^\mu$, with $d_J = 3 > 1$;
- $n_B = 2$ terms are limited by Lorentz invariance to $(\partial_\mu A^\mu)^2$, $\partial_\mu A_\nu \partial^\nu A^\mu$, $A_\nu \partial_\mu \partial^\nu A^\mu$, and $\Box A_\mu A^\mu$, but in this case $d_g = 0 \leq 2$ (naively) forbids them; and a mass term $A_\mu A^\mu$ with $d_g = 2$;
- $n_B = 3$ requires one derivative for Lorentz invariance, so possible terms are $g(\partial_\mu A^\nu) A_\nu A^\mu$ and $g(\partial_\mu A^\mu) A_\nu A^\nu$, but $d_g = 0 < 3 = n_B$ and so they are forbidden.

No renormalisable self-interaction exists for the Proca field.

Renormalised perturbation theory in the canonical formalism - back from the start∗
We started from the canonical quantisation of a theory, ran into troubles, and found that renormalisation can fix them. It may help clarify the procedure if we go back to the start having in mind that regularisation of the theory and a suitable redefinition of the parameters is going to be needed.

Instead of claiming that we are solving directly the theory defined by some Hamiltonian $H[\phi,\pi]$ for canonically conjugate field variables ϕ and π obeying Hamilton equations of motion and canonical commutation relations, we start from the implicitly regularised Hamiltonian $H[\phi_B,\pi_B]$ with canonical variables ϕ_B and π_B, again obeying Hamilton equations and canonical commutation relations. Having reduced the degrees of freedom to a finite number by imposing a UV and an IR cutoff, we are just doing quantum mechanics with a large number of canonical variables. For good measure, we also switch the interaction on and off adiabatically at large times, so that $H \to H_0$ and $\phi_B(t) \to \phi_0(t)$ as $t \to \pm\infty$, where ϕ_0 is a free field with the usual normalisation. This procedure automatically kills any bound state of the theory as a possible asymptotic states, and so is suitable only if the spectrum of the theory is not radically changed by the interactions (or if this radical change can be taken into account separately.)

In this setting, the Hamiltonian is time dependent and reads

$$H(t) = H_0[\phi_B(0),\pi_B(0)] + f_\epsilon(t) H_I[\phi_B(0),\pi_B(0)]\,, \tag{1.86}$$

where the adiabatic switching factor f_ϵ is a smooth, slowly varying function such that $f_\epsilon(t) = 1$ for $|t| < T_0$, and $f_\epsilon(t) \to 0$ for $t \to \pm\infty$. Notice that both H_0 and H_I are time-independent by construction. In H_0 one should use the physical mass m of the particle, and in H_I one should include $m_B^2 - m^2 = \delta m^2$, the difference between the bare and physical mass squared, to be tuned so that particles have mass m also in the integracting theory. Similarly, one should include a vacuum energy difference E_0 in H_I, to be tuned so that the vacuum has vanishing energy (i.e., is translation invariant) also in the interacting theory:

$$H_I = \delta m^2 \phi_B^2 + E_0 + V(\phi_B)\,. \tag{1.87}$$

The temporal evolution is given by

$$\mathcal{U}(t,t') = \mathrm{Texp}\left\{-i\int_{t'}^{t} d\tau\, H(\tau)\right\} = \mathrm{Texp}\left\{-i\int_{t'}^{t} d\tau\, \left(H_0 + f_\epsilon(\tau) H_I\right)\right\}\,, \tag{1.88}$$

and reduces to $\mathcal{U}(t,t') \to e^{-iH(t-t')}$ as $\epsilon \to 0$, i.e., as the switching on/off function is removed. The Møller operators read now

$$\Omega_\pm = \lim_{t\to\mp\infty} \mathcal{U}(t,0)^\dagger e^{-iH_0[\phi_B(0),\pi_B(0)]t}\,, \tag{1.89}$$

with the free theory at asymptotic times governed by $H_0[\phi_B(0),\pi_B(0)]$. We set $\phi_0(0) = \phi_B(0)$, $\pi_0(0) = \pi_B(0)$, and define the freely-evolving variables

$$\begin{aligned}
\phi_0(t) &= e^{iH_0[\phi_B(0),\pi_B(0)]t}\phi_B(0)e^{-iH_0[\phi_B(0),\pi_B(0)]t} = e^{iH_0[\phi_0(0),\pi_0(0)]t}\phi_0(0)e^{-iH_0[\phi_0(0),\pi_0(0)]t}\,,\\
\pi_0(t) &= e^{iH_0[\phi_B(0),\pi_B(0)]t}\pi_B(0)e^{-iH_0[\phi_B(0),\pi_B(0)]t} = e^{iH_0[\phi_0(0),\pi_0(0)]t}\pi_0(0)e^{-iH_0[\phi_0(0),\pi_0(0)]t}\,.
\end{aligned} \tag{1.90}$$

Then

$$\begin{aligned}
\phi_0(t) &= e^{iH_0[\phi_0(0),\pi_0(0)]t}\mathcal{U}(t,0)\phi_B(t)\mathcal{U}(t,0)^\dagger e^{-iH_0[\phi_0(0),\pi_0(0)]t} = U(t)\phi_B(t)U(t)^\dagger\,,\\
\pi_0(t) &= e^{iH_0[\phi_0(0),\pi_0(0)]t}\mathcal{U}(t,0)\pi_B(t)\mathcal{U}(t,0)^\dagger e^{-iH_0[\phi_0(0),\pi_0(0)]t} = U(t)\pi_B(t)U(t)^\dagger\,,
\end{aligned} \tag{1.91}$$

and $U(t)$ obeys the differential equation

$$\begin{aligned}\dot{U}(t) &= ie^{iH_0[\phi_0(0),\pi_0(0)]t}\left\{H_0[\phi_0(0),\pi_0(0)] - H(t)\right\}\mathcal{U}(t,0) \\ &= -ie^{iH_0[\phi_0(0),\pi_0(0)]t}f_\epsilon(t)H_I[\phi_0(0),\pi_0(0)]e^{-iH_0[\phi_0(0),\pi_0(0)]t}U(t) \equiv -iV_I(t)U(t)\,.\end{aligned} \tag{1.92}$$

Together with $U(0) = \mathbf{1}$, this yields

$$U(t) = \mathrm{Texp}\left\{-i\int_0^t d\tau\, V_I(\tau)\right\}\,. \tag{1.93}$$

Similarly,

$$\dot{U}(t)^\dagger = U(t)^\dagger iV_I(t) \Rightarrow U(t)^\dagger = \mathrm{Texp}\left\{-i\int_t^0 d\tau\, V_I(\tau)\right\}\,, \tag{1.94}$$

and combining the two results (and using uniqueness of the solution of the Cauchy problem) on finds

$$U(t)U(t')^\dagger = \mathrm{Texp}\left\{-i\int_{t'}^t d\tau\, V_I(\tau)\right\}\,. \tag{1.95}$$

The Møller operators can be obtained by solving an equation similar to Eqs. (1.92) and (1.94). Set

$$\Omega(t) = \mathcal{U}(t,0)^\dagger e^{-iH_0t}\,, \qquad \Omega_\pm = \lim_{t\to\mp\infty}\Omega(t)\,, \tag{1.96}$$

where we denoted simply $H_0 = H_0[\phi_B(0),\pi_B(0)]$, and take its time derivative,

$$\dot{\Omega}(t) = i\mathcal{U}(t,0)^\dagger(H(t)-H_0)e^{-iH_0t} = i\mathcal{U}(t,0)^\dagger e^{-iH_0t}e^{iH_0t}(H(t)-H_0)e^{-iH_0t} = \Omega(t)iV_I(t)\,. \tag{1.97}$$

Since $\Omega(0) = \mathbf{1}$, this is solved by

$$\Omega(t) = \mathrm{Texp}\left\{-i\int_t^0 d\tau V_I(\tau)\right\} = U(t)^\dagger \Rightarrow \Omega_\pm = U(\mp\infty)^\dagger\,. \tag{1.98}$$

Then one finds for the scattering matrix S

$$S = \Omega_-^\dagger\Omega_+ = U(+\infty)U(-\infty)^\dagger = \mathrm{Texp}\left\{-i\int_{-\infty}^{+\infty} d\tau\, V_I(\tau)\right\}\,. \tag{1.99}$$

This operator acts on the Fock space of the free particles created and annihilated by ϕ_0, starting from the free vacuum $|0\rangle_0$. In particular, ${}_0\langle 0|S|0\rangle_0$ is the vacuum-to-vacuum amplitude which is necessarily a phase due to uniqueness and Poincaré invariance of $|0\rangle_0$. This phase can be set to 1 without any loss of information, in practice by dividing out by ${}_0\langle 0|S|0\rangle_0$. The scattering amplitudes are then obtained as

$$\begin{aligned}S_{fi} &= \frac{{}_0\langle\varphi_f|S|\varphi_i\rangle_0}{{}_0\langle 0|S|0\rangle_0} \\ &= \int d\Omega_{p'}^{(n')}\,\varphi_f^1(p_1')^*\ldots\varphi_f^{n'}(p_{n'}')^*\int d\Omega_p^{(n)}\,\varphi_i^1(p_1)\ldots\varphi_i^n(p_n)\frac{{}_0\langle p_1',\ldots,p_{n'}'|S|p_1,\ldots,p_n\rangle_0}{{}_0\langle 0|S|0\rangle_0}\,,\end{aligned} \tag{1.100}$$

starting from the $n \to n'$ transition amplitudes

$$\frac{{}_0\langle p'_1,\dots,p'_{n'}|S|p_1,\dots,p_n\rangle_0}{{}_0\langle 0|S|0\rangle_0} = \frac{{}_0\langle p'_1,\dots,p'_{n'}|\Omega_-^\dagger\,\Omega_+|p_1,\dots,p_n\rangle_0}{{}_0\langle 0|S|0\rangle_0} = {}_{\rm out}\langle p'_1,\dots,p'_{n'}|p_1,\dots,p_n\rangle_{\rm in}\,. \tag{1.101}$$

In Eq. (1.100) the contribution from the vacuum energy counterterm gets cancelled between numerator and denominator and so can be ignored.

A better way to discuss this point is to notice that the adiabatic switching on and off of the interaction leads the free vacuum state to new states $\Omega_\pm|0\rangle_0 = \lim_{\epsilon\to 0}\Omega^\epsilon_\pm|0\rangle_0$, where the dependence on ϵ has been made explicit. These are the interacting in and out vacuum states, that are eigenvectors of H, obeying[12]

$$\begin{aligned} H\Omega_\pm|0\rangle_0 &= \lim_{\epsilon\to 0} \pm i\epsilon g\frac{\partial}{\partial g}\Omega^\epsilon_\pm(g)|0\rangle_0\Big|_{g=1}\,,\\ \Omega^\epsilon_\pm(g) &= {\rm Texp}\left\{-ig\int_{\mp\infty}^0 d\tau\, e^{-\epsilon|\tau|}e^{iH_0\tau}H_I e^{-iH_0\tau}\right\}\\ &= e^{\mp ig\frac{E_0}{\epsilon}}{\rm Texp}\left\{-ig\int_{\mp\infty}^0 d\tau\, e^{-\epsilon|\tau|}e^{iH_0\tau}(H_I-E_0)e^{-iH_0\tau}\right\}\,. \end{aligned} \tag{1.102}$$

This result is known as *Gell-Mann–Low theorem.*[13] Since $\Omega_\pm|0\rangle_0$ is the interacting (in and out) vacuum, one must have $H\Omega_\pm|0\rangle_0 = 0$, implying ${}_0\langle 0|H\Omega_\pm|0\rangle_0 = 0$, which in turn requires

$$0 = \lim_{\epsilon\to 0}\pm i\epsilon g\frac{\partial}{\partial g}\left[e^{\mp ig\frac{E_0}{\epsilon}}{}_0\langle 0|{\rm T}e^{-ig\int_{\mp\infty}^0 d\tau\, e^{-\epsilon|\tau|}e^{iH_0\tau}(H_I-E_0)e^{-iH_0\tau}}|0\rangle_0\right]_{g=1}\,. \tag{1.103}$$

This is achieved by tuning E_0 at finite ϵ as

$$e^{\pm ig\frac{E_0}{\epsilon}} = {}_0\langle 0|{\rm T}e^{-ig\int_{\mp\infty}^0 d\tau\, e^{-\epsilon|\tau|}e^{iH_0\tau}(H_I-E_0)e^{-iH_0\tau}}|0\rangle_0\,. \tag{1.104}$$

More symmetrically,

$$\begin{aligned} 0 &= 2\,{}_0\langle 0|\Omega_-^\dagger H\Omega_+|0\rangle_0 = {}_0\langle 0|\Omega_-^\dagger(+i\epsilon g\frac{\partial}{\partial g}\Omega_+) + (-i\epsilon g\frac{\partial}{\partial g}\Omega_-)^\dagger\Omega_+|0\rangle_0\\ &= i\epsilon g\frac{\partial}{\partial g}\,{}_0\langle 0|\Omega_-^\dagger\,\Omega_+|0\rangle_0 = i\epsilon g\frac{\partial}{\partial g}\,{}_0\langle 0|S|0\rangle_0\\ &= i\epsilon g\frac{\partial}{\partial g}e^{-2ig\frac{E_0}{\epsilon}}{}_0\langle 0|{\rm T}e^{-ig\int_{\mp\infty}^0 d\tau\, e^{-\epsilon|\tau|}e^{iH_0\tau}(H_I-E_0)e^{-iH_0\tau}}|0\rangle_0\,, \end{aligned} \tag{1.105}$$

which is obtained by setting

$$e^{-2ig\frac{E_0}{\epsilon}} = \frac{1}{{}_0\langle 0|{\rm T}e^{-ig\int_{-\infty}^{+\infty} d\tau\, e^{-\epsilon|\tau|}e^{iH_0\tau}(H_I-E_0)e^{-iH_0\tau}}|0\rangle_0}\,. \tag{1.106}$$

[12] An infinite phase should be removed by dividing by ${}_0\langle 0|\Omega^\epsilon_\pm|0\rangle_0$ before taking the limit, but this does not change the argument made here.

[13] M. Gell-Mann and F. Low, "Bound states in quantum field theory", Phys. Rev. 84 (1951) 350-354. See also J. Sucher, "S-matrix formalism for level-shift calculations", Phys. Rev. 107 (1957) 1448-1449.

One can then drop E_0 from V_I and include this factor in the S-matrix calculation, which precisely cancels out the contribution of vacuum bubble diagrams from every matrix element. Notice that

$$\begin{aligned}\mathcal{U}(s,0)\Omega(t) &= e^{-iH_0 s}U(s)U(t)^\dagger = e^{-iH_0 s}\mathrm{Texp}\left\{-i\int_t^s d\tau\, e^{iH_0\tau}f_\epsilon(\tau)H_I e^{-iH_0\tau}\right\}\\ &= e^{-iH_0 s}\mathrm{Texp}\left\{-i\int_{t-s}^0 d\tau\, e^{iH_0(\tau+s)}f_\epsilon(\tau+s)H_I e^{-iH_0(\tau+s)}\right\}\\ &= e^{-iH_0 s}e^{iH_0 s}\mathrm{Texp}\left\{-i\int_{t-s}^0 d\tau\, e^{iH_0\tau}f_\epsilon(\tau+s)H_I e^{-iH_0\tau}\right\}e^{-iH_0 s}\\ &= \mathrm{Texp}\left\{-i\int_{t-s}^0 d\tau\, e^{iH_0\tau}(f_\epsilon(\tau)+s\dot f_\epsilon(\tau)+\ldots)H_I e^{-iH_0\tau}\right\}e^{-iH_0 s}\\ &= (\Omega(t-s)+\ldots)e^{-iH_0 s}\,.\end{aligned} \tag{1.107}$$

Since f_ϵ is slowly varying, its derivatives can be neglected (and vanish in the adiabatic limit), so that

$$\mathcal{U}(s,0)\Omega_\pm = \lim_{t\to\pm\infty}\mathcal{U}(s,0)\Omega(t) = \lim_{t\to\pm\infty}\Omega(t-s)e^{-iH_0 s} = \Omega_\pm e^{-iH_0 s}\,, \tag{1.108}$$

up to terms that vanish in the adiabatic limit. In this limit,

$$\begin{aligned}H|p_1,\ldots,p_n\rangle_{\mathrm{in/out}} &= H\Omega_\pm|p_1,\ldots,p_n\rangle_0 = \Omega_\pm H_0|p_1,\ldots,p_n\rangle_0\\ &= E\Omega_\pm|p_1,\ldots,p_n\rangle_0 = E|p_1,\ldots,p_n\rangle_{\mathrm{in/out}}\,,\end{aligned} \tag{1.109}$$

i.e., the in/out states are eigenstates of the full Hamiltonian, in one-one correspondence with free multiparticle states. Moreover, if $U_0(a,\Lambda)$ are the unitary representatives of Poincaré transformations, then

$$\begin{aligned}\Omega_\pm U_0(a,\Lambda)|p_1,\ldots,p_n\rangle_0 &= e^{-ia\cdot\sum_j p_j}|\Lambda p_1,\ldots,\Lambda p_n\rangle_0 = e^{-ia\cdot\sum_j p_j}\Omega_\pm|\Lambda p_1,\ldots,\Lambda p_n\rangle_0\\ &= e^{-ia\cdot\sum_j p_j}|\Lambda p_1,\ldots,\Lambda p_n\rangle_{\mathrm{in/out}} = U_{\mathrm{in/out}}(a,\Lambda)|p_1,\ldots,p_n\rangle_{\mathrm{in/out}}\,,\end{aligned} \tag{1.110}$$

so that Poincaré transformations are defined on in and out states. Assuming that $[U_0(a,\Lambda),S]=0$, i.e., Poincaré invariance holds, then

$$\begin{aligned}&{}_{\mathrm{out}}\langle p'_1,\ldots,p'_{n'}|U_{\mathrm{out}}(a,\Lambda)^\dagger U_{\mathrm{in}}(a,\Lambda)|p_1,\ldots,p_n\rangle_{\mathrm{in}}\\ &= {}_0\langle p'_1,\ldots,p'_{n'}|U_0(a,\Lambda)^\dagger\Omega_-^\dagger\Omega_+U_0(a,\Lambda)|p_1,\ldots,p_n\rangle_0\\ &= {}_0\langle p'_1,\ldots,p'_{n'}|U_0(a,\Lambda)^\dagger SU_0(a,\Lambda)|p_1,\ldots,p_n\rangle_0\\ &= {}_0\langle p'_1,\ldots,p'_{n'}|S|p_1,\ldots,p_n\rangle_0 = {}_{\mathrm{out}}\langle p'_1,\ldots,p'_{n'}|p_1,\ldots,p_n\rangle_{\mathrm{in}}\,,\end{aligned} \tag{1.111}$$

i.e., $U_{\mathrm{out}}(a,\Lambda)=U_{\mathrm{in}}(a,\Lambda)$. In other words, if the interaction Hamiltonian is Poincaré invariant, then in and out states transform according to the same unitary representation of the Poincaré group, and transform precisely like free multiparticle states.

At this point one sets up perturbation theory and employs the usual Feynman rules to compute the (still regularised) perturbative series. An important point is that properly taking into account the presence of the adiabatic switch results into a modificiation of the naive Feynman rule for external lines. In general, diagrams contributing to a process with n incoming plus outgoing particles can be written as the product of a connected truncated n-point part and n

two-point parts, connecting the n-point part with the external particles. The n-point part and the n two-point parts can be resummed separately to all orders. The result for the full external lines is naively of the form

$$1 + D\Sigma + (D\Sigma)^2 + \ldots = \frac{1}{1 - D\Sigma} = \frac{p^2 - m^2}{p^2 - m^2 - \Sigma(p^2) + i\epsilon}\,, \tag{1.112}$$

where Σ is the sum of two-point 1PI diagrams, including the contributions of the mass counterterm $\delta m^2\phi^2$. For m to be the physical mass of the particle, one needs the full two-point function to have a pole there, which a similar calculations shows to be

$$D + D\Sigma D + (D\Sigma)^2 D + \ldots = \frac{1}{1 - D\Sigma} D = \frac{1}{p^2 - m^2 - \Sigma(p^2) + i\epsilon}\,. \tag{1.113}$$

One then needs $\Sigma(m^2) = 0$, which is achieved by suitably choosing δm^2. The fact that this may be divergent as the regularisation is removed is irrelevant from the conceptual point of view. One then finds

$$\frac{p^2 - m^2}{p^2 - m^2 - \Sigma(p^2)} \underset{p^2 \to m^2}{=} \frac{p^2 - m^2}{(p^2 - m^2)[1 - \Sigma'(m^2)]} = \frac{1}{[1 - \Sigma'(m^2)]} = Z\,. \tag{1.114}$$

Taking into account the adiabatic switching correctly, this is modified into[14]

$$Z \to \sqrt{Z}\,. \tag{1.115}$$

This factor is a leftover of the adiabating switching procedure: while free particle states are correctly representing the state of the system at asymptotic times when adiabating switching is present, in the physical theory there is no such a thing and the true asymptotic states are affected by the persistent effects of the interaction, responsible, e.g., for the true mass of the particle. At any intermediate stage, the true asymptotic states are built out of a cloud of particles surrounding the original free particle, which is implemented by the Møller operators. When representing in terms of momentum eigenvectors, however, it is not guaranteed that the correct normalisation is mantained - and in fact it is not. Formally, for one-particle states

$$\begin{aligned} \Omega_\pm |p\rangle_0 &= |p\rangle_0 + \int_0^{\pm\infty} dt\, e^{-\epsilon|t|} e^{iHt} i H_I e^{-iH_0 t} |p\rangle_0 \\ &= |p\rangle_0 - \frac{1}{H - E_p \pm i\epsilon} H_I |p\rangle_0 = \frac{\pm i\epsilon}{H - E_p \pm i\epsilon} |p\rangle_0\,. \end{aligned} \tag{1.116}$$

It is easy to show that as $\epsilon \to 0$, this becomes an eigenstate of H:

$$(H - E_p \pm i\epsilon)\Omega_\pm |p\rangle_0 = \pm i\epsilon |p\rangle_0 \Rightarrow (H - E_p)\Omega_\pm |p\rangle_0 = \pm i\epsilon\,(|p\rangle_0 - \Omega_\pm |p\rangle_0) \underset{\epsilon\to 0}{\to} 0\,. \tag{1.117}$$

This applies, more generally, to multiparticle states $|p_1, \ldots, p_n\rangle_0$, that are turned by $\Omega_\pm$ into eigenstates of H (in the limit $\epsilon \to 0$). In general, however, $\Omega_\pm |p\rangle_0$ does not have the usual

[14] F.J. Dyson, "The S matrix in quantum electrodynamics" Phys. Rev. 75 (1949) 1736-1755; "Heisenberg Operators in Quantum Electrodynamics. II", Phys. Rev. 83 (1951) 3, 608-627. See also, F.J. Dyson, "Advanced quantum mechanics", quant-ph/0608140, pp. 110-111; S. Schweber, "An introduction to relativistic quantum field theory", sec. 15c; F. Mandl and G. Shaw, "Quantum Field Theory", sec. 9.4.

relativistic normalisation even in this limit,[15] so we set

$$\sqrt{Z}|p\pm\rangle = \lim_{\epsilon\to 0}\Omega_\pm|p\rangle_0\,, \tag{1.118}$$

where $|p\pm\rangle$ are correctly normalised and Z is real positive (after suitably choosing phases), but in general $Z \neq 1$. Taking the scalar product of Eq. (1.116) with $|p\pm\rangle$ (assuming regularisation in a finite spatial box so that momentum eigenstates are normalisable), one finds

$$\sqrt{Z} = \langle p\pm|\sqrt{Z}|p\pm\rangle = \langle p\pm|\lim_{\epsilon\to 0}\Omega_\pm|p\rangle_0 = \langle p\pm|p\rangle_0\,, \tag{1.119}$$

so one sees that Z is the same for both $\Omega_\pm$. One can also argue that for multiparticle states one gets the same factor for each particle. This factor is the same factor discussed above: one can think about the fully dressed external lines as the processes turning $|p_1,\ldots,p_n\rangle_0$ into $|p_1,\ldots,p_n+\rangle$ for the incoming particles, before they interact with each other, and conversely $|p'_1,\ldots,p'_{n'}-\rangle$ into $|p'_1,\ldots,p'_{n'}\rangle_0$ for outgoing particles, after they have interacted. (Particles that do not interact with anything else are turned from free to interacting to free again without any loss, i.e., with probability 1. At finite ϵ there are parts of the wavefunction Ω^ϵ that will get lost as $\epsilon\to 0$, but since they are not disturbed they sum coherently and give back 1.)

One can then either ignore loop corrections to external lines entirely and simply include a factor $\sqrt{Z}$, or include loop corrections to external lines explicitly and include a factor $1/\sqrt{Z}$ for each external line. In either case, this boils down to the resummed external line being removed when put on shell, and a factor $\sqrt{Z}$ being attached to the connected truncated part. If one insists on keeping it in the game, one can treat it as being multiplied by $1/Z$, while a factor $\sqrt{Z}$ is attached to the connected truncated part. For the latter, the topological relation $E+2I=\sum_k nV_k$ implies that the overall factor $Z^{\frac{1}{2}E} = Z^{-I+\frac{1}{2}\sum_k kV_k}$ can be treated as a modification Z^{-1} for each (elementary) internal line and an effective redefinition $Z^{\frac{k}{2}}$ of the coupling $\lambda_{Bk}\to Z^{\frac{k}{2}}\lambda_{Bk}$ of the (elementary) vertex with k lines. The former effectively redefines the full internal propagators so that they have residue 1 at the particle pole; this removes self-energy divergences. The latter, after setting $\lambda_{Bk}=Z_k\lambda_k$, amounts effectively to having for each vertex a factor $Z^{\frac{k}{2}}Z_k\lambda_k$, so that only the combination $Z'_k = Z^{\frac{k}{2}}Z_k$ of renormalisation constants appears. Divergences can now be removed by suitably defining δm^2 and Z'_k, so that the physical mass and the renormalised coupling (suitably defined by some prescription) take their experimental values, while it is clear from the above that Z plays physically no role.

The treatment of external lines discussed above can be summarised as

$$\begin{aligned}{}_{\rm out}\langle p'_1,\ldots,p'_{n'}|p_1,\ldots,p_n\rangle_{\rm in} &= G_n(-p'_1,\ldots,-p'_{n'},p_1,\ldots,p_n)\\ &\quad\times[G_2(p'_1)\ldots G_2(p'_{n'})]^{-1}[G_2(p_1)\ldots G_2(p_n)]^{-1}\\ &\quad\times Z^{\frac{1}{2}}\bar u(p'_1)\ldots Z^{\frac{1}{2}}\bar u(p'_{n'})Z^{\frac{1}{2}}u(p_1)\ldots Z^{\frac{1}{2}}u(p_n)\,,\end{aligned} \tag{1.120}$$

i.e., the full n-point function is stripped of fully dressed external lines, replaced by $Z^{\frac{1}{2}}$ times the particle wave function, or equivalently

$$\begin{aligned}{}_{\rm out}\langle p'_1,\ldots,p'_{n'}|p_1,\ldots,p_n\rangle_{\rm in} &= G_n(-p'_1,\ldots,-p'_{n'},p_1,\ldots,p_n)\\ &\quad\times[G_2^{\rm free}(p'_1)\ldots G_2^{\rm free}(p'_{n'})]^{-1}[G_2^{\rm free}(p_1)\ldots G_2^{\rm free}(p_n)]^{-1}\\ &\quad\times Z^{-\frac{1}{2}}\bar u(p'_1)\ldots Z^{-\frac{1}{2}}\bar u(p'_{n'})Z^{-\frac{1}{2}}u(p_1)\ldots Z^{-\frac{1}{2}}u(p_n)\,,\end{aligned} \tag{1.121}$$

[15] See, e.g., Bryce S. DeWitt, "State-vector normalization in formal scattering theory", Phys. Rev. 100 (1955) 905-911.

i.e., the full n-point function is stripped of free external lines, replaced by $Z^{-\frac{1}{2}}$ times the particle wave function.

Renormalised perturbation theory∗ There is a practically more convenient way to implement the perturbative procedure. Internal lines including the renormalisation factor Z^{-1} can be further recast as

$$\begin{aligned}\frac{i}{p^2-m^2+i\epsilon}\frac{1}{Z} &= \frac{i}{p^2-m^2+i\epsilon}\frac{1}{1+(Z-1)} = \frac{i}{p^2-m^2+i\epsilon}\left[1+\sum_{n=1}^{\infty}(1-Z)^n\right] \\ &= \frac{i}{p^2-m^2+i\epsilon}\sum_{n=0}^{\infty}\left[i(p^2-m^2)(Z-1)\frac{i}{p^2-m^2+i\epsilon}\right]^n ,\end{aligned} \tag{1.122}$$

which is equivalent to the sum of insertions of a new vertex,

$$(Z-1)\frac{1}{2}\left[(\partial_\mu\phi)^2-m^2\phi^2\right] . \tag{1.123}$$

The Feynman rules can then be summarised as follows:

- usual factor for external lines;
- usual factor $i/(p^2-m^2+i\epsilon)$ with m physical for internal lines;
- factor $iZ^{\frac{k}{2}}Z_k\lambda_k$ for vertex k;
- factor $-i\delta m^2$ for two-point vertex $-\delta m^2\phi^2/2 = -(Z_m-1)Zm^2\phi^2/2$;
- factor $i(p^2-m^2)(Z-1)$ for two-point vertex $(Z-1)\frac{1}{2}\left[(\partial_\mu\phi)^2-m^2\phi^2\right]$.

Effectively, these can be derived from a new interaction Lagrangian that reads

$$\begin{aligned}\mathscr{L}_I &= (Z-1)\frac{1}{2}\left[(\partial_\mu\phi)^2-m^2\phi^2\right]-(Z_m-1)Zm^2\frac{1}{2}\phi^2+\sum_k Z^{\frac{k}{2}}Z_k\lambda_k\phi^k \\ &= \frac{Z-1}{2}(\partial_\mu\phi)^2-(Z_m-1)m^2\frac{Z}{2}\phi^2+\sum_k Z^{\frac{k}{2}}Z_k\lambda_k\phi^k ,\end{aligned} \tag{1.124}$$

employed as usual directly into Dyson's formula, replacing ϕ with a free field with standard normalisation $[\phi_0,\dot{\phi}_0]=i$, governed by the free Lagrangian

$$\mathscr{L}_0 = \frac{1}{2}\left[(\partial_\mu\phi)^2-m^2\phi^2\right] . \tag{1.125}$$

Combining together $\mathscr{L}=\mathscr{L}_0+\mathscr{L}_I$ one finds

$$\mathscr{L} = \frac{Z}{2}(\partial_\mu\phi)^2-Z_m m^2\frac{Z}{2}\phi^2+\sum_k Z^{\frac{k}{2}}Z_k\lambda_k\phi^k = \frac{Z}{2}(\partial_\mu\phi)^2-m_B^2\frac{Z}{2}\phi^2+\sum_k Z^{\frac{k}{2}}\lambda_{Bk}\phi^k . \tag{1.126}$$

The value of Z is determined by the condition that the full two-point propagator of ϕ at the particle pole has residue 1. The values of Z_m and Z_k are fixed instead by comparison with

experiments of m and λ_k, and so must reabsorb any remaining divergence in the two-point non-derivative and k-point vertices. At each order one then includes a suitable contribution in Z, Z_m and Z_k in order to fullfil the requirements.

Notice that redefining $Z\phi = \phi_B$, one ends up exactly with the original Lagrangian,

$$\mathscr{L} = \frac{1}{2}(\partial_\mu \phi_B)^2 - m_B^2 \frac{1}{2}\phi_B^2 + \sum_k \lambda_{Bk}\phi_B^k \,. \tag{1.127}$$

However, if one uses canonical quantisation on this Lagrangian one does not end up having standard commutation relations for ϕ and $\dot{\phi}$. Nonetheless, for the perturbative treatment, *in practice* one can simply rescale ϕ_B, split the desired free part, and use the rest as minus the interaction Hamiltonian in Dyson's formula. The resulting perturbative series, suitably modified for what concerns the external lines, gives the Green's functions of the *renormalised field* ϕ. This *does not* obey standard commutation relations $[\phi, \dot{\phi}] = i$.

As far as reabsorbing divergences goes, one can use a different set of prescriptions than the on-shell ones. For example, one can set $\phi_B = Z'^{\frac{1}{2}}\phi'$ and use Z' to reabsorb divergences proportional to $p^2 - m^2$, requiring that the residue at the pole be some finite value z; and set $m_B^2 = Z'_m m'^2$ and require that $m' = z_m m$ for some finite z_m - or something else which is, however, practically equivalent to this. The definition of the renormalised couplings is inherently arbitrary, and one can employ also unphysical conditions like, e.g., the value of the k-point function for some off-shell choice of momenta; for notational uniformity, let $\lambda_{Bk} = Z'_k \lambda'_k$. Again, at each perturbative order one includes contributions in Z', Z'_m and Z'_k in order to fullfil the renormalisation conditions. One ends up with finite values for m' and λ'_k, related by a finite renormalisation to the physical ones. Of course, this procedure cannot change the S-matrix - as long as the physical mass and couplings are fixed. On the other hand, it changes the Green's functions of the renormalised field ϕ'. Since ϕ_B is always the same if we fix the corresponding physical theory (i.e., the physical mass and coupling), so will be its Green's functions, and so

$$\langle 0|\mathrm{T}\{\phi_B(x_1)\dots\phi_B(x_n)\}|0\rangle = Z^{\frac{n}{2}}\langle 0|\mathrm{T}\{\phi(x_1)\dots\phi(x_n)\}|0\rangle = Z'^{\frac{n}{2}}\langle 0|\mathrm{T}\{\phi'(x_1)\dots\phi'(x_n)\}|0\rangle \,. \tag{1.128}$$

References

- The discussion of formal scattering theory and perturbative quantisation is rather standard and found in many textbooks, e.g.,

  M.E. Peskin and D.V. Schroeder, "An Introduction to Quantum Field Theory".

- The discussion of renormalisation is admittedly sketchy and aimed at giving an overview rather than a detailed presentation. For a thorough discussion consult

  D. Anselmi, "Renormalization", freely available at `www.renormalization.com`;

  J. Collins, "Renormalization".

- The discussion of renormalised perturbation theory in the canonical formalism using the adiabatic switching on and off procedure is assembled from bits and pieces found in most textbooks, but not presented organically. Besides the original literature cited in the text, I found the following books useful:

  F. J. Dyson, "Advanced quantum mechanics", quant-ph/0608140;

S. Schweber, "An introduction to relativistic quantum field theory";

F. Mandl and G. Shaw, "Quantum Field Theory".

2 Elements of non-perturbative quantum field theory

The perturbative quantisation procedure outlined above works quite well in practice, at least for certain theories, but theoretically it is not satisfactory. Its most appealing feature is that it indeed describes the physics of interacting particles in a manifestly local and Poincaré-invariant fashion, which is what we set out to do. Moreover, it allows to label the states of the fully interacting theory that describe the initial and final states of a scattering process in terms of free-particle quantum numbers (i.e., number and type of particles, energy, momentum, spin,...). On the other hand, it relies on the adiabatic switching procedure, which is somewhat physically justified (the actual scattering interaction takes place over a short time) and somewhat not (interactions have persistent effects that change the asymptotic states themselves), and on the bold assumption that a perturbative expansion can be done, i.e., that the theory is analytic at vanishing coupling (which is very likely *not* the case in most theories, most notably QED). While one could accept that as an approximation to the true theory, since the perturbative series is the very device that we are using to *define* the quantised theory itself, one is left with very shaky foundations.

It is then important to understand what would a quantum field theory look like under general assumptions, including symmetry and locality properties, and find out what are the general properties that one should expect independently of the quantisation procedure. This line of research is known as "axiomatic quantum field theory" (though nowadays the term "algebraic quantum field theory" is preferred), and was pursued among others by Lehmann, Symanzik, and Zimmermann; Wightman; Streater; Haag; Ruelle; Källén. While this is unlikely to help with practical calculations, it will help understanding QFT itself, and clarify the connection between the underlying objects, i.e., fields, and the observable entities, i.e., particles.

Wightman's axioms The starting point of the axiomatic approach is a set of physically motivated assumptions, or axioms, that a decent QFT has to satisfy. Without any pretense to mathematical rigour, these are the main basic assumptions on which one wants to build (*Wightman's axioms*). It is understood that the theory is formulated in some (separable) Hilbert space $\mathcal{H}$, and that fields $\phi_i(x)$ are associated with the points x of spacetime.

1. The theory is symmetric under translations, with translation symmetry implemented by unitary operators $U(a) = e^{-iP\cdot a}$, whose Hermitean generators $P_\mu = P_\mu^\dagger$ are identified with the four-momentum operator.

2. There is a *unique* translation-invariant normalisable vacuum state $|0\rangle$,

$$P_\mu|0\rangle = 0\,, \qquad \langle 0|0\rangle = 1\,. \tag{2.129}$$

3. Fields build the Hilbert space out of the vacuum, i.e., all the states (or at least a dense set of states) is obtained by applying polynomials $P[\phi]$ of fields on the vacuum, $\{P[\phi]|0\rangle\} = \mathcal{H}$.

4. The theory has a positive energy-momentum spectrum, i.e., the eigenvalues p_μ of P_μ satisfy $p^2 \geq 0$, $p_0 \geq 0$. It follows that $|0\rangle$ is also the unique state of minimal energy $p_0 = 0$.

5. Lorentz symmetry is implemented by unitary operators $U(\Lambda)$, and so full Poincaré symmetry is implemented by unitary operators. It follows from group composition properties that $|0\rangle$ is also Lorentz invariant. In fact

$$U(a)U(\Lambda)|0\rangle = U(\Lambda)U(\Lambda^{-1})U(a)U(\Lambda)|0\rangle = U(\Lambda)U(\Lambda^{-1}a)|0\rangle = U(\Lambda)|0\rangle = |0\rangle\,, \tag{2.130}$$

where the last passage follows since $U(\Lambda)|0\rangle$ is translation-invariant, but such a state is unique.

6. Fields transform covariantly under Poincaré symmetry,

$$U(a)^\dagger U(\Lambda)^\dagger \phi_i(x) U(\Lambda)U(a) = S_{ij}(\Lambda)\phi_j(\Lambda^{-1}x + a)\,, \tag{2.131}$$

where $S_{ij}(\Lambda)$ is some finite-dimensional irreducible representation of the proper orthocronous Lorentz group. This is a technical assumption that is not strictly necessary, but which greatly simplifies things.

7. Fields obey the microcausality (locality) condition

$$[\phi_i(x), \phi_j(y)]_\pm = 0 \text{ for } (x-y)^2 < 0\,, \tag{2.132}$$

where commutators $[\cdot,\cdot]_-$ or anticommutators $[\cdot,\cdot]_+$ are used depending on the spin of the representation $S(\Lambda)$.

From this set of physically motivated axioms one can derive rigorously many appealing properties. An important one is the *cluster property* of vacuum expectation values of products of fields (*Wightman's functions*),

$$\begin{aligned} & \langle 0|\phi(x_1)\dots\phi(x_n)\phi(y_1+\lambda a)\dots\phi(y_m+\lambda a)|0\rangle \\ \underset{\lambda\to\infty}{\to} & \langle 0|\phi(x_1)\dots\phi(x_n)|0\rangle\langle 0|\phi(y_1+\lambda a)\dots\phi(y_m+\lambda a)|0\rangle \\ = & \langle 0|\phi(x_1)\dots\phi(x_n)|0\rangle\langle 0|\phi(y_1)\dots\phi(y_m)|0\rangle\,. \end{aligned} \tag{2.133}$$

Wightman's reconstruction theorem shows how to reconstruct the full field theory from the Wightman's functions $\langle 0|\phi(x_1)\dots\phi(x_n)|0\rangle$. One can also prove the well-known spin/statistics theorem and CPT theorem. Moreover, the Haag-Ruelle theory of scattering shows the existence of asymptotic fields and the validity of the LSZ asymptotic condition, that we will discuss below.

While most of what we need can actually be derived from the axioms, for simplicity we will make further, more detailed assumptions that will make our life simpler. One such assumption concerns the spectrum of the theory. We will assume that single-particle states $|p;\alpha\rangle$ exist, with $P_\mu|p;\alpha\rangle = p_\mu|p;\alpha\rangle$ and $p_\mu p^\mu = m_\alpha^2$, and normalised according to

$$\langle p';\alpha'|p;\alpha\rangle = \delta_{\alpha'\alpha} 2p^0 (2\pi)^3 \delta^{(3)}(\vec{p}' - \vec{p})\,; \tag{2.134}$$

and furthermore that the vacuum and the single-particle states are discrete points in the spectrum of $P_\mu P^\mu$, with $m_g = \min_\alpha m_\alpha > 0$ (mass gap), and the continuous spectrum of $P_\mu P^\mu$ starting at $(2m_g)^2$. We also assume that the are no other discrete points in the spectrum of $P_\mu P^\mu$ (bound states).

Spectral (Källén-Lehmann) representation of the propagator We now derive an important property of the two-point function of an interacting field that we have actually used several times already. Consider a single Hermitean scalar field $\phi = \phi^\dagger$, and its time-ordered two-point function

$$D(x) \equiv \langle 0|T\{\phi(x)\phi(0)\}|0\rangle = \theta(x^0)\langle 0|\phi(x)\phi(0)|0\rangle + \theta(-x^0)\langle 0|\phi(0)\phi(x)|0\rangle\,. \tag{2.135}$$

Inserting a complete set of energy-momentum eigenstates, including the single-particle states, one finds

$$\begin{aligned}\langle 0|\phi(x)\phi(0)|0\rangle &= \sum_n \langle 0|\phi(x)|n\rangle\langle n|\phi(0)|0\rangle \\ &= \sum_n \langle 0|e^{iP\cdot x}\phi(0)e^{-iP\cdot x}|n\rangle\langle n|\phi(0)|0\rangle \qquad \text{by translation invariance} \\ &= \sum_n e^{-ip_n\cdot x}|\langle 0|\phi(0)|n\rangle|^2 \qquad P_\mu \text{ eigenstates}\,.\end{aligned} \tag{2.136}$$

Plug this back in one finds

$$\begin{aligned}D(x) &= \sum_n \left[\theta(x^0)e^{-ip_n\cdot x} + \theta(-x^0)e^{ip_n\cdot x}\right]|\langle 0|\phi(0)|n\rangle|^2 \\ &= \int \frac{d^4p}{(2\pi)^4}\,\left[\theta(x^0)e^{-ip\cdot x} + \theta(-x^0)e^{ip\cdot x}\right]\varrho(p) \\ \varrho(p) &\equiv \sum_n (2\pi)^4\delta^{(4)}(p_n - p)|\langle 0|\phi(0)|n\rangle|^2\,.\end{aligned} \tag{2.137}$$

We can say more about ϱ. First of all, one clearly has $\varrho \geq 0$. Next, using Lorentz invariance and covariance of the field, $U(\Lambda)^\dagger\phi(x)U(\Lambda) = \phi(\Lambda^{-1}x)$, one finds

$$\begin{aligned}\varrho(\Lambda p) &= \sum_n (2\pi)^4\delta^{(4)}(p_n - \Lambda p)|\langle 0|\phi(0)|n\rangle|^2 \\ &= \sum_{n_\Lambda} (2\pi)^4\delta^{(4)}(p_{n_\Lambda} - \Lambda p)|\langle 0|\phi(0)|n_\Lambda\rangle|^2 \\ &= \sum_n (2\pi)^4\delta^{(4)}(\Lambda p_n - \Lambda p)|\langle 0|\phi(0)U(\Lambda)|n\rangle|^2 \\ &= \sum_n (2\pi)^4\delta^{(4)}(p_n - p)|\langle 0|\phi(0)|n\rangle|^2 = \varrho(p)\,,\end{aligned} \tag{2.138}$$

i.e., $\varrho(p)$ is a Lorentz-invariant function of p. Together with positivity of the energy spectrum this implies

$$\varrho(p) = 2\pi\theta(p^0)\rho(p^2)\,, \tag{2.139}$$

with $\rho \geq 0$. Notice that for single-particle states one has

$$\langle 0|\phi(0)|p\rangle = \langle 0|\phi(0)|\Lambda p\rangle = f(p^2) = f(m^2) \equiv \sqrt{Z}\,, \tag{2.140}$$

i.e., a p-independent constant, that can be chosen real positive by suitably choosing the phase of one-particle states. It is then implicitly assumed that $Z > 0$ and that the positive determination

of the square root is used. Using now the properties of ϱ we obtain

$$\begin{aligned} D(x) &= \int \frac{d^4p}{(2\pi)^4} \left[\theta(x^0)e^{-ip\cdot x} + \theta(-x^0)e^{ip\cdot x}\right] 2\pi\theta(p^0)\rho(p^2) \\ &= \int_0^\infty ds\,\rho(s) \int \frac{d^4p}{(2\pi)^4} \left[\theta(x^0)e^{-ip\cdot x} + \theta(-x^0)e^{ip\cdot x}\right] 2\pi\theta(p^0)\delta(p^2-s) \\ &= \int_0^\infty ds\,\rho(s)\Delta_F(x;s) = \int_0^\infty ds\,\rho(s) \int \frac{d^4p}{(2\pi)^4}\, e^{-ip\cdot x} \frac{i}{p^2 - s + i\epsilon} \end{aligned} \tag{2.141}$$

where $\Delta_F(x;s)$ is the free causal (Feynman) propagator for a particle of mass squared s. This is the spectral, or Källén-Lehmann representation of the propagator. We now use our assumption on the spectrum, i.e., that there are isolated single-particle states at $p^2 = m^2$, and continuous spectrum starting at the "two-particle threshold" $p^2 = 4m^2$, and find

$$\begin{aligned} \rho(s) &= Z\delta(s-m^2) + \theta(s-4m^2)\sigma(s) \\ \tilde{D}(p) &\equiv \int d^4x\, e^{ip\cdot x} D(x) = \frac{iZ}{p^2 - m^2 + i\epsilon} + \int_{4m^2}^\infty ds\,\sigma(s) \frac{i}{p^2 - s + i\epsilon}\,. \end{aligned} \tag{2.142}$$

This shows that the full propagator (in momentum space) $\tilde{\Delta}_F(p)$ has a pole at the physical value of the particle mass, with residue equal to $Z > 0$. Keeping the position of the pole at the physical value was used as a requirement in the perturbative approach, and required the introduction of a suitable mass counterterm, or in other words, a tuning of the mass parameter in the Lagrangian so that the actual mass of the particle took the desired value. While intuitively understandable, the reason why one should do that is formalised by this result. Moreover, the meaning of the residue is now clear: $\sqrt{Z}$ is the matrix element of the field (at $x = 0$) between the vacuum and the one-particle states. In other words, ϕ can create $\sqrt{Z}$-times a one-particle state, with $\sqrt{Z}$ generally different from 1, since ϕ can also create multiparticle states.

In and out states As we have already discussed, at $t \to \mp\infty$ the states of our system should look like those of a set of non-interacting particles. In the approach based on the adiabatic switching procedure, we saw how in and out states are obtained from free particle states via the Møller operators. However, here we want to avoid using the unphysical adiabatic switching, so working with a time-translation invariant system all along. In this case the interaction picture becomes problematic (recall Haag's theorem), and basically one cannot use both H_0 and H in the same Hilbert space. We thus want to avoid entirely the introduction of a free Hamiltonian H_0 in our formalism.

At the same time, we want to make use the experimental fact that the states of a real, interacting scattering system can be labelled by momenta and spin, precisely like the continuum states of a free field theory. We then just *postulate* the existence of *complete sets* of in and out states $|p_1, \ldots, p_n\rangle_{\text{in,out}}$, corresponding to states that look like non-interacting multiparticle states in the far past or in the far future. This means that these states must transform like multiparticle states under translations and Lorentz transformations,

$$U(\Lambda)U(a)|p_1, \ldots, p_n\rangle_{\text{in,out}} = e^{-i(\sum_j p_j)\cdot a}|\Lambda p_1, \ldots, \Lambda p_n\rangle_{\text{in,out}}\,, \qquad p_j^2 = m^2\,, \tag{2.143}$$

so that they can be labelled precisely like non-interacting multiparticle states by momenta and spin (omitted here for simplicity); and provide bases to expand the initial and final (exact!)

states of the system,

$$
\begin{aligned}
|\Psi+\rangle &= \int d\Omega_{p_1} \dots \int d\Omega_{p_n}\, f_1(p_1)\dots f_n(p_n)|p_1,\dots,p_n\rangle_{\rm in}\,, \\
|\Psi'-\rangle &= \int d\Omega_{p'_1} \dots \int d\Omega_{p'_{n'}}\, f'_1(p'_1)\dots f'_{n'}(p'_{n'})|p'_1,\dots,p'_{n'}\rangle_{\rm out}\,.
\end{aligned}
\tag{2.144}
$$

Such states include invariant, vacuum in and out states as well, which under the assumption of uniqueness must then be the same state as $|0\rangle$, so up to phase factors that can be set to 1, $|0\rangle_{\rm in} = |0\rangle_{\rm out} = |0\rangle$. Moreover, $|p\rangle_{\rm in}$ and $|p\rangle_{\rm out}$ are both eigenstates of P_μ with the same eigenvalues, in particular with $p^2 = m^2$, and since there are only one-particle states with this property, $|p\rangle_{\rm in}$ and $|p\rangle_{\rm out}$ can differ at most by a phase factor that can be set to 1, and so $|p\rangle_{\rm in} = |p\rangle_{\rm out} = |p\rangle$.

The existence of these states can be actually derived under Wightman's axioms using the so-called *Haag-Ruelle theory of scattering*. On the other hand, completeness of these states is a separate (and difficult to prove) matter, and it is usually *assumed* that in and out states form two (generally different) complete sets of states in the Hilbert space of the system (*asymptotic completeness condition*).

Finally, scattering amplitudes are obtained as

$$
\begin{aligned}
\langle \Psi' - |\Psi+\rangle = \int d\Omega_{p'_1} \dots \int d\Omega_{p'_{n'}}\, f'_1(p'_1)^* \dots f'_{n'}(p'_{n'})^* \int d\Omega_{p_1} \dots \int d\Omega_{p_n}\, f_1(p_1)\dots f_n(p_n) \\
\times\, {}_{\rm out}\langle p'_1,\dots,p'_{n'}|p_1,\dots,p_n\rangle_{\rm in}\,.
\end{aligned}
\tag{2.145}
$$

As a shorthand notation, we denote the S-matrix elements as

$$
S_{\beta\alpha} = {}_{\rm out}\langle p'_1,\dots,p'_{n'}|p_1,\dots,p_n\rangle_{\rm in} = {}_{\rm out}\langle\beta|\alpha\rangle_{\rm in}\,. \tag{2.146}
$$

Since in/out states are assumed to be complete, $S_{\beta\alpha}$ is a unitary matrix. Defining the S operator via

$$
{}_{\rm out}\langle\beta| = \sum_\alpha (S_{\beta\alpha})\ {}_{\rm in}\langle\alpha| \equiv {}_{\rm in}\langle\beta|S\,, \tag{2.147}
$$

one has from completeness

$$
\begin{aligned}
\delta_{\beta\alpha} = {}_{\rm out}\langle\beta|\alpha\rangle_{\rm out} &= {}_{\rm in}\langle\beta|SS^\dagger|\alpha\rangle_{\rm in} && \Longrightarrow SS^\dagger = \mathbf{1}\,, \\
{}_{\rm out}\langle\beta|S^\dagger S|\alpha\rangle_{\rm out} &= {}_{\rm in}\langle\beta|SS^\dagger S|\alpha\rangle_{\rm out} = {}_{\rm in}\langle\beta|S|\alpha\rangle_{\rm out} && \\
&= {}_{\rm out}\langle\beta|\alpha\rangle_{\rm out} = \delta_{\beta\alpha} && \Longrightarrow S^\dagger S = \mathbf{1}\,,
\end{aligned}
\tag{2.148}
$$

implying that S is a unitary operator. Moreover, S is Poincaré invariant, $U(a,\Lambda)^\dagger S U(a,\Lambda) = S$, since

$$
\begin{aligned}
S_{(\Lambda\beta)(\Lambda\alpha)} &= {}_{\rm out}\langle\Lambda\beta|\Lambda\alpha\rangle_{\rm in} = {}_{\rm out}\langle\beta|U(\Lambda)^\dagger U(\Lambda)|\alpha\rangle_{\rm in} = S_{\beta\alpha}\,, \\
S_{(a\beta)(a\alpha)} &= {}_{\rm out}\langle\beta|e^{i\sum_{j'} p'_{j'} a} e^{-i\sum_j p_j a}|\alpha\rangle_{\rm in} = {}_{\rm out}\langle\beta|U(a)^\dagger U(a)|\alpha\rangle_{\rm in} = S_{\beta\alpha}\,.
\end{aligned}
\tag{2.149}
$$

Stability of the vacuum and of the 1-particle states implies

$$
\begin{aligned}
S_{00} &= {}_{\rm out}\langle 0|0\rangle_{\rm in} = \langle 0|0\rangle = 1\,, \\
S_{p'p} &= {}_{\rm out}\langle p'|p\rangle_{\rm in} = \langle p'|p\rangle = (2\pi)^3 2p^0 \delta^{(3)}(\vec{p}' - \vec{p})\,.
\end{aligned}
\tag{2.150}
$$

Finally, S connects in and out creation and annihilation operators: since $|\beta\rangle_{\rm out}$ is a complete set,

$$ {}_{\rm out}\langle\beta|a_{\rm out}(p) = {}_{\rm out}\langle\beta p| = {}_{\rm in}\langle\beta p|S = {}_{\rm in}\langle\beta|a_{\rm in}(p)S = {}_{\rm in}\langle\beta|SS^\dagger a_{\rm in}(p)S = {}_{\rm out}\langle\beta|S^\dagger a_{\rm in}(p)S\,, \quad (2.151) $$

and so $S^\dagger a_{\rm in}(p)S = a_{\rm out}(p)$, and $S^\dagger a_{\rm in}(p)^\dagger S = a_{\rm out}(p)^\dagger$.

It should be noted that this S operator differs from the one appearing in the approach based on the interaction picture. In fact, in that case S acts on free-particle states, eigenstates of some free Hamiltonian H_0. Here, instead, it connects the in and out states, that are eigenstates of the *full* Hamiltonian H.

In and out fields From the multiparticle in and out states one defines as usual the in and out creation operators, i.e.,

$$ a_{\rm in/out}(p)^\dagger|0\rangle = |p\rangle_{\rm in/out}\,, \qquad a_{\rm in/out}(p)|0\rangle = 0\,, \quad (2.152) $$

and so on. These obey the usual commutation relations,

$$ [a_{\rm in/out}(p), a_{\rm in/out}(q)^\dagger] = 2p^0(2\pi)^3\delta^{(3)}(\vec{p}-\vec{q}) \qquad [a_{\rm in/out}(p), a_{\rm in/out}(q)] = 0\,. \quad (2.153) $$

Their transformation properties under translations and Lorentz transformations follow from Eq. (2.143): for an arbitary set of moments $p_1, \ldots, p_n$,

$$ \begin{aligned} &[e^{-ip\cdot a}a(\Lambda p)^\dagger_{\rm in/out}]e^{-i\sum_j p_j\cdot a}|\Lambda p_1, \ldots, \Lambda p_n\rangle = e^{-ip\cdot a}e^{-i\sum_j p_j\cdot a}|\Lambda p, \Lambda p_1, \ldots, \Lambda p_n\rangle_{\rm in/out} \\ &= U(\Lambda)U(a)|p, p_1, \ldots, p_n\rangle_{\rm in/out} = U(\Lambda)U(a)a_{\rm in/out}(p)^\dagger|p_1, \ldots, p_n\rangle \\ &= U(\Lambda)U(a)a_{\rm in/out}(p)^\dagger U(a)^\dagger U(\Lambda)^\dagger U(\Lambda)U(a)|p_1, \ldots, p_n\rangle \\ &= [U(\Lambda)U(a)a_{\rm in/out}(p)^\dagger U(a)^\dagger U(\Lambda)^\dagger]e^{-i\sum_j p_j\cdot a}|\Lambda p_1, \ldots, \Lambda p_n\rangle\,, \end{aligned} \quad (2.154) $$

and so

$$ \begin{aligned} U(\Lambda)U(a)a_{\rm in/out}(p)^\dagger U(a)^\dagger U(\Lambda)^\dagger &= e^{-ip\cdot a}a(\Lambda p)^\dagger_{\rm in/out}\,, \\ U(\Lambda)U(a)a_{\rm in/out}(p)U(a)^\dagger U(\Lambda)^\dagger &= e^{ip\cdot a}a(\Lambda p)_{\rm in/out}\,; \\ U(a)^\dagger U(\Lambda)^\dagger a_{\rm in/out}(p)^\dagger U(\Lambda)U(a) &= e^{i\Lambda^{-1}p\cdot a}a(\Lambda^{-1}p)^\dagger_{\rm in/out}\,, \\ U(a)^\dagger U(\Lambda)^\dagger a_{\rm in/out}(p)U(\Lambda)U(a) &= e^{-i\Lambda^{-1}p\cdot a}a(\Lambda^{-1}p)_{\rm in/out}\,. \end{aligned} \quad (2.155) $$

In turn, from creation and annihilation operators one defines the in and out fields,

$$ \phi_{\rm in/out}(x) = \int d\Omega_p \left\{a_{\rm in/out}(p)e^{-ip\cdot x} + a_{\rm in/out}(p)^\dagger e^{ip\cdot x}\right\}\,, \quad (2.156) $$

whose transformation properties are inherited from those of a and $a^\dagger$,

$$ \begin{aligned} &U(a)^\dagger U(\Lambda)^\dagger\phi_{\rm in/out}(x)U(\Lambda)U(a) \\ &= \int d\Omega_p \left\{e^{-i\Lambda^{-1}p\cdot a}a_{\rm in/out}(\Lambda^{-1}p)e^{-ip\cdot x} + e^{i\Lambda^{-1}p\cdot a}a_{\rm in/out}(\Lambda^{-1}p)^\dagger e^{ip\cdot x}\right\} \\ &= \int d\Omega_p \left\{e^{-ip\cdot a}a_{\rm in/out}(p)e^{-ip\cdot\Lambda^{-1}x} + e^{ip\cdot a}a_{\rm in/out}(p)^\dagger e^{ip\cdot\Lambda^{-1}x}\right\} = \phi(\Lambda^{-1}x + a)\,. \end{aligned} \quad (2.157) $$

Moreover, they obey the standard commutation relations of free fields, as a consequence of Eq. (2.153),

$$[\phi_{\rm in/out}(x), \phi_{\rm in/out}(y)] = \int d\Omega_p \left\{ e^{-ip\cdot(x-y)} - e^{ip\cdot(x-y)} \right\} \equiv \Delta(x-y)\,, \tag{2.158}$$

so in particular

$$\begin{aligned} [\phi_{\rm in/out}(x), \dot{\phi}_{\rm in/out}(y)]|_{y^0=x^0} &= \frac{\partial}{\partial y^0} [\phi_{\rm in/out}(x), \phi_{\rm in/out}(y)]|_{y^0=x^0} \\ &= i \int d\Omega_p\, p^0 \left\{ e^{-ip\cdot(x-y)} + e^{ip\cdot(x-y)} \right\}_{y^0=x^0} = i\delta(\vec{x}-\vec{y})\,. \end{aligned} \tag{2.159}$$

Finally, they obey by construction the free Klein-Gordon equation,

$$(\Box + m^2)\phi_{\rm in/out}(x) = 0\,. \tag{2.160}$$

One could conversely assume the existence of fields $\phi_{\rm in/out}(x)$ that (1.) transform covariantly under $U(\Lambda)U(a)$, (2.) obey the free Klein-Gordon equation, and (3.) obey the free-field commutation relations,[16] and obtain their representation Eq. (2.156), and so the in and out states of Eq. (2.143). In particular, a field obeying (1.) and (2.) necessarily creates only one-particle states out of the vacuum. In fact, from covariance it follows

$$\partial_\mu \phi_{\rm in}(x) = \partial_\mu e^{iP\cdot x} \phi_{\rm in}(0) e^{-iP\cdot x} = e^{iP\cdot x}[iP_\mu, \phi_{\rm in}(0)]e^{-iP\cdot x} = [iP_\mu, \phi_{\rm in}(x)]\,, \tag{2.161}$$

and so using (2.)

$$-\Box\phi_{\rm in}(x) = [P_\mu, [P^\mu, \phi_{\rm in}(x)]] = m^2\phi_{\rm in}(x)\,. \tag{2.162}$$

But then for any P_μ eigenstate, $P_\mu|\bar{p}\rangle = \bar{p}_\mu|\bar{p}\rangle$, one finds

$$\begin{aligned} m^2\langle 0|\phi_{\rm in}(x)|\bar{p}\rangle &= \langle 0|[P_\mu, [P^\mu, \phi_{\rm in}(x)]]|\bar{p}\rangle = -\langle 0|[P^\mu, \phi_{\rm in}(x)]P_\mu|\bar{p}\rangle \\ &= \langle 0|\phi_{\rm in}(x)P^\mu P_\mu|\bar{p}\rangle = \bar{p}^2\langle 0|\phi_{\rm in}(x)|\bar{p}\rangle\,, \end{aligned} \tag{2.163}$$

i.e., $\langle 0|\phi_{\rm in}(x)|\bar{p}\rangle \neq 0$ only if $|\bar{p}\rangle$ is a single-particle state, and so

$$\phi_{\rm in}(0)|0\rangle = \int d\Omega_p\, |p\rangle\langle p|\phi_{\rm in}(0)|0\rangle\,, \tag{2.164}$$

with $C = \langle p|\phi_{\rm in}(0)|0\rangle$ a p-independent constant due to Lorentz invariance. The same applies to $\phi_{\rm out}$. Since by construction $\phi_{\rm in/out}$ only creates one-particle in/out states out of the vacuum, one also has

$$\phi_{\rm in}(0)|0\rangle = \int d\Omega_p\, |p\rangle_{\rm in\ in}\langle p|\phi_{\rm in}(0)|0\rangle\,, \tag{2.165}$$

again with $C_{\rm in} = {}_{\rm in}\langle p|\phi_{\rm in}(0)|0\rangle$ a p-independent constant. But both $|p\rangle$ and $|p\rangle_{\rm in}$ are eigenstates of P_μ with the same eigenvalues, so $|p\rangle \propto |p\rangle_{\rm in}$, and since they have the same normalisation the proportionality factor is just a phase factor. The same applies to $|p\rangle_{\rm out}$ as well, so one concludes again $|p\rangle_{\rm in} = |p\rangle_{\rm out} = |p\rangle$.

[16] Under Wightman's axioms, the Jost-Schroer theorem implies that obeying the free Klein-Gordon equation automatically implies free-field commutation relations.

The in and out fields are connected by the S operator discussed above. In fact, since $S^\dagger a_{\rm in}(p)S = a_{\rm out}(p)$, one has immediately that

$$S^\dagger \phi_{\rm in}(x) S = \phi_{\rm out}(x)\,. \tag{2.166}$$

It is worth mentioning again that while being created out of the vacuum by the free in and out fields, the in and out states are eigenstates of the full Hamiltonian H, and not of some other free Hamiltonian H_0. As pointed out above, the in and out fields evolve in time with the full Hamiltonian H. At the same time, being free fields with the decomposition Eq. (2.156), their temporal evolution is equally well described in terms of free-field Hamiltonians $H_{\rm in/out}$. This apparent contradiction is resolved by noticing that in fact the full Hamiltonian is a functional of the interacting field ϕ, $H = H[\phi, \partial\phi]$, while the in and out Hamiltonians $H_{\rm in/out} = H_{\rm in/out}[\phi_{\rm in/out}, \partial\phi_{\rm in/out}]$ are functionals of $\phi_{\rm in/out}$, and one simply has $H[\phi, \partial\phi] = H_{\rm in/out}[\phi_{\rm in/out}, \partial\phi_{\rm in/out}]$.

Asymptotic (LSZ) condition The existence of the free fields $\phi_{\rm in/out}(x)$, Eq. (2.156) is entirely equivalent to that of the in and out states, Eq. (2.143). The crucial point is assuming now that these fields are somehow related to the basic fields of our theory in the limit of large times, so that also the in and out states get related to the basic field. Again, the existence and the nature of this relation is proven in the Haag-Ruelle theory of scattering: we will be happy with assuming it.

One could naively think that $\phi(x) \to \phi_{\rm in/out}(x)$ as $x^0 \to \mp\infty$ as an operator relation, or more generally that $\phi(x) \to \sqrt{Z}\phi_{\rm in/out}(x)$ for some constant Z. This, however, leads to contradictions: for example, for the two-point function one would find

$$\begin{aligned} W(x-y) &\equiv \langle 0|\phi(x^0+\tau,\vec{x})\phi(y^0+\tau,\vec{y})|0\rangle \\ &\underset{\tau\to-\infty}{\to} \langle 0|\phi_{\rm in}(x^0+\tau,\vec{x})\phi_{\rm in}(y^0+\tau,\vec{y})|0\rangle = W_{\rm free}(x-y)\,, \end{aligned} \tag{2.167}$$

but since the LHS is τ-independent one would have $W(x) = W_{\rm free}$. But the Jost-Schroer theorem states that a field obeying $W(x) = W_{\rm free}$ is necessarily a free field. This also shows that the limit cannot be a strong limit either, for otherwise the vector $\phi(x^0+\tau,\vec{x})|0\rangle$ would tend to $\phi(x^0+\tau,\vec{x})|0\rangle \to \phi_{\rm in}(x^0+\tau,\vec{x})|0\rangle$, and the same argument as above leads to ϕ being a free field.

The correct asymptotic condition is the following. For any normalisable solutions $f(x)$ of Klein-Gordon equation, $(\Box + m^2)f = 0$, define

$$\phi^f(t) \equiv i\int d^3x\, f(x)^* \overset{\leftrightarrow}{\partial}_0 \phi(t,\vec{x})\,, \qquad \phi^f_{\rm in,out} \equiv i\int d^3x\, f(x)^* \overset{\leftrightarrow}{\partial}_0 \phi_{\rm in,out}(t,\vec{x})\,. \tag{2.168}$$

This procedure smears the fields in space, provides a Lorentz-invariant quantity, and results in a t-independent object for the free in/out fields (see below). For any normalisable states $|\alpha\rangle, |\beta\rangle$ and Klein-Gordon solution f, we assume that ϕ obeys the *asymptotic LSZ condition*,

$$\begin{aligned} \lim_{t\to-\infty} \langle\alpha|\phi^f(t)|\beta\rangle &= \sqrt{Z}\langle\alpha|\phi^f_{\rm in}|\beta\rangle\,, \\ \lim_{t\to+\infty} \langle\alpha|\phi^f(t)|\beta\rangle &= \sqrt{Z}\langle\alpha|\phi^f_{\rm out}|\beta\rangle\,. \end{aligned} \tag{2.169}$$

Here $\sqrt{Z}$ must be the same for in/out fields, and equals $\langle 0|\phi(0)|p\rangle = \sqrt{Z}$, which is a p-independent constant due to Lorentz invariance. In fact, taking $|\beta\rangle = |0\rangle$ and $|\alpha\rangle = \int d\Omega_p\, \tilde{g}(p)|p\rangle$,

one has

$$\begin{aligned}\langle\alpha|\phi^f(t)|0\rangle &= \int d\Omega_p\,\tilde g(p)\langle p|\phi^f(t)|0\rangle = i\int d\Omega_p\,\langle p|\phi(0)|0\rangle\tilde g(p)\int d^3x\,f(x)^*\overset{\leftrightarrow}{\partial}_0 e^{ip\cdot x}\\ &= i\sqrt{Z}\int d^3x\,f(x)^*\overset{\leftrightarrow}{\partial}_0\int d\Omega_p\,\tilde g(p)e^{ip\cdot x}\,.\end{aligned} \tag{2.170}$$

But

$$g(x) = \int d\Omega_p\,\tilde g(p)e^{ip\cdot x} \tag{2.171}$$

is also a normalisable solution of the Klein-Gordon equation, and so

$$\langle\alpha|\phi^f(t)|0\rangle = i\sqrt{Z}\int d^3x\,f(x)^*\overset{\leftrightarrow}{\partial}_0 g(x) \tag{2.172}$$

is t-independent and so

$$\begin{aligned}\langle\alpha|\phi^f(t)|0\rangle &= i\sqrt{Z}\int d^3x\,f(x)^*\overset{\leftrightarrow}{\partial}_0 g(x) = \sqrt{Z_{\rm in,out}}\langle\alpha|\phi^f_{\rm in,out}|0\rangle\\ &= \sqrt{Z_{\rm in,out}}\int d\Omega_p\,\tilde g(p)\langle p|\phi^f_{\rm in,out}|0\rangle = i\sqrt{Z_{\rm in,out}}\int d\Omega_p\,\tilde g(p)\int d^3x\,f(x)^*\overset{\leftrightarrow}{\partial}_0 e^{ip\cdot x}\\ &= i\sqrt{Z_{\rm in,out}}\int d^3x\,f(x)^*\overset{\leftrightarrow}{\partial}_0 g(x)\,,\end{aligned} \tag{2.173}$$

having used $\langle p|\phi_{\rm in,out}(0)|0\rangle = 1$.

We now show the Lorentz invariance of $(f,g)\equiv\int d^3x\,f(x)^*\overset{\leftrightarrow}{\partial}_0 g(x)$, for any f,g. Rotation invariance is obvious. Consider a boost in direction 1,

$$x'^0 = \gamma(x^0-\beta x^1)\,,\qquad x'^1 = \gamma(x^1-\beta x^0)\,,\qquad x'^{2,3} = x^{2,3}\,. \tag{2.174}$$

It is easy to see that

$$d^3x = \frac{1}{\gamma}d^3x'\,,\qquad \frac{\partial}{\partial x^0} = \frac{\partial x'^0}{\partial x^0}\frac{\partial}{\partial x'^0} = \gamma\frac{\partial}{\partial x'^0}\,. \tag{2.175}$$

Changing now integration variables, $\vec x\to\vec x'$, and denoting $f_\Lambda(x)\equiv f(\Lambda x)$, we find

$$\begin{aligned}(f_\Lambda,g_\Lambda) = \int d^3x\,f(\Lambda x)^*\overset{\leftrightarrow}{\partial}_0 g(\Lambda x) &= \int d^3x\,f(\Lambda x)^*\frac{\overset{\leftrightarrow}{\partial}}{\partial x^0}g(\Lambda x) = \int d^3x'\,\frac{1}{\gamma}f(x')^*\gamma\frac{\overset{\leftrightarrow}{\partial}}{\partial x'^0}g(x')\\ &= \int d^3x\,f(x)^*\overset{\leftrightarrow}{\partial}_0 g(x) = (f,g)\,.\end{aligned} \tag{2.176}$$

If we now take f,g to be solutions of the Klein-Gordon equation, with (at least) f vanishing sufficiently fast at infinity, one has that (f,g) is time-independent. In fact,

$$\begin{aligned}\partial_0\int d^3x\,f(x)\overset{\leftrightarrow}{\partial}_0 g(x) &= \int d^3x\,\{f(x)[\partial_0^2 g(x)] - [\partial_0^2 f(x)]g(x)\}\\ &= \int d^3x\,f(x)[(\vec\nabla^{\,2}-m^2)g(x)] - [(\vec\nabla^{\,2}-m^2)f(x)]g(x)\\ &= \int d^3x\,\vec\nabla\cdot\Big\{f(x)[\vec\nabla g(x)] - [\vec\nabla f(x)]g(x)\Big\}\\ &= \lim_{R\to\infty}\int_{\partial B_R} d^2\vec\Sigma\cdot\Big\{f(x)[\vec\nabla g(x)] - [\vec\nabla f(x)]g(x)\Big\} = 0\,,\end{aligned} \tag{2.177}$$

where B_R is the ball of radius R. This result applies in particular if g is a free field and f is normalisable.

Reduction formula The asymptotic condition allows one to express S-matrix elements entirely in terms of vacuum expectation values of fields. Consider the matrix element ${}_{\rm out}\langle\beta|\alpha p\rangle_{\rm in}$, where α and β denote the remaining particles. One has

$$\begin{aligned}
{}_{\rm out}\langle\beta|\alpha p\rangle_{\rm in} &= {}_{\rm out}\langle\beta|a_{\rm in}(p)^\dagger|\alpha\rangle_{\rm in} \\
&= {}_{\rm out}\langle\beta|a_{\rm out}(p)^\dagger|\alpha\rangle_{\rm in} + {}_{\rm out}\langle\beta|a_{\rm in}(p)^\dagger - a_{\rm out}(p)^\dagger|\alpha\rangle_{\rm in} \\
&= {}_{\rm out}\langle\beta - p|\alpha\rangle_{\rm in} - i\int d^3x\, e^{-ip\cdot x} \overset{\leftrightarrow}{\partial}_0 \, {}_{\rm out}\langle\beta|\phi_{\rm in}(x) - \phi_{\rm out}(x)|\alpha\rangle_{\rm in}
\end{aligned} \tag{2.178}$$

where in the last passage we used the usual relation between free fields and creation operators,

$$a_{\rm in/out}(p) = i\int d^3x\, e^{ip\cdot x} \overset{\leftrightarrow}{\partial}_0 \, \phi_{\rm in/out}(x)\,, \qquad a_{\rm in/out}(p)^\dagger = -i\int d^3x\, e^{-ip\cdot x} \overset{\leftrightarrow}{\partial}_0 \, \phi_{\rm in/out}(x)\,, \tag{2.179}$$

and $|\beta - p\rangle_{\rm out}$ denotes the state with particle content β from which a particle of momentum p is removed (if at all present). In general one is interested in the case $\beta \neq \alpha$, so this disconnected term is not our main focus. We now use the t-independence of Eq. (2.179) together with the LSZ condition to write

$$\begin{aligned}
&{}_{\rm out}\langle\beta|\alpha p\rangle_{\rm in} - {}_{\rm out}\langle\beta - p|\alpha\rangle_{\rm in} \\
&= -i\lim_{x_0\to-\infty}\int d^3x\, e^{-ip\cdot x} \overset{\leftrightarrow}{\partial}_0 \, {}_{\rm out}\langle\beta|\phi_{\rm in}(x)|\alpha\rangle_{\rm in} + i\lim_{x_0\to+\infty}\int d^3x\, e^{-ip\cdot x} \overset{\leftrightarrow}{\partial}_0 \, {}_{\rm out}\langle\beta|\phi_{\rm out}(x)|\alpha\rangle_{\rm in} \\
&= -\frac{i}{\sqrt{Z}}\lim_{x_0\to-\infty}\int d^3x\, e^{-ip\cdot x} \overset{\leftrightarrow}{\partial}_0 \, {}_{\rm out}\langle\beta|\phi(x)|\alpha\rangle_{\rm in} + \frac{i}{\sqrt{Z}}\lim_{x_0\to+\infty}\int d^3x\, e^{-ip\cdot x} \overset{\leftrightarrow}{\partial}_0 \, {}_{\rm out}\langle\beta|\phi(x)|\alpha\rangle_{\rm in} \\
&= \frac{i}{\sqrt{Z}}\int d^4x\, \partial_0 \left\{ e^{-ip\cdot x} \overset{\leftrightarrow}{\partial}_0 \, {}_{\rm out}\langle\beta|\phi(x)|\alpha\rangle_{\rm in} \right\} .
\end{aligned} \tag{2.180}$$

Next, we exploit the fact that $e^{-ip\cdot x}$ is a solution of the Klein-Gordon equation to show that[17]

$$\begin{aligned}
&{}_{\rm out}\langle\beta|\alpha p\rangle_{\rm in} - {}_{\rm out}\langle\beta - p|\alpha\rangle_{\rm in} \\
&= \frac{i}{\sqrt{Z}}\int d^4x \left\{ e^{-ip\cdot x}\, \partial_0^2 \, {}_{\rm out}\langle\beta|\phi(x)|\alpha\rangle_{\rm in} - {}_{\rm out}\langle\beta|\phi(x)|\alpha\rangle_{\rm in} \partial_0^2 e^{-ip\cdot x} \right\} \\
&= \frac{i}{\sqrt{Z}}\int d^4x \left\{ e^{-ip\cdot x}\, \partial_0^2 \, {}_{\rm out}\langle\beta|\phi(x)|\alpha\rangle_{\rm in} - {}_{\rm out}\langle\beta|\phi(x)|\alpha\rangle_{\rm in} (\vec{\nabla}^2 - m^2) e^{-ip\cdot x} \right\} \\
&= \frac{i}{\sqrt{Z}}\int d^4x\, e^{-ip\cdot x} \left(\partial_0^2 - \vec{\nabla}^2 + m^2\right) {}_{\rm out}\langle\beta|\phi(x)|\alpha\rangle_{\rm in} \\
&= \frac{i}{\sqrt{Z}}\int d^4x\, e^{-ip\cdot x} \left(\Box + m^2\right) {}_{\rm out}\langle\beta|\phi(x)|\alpha\rangle_{\rm in} .
\end{aligned} \tag{2.181}$$

This is the essence of the reduction formula: particles get replaced by fields, with a suitable integro/differential operator acting on them. Writing $|\beta\rangle_{\rm out} = |\gamma p'\rangle_{\rm out}$, we now apply the same

[17] Here one should use a normalisable solution of the equation in order to drop boundary terms when using partial integration in space. Notice that boundary terms could not be dropped if one used partial integration in time since even a normalisable solution does not vanish at large times.

procedure to an out particle, and find

$$\begin{aligned}
&{}_{\rm out}\langle\beta|\phi(x)|\alpha\rangle_{\rm in} = {}_{\rm out}\langle\gamma p'|\phi(x)|\alpha\rangle_{\rm in} = {}_{\rm out}\langle\gamma|a_{\rm out}(p')\phi(x)|\alpha\rangle_{\rm in} \\
&= {}_{\rm out}\langle\gamma|a_{\rm out}(p')\phi(x) - \phi(x)a_{\rm in}(p')|\alpha\rangle_{\rm in} + {}_{\rm out}\langle\gamma|\phi(x)a_{\rm in}(p')|\alpha\rangle_{\rm in} \\
&= {}_{\rm out}\langle\gamma|a_{\rm out}(p')\phi(x) - \phi(x)a_{\rm in}(p')|\alpha\rangle_{\rm in} + {}_{\rm out}\langle\gamma|\phi(x)|\alpha - p'\rangle_{\rm in}\,.
\end{aligned} \tag{2.182}$$

The last term is again an uninteresting disconnected term. For the interesting part we have

$$\begin{aligned}
&{}_{\rm out}\langle\beta|\phi(x)|\alpha\rangle_{\rm in} - {}_{\rm out}\langle\gamma|\phi(x)|\alpha - p'\rangle_{\rm in} \\
&= i\int d^3y\, e^{ip\cdot y}\overset{\leftrightarrow}{\partial}{}^y_0\, {}_{\rm out}\langle\gamma|\phi_{\rm out}(y)\phi(x) - \phi(x)\phi_{\rm in}(y)|\alpha\rangle_{\rm in} \\
&= \lim_{y^0\to+\infty} i\int d^3y\, e^{ip\cdot y}\overset{\leftrightarrow}{\partial}{}^y_0\, {}_{\rm out}\langle\gamma|\phi_{\rm out}(y)\phi(x)|\alpha\rangle_{\rm in} - \lim_{y^0\to-\infty} i\int d^3y\, e^{ip\cdot y}\overset{\leftrightarrow}{\partial}{}^y_0\, {}_{\rm out}\langle\gamma|\phi(x)\phi_{\rm in}(y)|\alpha\rangle_{\rm in} \\
&= \lim_{y^0\to+\infty} \frac{i}{\sqrt{Z}}\int d^3y\, e^{ip\cdot y}\overset{\leftrightarrow}{\partial}{}^y_0\, {}_{\rm out}\langle\gamma|\phi(y)\phi(x)|\alpha\rangle_{\rm in} - \lim_{y^0\to-\infty} \frac{i}{\sqrt{Z}}\int d^3y\, e^{ip\cdot y}\overset{\leftrightarrow}{\partial}{}^y_0\, {}_{\rm out}\langle\gamma|\phi(x)\phi(y)|\alpha\rangle_{\rm in} \\
&= \frac{i}{\sqrt{Z}}\int d^4y\, \partial^y_0\big\{e^{ip\cdot y}\overset{\leftrightarrow}{\partial}{}^y_0\, {}_{\rm out}\langle\gamma|{\rm T}\{\phi(y)\phi(x)\}|\alpha\rangle_{\rm in}\big\}\,.
\end{aligned} \tag{2.183}$$

As before, we use integration by parts to get

$$\begin{aligned}
&{}_{\rm out}\langle\beta|\phi(x)|\alpha\rangle_{\rm in} - {}_{\rm out}\langle\gamma|\phi(x)|\alpha - p'\rangle_{\rm in} \\
&= \frac{i}{\sqrt{Z}}\int d^4y\, \partial^y_0\big\{e^{ip'\cdot y}\overset{\leftrightarrow}{\partial}{}^y_0\, {}_{\rm out}\langle\gamma|{\rm T}\{\phi(y)\phi(x)\}|\alpha\rangle_{\rm in}\big\} \\
&= \frac{i}{\sqrt{Z}}\int d^4y\, \big\{e^{ip'\cdot y}(\partial^y_0)^2\, {}_{\rm out}\langle\gamma|{\rm T}\{\phi(y)\phi(x)\}|\alpha\rangle_{\rm in} - {}_{\rm out}\langle\gamma|{\rm T}\{\phi(y)\phi(x)\}|\alpha\rangle_{\rm in}(\vec{\nabla}^2_y - m^2)e^{ip'\cdot y}\big\} \\
&= \frac{i}{\sqrt{Z}}\int d^4y\, e^{ip'\cdot y}(\Box_y + m^2)_{\rm out}\langle\gamma|{\rm T}\{\phi(y)\phi(x)\}|\alpha\rangle_{\rm in}\,.
\end{aligned} \tag{2.184}$$

The only difference between an incoming and an outgoing particle is the sign of the exponent in the phase factor. If we now assume for simplicity that $\alpha p \cap \gamma p' = \emptyset$, we have putting toghether the two results above

$${}_{\rm out}\langle\gamma p'|\alpha p\rangle_{\rm in} = \left(\frac{i}{\sqrt{Z}}\right)^2\int d^4x\, e^{-ip\cdot x}\int d^4y\, e^{ip'\cdot y}(\Box_x + m^2)(\Box_y + m^2)\, {}_{\rm out}\langle\gamma|{\rm T}\{\phi(y)\phi(x)\}|\alpha\rangle_{\rm in}\,. \tag{2.185}$$

One can now repeat the procedure for all the particles. Assuming $\{p'_1,\ldots,p'_{n'}\}\cap\{p_1,\ldots,p_n\} = \emptyset$, so that one does not have to worry about disconnected pieces, one finds the *LSZ reduction formula*

$$\begin{aligned}
&{}_{\rm out}\langle p'_1,\ldots,p'_{n'}|p_1,\ldots,p_n\rangle_{\rm in} \\
&\quad = \prod_{j=1}^{n}\int d^4x_j\, e^{-ip_j\cdot x_j}\left(\frac{\Box_{x_j} + m^2}{-i\sqrt{Z}}\right)\prod_{j'=1}^{n'}\int d^4y_{j'}\, e^{ip'_{j'}\cdot y_{j'}}\left(\frac{\Box_{y_{j'}} + m^2}{-i\sqrt{Z}}\right) \\
&\qquad\qquad \times\ \langle 0|{\rm T}\{\phi(y_1)\ldots\phi(y_{n'})\phi(x_1)\ldots\phi(x_n)\}|0\rangle\,.
\end{aligned} \tag{2.186}$$

A few comments are in order.

- The S-matrix is obtained from the Green's functions of the interacting fields,

$$G_n(x) = \langle 0|\mathrm{T}\{\phi(x_1)\dots\phi(x_n)\}|0\rangle\,. \tag{2.187}$$

- Green's functions are manifestly symmetric, manifestly implying crossing symmetry.
- The S-matrix is invariant under a field rescaling $\phi \to \sqrt{z}\phi$, since also the value of the matrix element between the vacuum and the one-particle states also gets rescaled, $\sqrt{Z} \to \sqrt{zZ}$.
- In the reduction formula, any local operator $\mathcal{O}(x)$ with $\sqrt{Z}_{\mathcal{O}} = \langle 0|\mathcal{O}(0)|p\rangle \neq 0$ can be used, provided this normalisation constant is used instead of $\sqrt{Z}$.

In momentum space, denoting

$$\begin{aligned} G_{n+n'}(y,x) &= \langle 0|\mathrm{T}\{\phi(y_1)\dots\phi(y_{n'})\phi(x_1)\dots\phi(x_n)\}|0\rangle\,, \\ (2\pi)^4\delta^{(4)}(p'-p)\tilde{G}_{n+n'}(-p',p) &= \prod_{j=1}^{n}\int d^4x_j e^{-ip_j\cdot x_j}\prod_{j'=1}^{n'}\int d^4y_{j'}e^{ip'_{j'}\cdot y_{j'}}G_{n+n'}(y,x)\,, \end{aligned} \tag{2.188}$$

we find

$$\begin{aligned} &{}_{\mathrm{out}}\langle p'_1,\dots,p'_{n'}|p_1,\dots,p_n\rangle_{\mathrm{in}} \\ &= (2\pi)^4\delta^{(4)}(p'-p)\lim_{p^2,p'^2\to m^2}\prod_{j=1}^{n}\left(\frac{p_j^2-m^2}{i\sqrt{Z}}\right)\prod_{j'=1}^{n'}\left(\frac{p'^2_{j'}-m^2}{i\sqrt{Z}}\right)\tilde{G}_{n+n'}(-p',p)\,. \end{aligned} \tag{2.189}$$

This shows that the S-matrix elements are the residues of the multi-poles of momentum-space Green's functions at $p_j^2, p'^2_{j'} \to m^2$, i.e., as the external momenta go on-shell for physical values of the masses. The factors in front of the n-point function are the inverses of $\sqrt{Z}$ times free propagators D_{free}. As we showed above, in the on-shell limit the full propagator is Z times the free propagator. The reduction procedure then boils down to stripping a full unrenormalised propagator D_{u} and multiplying by $\sqrt{Z}$ for each external line; or stripping a full renormalised propagator $D_{\mathrm{r}} = D_{\mathrm{u}}/Z$ and further dividing by $\sqrt{Z}$ for each external line.

Perturbation theory The discussion above provides more solid ground for scattering theory (in particular clarifying the origin of the $\sqrt{Z}$ factors), but does not really help frm the point of view of calculations. To this end, one has to set up again some approximation scheme to compute G_n, and perturbation theory is the first thing that comes to mind.

In the discussion above we did not say much about how the fields ϕ are constructed. We now assume that they are canonically quantised fields. By construction, also $\phi_{\mathrm{in,out}}$ and $\pi_{\mathrm{in,out}} = \dot{\phi}_{\mathrm{in,out}}$ obey canonical commutation relations. We then look for a unitary transformation $U(t)$ connecting the interacting field and momentum, ϕ and π, and the free field and momentum, ϕ_{in} and π_{in},

$$\phi(t) = U(t)^\dagger\phi_{\mathrm{in}}(t)U(t)\,, \qquad \pi(t) = U(t)^\dagger\pi_{\mathrm{in}}(t)U(t)\,. \tag{2.190}$$

Being free canonical fields, $\phi_{\rm in}$ and $\pi_{\rm in}$ obey[18]

$$\begin{aligned}\dot\phi_{\rm in}(x) &= i[H_{\rm in}(\phi_{\rm in},\pi_{\rm in}),\phi_{\rm in}(x)]\,,\\ \dot\pi_{\rm in}(x) &= i[H_{\rm in}(\phi_{\rm in},\pi_{\rm in}),\pi_{\rm in}(x)]\,,\end{aligned} \tag{2.191}$$

with

$$H_{\rm in}(\phi_{\rm in},\pi_{\rm in}) = \frac{1}{2}\int d^3x\left\{\pi_{\rm in}^2 + \vec\nabla\phi_{\rm in}^2 + m^2\phi_{\rm in}^2\right\}. \tag{2.192}$$

For the interacting (or Heisenberg) field instead

$$\begin{aligned}\dot\phi(x) &= i[H(\phi,\pi),\phi(x)]\,,\\ \dot\pi(x) &= i[H(\phi,\pi),\pi(x)]\,.\end{aligned} \tag{2.193}$$

Finally, let

$$H(\phi,\pi) = H_{\rm in}(\phi,\pi) + [H(\phi,\pi) - H_{\rm in}(\phi,\pi)] \equiv H_{\rm in}(\phi,\pi) + H_I(\phi,\pi)\,. \tag{2.194}$$

Taking now the time derivative of $\phi_{\rm in}(t)$ we find

$$\begin{aligned}\dot\phi_{\rm in}(t) &= \tfrac{\partial}{\partial t}[U(t)\phi(t)U(t)^\dagger]\\ &= \dot U(t)\phi(t)U(t)^\dagger - U(t)\phi(t)U(t)^\dagger\dot U(t)U(t)^\dagger + U(t)\dot\phi(t)U(t)^\dagger\\ &= [\dot U(t)U(t)^\dagger,\phi_{\rm in}(t)] + iU(t)[H(\phi(t),\pi(t)),\phi(t)]U(t)^\dagger\\ &= [\dot U(t)U(t)^\dagger,\phi_{\rm in}(t)] + i[H(\phi_{\rm in}(t),\pi_{\rm in}(t)),\phi_{\rm in}(t)]\\ &= i[H_{\rm in}(\phi_{\rm in},\pi_{\rm in}),\phi_{\rm in}(t)] + [\dot U(t)U(t)^\dagger + iH_I(\phi_{\rm in}(t),\pi_{\rm in}(t)),\phi_{\rm in}(t)]\\ &= \dot\phi_{\rm in}(t) + [\dot U(t)U(t)^\dagger + iH_I(\phi_{\rm in}(t),\pi_{\rm in}(t)),\phi_{\rm in}(t)]\,.\end{aligned} \tag{2.195}$$

An identical calculation shows also that

$$\dot\pi_{\rm in}(t) = \dot\pi_{\rm in}(t) + [\dot U(t)U(t)^\dagger + iH_I(\phi_{\rm in}(t),\pi_{\rm in}(t)),\pi_{\rm in}(t)]\,. \tag{2.196}$$

As a consequence

$$\frac{\delta}{\delta\phi_{\rm in}(t,\vec x)}[\dot U(t)U(t)^\dagger + iH_I(\phi_{\rm in}(t),\pi_{\rm in}(t))] = \frac{\delta}{\delta\pi_{\rm in}(t,\vec x)}[\dot U(t)U(t)^\dagger + iH_I(\phi_{\rm in}(t),\pi_{\rm in}(t))] = 0\,, \tag{2.197}$$

meaning that

$$i\dot U(t)U(t)^\dagger = H_I(\phi_{\rm in}(t),\pi_{\rm in}(t)) + \mathcal{E}_0(t) \equiv H_I'(\phi_{\rm in}(t),\pi_{\rm in}(t)) \equiv V_I(t) + \mathcal{E}_0(t) \equiv V_I'(t)\,, \tag{2.198}$$

where $\mathcal{E}_0(t)$ is a c-number function of time.

To find out what $U(t)$ looks like, define $\mathcal{U}(t,t') = U(t)U(t')^\dagger$, which obeys the obvious boundary condition $\mathcal{U}(t,t) = \mathbf{1}$, and the differential equation

$$\partial_t\mathcal{U}(t,t') = -iV_I'(t)\mathcal{U}(t,t')\,. \tag{2.199}$$

[18]Notice that the temporal evolution of $\phi_{\rm in}$ is governed by $H(\phi,\pi)$,

$$\begin{aligned}\dot\phi_{\rm in}(x) &= i[H(\phi,\pi),\phi_{\rm in}(x)]\,,\\ \dot\pi_{\rm in}(x) &= i[H(\phi,\pi),\pi_{\rm in}(x)]\,,\end{aligned}$$

which means that $H(\phi,\pi) = H_{\rm in}(\phi_{\rm in},\pi_{\rm in})$ – but not $H(\phi_{\rm in},\pi_{\rm in}) = H_{\rm in}(\phi_{\rm in},\pi_{\rm in})$!

We already know the solution of this equation

$$\mathcal{U}(t,t') = U(t)U(t')^\dagger = \mathrm{Texp}\left\{-i\int_{t'}^{t} d\tau V_I'(\tau)\right\} = \mathrm{Texp}\left\{-i\int_{t'}^{t} d\tau V_I(\tau)\right\} e^{-i\int_{t'}^{t} d\tau \mathcal{E}_0(\tau)}\,. \quad (2.200)$$

We will not really need $U(t)$ itself. Plugging this into Green's function (taking $t \geq \max_i t_i \geq -t$)

$$\begin{aligned}
&\langle 0|\mathrm{T}\{\phi(x_1)\phi(x_2)\dots\phi(x_n)\}|0\rangle \\
&= \langle 0|\mathrm{T}\{U(t_1)^\dagger\phi_{\mathrm{in}}(x_1)U(t_1)U(t_2)^\dagger\phi_{\mathrm{in}}(x_2)U(t_2)\dots U(t_n)^\dagger\phi_{\mathrm{in}}(x_n)U(t_n)\}|0\rangle \\
&= \langle 0|U(t)^\dagger\mathrm{T}\{\mathcal{U}(t,t_1)\phi_{\mathrm{in}}(x_1)\mathcal{U}(t_1,t_2)\phi_{\mathrm{in}}(x_2)\dots\mathcal{U}(t_{n-1},t_n)^\dagger\phi_{\mathrm{in}}(x_n)\mathcal{U}(t_n,-t))\}U(-t)|0\rangle \\
&= \langle 0|U(t)^\dagger\mathrm{T}\{\phi_{\mathrm{in}}(x_1)\dots\phi_{\mathrm{in}}(x_n)\mathrm{exp}\left\{-i\int_{-t}^{t} d\tau V_I'(\tau)\right\}\}U(-t)|0\rangle \\
&= \lim_{t\to\infty}\langle 0|U(t)^\dagger\mathrm{T}\{\phi_{\mathrm{in}}(x_1)\dots\phi_{\mathrm{in}}(x_n)\mathrm{exp}\left\{-i\int_{-t}^{t} d\tau V_I'(\tau)\right\}\}U(-t)|0\rangle
\end{aligned} \quad (2.201)$$

We now show that

$$\begin{aligned}
&\lim_{t\to\infty}\langle 0|U(t)^\dagger\mathrm{T}\{\phi_{\mathrm{in}}(x_1)\dots\phi_{\mathrm{in}}(x_n)\mathrm{exp}\left\{-i\int_{-t}^{t} d\tau V_I'(\tau)\right\}\}U(-t)|0\rangle \\
&= \lim_{t\to\infty}\langle 0|\mathrm{T}\{\phi_{\mathrm{in}}(x_1)\dots\phi_{\mathrm{in}}(x_n)\mathrm{exp}\left\{-i\int_{-t}^{t} d\tau V_I'(\tau)\right\}\}|0\rangle\langle 0|U(t)^\dagger|0\rangle\langle 0|U(-t)|0\rangle\,.
\end{aligned} \quad (2.202)$$

To do this, consider for a generic particle content α

$$\begin{aligned}
{}_{\mathrm{in}}\langle p\alpha|U(-t)|0\rangle &= -i\int d^3x\, e^{ip\cdot x}\overset{\leftrightarrow}{\partial}_0\ {}_{\mathrm{in}}\langle\alpha|\phi_{\mathrm{in}}(x)U(-t)|0\rangle \\
&= -i\int d^3x\, e^{ip\cdot x}\overset{\leftrightarrow}{\partial}_0\ {}_{\mathrm{in}}\langle\alpha|U(x^0)\phi(x)U(x^0)^\dagger U(-t)|0\rangle \\
&= -i\int d^3x\ {}_{\mathrm{in}}\langle\alpha|U(x^0)[e^{ip\cdot x}\overset{\leftrightarrow}{\partial}_0\phi(x)]U(x^0)^\dagger U(-t)|0\rangle \\
&\quad - i\int d^3x\, e^{ip\cdot x}{}_{\mathrm{in}}\langle\alpha|[\dot{U}(x^0)U(x^0)^\dagger, U(x^0)\phi(x)U(x^0)^\dagger]U(-t)|0\rangle
\end{aligned} \quad (2.203)$$

Setting now $x^0 = -t$, since V_I depend only on ϕ_{in} but not on π_{in}, we have

$$\begin{aligned}
{}_{\mathrm{in}}\langle p\alpha|U(-t)|0\rangle &= -i\int d^3x\ {}_{\mathrm{in}}\langle\alpha|U(-t)[e^{ip\cdot x}\overset{\leftrightarrow}{\partial}_0\phi(x)]|0\rangle \\
&\quad - i\int d^3x\, e^{ip\cdot x}\ {}_{\mathrm{in}}\langle\alpha|[-iV_I(-t),\phi_{\mathrm{in}}(x)]U(-t)|0\rangle \\
&= -i\int d^3x\ {}_{\mathrm{in}}\langle\alpha|U(-t)[e^{ip\cdot x}\overset{\leftrightarrow}{\partial}_0\phi(x)]|0\rangle \\
&\underset{t\to\infty}{\to} -i\int d^3x\ {}_{\mathrm{in}}\langle\alpha|U(-t)[e^{ip\cdot x}\overset{\leftrightarrow}{\partial}_0\sqrt{Z}\phi_{\mathrm{in}}(x)]|0\rangle = \sqrt{Z}\ {}_{\mathrm{in}}\langle\alpha|U(-t)a(p)_{\mathrm{in}}|0\rangle = 0\,.
\end{aligned} \quad (2.204)$$

An entirely analogous result holds for ${}_{\mathrm{out}}\langle p\alpha|U(t)|0\rangle$ in the limit $t\to\infty$. It follows then that

$$\lim_{t\to\infty} U(\pm t)|0\rangle = \lambda_\pm|0\rangle\,, \quad (2.205)$$

for some constants $\lambda_\pm = \lim_{t\to\infty}\langle 0|U(\pm t)|0\rangle$. But then

$$\begin{aligned}
&\lim_{t\to\infty}\langle 0|U(t)^\dagger|0\rangle\langle 0|U(-t)|0\rangle = \lim_{t\to\infty}\langle 0|U(-t)|0\rangle\langle 0|U(t)^\dagger|0\rangle \\
&= \lim_{t\to\infty}\langle 0|U(-t)U(t)^\dagger|0\rangle = \lim_{t\to\infty}\langle 0|U(t)U(-t)^\dagger|0\rangle^* \\
&= \lim_{t\to\infty}\langle 0|\mathrm{Texp}\left\{-i\int_{-t}^{t} d\tau V_I'(\tau)\right\}|0\rangle^*
\end{aligned} \tag{2.206}$$

With this result we complete the derivation of the *Gell-Mann–Low formula*,

$$\begin{aligned}
\langle 0|\mathrm{T}\{\phi(x_1)\phi(x_2)\dots\phi(x_n)\}|0\rangle &= \lim_{t\to\infty}\frac{\langle 0|\mathrm{T}\{\phi_{\mathrm{in}}(x_1)\dots\phi_{\mathrm{in}}(x_n)\mathrm{exp}\left\{-i\int_{-t}^{t} d\tau V_I'(\tau)\right\}\}|0\rangle}{\langle 0|\mathrm{Texp}\left\{-i\int_{-t}^{t} d\tau V_I'(\tau)\right\}|0\rangle} \\
&= \frac{\langle 0|\mathrm{T}\{\phi_{\mathrm{in}}(x_1)\dots\phi_{\mathrm{in}}(x_n)\mathrm{exp}\left\{-i\int_{-\infty}^{+\infty} d\tau V_I'(\tau)\right\}\}|0\rangle}{\langle 0|\mathrm{Texp}\left\{-i\int_{-\infty}^{+\infty} d\tau V_I'(\tau)\right\}|0\rangle} \\
&= \frac{\langle 0|\mathrm{T}\{\phi_{\mathrm{in}}(x_1)\dots\phi_{\mathrm{in}}(x_n)\mathrm{exp}\left\{-i\int_{-\infty}^{+\infty} d\tau V_I(\tau)\right\}\}|0\rangle}{\langle 0|\mathrm{Texp}\left\{-i\int_{-\infty}^{+\infty} d\tau V_I(\tau)\right\}|0\rangle},
\end{aligned} \tag{2.207}$$

where in the last passage we dropped the contribution of $\mathcal{E}_0$ since it cancels out anyway. This is the starting point of the perturbative expansion:

$$\begin{aligned}
&\langle 0|\mathrm{T}\{\phi(x_1)\phi(x_2)\dots\phi(x_n)\}|0\rangle \\
&= \frac{\sum_N \frac{(-i)^N}{N!}\langle 0|\mathrm{T}\{\phi_{\mathrm{in}}(x_1)\dots\phi_{\mathrm{in}}(x_n)\int_{-\infty}^{+\infty} d\tau_1 V_I(\tau_1)\dots\int_{-\infty}^{+\infty} d\tau_N V_I(\tau_N)\}|0\rangle}{\sum_M \frac{(-i)^M}{M!}\langle 0|\mathrm{T}\{\int_{-\infty}^{+\infty} d\tau_1 V_I(\tau_1)\dots\int_{-\infty}^{+\infty} d\tau_M V_I(\tau_M)\}|0\rangle},
\end{aligned} \tag{2.208}$$

to which one applies the usual machinery of Feynman diagrams. The numerator equas all diagrams (connected and disconnected) with N external sources, corresponding to a vertex $J\phi$. The denominator equals the sum vacuum-to-vacuum diagrams, and so cancels out disconnected vacuum bubbles in the numerator. Putting together the LSZ reduction formula and the Gell-Mann–Low formula we find (for $\{p_1',\dots,p_{n'}'\}\cap\{p_1,\dots,p_n\}=\emptyset$)

$$\begin{aligned}
&{}_{\mathrm{out}}\langle p_1',\dots,p_{n'}'|p_1,\dots,p_n\rangle_{\mathrm{in}} \\
&= (2\pi)^4\delta^{(4)}(p'-p)\lim_{p^2,p'^2\to m^2}\prod_{j=1}^{n}\left(\frac{p_j^2-m^2}{i\sqrt{Z}}\right)\prod_{j'=1}^{n'}\left(\frac{p_{j'}'^2-m^2}{i\sqrt{Z}}\right) \\
&\qquad\qquad \times\frac{\{\sum\text{diagrams with } n'+n \text{ legs } (-p',p)\}}{\{\sum\text{vacuum-to-vacuum diagrams}\}} \\
&= (2\pi)^4\delta^{(4)}(p'-p)Z^{-\frac{n+n'}{2}}\{\sum\text{connected amputated diagrams with } n'+n \text{ legs } (-p',p)\} \\
&= (2\pi)^4\delta^{(4)}(p'-p)Z^{\frac{n+n'}{2}}\{\sum\text{connected fully amputated diagrams with } n'+n \text{ legs } (-p',p)\}.
\end{aligned} \tag{2.209}$$

Since for scalar particles the wave function read $u(p)=\bar{u}(p)=1$, the $(p^2-m^2)/i\times 1$ factors correspond to removing the last free propagator from each external line and replacing it with the

particles' wave functions. Including the factor $1/\sqrt{Z}$ one precisely recovers the rules discussed before when using adiabatic switching.

As we already know, this expansion needs renormalisation. After renormalising to the (physical) mass $m_B = Z_m m$, in order for the pole of the two-point function to be at the right place, one still has a (possibly divergent) residue Z in the propagator, and further divergences associated with the vertices. With $E = n + n'$ lines one has for vertices and internal lines the relation $E = \sum_k kV_k - 2I$, and so the Z factors coming from the reduction formula read

$$Z^{\frac{n+n'}{2}} = Z^{\frac{E}{2}} = Z^{-I+\frac{\sum_k kV_k}{2}} \,. \tag{2.210}$$

Introducing the renormalised couplings $\lambda_{Bk} = Z_k \lambda_k$, one has an overall factor

$$Z^{-I+\frac{\sum_k kV_k}{2}} \prod_k Z_k^{V_k} = Z^{-I} \prod_k \left(Z_k Z^{\frac{k}{2}} \right)^{V_k} \,, \tag{2.211}$$

where Z^{-I} takes care of renormalising (fully dressed) internal lines, and the combinations $Z_k Z^{\frac{k}{2}}$ take care of renormalising the vertex functions.

References

- Wightman's axioms and its consequences are nicely described in

  F. Strocchi, "An introduction to the non-perturbative foundations of quantum field theory".

- The treatment of in and out fields, and the derivation of the LSZ reduction formula and of the Gell-Mann–Low formula is adapted from

  J.D. Bjorken, S.D. Drell, "Relativistic quantum fields"

3 Path-integral techniques

Green's functions can be represented in terms of path integrals as follows,

$$G_n(x_1, \ldots, x_n) = \langle 0 | \mathrm{T}\{\hat{\phi}(x_1) \ldots \hat{\phi}(x_n)\} | 0 \rangle = \frac{\int [\mathrm{D}\phi]\, e^{iS[\phi]} \phi(x_1) \ldots \phi(x_n)}{\int [\mathrm{D}\phi]\, e^{iS[\phi]}} \,, \tag{3.212}$$

where formally[19]

$$\int [\mathrm{D}\phi] = \int_{\substack{\phi(+\infty,\vec{x}) \\ = \phi(-\infty,\vec{x})}} \prod_x d\phi(x) \,. \tag{3.213}$$

[19] This should be understood as the limit of integrals over a discrete lattice, i.e.,

$$\int [\mathrm{D}\phi] = \lim_{T,L\to\infty} \lim_{N_t,N_s\to\infty} \int \prod_{i_{1,2,3}=-N_s,\ldots,N_s} \left\{ \prod_{i_t=-N_t,\ldots,N_t} d\phi\left(i_t \tfrac{T}{N_t}, \vec{\imath} \tfrac{L}{N_s} \right) \right\} \delta\left(\phi\left(T, \vec{\imath} \tfrac{L}{N_s} \right) - \phi\left(-T, \vec{\imath} \tfrac{L}{N_s} \right) \right) \,.$$

The G_n can be obtained by functional differentiation from the generating functional $Z[J]$,

$$Z[J] \equiv \int [\mathrm{D}\phi]\, e^{iS[\phi]+iJ\cdot\phi}\,, \qquad J\cdot\phi \equiv \int d^4x\, J(x)\phi(x)\,. \tag{3.214}$$

In fact, defining functional derivatives via the relation

$$\int d^4x\, \frac{\delta F[J]}{\delta J(x)} q(x) \equiv \lim_{\epsilon\to 0} \frac{F[J+\epsilon q]-F[J]}{\epsilon}\,, \tag{3.215}$$

where $q = q(x)$ is arbitrary, we have

$$G_n(x_1,\ldots,x_n) = \frac{1}{Z[0]}\left(-i\frac{\delta}{\delta J(x_1)}\right)\ldots\left(-i\frac{\delta}{\delta J(x_n)}\right) Z[J]\Big|_{J=0}\,. \tag{3.216}$$

Notice that in operator language

$$\begin{aligned}\frac{Z[J]}{Z[0]} &= \langle 0|\mathrm{Texp}\{iJ\cdot\hat\phi\}|0\rangle = \langle 0|\mathrm{Texp}\left\{i\int d^4x\, J(x)\hat\phi(x)\right\}|0\rangle \\ &= \langle 0|\mathrm{Texp}\left\{i\int dt\, e^{iHt}\left[\int d^3x\, J(t,\vec x)\hat\phi(0,\vec x)\right]e^{-iHt}\right\}|0\rangle\,.\end{aligned} \tag{3.217}$$

For a time-dependent Hamiltonian

$$H_J(t) \equiv H - \int d^3x\, J(t,\vec x)\hat\phi(0,\vec x)\,, \tag{3.218}$$

the temporal evolution operator $\mathcal{U}(t,t')$, obeying

$$\frac{\partial}{\partial t}\mathcal{U}_J(t,t') = -iH_J(t)\mathcal{U}(t,t')\,, \qquad \mathcal{U}_J(t,t) = \mathbf{1}\,, \tag{3.219}$$

reads

$$\begin{aligned}\mathcal{U}_J(t,t') &= \mathrm{Texp}\left\{-i\int_{t'}^{t} dt\, H_J(t)\right\} = \mathrm{Texp}\left\{-i\int_{t'}^{t} dt\,\left[H - \int d^3x\, J(t,\vec x)\hat\phi(0,\vec x)\right]\right\} \\ &= e^{-iHt}\,\mathrm{Texp}\left\{i\int_{t'}^{t} dt\, e^{iHt}\left[\int d^3x\, J(t,\vec x)\hat\phi(0,\vec x)\right]e^{-iHt}\right\}\,.\end{aligned} \tag{3.220}$$

In fact, the first expression clearly obeys the differential equation and boundary condition in Eq. (3.219), while for the last expression

$$\begin{aligned}&\frac{\partial}{\partial t} e^{-iHt}\,\mathrm{Texp}\left\{i\int_{t'}^{t} dt\int d^3x\, J(t,\vec x)e^{iHt}\hat\phi(0,\vec x)e^{-iHt}\right\} \\ &= -ie^{-iHt}\left(H - \int d^3x\, J(t,\vec x)e^{iHt}\hat\phi(0,\vec x)e^{-iHt}\right) \\ &\quad\times \mathrm{Texp}\left\{i\int_{t'}^{t} dt\int d^3x\, J(t,\vec x)e^{iHt}\hat\phi(0,\vec x)e^{-iHt}\right\} \\ &= -i\left(H - \int d^3x\, J(t,\vec x)\hat\phi(0,\vec x)\right) \\ &\quad\times e^{-iHt}\mathrm{Texp}\left\{i\int_{t'}^{t} dt\int d^3x\, J(t,\vec x)e^{iHt}\hat\phi(0,\vec x)e^{-iHt}\right\} \\ &= -iH_J(t)e^{-iHt}\mathrm{Texp}\left\{i\int_{t'}^{t} dt\int d^3x\, J(t,\vec x)e^{iHt}\hat\phi(0,\vec x)e^{-iHt}\right\}\,,\end{aligned} \tag{3.221}$$

so the two expressions muts be equal due to uniqueness of the solution of the initial-value problem. Then, since $H|0\rangle = 0$, we have

$$\langle 0|\mathcal{U}_J(+\infty,-\infty)|0\rangle = \langle 0|\mathrm{Texp}\left\{ i\int dt\, e^{iHt}\left[\int d^3x\, J(t,\vec{x})\hat{\phi}(0,\vec{x})\right] e^{-iHt}\right\}|0\rangle = \frac{Z[J]}{Z[0]}\,, \quad (3.222)$$

i.e., $Z[J]/Z[0]$ is the amplitude for the transition from the vacuum state (i.e., $|0\rangle$) at $t=-\infty$ to the vacuum state at $t=\infty$ in the presence of an external source J. This will be used later when giving a physical interpretation to the generating functional.

Perturbative expansion∗ The path integral representation is particularly suited for a perturbative expansion, and makes the bookkeeping transparent. Separating the Lagrangian into a free, quadratic part $\mathscr{L}_0$ and an interaction part, $\mathscr{L} = \mathscr{L}_0 + \mathscr{L}_I$, and the action accordingly, $S = S_0 + S_I$, one has

$$\begin{aligned} Z[J] &= \int [\mathrm{D}\phi]\, e^{i(S_0[\phi]+S_I[\phi])+iJ\cdot\phi} = \int [\mathrm{D}\phi]\, e^{iS_0[\phi]+iJ\cdot\phi}\sum_{n=0}^{\infty}\frac{i^n}{n!}S_I[\phi]^n \\ &= \sum_{n=0}^{\infty}\frac{i^n}{n!}S_I\left[-i\tfrac{\delta}{\delta J}\right]^n\int [\mathrm{D}\phi]\, e^{iS_0[\phi]+iJ\cdot\phi} = e^{iS_I\left[-i\frac{\delta}{\delta J}\right]}\int [\mathrm{D}\phi]\, e^{iS_0[\phi]+iJ\cdot\phi} \\ &= e^{iS_I\left[-i\frac{\delta}{\delta J}\right]}Z_0[J]\,. \end{aligned} \quad (3.223)$$

The free generating functional Z_0 can be computed explicitly. Since the quadratic part of the action reads in general

$$S_0 = \frac{1}{2}\int d^4x\int d^4y\,\phi(x)K(x,y)\phi(y) + \int d^4x\, c(x)\phi(x) = \frac{1}{2}\phi^T\cdot K\cdot\phi + c\cdot\phi\,, \quad (3.224)$$

for some kernel K and function c, one has

$$\begin{aligned} S_0 + J\cdot\phi &= \tfrac{1}{2}\phi^T\cdot K\cdot\phi + (J+c)\cdot\phi \\ &= \frac{1}{2}[\phi + K^{-1}(J+c)]^T\cdot K\cdot[\phi+K^{-1}(J+c)] - \frac{1}{2}(J+c)^T\cdot K^{-1}\cdot(J+c)\,, \end{aligned} \quad (3.225)$$

and so performing the Gaussian integral leads to

$$\frac{Z_0[J]}{Z_0[0]} = \frac{e^{-\frac{i}{2}(J+c)^T\cdot K^{-1}\cdot(J+c)}}{e^{-\frac{i}{2}c^T\cdot K^{-1}\cdot c}} = e^{-\frac{i}{2}J^T\cdot K^{-1}\cdot J - iJ^T\cdot K^{-1}\cdot c}\,. \quad (3.226)$$

The quantity $Z_0[0]$ is just a constant and plays no role. The expectation value of the field reads

$$\langle\phi\rangle_0 = \frac{1}{i}\frac{\delta}{\delta J(x)}\frac{Z_0[J]}{Z_0[0]}\bigg|_{J=0} = -K^{-1}c\,. \quad (3.227)$$

Then

$$\frac{Z_0[J]}{Z_0[0]}e^{-iJ\langle\phi\rangle_0} = \int [\mathrm{D}\phi]\, e^{iS_0[\phi]+iJ\cdot(\phi-\langle\phi\rangle_0)} = e^{-\frac{i}{2}J^T\cdot K^{-1}\cdot J} \quad (3.228)$$

is the generating functional of the correlation functions of $\bar{\phi} = \phi - \langle\phi\rangle_0$. The free two-point function of this field reads

$$\langle\bar{\phi}(x)\bar{\phi}(y)\rangle_0 = \langle\phi(x)\phi(y)\rangle_0 - \langle\phi(x)\rangle_0\langle\phi(y)\rangle_0 = (-i)^{-2}(-i)K^{-1} = iK^{-1}\,. \quad (3.229)$$

In the standard case $K = -(\Box + m^2) + i\epsilon$, so in momentum space

$$\widetilde{iK^{-1}} = \frac{i}{p^2 - m^2 + i\epsilon}\,. \tag{3.230}$$

The perturbative expansion of the generating functional is obtained by expanding $e^{iS_I\left[-i\frac{\delta}{\delta J}\right]}$ in Eq. (3.223) in powers of the coupling and acting with the result on $Z_0[J]$ from Eq. (3.228). For example, for a ϕ^4 interaction

$$e^{iS_I\left[-i\frac{\delta}{\delta J}\right]} = \sum_{n=0}^{\infty} \frac{i^n}{n!}\left(\frac{\lambda}{4!}\right)^n \int d^4x_1\, \frac{1}{i}\frac{\delta^4}{\delta J(x_1)^4} \cdots \int d^4x_n\, \frac{1}{i}\frac{\delta^4}{\delta J(x_n)^4}\,. \tag{3.231}$$

Each derivative removes a source factor J, leaving a sum of products of factors $K^{-1}(x_i, x_j)$ and $K^{-1}(x_i, y_k)J(y_k)$, integrated over x_i and y_k. This can be represented graphically by associating each x_i with an interaction vertex with four lines coming out of it, each y_k with a source term where a single line ends, and each K^{-1} with a line. For a fixed number E of sources J, and at order V in the perturbative expansion, the total number of K^{-1} factors (i.e., of lines) appearing is $E + I$, with E equal to the number of K^{-1} factors paired ot a source (i.e., external lines), and I equal to the number of K^{-1}s not paired to a source (i.e., internal lines). The number of derivatives appearing in the procedure is equal to $E + 2I$, since two are required to produce an internal line, and one is required to produce an external line; but it is also equal to $4V$, hence $E + 2I = 4V$.

Going over to momentum space [see Eq. (3.230)],

$$\begin{aligned} iK^{-1}(x,y) &= \int \frac{d^4p}{(2\pi)^4}\, e^{-ip\cdot(x-y)} \frac{i}{p^2 - m^2 + i\epsilon} = \int \frac{d^4p}{(2\pi)^4}\, e^{-ip\cdot(x-y)} \tilde{D}_0(p)\,, \\ J(x) &= \int \frac{d^4q}{(2\pi)^4}\, e^{-iq\cdot x} \tilde{J}(q)\,, \end{aligned} \tag{3.232}$$

one associates a momentum p with each internal or external line, and integration over the position of the vertices leads to momentum-conserving delta functions. Since one of these simply expresses conservation of total momentum, i.e., $\sum_k q_k = 0$ with the sum extending over the sources, one is left with a number of momentum integrals equal to $I - V + 1 \equiv L$. This is by definition the number of *loops* of the diagram.

The formulation of renormalised perturbation theory is straightforward in the path integral formalism. In fact, focussing for simplicity on the ϕ^4 scalar theory,

$$\mathscr{L}(\phi) = \frac{1}{2}(\partial_\mu \phi_B)^2 - \frac{1}{2}m_B^2\phi_B^2 + \frac{\lambda_B}{4!}\phi_B^4\,, \qquad S[\phi] = \int d^4x\, \mathscr{L}(\phi)\,, \tag{3.233}$$

one first changes variables to $\phi_B = \sqrt{Z}\phi$, so that

$$Z[J] = \int [\mathrm{D}\phi_B]\, e^{iS[\phi_B] + iJ\cdot\phi_B} = \int [\mathrm{D}\phi]\, e^{iS[\sqrt{Z}\phi] + i\sqrt{Z}J\cdot\phi}\,, \tag{3.234}$$

up to an irrelevant proportionality factor, and then sets $m_B^2 = Z_m m^2$ and $\lambda_B = Z_\lambda \lambda$ and splits[20]

$$\begin{aligned}
\mathscr{L}(\sqrt{Z}\phi) &= \frac{Z}{2}(\partial_\mu\phi)^2 - \frac{Z}{2}Z_m m^2\phi^2 + \frac{\lambda Z_\lambda Z^2}{4!}\phi^4 = \mathscr{L}_0(\phi) + \mathscr{L}_I(\phi) + \mathscr{L}_{\text{c.t.}}(\phi)\,, \\
\mathscr{L}_0(\phi) &= \frac{1}{2}(\partial_\mu\phi)^2 - \frac{1}{2}m^2\phi^2\,, \\
\mathscr{L}_I(\phi) &= \frac{\lambda}{4!}\phi^4\,, \\
\mathscr{L}_{\text{c.t.}}(\phi) &= (Z-1)\frac{1}{2}\left[(\partial_\mu\phi)^2 - m^2\phi^2\right] - (Z_m - 1)Zm^2\frac{1}{2}\phi^2 + \frac{\lambda(Z_\lambda Z^2 - 1)}{4!}\phi^4\,.
\end{aligned} \tag{3.235}$$

The free Lagrangean $\mathscr{L}_0(\phi)$ has the same form as the free part of the initial Lagrangean, but it contains the renormalised field ϕ and renormalised mass m, and is used to define the free propagator to be employed in the perturbative expansion. The interaction part of the Lagrangean is split into an interaction part proper, $\mathscr{L}_I(\phi)$, identical in form to the original interaction Lagrangean but depending on ϕ and on the renormalised coupling λ, and a counterterm Lagrangean, $\mathscr{L}_{\text{c.t.}}(\phi)$, which contains all the renormalisation constants. In practice, the coefficients $C_1 = Z - 1$, $C_2 = (Z_m - 1)Zm^2$, and $C_3 = (Z_\lambda Z^2 - 1)\lambda$ are determined at each perturbative order by imposing suitable renormalisation conditions [see Eqs. (1.60) and (1.61) and the subsequent discussion], and incidentally cancel out the divergences appearing in loop diagrams. The treatment of $\mathscr{L}_{\text{c.t.}}(\phi)$ as an interaction Lagrangean is justified since this procedure leads to $C_{1,2,3} = \mathcal{O}(\lambda)$.

Generating functional of connected Green's functions From the generating functional of the Green's functions, $Z[J]$, one obtains the generating functional of the *connected* Green's functions, $W[J]$, via

$$Z[J] = e^{iW[J]}\,. \tag{3.236}$$

This is understood immediately in terms of Feynman diagrams, for which the concept of connectedness is directly related to connectedness as a graph. In general, $Z[J]$ is the sum of all Fenyman diagrams with any number of external legs ending at the position x_i of sources $J(x_i)$, and each diagram can be written as the product of its connected parts. A graph is connected if for any pair of vertices (including those coupling the field to the external source) one can find a path (i.e., a sequence of internal lines in the graph – including those going from a vertex to a source) that goes from one to the other. Then

$$\begin{aligned}
Z[J] &= \sum_{g\in\text{graphs}} Z_g = \sum_{g\in\text{graphs}} \prod_{g^{(c)}\in g} Z_{g^{(c)}} \\
&= \sum_{N=0}^{\infty} \frac{1}{N!}\left(\sum_{g^{(c)}\in\text{conn. graphs}} Z_{g^{(c)}}\right)^N = e^{\sum_{g^{(c)}\in\text{conn. graphs}} Z_{g^{(c)}}}\,.
\end{aligned} \tag{3.237}$$

Then $iW[J]$ is the sum of all *connected* graphs with any number of external lines attached to sources $J(x)$.

[20] In principle one should set $m_B^2 = \delta m^2 + Z_m m^2$, allowing for additive renormalisation of the mass. In general, divergences corresponding to the insertion of an interaction term $(\text{DIV})\phi^2$ read in terms of the UV cutoff Λ as $(\text{DIV}) = a\Lambda^2 + bm^2\log\Lambda$, for dimensionless coefficients a, b. However, if one employs dimensional regularisation there are no power divergences, only logarithmic ones, and so only multiplicative renormalisation is required.

One can define connectedness independently of Feynman diagrams in a recursive manner. The idea is to isolate the contributions to a correlation function $\langle\phi(x_1)\dots\phi(x_n)\rangle$ that vanish when one or more of the points x_i, say, $\{x_1,\dots,x_j\}$ are far from the others. From the cluster property one has

$$\langle\phi(x_1)\dots\phi(x_j)\phi(x_{j+1})\dots\phi(x_n)\rangle \to \langle\phi(x_1)\dots\phi(x_j)\rangle\langle\phi(x_{j+1})\dots\phi(x_n)\rangle\,, \tag{3.238}$$

so that $\langle\phi(x_1)\dots\phi(x_j)\phi(x_{j+1})\dots\phi(x_n)\rangle - \langle\phi(x_1)\dots\phi(x_j)\rangle\langle\phi(x_{j+1})\dots\phi(x_n)\rangle$ vanishes in the limit. The plan is to do this systematically. One then starts by defining $\langle\phi(x)\rangle_c \equiv \langle\phi(x)\rangle$, since being there only one point it can only be close to itself. Then, for the two point function,

$$\langle\phi(x_1)\phi(x_2)\rangle \equiv \langle\phi(x_1)\phi(x_2)\rangle_c + \langle\phi(x_1)\rangle_c\langle\phi(x_2)\rangle_c = \langle\phi(x_1)\phi(x_2)\rangle_c + \langle\phi(x_1)\rangle\langle\phi(x_2)\rangle\,, \tag{3.239}$$

where the first equality defines the two-point connected component. One then proceeds to the three-point function, defining its connected component by the relation

$$\begin{aligned}\langle\phi(x_1)\phi(x_2)\phi(x_3)\rangle \equiv{}& \langle\phi(x_1)\phi(x_2)\phi(x_2)\rangle_c \\ &+ \langle\phi(x_1)\phi(x_2)\rangle_c\langle\phi(x_3)\rangle_c + \langle\phi(x_2)\phi(x_3)\rangle_c\langle\phi(x_1)\rangle_c + \langle\phi(x_3)\phi(x_1)\rangle_c\langle\phi(x_2)\rangle_c \\ &+ \langle\phi(x_1)\rangle_c\langle\phi(x_2)\rangle_c\langle\phi(x_3)\rangle_c\,,\end{aligned} \tag{3.240}$$

where the two-point and one-point connected functions have already been defined at the previous stages. In general,

$$\langle\phi(x_1)\dots\phi(x_n)\rangle \equiv \sum_{\substack{P=\{P_i\}\\ P_i\neq\emptyset,\, P_i\cap P_j=\emptyset\\ \cup_i P_i=\{1,\dots,n\}}} \prod_{\{P_i\}} \left\langle \prod_{j\in P_i}\phi(x_j)\right\rangle_c\,, \tag{3.241}$$

where the sum is over partitions of all the partitions of $\{1,\dots,n\}$ into nonempty disjoint sets P_i (parts), the first product is over the parts P_i of the partition, and the second product is over the elements $j\in P_i$. All but one of the terms on the right-hand side have been defined already when dealing with the correlation functions of order $n-1$ and lower, so Eq. (3.241) provides the definition of $\langle\phi(x_1)\dots\phi(x_n)\rangle_c$. Clearly, this can be expressed entirely in terms of ordinary correlation functions $\langle\phi(x_1)\dots\phi(x_n)\rangle$. For example, for the two-point and three-point functions one has

$$\begin{aligned}\langle\phi(x_1)\phi(x_2)\rangle_c &= \langle\phi(x_1)\phi(x_2)\rangle - \langle\phi(x_1)\rangle\langle\phi(x_2)\rangle\,,\\ \langle\phi(x_1)\phi(x_2)\phi(x_2)\rangle_c &= \langle\phi(x_1)\phi(x_2)\phi(x_3)\rangle \\ &\quad - \langle\phi(x_1)\phi(x_2)\rangle\langle\phi(x_3)\rangle - \langle\phi(x_2)\phi(x_3)\rangle\langle\phi(x_1)\rangle - \langle\phi(x_3)\phi(x_1)\rangle\langle\phi(x_2)\rangle \\ &\quad + 2\langle\phi(x_1)\rangle\langle\phi(x_2)\rangle\langle\phi(x_3)\rangle\,.\end{aligned} \tag{3.242}$$

By construction, each connected part vanishes when any two of the spacetime points to which the fields are attached are far apart. This can be verified explicitly in Eq. (3.242) by using the cluster property. The same construction applies to the correlation functions in the presence of a source, defined as

$$\langle\phi(x_1)\dots\phi(x_n)\rangle_J = \frac{\displaystyle\int [\mathrm{D}\phi]\, e^{iS[\phi]+iJ\cdot\phi}\phi(x_1)\dots\phi(x_n)}{\displaystyle\int [\mathrm{D}\phi]\, e^{iS[\phi]+iJ\cdot\phi}} = \frac{1}{Z[J]}\frac{1}{i}\frac{\delta}{\delta J(x_1)}\dots\frac{1}{i}\frac{\delta}{\delta J(x_n)}Z[J]\,, \tag{3.243}$$

that can be decomposed into connected components starting from $\langle\phi(x)\rangle_{J\,c} = \langle\phi(x)\rangle_J$ and using the recursive procedure.

To recover the generating functional $Z[J]$ one has to add up all the n-point functions. Using a source J_0 as the expansion point, one has

$$\begin{aligned}\frac{Z[J]}{Z[0]} &= \sum_{n=0}^{\infty}\frac{1}{n!}\int d^4x_1\, i(J(x_1)-J_0(x_1))\ldots\int d^4x_n\, i(J(x_n)-J_0(x_n))\langle\phi(x_1)\ldots\phi(x_n)\rangle_{J_0}\\ &= \sum_{n=0}^{\infty}\frac{1}{n!}\int d^4x_1\, i\Delta J(x_1)\ldots\int d^4x_n\, i\Delta J(x_n)\langle\phi(x_1)\ldots\phi(x_n)\rangle_{J_0}\\ &= \sum_{n}\frac{1}{n!}\sum_{\substack{P=\{P_i\}\\ P_i\neq\emptyset,\, P_i\cap P_j=\emptyset\\ \cup_i P_i=\{1,\ldots,n\}}}\prod_{\{P_i\}}\left\langle\prod_{j\in P_i}\int d^4x_j\, i\Delta J(x_j)\phi(x_j)\right\rangle_{J_0\,c},\end{aligned} \tag{3.244}$$

where the $n=0$ term corresponds to $\langle 1\rangle_J = 1$, and in the last passage we used the decomposition in connected components. Since coordinates are integrated over, the only feature of the partitions that enters Eq. (3.244) is the number n_k of subsets of $\{1,\ldots,n\}$ of size $k=1,\ldots,n$ appearing in it, with partitions differing only by a permutation of the x_j giving the same contribution. For a given set of $\{n_k\}$, $\sum_{k=1}^n kn_k = n$ one finds $\frac{n!}{\prod_k n_k!(k!)^{n_k}}$ identical contributions to $Z[J]/Z[0]$, and so

$$\frac{Z[J]}{Z[0]} = \sum_{n=0}^{\infty}\frac{1}{n!}\sum_{\substack{n_k=0,\ldots,n\\ \sum_{k=1}^n kn_k=n}}\frac{n!}{\prod_k n_k!(k!)^{n_k}}\prod_k\left\langle\left(\int d^4x\, i\Delta J(x)\phi(x)\right)^k\right\rangle_{J_0\,c}^{n_k}. \tag{3.245}$$

The sum over k can be extended from $k=0$, since $k=0$ and will not contribute anyway to $\sum_{k=1}^n kn_k$. Moreover, since we are summing over n, we can drop the constraint and allow k to go from 0 to ∞. We find

$$\begin{aligned}\frac{Z[J]}{Z[0]} &= \sum_{n=0}^{\infty}\sum_{\substack{\{n_k\}\\ n_k\geq 0}}\delta_{\sum_{k=0}^{\infty}kn_k,n}\frac{1}{\prod_k n_k!(k!)^{n_k}}\prod_{k=0}^{\infty}\left\langle\left(\int d^4x\, i\Delta J(x)\phi(x)\right)^k\right\rangle_{J_0\,c}^{n_k}\\ &= \prod_{k=0}^{\infty}\sum_{n_k=0}^{\infty}\frac{1}{n_k!}\left\{\frac{1}{k!}\left\langle\left(\int d^4x\, i\Delta J(x)\phi(x)\right)^k\right\rangle_{J_0\,c}\right\}^{n_k}\\ &= \prod_{k=0}^{\infty}\exp\left\{\frac{1}{k!}\left\langle\left(\int d^4x\, i\Delta J(x)\phi(x)\right)^k\right\rangle_{J_0\,c}\right\}\\ &= \exp\left\{\sum_{k=0}^{\infty}\frac{1}{k!}\int d^4x_1\, i\Delta J(x_1)\ldots\int d^4x_k\, i\Delta J(x_k)\langle\phi(x_1)\ldots\phi(x_k)\rangle_{J_0\,c}\right\},\end{aligned} \tag{3.246}$$

and so from the definition Eq. (3.236)

$$\begin{aligned} & i(W[J]-W[0]) \\ &= \sum_{k=0}^{\infty} \frac{1}{k!} \int d^4x_1\, i\Delta J(x_1) \dots \int d^4x_k\, i\Delta J(x_k) \langle \phi(x_1) \dots \phi(x_k) \rangle_{J_0\, c} \\ &= \sum_{k=0}^{\infty} \frac{1}{k!} \int d^4x_1\, i(J(x_1)-J_0(x_1)) \dots \int d^4x_k\, i(J(x_k)-J_0(x_k)) \langle \phi(x_1) \dots \phi(x_k) \rangle_{J_0\, c} \,. \end{aligned} \tag{3.247}$$

The quantity $W[0]$ is the sum of connected vacuum bubbles, and plays no role in correlation functions.

For the skeptics, here is an explicit calculation. Using the definition Eq. (3.243),

$$\begin{aligned} \frac{1}{i}\frac{\delta}{J(x)} iW[J] &= \frac{1}{i}\frac{\delta}{J(x)} \log Z[J] = \frac{1}{Z[J]}\frac{1}{i}\frac{\delta Z[J]}{\delta J(x)} = \langle \phi(x) \rangle_J = \langle \phi(x) \rangle_{J\, c} \,, \\ \frac{1}{i}\frac{\delta}{\delta J(x_1)}\frac{1}{i}\frac{\delta}{\delta J(x_2)} iW[J] &= \frac{1}{i}\frac{\delta}{\delta J(x_1)}\frac{1}{i}\frac{\delta}{\delta J(x_2)} \log Z[J] = \frac{1}{i}\frac{\delta}{\delta J(x_1)} \left(\frac{1}{Z[J]}\frac{1}{i}\frac{\delta Z[J]}{\delta J(x_2)} \right) \\ &= \frac{1}{Z[J]}\frac{1}{i^2}\frac{\delta^2 Z[J]}{\delta J(x_1)\delta J(x_2)} - \frac{1}{Z[J]^2} \left(\frac{1}{i}\frac{\delta Z[J]}{\delta J(x_1)} \right) \left(\frac{1}{i}\frac{\delta Z[J]}{\delta J(x_2)} \right) \\ &= \langle \phi(x_1)\phi(x_2) \rangle_J - \langle \phi(x_1) \rangle_J \langle \phi(x_2) \rangle_J = \langle \phi(x_1)\phi(x_2) \rangle_{J\, c} \,, \end{aligned} \tag{3.248}$$

and in general

$$\frac{1}{i^{n-1}} \frac{\delta^n W[J]}{\delta J(x_1) \dots \delta J(x_n)} = \langle \phi(x_1) \dots \phi(x_n) \rangle_{J\, c} \,. \tag{3.249}$$

Effective action There is one more generating functional of great importance. Let us denote

$$\varphi_J(x) = \langle \phi(x) \rangle_J = \frac{\delta W[J]}{\delta J(x)} \,. \tag{3.250}$$

The classical field $\varphi_J(x)$ corresponds to the expectation value of the quantum field $\phi(x)$ in the presence of a source $J(x)$. One can invert the relation, and for a prescribed $\varphi(x)$ find the source $J_\varphi(x)$ that produces it, i.e., $\langle \phi(x) \rangle_{J_\varphi} = \varphi(x)$. We then define the *effective action* by means of a Legendre transform as

$$\Gamma[\varphi] \equiv W[J_\varphi] - J_\varphi \cdot \varphi \,. \tag{3.251}$$

It is straightforward to show that

$$\begin{aligned} \frac{\delta\Gamma[\varphi]}{\delta\varphi(x)} &= \int d^4y \frac{\delta J_\varphi(y)}{\delta\varphi(x)} \frac{\delta W[J]}{\delta J(y)}\bigg|_{J=J_\varphi} - \int d^4y \frac{\delta J_\varphi(y)}{\delta\varphi(x)} \varphi(y) - J_\varphi(x) \\ &= \int d^4y \frac{\delta J_\varphi(y)}{\delta\varphi(x)} \varphi(y) - \int d^4y \frac{\delta J_\varphi(y)}{\delta\varphi(x)} \varphi(y) - J_\varphi(x) = -J_\varphi(x) \end{aligned} \tag{3.252}$$

or in compact notation

$$\frac{\delta\Gamma[\varphi]}{\delta\varphi}\bigg|_{\varphi=\varphi_J} = \frac{\delta J_\varphi}{\delta\varphi} \cdot \frac{\delta W[J]}{\delta J}\bigg|_{J=J_\varphi} - \frac{\delta J_\varphi}{\delta\varphi} \cdot \varphi - J_\varphi = \frac{\delta J_\varphi}{\delta\varphi} \cdot \varphi - \frac{\delta J_\varphi}{\delta\varphi} \cdot \varphi - J_\varphi = -J_\varphi \,. \tag{3.253}$$

The inverse transformation reads

$$W[J] = \Gamma[\varphi_J] + J \cdot \varphi_J \,, \tag{3.254}$$

since clearly

$$\frac{\delta W[J]}{\delta J} = \frac{\delta \Gamma[\varphi_J]}{\delta \varphi_J} \cdot \frac{\delta \varphi_J}{\delta J} + J \cdot \frac{\delta \varphi_J}{\delta J} + \varphi_J = -J \cdot \frac{\delta \varphi_J}{\delta J} + J \cdot \frac{\delta \varphi_J}{\delta J} + \varphi_J = \varphi_J \,, \tag{3.255}$$

and so $\varphi_{J_\varphi} = \varphi$.

The field $\varphi_J = \langle \phi \rangle_J$, which is a c-number field but of quantum origin, obeys the quantum-corrected equation of motion

$$\left. \frac{\delta \Gamma[\varphi]}{\delta \varphi} \right|_{\varphi = \varphi_J} + J = 0 \,. \tag{3.256}$$

In particular, in the absence of an external source, the possible vacuum expectation values $\varphi_0 = \langle \phi \rangle_{J=0}$ of the quantum field ϕ must obey

$$\left. \frac{\delta \Gamma[\varphi]}{\delta \varphi} \right|_{\varphi = \varphi_0} = 0 \,. \tag{3.257}$$

This should be compared with the classical case, in which the equations of motion in the presence of an external source read

$$\left. \frac{\delta S[\varphi_c]}{\delta \varphi_c} \right|_{\varphi_c = \varphi_{cJ}} + J = 0 \,, \tag{3.258}$$

and in particular $\frac{\delta S[\varphi_c]}{\delta \varphi_c} = 0$ are the equations of motion without a source.

Besides providing the equations of motion for φ_J, the effective action has a second interpretation as the generating functional of one-particle-irreducible (1PI) Feynman diagrams. These are diagrams that cannot be made disconnected by cutting a single internal line. Clearly, the most general connected diagram can be built out of 1PI diagrams with at least three external legs, connected by fully dressed propagators, which in turn are obtained from 1PI diagrams by simply resumming a geometric series. Denoting

$$\begin{aligned} W^{(2)}(x_1, x_2) &= \left. \frac{\delta^2 W[J]}{\delta J(x_1) \delta J(x_2)} \right|_{J=0} = i \langle \phi(x_1) \phi(x_2) \rangle_c = i D(x_1 - x_2) \,, \\ W_0^{(2)}(x_1, x_2) &= \left. \frac{\delta^2 W_0[J]}{\delta J(x_1) \delta J(x_2)} \right|_{J=0} = i \langle \phi(x_1) \phi(x_2) \rangle_{0\,c} = i D_0(x_1 - x_2) \,, \end{aligned} \tag{3.259}$$

with W_0 the generating functional of the free theory, one has

$$\begin{aligned} W^{(2)} &= W_0^{(2)} + W_0^{(2)} \cdot (1\mathrm{PI})_2 \cdot W_0^{(2)} + W_0^{(2)} \cdot (1\mathrm{PI})_2 \cdot W_0^{(2)} \cdot (1\mathrm{PI}) \cdot W_0^{(2)} + \dots \\ &= W_0^{(2)} \cdot \frac{1}{1 - (1\mathrm{PI})_2 \cdot W_0^{(2)}} = \frac{1}{[W_0^{(2)}]^{-1} - (1\mathrm{PI})_2} \,, \end{aligned} \tag{3.260}$$

where $(1\mathrm{PI})_2$ denotes the sum of 1PI diagrams with two external legs. On the other hand, from the definitions of W and Γ,

$$\frac{\delta^2 W[J]}{\delta J(x) \delta J(y)} = \frac{\delta \varphi_J(x)}{\delta J(y)} \,, \qquad \frac{\delta^2 \Gamma[\varphi]}{\delta \varphi(x) \delta \varphi(y)} = -\frac{\delta J_\varphi(x)}{\delta \varphi(y)} \tag{3.261}$$

and so

$$\int d^4z \frac{\delta^2 W[J]}{\delta J(x)\delta J(z)}\bigg|_{J=J_\varphi} \frac{\delta^2\Gamma[\varphi]}{\delta\varphi(z)\delta\varphi(y)} = -\int d^4z \frac{\delta\varphi_J(x)}{\delta J(z)}\bigg|_{J=J_\varphi} \frac{\delta J_\varphi(z)}{\delta\varphi(y)} \\ = -\frac{\delta\varphi_{J_\varphi}(x)}{\delta\varphi(y)} = -\frac{\delta\varphi(x)}{\delta\varphi(y)} = -\delta^{(4)}(x-y)\,. \tag{3.262}$$

This means that, denoting

$$\Gamma^{(2)}(x_1,x_2) = \frac{\delta^2\Gamma[\varphi]}{\delta\varphi(x_1)\delta\varphi(x_2)}\bigg|_{\varphi=0}\,, \tag{3.263}$$

one has

$$\Gamma^{(2)} = -[W^{(2)}]^{-1} = -\Big([W_0^{(2)}]^{-1} - (1\mathrm{PI})_2\Big) = -[W_0^{(2)}]^{-1} + (1\mathrm{PI})_2\,. \tag{3.264}$$

Going over to momentum space,

$$\tilde\Gamma^{(2)} = -\frac{1}{i\tilde D_0} + \widetilde{(1\mathrm{PI})_2} = p^2 - m^2 + i\epsilon + \widetilde{(1\mathrm{PI})_2}\,. \tag{3.265}$$

To show that Γ generates the 1PI diagrams, we follow Coleman's approach and define a new theory by means of

$$e^{iW_\Gamma[J,g]} \equiv \int [\mathrm{D}\phi]\, e^{\frac{i}{g}(\Gamma[\phi]+J\cdot\phi)}\,. \tag{3.266}$$

This means that we build our interactions using as propagators and vertices those appearing in Γ,

$$\Gamma[\phi] = \sum_{n=0}^\infty \frac{1}{n!}\int d^4x_1 \ldots \int d^4x_n\, \Gamma^{(n)}(x_1,\ldots,x_n)\phi(x_1)\ldots\phi(x_n) \\ = \Gamma[0] + \int d^4x\, \Gamma^{(1)}(x)\phi(x) + \frac{1}{2}\int d^4x_1 \int d^4x_2\, \Gamma^{(2)}(x_1,x_2)\phi(x_1)\phi(x_2) \\ + \sum_{n=3}^\infty \frac{1}{n!}\int d^4x_1 \ldots \int d^4x_n\, \Gamma^{(n)}(x_1,\ldots,x_n)\phi(x_1)\ldots\phi(x_n)\,. \tag{3.267}$$

Ignoring $\Gamma[0]$, which is just a constant that gets cancelled out in correlation functions, and subtracting the vacuum expectation value $-[\Gamma^{(2)}]^{-1}\cdot\Gamma^{(1)}$ [see Eq. (3.227)] from the field, correlation functions are built perturbatively using the propagator $g[\Gamma^{(2)}]^{-1}$, which plays here the same role as K^{-1} did before, and the vertices $g^{-1}\Gamma^{(n)}$ and $g^{-1}J$, with the latter a single-line vertex that corresponds to external lines in a diagrammatic representation. For a fixed number V of vertices with $n \geq 3$, I internal lines, and E external lines, the corresponding power of g is equal to the number of propagators (including those ending in a source) minus the total number of vertices (including those associated with sources), and so

$$g^{I+E} g^{-(V+E)} = g^{I-V}\,. \tag{3.268}$$

A generic, connected L-loop diagrams, $L = I - V + 1$, comes then with a power g^{L-1}. The expansion in powers of g is then an expansion in the number of loops. This device can be used also in the ordinary case, introducing a formal parameter g that is eventually set to 1.

In the case at hand, the loop expansion reads

$$W_\Gamma[J,g] = \sum_{L=0}^{\infty} g^{L-1} W_\Gamma^{(L)}[J]\,, \tag{3.269}$$

with $W_\Gamma^{(L)}[J]$ the sum of connected graphs with L loops obtained from the functional Eq. (3.266), i.e., using $\Gamma^{(n)}$ as the coefficient of the n-point vertex. In particular, $W_\Gamma^{(0)}[J]$ is the sum of tree graphs (i.e., graphs with no loops) obtained in this way, and dominates the sum in the limit $g \to 0$. On the other hand, $W_\Gamma[J,g]$ in the limit $g \to 0$ can be obtained also via a saddle-point calculation. One has, setting $\phi = \phi_{\rm s.p.} + \sqrt{g}\chi$,

$$\begin{aligned} e^{iW_\Gamma[J,g]} &= \int [\mathrm{D}\sqrt{g}\chi]\, e^{\frac{i}{g}\left(\Gamma[\phi_{\rm s.p.}+\sqrt{g}\chi]+J\cdot(\phi_{\rm s.p.}+\sqrt{g}\chi)\right)} \\ &= e^{\frac{i}{g}(\Gamma[\phi_{\rm s.p.}]+J\cdot\phi_{\rm s.p.})} \int [\mathrm{D}\sqrt{g}\chi]\, e^{\frac{i}{g}\left(\sqrt{g}(\Gamma'[\phi_{\rm s.p.}]+J)\cdot\chi+\frac{1}{2}g\chi^T\cdot\Gamma''[\phi_{\rm s.p.}]\cdot\chi+\mathcal{O}(g^{\frac{3}{2}}\chi^3)\right)}\,. \end{aligned} \tag{3.270}$$

Choosing $\phi_{\rm s.p.}$ to satisfy the saddle-point equation $\Gamma'[\phi_{\rm s.p.}] + J = 0$, one has

$$e^{iW_\Gamma[J,g]} = e^{\frac{i}{g}(\Gamma[\phi_{\rm s.p.}]+J\cdot\phi_{\rm s.p.})} \int [\mathrm{D}\sqrt{g}\chi]\, e^{\frac{i}{2}\chi^T\cdot\Gamma''[\phi_{\rm s.p.}]\cdot\chi}\left(1+\mathcal{O}(g\chi^4)\right)\,, \tag{3.271}$$

where the correction are proportional to integer powers of g, since only even powers of the field χ contribute. Then

$$\begin{aligned} e^{i(W_\Gamma[J,g]-W_\Gamma[0,g])} &= \frac{e^{\frac{i}{g}(\Gamma[\phi_{\rm s.p.}[J]]+J\cdot\phi_{\rm s.p.})} \int [\mathrm{D}\sqrt{g}\chi]\, e^{\frac{i}{2}\chi^T\cdot\Gamma''[\phi_{\rm s.p.}[J]]\cdot\chi}\left(1+\mathcal{O}(g\chi^4)\right)}{e^{\frac{i}{g}(\Gamma[\phi_{\rm s.p.}[0]])} \int [\mathrm{D}\sqrt{g}\chi]\, e^{\frac{i}{2}\chi^T\cdot\Gamma''[\phi_{\rm s.p.}[0]]\cdot\chi}\left(1+\mathcal{O}(g\chi^4)\right)} \\ &= e^{\frac{i}{g}(\Gamma[\phi_{\rm s.p.}[J]]+J\cdot\phi_{\rm s.p.}-\Gamma[\phi_{\rm s.p.}[0]]+\mathcal{O}(1))}\,, \end{aligned} \tag{3.272}$$

and so

$$W_\Gamma^{(0)}[J] - W_\Gamma^{(0)}[0] = \Gamma[\phi_{\rm s.p.}[J]] + J\cdot\phi_{\rm s.p.} - \Gamma[\phi_{\rm s.p.}[0]]\,, \tag{3.273}$$

but by the definition of $\phi_{\rm s.p.}$ and the relation between W and Γ

$$W_\Gamma^{(0)}[J] - W_\Gamma^{(0)}[0] = W[J] - W[0]\,. \tag{3.274}$$

Then, ignoring the J-independent terms that do not contribute to correlation functions, $W[J]$ equals the sum of connected *tree* diagrams built using $\frac{i}{n!}\Gamma^{(n)}\phi^n$, $n \geq 3$, as vertices and $i[\Gamma^{(2)}]^{-1} = -iW^{(2)} = D$ as propagator. On the other hand, $W[J]$ also equals the sum of connected tree diagrams built using the sum of 1PI diagrams with n external lines as vertices, connected by fully dressed propagators $D = -iW^{(2)}$. It then follows that $i\Gamma^{(n)}$ equals the sum of 1PI diagrams with n legs, and so $i\Gamma$ is the generating functional of 1PI diagrams.

The identification of $i\Gamma^{(n)}$ with the sum of 1PI diagrams with n legs follows from the fact that a tree diagram with E external lines cannot be built using vertices with more than E lines attached, and using at most one vertex with E lines attached. Then, if one has identified $i\Gamma^{(n)}$ with the sum of 1PI diagrams with n legs for $n \leq N$, at $n = N+1$ there is only one possible diagram containing the sum of 1PI diagrams with $N+1$ legs, namely the diagram made out of the sum of 1PI diagrams with $N+1$ legs to which $N+1$ full propagators are attached; and only

one possible diagram containing $i\Gamma^{(N+1)}$, namely that having a single vertex $i\Gamma^{(N+1)}$ with $N+1$ full propagators attached; and therefore $i\Gamma^{(N+1)}$ is identified with the sum of 1PI diagrams with $N+1$ legs. Since the 3-point function is necessarily built out of the sum of 1PI diagrams with three full propagators attached, and, parallelly, out of $\Gamma^{(3)}$ with three full propagators attached, the identification is complete (this is true even if the three point function vanishes).

It remains to show the initial statement. It follows from the relations $E+2I=\sum_n nV_n$ and $I-V+1=L$ that

$$\begin{aligned} 2L = 2I-2V+2 &= \sum_n nV_n - 2\sum_n V_n + 2 - E = \sum_n (n-2)V_n + 2 - E \\ &= \sum_{n\le E}(n-2)V_n + \sum_{n>E}(n-2)V_n + 2 - E \\ &> \sum_{n\le E}(n-2)V_n + (E-2)\left(-1+\sum_{n>E}V_n\right) . \end{aligned} \tag{3.275}$$

For $E>2$, if there is at least one vertex with $n>E$ then the last term is non-negative, and since the first one is also non-negative (since $n\ge 2$), one has necessarily $L>0$. Then no vertices with more than E lines can appear in a tree diagram with E external lines. Therefore for such a diagram

$$\begin{aligned} 0 &= 2-E+\sum_{n\le E}(n-2)V_n = 2-E+(E-2)V_E+\sum_{n<E}(n-2)V_n \\ &= (E-2)(V_E-1)+\sum_{n<E}(n-2)V_n . \end{aligned} \tag{3.276}$$

Since the second term is non-negative, for $E>2$ this equation can hold only if $V_E=1$ and $V_{n<E}=0$, or otherwise if $V_E=0$ and $E-2=\sum_{n<E}(n-2)V_n$. In particular, no more than one E-point vertex can appear, and if it does then it is the only vertex.[21]

Background field method A practically convenient method to compute Γ is provided by the *background field method*. Define the following generating functional,

$$e^{i\tilde{W}_{\phi_0}[J]} = \int [\mathrm{D}\phi]\, e^{iS[\phi+\phi_0]+J\cdot\phi} . \tag{3.277}$$

A simple change of variables shows that

$$e^{i\tilde{W}_{\phi_0}[J]} = \int [\mathrm{D}\phi]\, e^{iS[\phi]+J\cdot(\phi-\phi_0)} = e^{iW[J]-iJ\cdot\phi_0} , \tag{3.278}$$

i.e.,

$$\tilde{W}_{\phi_0}[J] = W[J] - J\cdot\phi_0 . \tag{3.279}$$

Define now the associated effective action. One has

$$\tilde{\varphi}_J = \frac{\delta\tilde{W}_{\phi_0}[J]}{\delta J} = \frac{\delta W[J]}{\delta J} - \phi_0 = \varphi_J - \phi_0 , \tag{3.280}$$

[21] It is possible that for the lowest nonzero n-point function one has $n>3$. From the above, for $E=3$ only a 3-point vertex is possible, and so 3-point 1PI and $\Gamma^{(3)}$ coincide. If one vanihses, so does the other. Then one should look at $E=4$, where only 4- and 3-point vertices are possible, but since the three-point function vanishes one has only the 4-point vertex, and so 4-point 1PI and $\Gamma^{(4)}$ coincide. If this function vanishes one continue until the first nonzero one.

and so

$$\tilde{\Gamma}_{\phi_0}[\tilde{\varphi}_J] = \tilde{W}_{\phi_0}[J] - J\cdot\tilde{\varphi}_J = W[J] - J\cdot\phi_0 - J\cdot(\varphi_J - \phi_0) = W[J] - J\cdot\varphi_J = \Gamma[\varphi_J]\,. \quad (3.281)$$

In general then

$$\tilde{\Gamma}_{\phi_0}[\varphi - \phi_0] = \Gamma[\varphi]\,, \quad (3.282)$$

and choosing $\varphi = \phi_0$

$$\Gamma[\phi_0] = \tilde{\Gamma}_{\phi_0}[0]\,. \quad (3.283)$$

The left-hand side of this equation is the generating functional we are after. The right-hand side is the sum of connected, one-particle irreducible vacuum diagrams (i.e., no external lines) for the theory defined by the shifted action $S[\phi + \phi_0]$. In particular, the sum of 1PI diagrams with n external lines of the original theory is equal to the sum of connected 1PI vacuum diagrams of the shifted theory where n factors of ϕ_0 appear.

Symmetries of the effective action Symmetries of the classical action S reflect into symmetries of the quantum effective action Γ. Let S be invariant under the infinitesimal transformation

$$\phi_a \to \phi_a + \delta_s\phi_a\,, \qquad \delta_s\phi_a(x) = \epsilon F_a[\phi; x]\,, \quad (3.284)$$

with F depending functionally on the fields at x, e.g.,

$$F_a[\phi; x] = A_{ab}\phi_b(x) + B_{ab}x^\mu\partial_\mu\phi_b(x) + C_{abc}\phi_b(x)\phi_c(x) + \dots\,. \quad (3.285)$$

The simplest case is that of a linear transformation, $F_a^{(L)}[\phi; x] = L_{ab}\phi_b(x)$. Let the functional integration measure be invariant as well under the transformation Eq. (3.284).[22] Symmetry of S and $[\mathrm{D}\phi]$ implies

$$\begin{aligned} Z[J] &= \int[\mathrm{D}\phi]\, e^{iS[\phi]+iJ\cdot\phi} = \int[\mathrm{D}\phi]\, e^{iS[\phi+\delta_s\phi]+iJ\cdot(\phi+\delta_s\phi)} = \int[\mathrm{D}\phi]\, e^{iS[\phi]+iJ\cdot(\phi+\delta_s\phi)} \\ &= \int[\mathrm{D}\phi]\, e^{iS[\phi]+iJ\cdot\phi}(1 + J\cdot\delta_s\phi) = Z[J](1 + \epsilon J\cdot\langle F[\phi; x]\rangle_J)\,, \end{aligned} \quad (3.286)$$

and since ϵ is arbitrary

$$J\cdot\langle F[\phi; x]\rangle_J = 0\,. \quad (3.287)$$

On the other hand, for J_φ such that $\langle\phi\rangle_{J_\varphi} = \varphi$ one has $J_\varphi = -\frac{\delta\Gamma}{\delta\varphi}$, and so

$$0 = J_\varphi\cdot\langle F[\phi; x]\rangle_{J_\varphi} = -\frac{\delta\Gamma[\varphi]}{\delta\varphi}\langle F[\phi; x]\rangle_{J_\varphi}\,. \quad (3.288)$$

This can be equivalently written as

$$\Gamma[\varphi + \epsilon\langle F[\phi; x]\rangle_{J_\varphi}] = \Gamma[\varphi]\,, \quad (3.289)$$

known as *Slavnov-Taylor* identity. This identity is particularly transparent if F is a linear transformation. In this case in fact

$$\langle F[\phi; x]\rangle_{J_\varphi} = \langle L\phi(x)\rangle_{J_\varphi} = L\langle\phi(x)\rangle_{J_\varphi} = L\varphi\,, \quad (3.290)$$

[22] It would actually suffice that $[\mathrm{D}\phi]\, e^{iS[\phi]}$ be invariant.

and the Slavnov-Taylor identity reads

$$\Gamma[\varphi + \epsilon L\varphi] = \Gamma[\varphi] \Rightarrow \Gamma[\varphi + \delta_s\varphi] = \Gamma[\varphi]\,, \tag{3.291}$$

i.e., the same transformation δ_s but applied to the fields φ is a symmetry of Γ. In more general cases $\langle F[\phi;x]\rangle_{J_\varphi} \neq F[\langle\phi\rangle_{J_\varphi};x] = F[\varphi;x]$, so the form of the symmetry transformation is modified.

Goldstone's theorem The effective action formalism can be used to provide a proof of Goldstone's theorem about the presence of massless particles (Nambu-Goldstone bosons) in the spectrum of theories where a continuous symmetry is spontaneously broken.

Assume that the action $S = S[\phi]$, with ϕ_a a set of N real scalar fields, is symmetric under linear transformations L, $\phi'_j = L_{jk}\phi_k$, providing a unitary representation $L = L(g)$, $g \in G$, of some continuous Lie group G, i.e., $L(g_1g_2) = L(g_1)L(g_2)$, $g_{1,2} \in G$. Since we are dealing here with real fields, the representation is actually orthogonal, i.e., $L(g^{-1}) = L(g)^{-1} = L(g)^T$. As we discussed above, for linear transformations $S[L\phi] = S[\phi]$ implies $\Gamma[L\varphi] = \Gamma[\varphi]$. The first implication of this fact is that if φ_0 is a possible vacuum of the theory, satisfying $\Gamma'[\varphi_0] = 0$, then so is $L\varphi_0$: since $\Gamma[L\varphi_0] = \Gamma[\varphi_0]$, taking derivatives with respect to $\varphi_{0a}(x)$

$$\begin{aligned} 0 = \frac{\delta\Gamma[\varphi]}{\delta\varphi_j(x)}\bigg|_{\varphi=\varphi_0} &= \int d^4y\, \frac{\delta\Gamma[\varphi]}{\delta\varphi_k(y)}\bigg|_{\varphi=L\varphi_0} \frac{\delta(L\varphi_0(y))_k}{\delta\varphi_{0j}(x)} \\ &= \int d^4y\, \frac{\delta\Gamma[\varphi]}{\delta\varphi_k(y)}\bigg|_{\varphi=L\varphi_0} L_{kj}\delta^{(4)}(y-x) = \frac{\delta\Gamma[\varphi]}{\delta\varphi_k(x)}\bigg|_{\varphi=L\varphi_0} L_{kj}\,, \end{aligned} \tag{3.292}$$

and since L are invertible matrices it follows that $\Gamma'[L\varphi_0] = 0$. If $L\varphi_0 \neq \varphi_0$, this provides a different solution to the quantum equations of motion.

We will now assume that all the vacua, i.e., the solutions $\bar\varphi_0$ of $\Gamma'[\bar\varphi_0] = 0$, can be obtained from each other by a symmetry transformation, and so $\bar\varphi_0 = L(g)\varphi_0$ for some g and for some chosen vacuum φ_0. Let furthermore $H \subseteq G$ be the (largest) subgroup of G that leaves φ_0 invariant, $L(h)\varphi_0 = \varphi_0\ \forall h \in H$. This is called the *stability subgroup*, and in the setup we are considering it is independent of φ_0.[23] Choose now the generators T^a_G of G to be $\{T^a_G\} = \{T^a_H\}\cup\{T^a\}$, with $\{T^a_H\}$ generators of H, and $\{T^a\}$ a basis of the complement of the linear space spanned by $\{T^a_H\}$ within the Lie algebra of G.[24] Let $\{t^a_G\} = \{t^a_H\}\cup\{t^a\}$ be the corresponding representatives of the generators induced by the representation L, i.e., given $g = \exp\{i\alpha_a T^a_G\}$ one has $L(g) = \exp\{i\alpha_a t^a_G\}$. Since $L(h)\varphi_0 = \varphi_0\ \forall h \in H$, one has that the (representatives of) its generators annihilate the vacuum, $t^a_H\varphi_0 = 0$. On the other hand, $t^a\varphi_0 \neq 0$ (for otherwise the algebra of the stability group would contain another generator and H would not be the largest group leaving φ_0 invariant).

Let us now work out further consequences of the symmetry. Starting from $\Gamma[L\varphi] = \Gamma[\varphi]$ for generic φ and $L = \exp\{i\alpha_a t^a_G\}$, and taking the derivative with respect to α_a and then setting

[23] If $L(h)\varphi_0 = \varphi_0\ \forall h \in H_{\varphi_0}$, then for any other vacuum $\bar\varphi_0 = L(g)\varphi_0$ one has

$$\bar\varphi_0 = L(g)\varphi_0 = L(g)L(h)\varphi_0 = L(gh)L(g^{-1})L(g)\varphi_0 = L(ghg^{-1})\bar\varphi_0 = L(\bar h)\bar\varphi_0\,,$$

i.e., $L(\bar h)\bar\varphi_0 = \bar\varphi_0\ \forall \bar h \in H_{\bar\varphi_0} = gH_{\varphi_0}g^{-1} \sim H_{\varphi_0}$, i.e., the stability groups are all isomorphic to each other.

[24] Recall that the Lie algebra $\mathfrak{g}$ of a Lie group G is first of all a real linear space, for which one can choose a basis $\{t^a_G\}$. We choose this basis to contain a basis $\{T^a_H\}$ of the Lie algebra $\mathfrak{h}$ of H, which is a subspace of $\mathfrak{g}$, and complete it with a basis of the complement of $\mathfrak{h}$ in $\mathfrak{g}$.

all α_b to 0, we find

$$0 = \int d^4x \, \frac{\delta\Gamma[\bar\varphi]}{\delta\bar\varphi_j(x)}\bigg|_{\bar\varphi=L\varphi} \frac{\partial(L\varphi(x))_j}{\partial\alpha_a}\bigg|_{\{\alpha_b\}=0} = \int d^4x \, \frac{\delta\Gamma[\varphi]}{\delta\varphi_j(x)}(t^a_G)_{jk}\varphi_k(x)\,. \tag{3.293}$$

Taking now the functional derivative with respect to $\varphi_k(y)$, we find

$$\begin{aligned} 0 &= \int d^4x \, \left[\frac{\delta^2\Gamma[\varphi]}{\delta\varphi_l(y)\delta\varphi_j(x)}(t^a_G)_{jk}\varphi_k(x) + \frac{\delta\Gamma[\varphi]}{\delta\varphi_j(x)}(t^a_G)_{jk}\delta_{kl}\delta^{(4)}(y-x)\right] \\ &= \frac{\delta\Gamma[\varphi]}{\delta\varphi_j(y)}(t^a_G)_{jl} + \int d^4x \, \frac{\delta^2\Gamma[\varphi]}{\delta\varphi_l(y)\delta\varphi_j(x)}(t^a_G)_{jk}\varphi_k(x)\,. \end{aligned} \tag{3.294}$$

If we now set $\varphi = \varphi_0$, the first term vanishes and we obtain

$$\int d^4x \, \frac{\delta^2\Gamma[\varphi]}{\delta\varphi_l(y)\delta\varphi_j(x)}\bigg|_{\varphi=\varphi_0} (t^a_G)_{jk}\varphi_{0k}(x) = 0\,, \tag{3.295}$$

or in compact notation

$$\frac{\delta^2\Gamma[\varphi_0]}{\delta\varphi^2}\cdot(t^a_G\varphi_0) = 0\,. \tag{3.296}$$

As a matrix equation, Eq. (3.296) tells us that $\Gamma''[\varphi_0] = -(W''[0])^{-1}$ has zero modes provided by $t^a\varphi_0$ (while $t^a_H\varphi_0 = 0$ and so give a trivial identity). For a translation-invariant theory, the vacua are x-independent, $\varphi_0(x) = \varphi_0$, and so denoting with $D_{jk}(x,y) = D_{jk}(x-y)$ the coordinate-space propagator,

$$D_{jk}(x-y) = \langle\phi_j(x)\phi_k(y)\rangle - \langle\phi_j(x)\rangle\langle\phi_k(y)\rangle = -i(W''[0])_{jk}(x,y)\,, \tag{3.297}$$

and with $\tilde D_{jk}(p)$ the momentum-space propagator,

$$D_{jk}(x) = \int \frac{d^4p}{(2\pi)^4}\, e^{-ip\cdot x}\tilde D_{jk}(p)\,, \tag{3.298}$$

then Eqs. (3.295) and (3.296) tell us that

$$\begin{aligned} 0 &= \left(\int d^4x \, \frac{\delta^2\Gamma[\varphi]}{\delta\varphi_l(y)\delta\varphi_j(x)}\bigg|_{\varphi=\varphi_0}\right)(t^a)_{jk}\varphi_{0k} \\ &= \tilde\Gamma^{(2)}_{lj}[\varphi_0](p=0)(t^a)_{jk}\varphi_{0k} = i(\tilde D(p=0))^{-1}_{jk}(t^a)_{jk}\varphi_{0k}\,, \end{aligned} \tag{3.299}$$

i.e., $(t^a)_{jk}\varphi_{0k}$ are zero modes of the inverse propagator at zero momentum, $[\tilde D(0)]^{-1}$. There are then at least as many zero modes of $D(0)^{-1}$ as the number n_0 of "broken generators", i.e., group generators for which $t^a\varphi_0 \neq 0$. Clearly, if $[\tilde D(0)]^{-1}$ has zero modes it cannot be inverted, and so the propagator $\tilde D(0)$ does not exist in the (at least) n_0-dimensional zero-mode subspace, signaling a singularity at $p = 0$ and the presence of at least n_0 massless particles in the theory. This is the content of Goldstone's theorem.

To see this in more detail, notice that from $\Gamma[L\varphi] = \Gamma[\varphi]$ one finds, expanding $\Gamma[\varphi]$ around a generic φ_0 and $\Gamma[L\varphi]$ around $L\varphi_0$, that

$$\begin{aligned}\Gamma[\varphi] &= \Gamma[\bar\varphi_0] + \Gamma'[\bar\varphi_0]\cdot(\varphi-\bar\varphi_0) + \frac{1}{2}(\varphi-\bar\varphi_0)^T\cdot\Gamma''[\bar\varphi_0]\cdot(\varphi-\bar\varphi_0)\\ &\quad + \sum_{n\geq 3}\Gamma^{(n)}[\bar\varphi_0](\varphi-\bar\varphi_0)^n\\ = \Gamma[L\varphi] &= \Gamma[L\bar\varphi_0] + \Gamma'[L\bar\varphi_0]\cdot(L\varphi-L\bar\varphi_0) + \frac{1}{2}(L\varphi-L\bar\varphi_0)^T\cdot\Gamma''[L\bar\varphi_0]\cdot(L\varphi-L\bar\varphi_0)\\ &\quad + \sum_{n\geq 3}\Gamma^{(n)}[L\bar\varphi_0](L\varphi-L\bar\varphi_0)^n\,.\end{aligned} \tag{3.300}$$

Taking $\bar\varphi_0$ to be our vacuum, $\bar\varphi_0 = \varphi_0$, for every $L_h = L(h)$ the representative of an element of the stability group, $L_h\varphi_0 = \varphi_0$, this equation becomes

$$\begin{aligned}&\Gamma[\varphi_0] + \frac{1}{2}(\varphi-\varphi_0)^T\cdot\Gamma''[\varphi_0]\cdot(\varphi-\varphi_0) + \sum_{n\geq 3}\Gamma^{(n)}[\varphi_0](\varphi-\bar\varphi_0)^n\\ &= \Gamma[\varphi_0] + \frac{1}{2}(\varphi-\varphi_0)^T\cdot(L_h^T\Gamma''[\varphi_0]L_h)\cdot(\varphi-\varphi_0) + \sum_{n\geq 3}\Gamma^{(n)}[\varphi_0](L_h(\varphi-\bar\varphi_0))^n\,,\end{aligned} \tag{3.301}$$

so in particular for the second-order term

$$L_h^T\Gamma''[\varphi_0]L_h = \Gamma''[\varphi_0]\,, \tag{3.302}$$

or in other words

$$D(p)^{-1} = L_h^T D(p)^{-1} L_h\,. \tag{3.303}$$

The subspace of zero modes is invariant under L_h, since given $D(0)^{-1}v = 0$ one has

$$D(0)^{-1}(L_h v) = L_h(L_h^T D(0)^{-1}L_h)v = L_h D(0)^{-1}v = 0\,. \tag{3.304}$$

Splitting $\mathbb{R}^N$ into the subspace of zero modes of $D(0)^{-1}$ and its complement, one has for $D(p)^{-1}$

$$D(p)^{-1} = \left(\begin{array}{c|c} d_1(p^2)^{-1} & 0 \\ \hline 0 & d_0(p^2)^{-1}\end{array}\right)\,, \tag{3.305}$$

with $[L_h, d_{0,1}(p^2)^{-1}] = 0$,[25] and where Lorentz invariance has been used to write $D(p)^{-1}$ as a function of p^2 only. For small p^2 we find

$$D(p)^{-1} = \left(\begin{array}{c|c} a_1 + b_1 p^2 + \dots & 0 \\ \hline 0 & b_0 p^2 + \dots\end{array}\right)\,, \tag{3.306}$$

and so

$$D(p) \underset{p^2\to 0}{\simeq} \left(\begin{array}{c|c} a_1^{-1} & 0 \\ \hline 0 & b_0^{-1}\frac{1}{p^2}\end{array}\right)\,, \tag{3.307}$$

having assumed that b_0 is invertible, while a_1 must be so (otherwise the corresponding zero modes should have been included in the zero-mode subspace). As we know from the Källén-Lehmann representation, the poles of $D(p)$ correspond to the masses of the particles that appear in the theory. The dimension of the lower right block is at least $n_0 \times n_0$ with n_0 the number of broken generators, so the corresponding pole at $p^2 = 0$ is of rank at least n_0, corresponding to at least n_0 massless modes.

[25] In general, the induced representation of H is not irreducible even if the representation of G is, so we cannot conclude that $d_{0,1}$ are multiples of the identity in $\mathbb{R}^N$.

Energy interpretation of the effective action If we smoothly turn on a source $J(t,\vec{x})$ in the distant past, leading up to a time-independent source $j(\vec{x})$ between $t=-T/2$ and $t=+T/2$, that we subsequently turn off smoothly in the distant future, the vacuum $|0\rangle$ in the absence of a source is adiabatically transformed into the ground state $|j\rangle$ in the presence of a time-independent source j, which is then adiabatically transformed back to the vacuum $|0\rangle$. The vacuum-to-vacuum transition amplitude is given in general by Eq. (3.222), and in the case at hand, since we can neglect the contribution from the switching on and the switching off of the source (assumed to take place in a time much smaller than T), we have

$$\begin{aligned} e^{i(W[J]-W[0])} = \frac{Z[J]}{Z[0]} &= \langle 0|\mathcal{U}_J(+\infty,-\infty)|0\rangle = \langle j|\mathcal{U}_J\left(+\tfrac{T}{2},-\tfrac{T}{2}\right)|j\rangle \\ &= \langle j|\mathrm{Texp}\Big\{-i\int_{-\frac{T}{2}}^{+\frac{T}{2}} dt\,\Big[H-\int d^3x\, j(\vec{x})\hat{\phi}(0,\vec{x})\Big]\Big\}|j\rangle \\ &= \langle j|e^{-iH_jT}|j\rangle = e^{-iE_jT}\,, \end{aligned} \tag{3.308}$$

where

$$\begin{aligned} H_j &\equiv H-\int d^3x\, j(\vec{x})\hat{\phi}(0,\vec{x})\,, \\ H_j|j\rangle &= E_j|j\rangle\,, \end{aligned} \tag{3.309}$$

and so

$$W[J]-W[0] = -E_jT\,. \tag{3.310}$$

Consider now a different line of thought. We want to find the state $|\Omega\rangle$ that minimises the energy expectation value,

$$\langle H\rangle_\Omega = \frac{\langle\Omega|H|\Omega\rangle}{\langle\Omega|\Omega\rangle}\,, \tag{3.311}$$

subject to the constraint that the fields have prescribed time-independent expectation values,

$$\langle\hat{\phi}(0,\vec{x})\rangle_\Omega = \frac{\langle\Omega|\hat{\phi}(0,\vec{x})|\Omega\rangle}{\langle\Omega|\Omega\rangle} = \varphi(\vec{x})\,. \tag{3.312}$$

Minimisation could of course be performed for $\langle\Omega|H|\Omega\rangle$ with the constraints Eq. (3.312) and $\langle\Omega|\Omega\rangle=1$. This problem is equivalently formulated using Lagrange multipliers, as the unconstrained minimisation over Ω, α and $\beta(\vec{x})$ of the quantity

$$\langle\Omega|H|\Omega\rangle - \alpha\langle\Omega|\Omega\rangle - \int d^3x\,\beta(\vec{x})\langle\Omega|\hat{\phi}(0,\vec{x})|\Omega\rangle\,. \tag{3.313}$$

Minimisation over $|\Omega\rangle$ gives the equation

$$\left(H-\int d^3x\,\beta(\vec{x})\hat{\phi}(0,\vec{x})\right)|\Omega\rangle = \alpha|\Omega\rangle\,. \tag{3.314}$$

On the other hand, we know that the state $|j\rangle$ provides a solution to this equation with $\alpha=E_j$, $\beta(\vec{x})=j(\vec{x})$, if the prescribed values of the fields in Eq. (3.312) are chosen to be $\varphi(\vec{x})=\langle\phi\rangle_J=\varphi_J(\vec{x})$ with the source J described above, i.e., constant and equal to j for $t\in[-T/2,T/2]$:

$$\begin{aligned} &\left(H-\int d^3x\, j(\vec{x})\hat{\phi}(0,\vec{x})\right)|j\rangle = E_j|j\rangle\,, \qquad \langle j|j\rangle = 1\,, \\ &\langle j|\hat{\phi}(x)|j\rangle = \langle\phi\rangle_J = \left.\frac{\delta W[\bar{J}]}{\delta\bar{J}}\right|_{\bar{J}=J}\,. \end{aligned} \tag{3.315}$$

To find out what the corresponding minimum of $\langle H\rangle_\Omega$ is, notice that

$$\begin{aligned}\min\langle H\rangle_\Omega = \langle H\rangle_{\Omega=j} &= \int d^3x\, j(\vec{x})\langle j|\hat{\phi}(0,\vec{x})|j\rangle + E_j\langle j|j\rangle = E_j + \int d^3x\, j(\vec{x})\varphi_J(0,\vec{x}) \\ &= \frac{1}{T}\left(TE_j + \int d^4x\, j(\vec{x})\varphi_J(0,\vec{x})\right) = \frac{1}{T}\left(-W[J] + J\cdot\varphi_J + W[0] - 0\cdot 0\right) \\ &= -\frac{1}{T}(\Gamma[\varphi_J] - \Gamma[0])\,.\end{aligned} \tag{3.316}$$

Then, ignoring $W[0]$ and $\Gamma[0]$ which are respectively J-independent and φ-independent constants that can be set to zero without any loss of information, one has that

- $-W[J]/T = E_j$ is the energy of the ground state in the presence of a time-independent source j;
- $-\Gamma[\varphi]/T = \min\langle H\rangle_\Omega$ is the minimal expectation value of the energy over normalised states $|\Omega\rangle$ under the constraint that quantum fields have the prescribed time-independent expectation value $\langle\Omega|\hat{\phi}|\Omega\rangle = \varphi$.

For translation-invariant theories, the n-point functions $W^{(n)}$ depend only on the coordinate differences, and therefore so do the functions $\Gamma^{(n)}$ that are derived from them. Regularising the effective action in a finite four-dimensional box of size $V_4 = T\times V$, we have for an x-independent field configuration φ_0 that

$$\Gamma[\varphi_0] = V_4\mathcal{V}[\varphi_0] = TV\mathcal{V}[\varphi_0]\,. \tag{3.317}$$

According to the discussion above, $\mathcal{V}[\varphi_0]$ is then the minimal expectation value of the energy density on states for which the expectation value of the field is φ_0.[26] This happens for example for the solutions of $\Gamma'[\varphi_0] = 0$, i.e., for the vacua of the theory (in the absence of external sources), which are x-independent for translation-invariant theories.

References

- Generating functionals are discussed in detail in

  S. Weinberg, "The Quantum Theory of Fields – Vol. 2: Modern Applications", chapter 16;

  J. Zinn-Justin, "Quantum Field Theory and Critical Phenomena", chapter 7.

- Coleman's argument for one-particle irreducibility is found in

  S. Coleman, "Aspects of symmetry", section 3.4;

  S. Weinberg, *op. cit.* , section 16.1;

[26] As a matter of fact, the actual definition of Γ is $\Gamma[\varphi] = \inf_J W[J] - J\cdot\varphi$, which makes it a convex function. This does not always coincide with the definition given above, but it is the case in a finite volume or when the classical potential appearing in the classical action S is convex. In this case the minimum of Γ is unique and identifies the vacuum of the theory. For theories with spontaneously broken symmetry the classical potential is not convex, the minimum is not unique, and the vacuum is determined also by how the spontaneous breaking is realised, i.e., by what small explicit breaking one introduces first and then removes to define the theory. See, e.g., L. O'Raifeartaigh, A. Wipf and H. Yoneyama, "The constraint effective potential", Nucl. Phys. B **271** (1986) 653–680.

- the energy interpretation of Γ is discussed in

  S. Coleman, "Aspects of symmetry", section 3.7;

  S. Weinberg, *op. cit.* , section 16.3.

4 Non-Abelian gauge theories

The symmetry properties of a system impose strong restrictions on its dynamics. This is even more so when the symmetry is local, i.e., the system is invariant under transformations that depend on the spacetime point. We will consider field theories defined by Lagrangeans $\mathscr{L}$ involving one or more sets of fields $\phi_i^{(R)}(x)$, $i = 1, \ldots, N_R$, that are transformed into each other by the symmetry transformations. The label R indicates explicitly the representation D_R of the symmetry group G under according to which they transform. We restrict our attention to matrix Lie groups G, that we now briefly review.

Matrix Lie groups and Lie algebras A matrix Lie group G is a matrix group that is at the same time a smooth manifold, that can be parameterised (at least locally) by $\mathcal{D}_G$ real parameters α_a, $a = 1, \ldots, \mathcal{D}_G$; $\mathcal{D}_G$ is called the dimension of the group. This means that every $g \in G$ is a function $g = g(\alpha)$ of the parameters $\{\alpha\}$. The parameterisation is chosen so that $g(0) = e$ is the identity element, $eg = ge = g$, $\forall g \in G$. The Lie algebra $\mathfrak{g}$ of G is the real vector space $X = X^a L_a$, $X^a \in \mathbb{R}$ spanned by the group generators $L_a \equiv -i\partial g(\alpha)/\partial\alpha^a|_{\alpha=0}$, equipped with the commutator. It is a property of Lie groups that $[X, Y] \in \mathfrak{g}$, $\forall X, Y \in \mathfrak{g}$, a property that thanks to linearity is equivalently expressed by the relations

$$[L_a, L_b] = i f^c{}_{ab} L_c \,. \tag{4.318}$$

The real numbers $f^c{}_{ab}$ are the *structure constants* of the group, and are completely determined once that a parameterisation $\{\alpha\}$ of the group near the identity is given.[27] Explicitly,

$$\begin{aligned}
[L_a, L_b] &= [(-i)\tfrac{\partial}{\partial\alpha_a} g(\alpha)\big|_{\alpha=0}, (-i)\tfrac{\partial}{\partial\beta_b} g(\beta)\big|_{\beta=0}] \\
&= -\tfrac{\partial^2}{\partial\alpha_a\partial\beta_b}[g(\alpha), g(\beta)]\big|_{\alpha=0,\beta=0} = -\tfrac{\partial^2}{\partial\alpha_a\partial\beta_b}\left(g(\alpha)g(\beta) - g(\beta)g(\alpha)\right)\big|_{\alpha=0,\beta=0} \\
&= -\tfrac{\partial^2}{\partial\alpha_a\partial\beta_b}\left[g(\gamma(\alpha,\beta)) - g(\gamma(\beta,\alpha)\right]\big|_{\alpha=0,\beta=0} \\
&= -\left(\frac{\partial^2\gamma^c(\alpha,\beta)}{\partial\alpha_a\partial\beta_b} - \frac{\partial^2\gamma^c(\beta,\alpha)}{\partial\alpha_a\partial\beta_b}\right)\Big|_{\alpha=0,\beta=0} \frac{\partial g(\gamma)}{\partial\gamma^c}\Big|_{\gamma=0} \\
&= -i\left(\frac{\partial^2\gamma^c(\alpha,\beta)}{\partial\alpha_a\partial\beta_b} - \frac{\partial^2\gamma^c(\alpha,\beta)}{\partial\alpha_b\partial\beta_a}\right)\Big|_{\alpha=0,\beta=0} (-i)\frac{\partial g(\gamma)}{\partial\gamma^c}\Big|_{\gamma=0} \\
&= i\left(-\frac{\partial^2\gamma^c(\alpha,\beta)}{\partial\alpha_a\partial\beta_b} + \frac{\partial^2\gamma^c(\alpha,\beta)}{\partial\alpha_b\partial\beta_a}\right)\Big|_{\alpha=0,\beta=0} L_c = i f^c{}_{ab} L_c \,,
\end{aligned} \tag{4.319}$$

where the group property has been used to express $g(\alpha)g(\beta)$ as $g(\gamma(\alpha,\beta))$ for suitable functions γ^c, $c = 1, \ldots, \mathcal{D}_G$, that obey $\gamma^c(0,0) = 0$.

[27] A change in parameterisation corresponds to a change of basis in $\mathfrak{g}$.

Representations of Lie groups and algebras Representations of G are maps of G on the space of invertible $N_R \times N_R$ complex matrices that preserve the group multiplication law, i.e., there is a $D_R(g)$ for any $g \in G$, and furthermore

$$D_R(g_1)D_R(g_2) = D_R(g_1 g_2), \quad \forall g_{1,2} \in G\,. \tag{4.320}$$

A representation of the group induces a representation $d_R(X)$ of the algebra, via

$$-i\frac{\partial}{\partial\alpha_a} D_R(g(\alpha))\Big|_{\alpha=0} \equiv d_R(L_a) \equiv t^a_R\,, \tag{4.321}$$

extended by linearity, i.e., $d_R(X) = d_R(X^a L_a) = X^a d_R(L_a) = X^a t^a_R$. A representation of the algebra is a linear mapping of $\mathfrak{g}$ on a space complex matrices that preserves the commutator, i.e., $d_R([X,Y]) = [d_R(X), d_R(Y)]$. Using Eq. (4.321) and repeating the calculation of Eq. (4.319), we find

$$\begin{aligned}
[t^a_R, t^b_R] &= [(-i)\tfrac{\partial}{\partial\alpha_a} D_R(g(\alpha))\big|_{\alpha=0}, (-i)\tfrac{\partial}{\partial\beta_b} D_R(g(\beta))\big|_{\beta=0}] \\
&= -\tfrac{\partial^2}{\partial\alpha_a\partial\beta_b}[D_R(g(\alpha)), D_R(g(\beta))]\big|_{\alpha=0,\beta=0} \\
&= -\tfrac{\partial^2}{\partial\alpha_a\partial\beta_b}\left(D_R(g(\alpha)g(\beta)) - D_R(g(\beta)g(\alpha))\right)\big|_{\alpha=0,\beta=0} \\
&= -\tfrac{\partial^2}{\partial\alpha_a\partial\beta_b}\left(D_R(g(\gamma(\alpha,\beta))) - D_R(g(\gamma(\beta,\alpha)))\right)\big|_{\alpha=0,\beta=0} \\
&= -\left(\tfrac{\partial^2\gamma^c(\alpha,\beta)}{\partial\alpha_a\partial\beta_b} - \tfrac{\partial^2\gamma^c(\beta,\alpha)}{\partial\alpha_a\partial\beta_b}\right)\big|_{\alpha=0,\beta=0} \frac{\partial D_R(\gamma)}{\partial\gamma^c}\bigg|_{\gamma=0} \\
&= -i\left(\tfrac{\partial^2\gamma^c(\alpha,\beta)}{\partial\alpha_a\partial\beta_b} - \tfrac{\partial^2\gamma^c(\alpha,\beta)}{\partial\alpha_b\partial\beta_a}\right)\big|_{\alpha=0,\beta=0}(-i)\frac{\partial D_R(\gamma)}{\partial\gamma^c}\bigg|_{\gamma=0} = i f^c{}_{ab} t^c_R\,,
\end{aligned} \tag{4.322}$$

with the same coefficients $f^c{}_{ab}$ as in Eq. (4.319). Here we used the fact that D_R is a representation to go from the second to the third line.

Global and local symmetries The statement that $\mathscr{L} = \mathscr{L}(\phi)$ is *globally* invariant under the symmetry group G is expressed mathematically as follows,

$$\mathscr{L}(D_R(g)\phi^{(R)}) = \mathscr{L}(\phi^{(R)}), \quad \forall g \in G\,, \tag{4.323}$$

where g is an x-independent group element. With ϕ without a superscript we denote callectively all the fields present in the theory. In infinitesimal form, the invariance condition $\delta\mathscr{L} = \mathscr{L}(\phi + \delta\phi) - \mathscr{L}(\phi) = 0$, where

$$\delta\phi^{(R)}_j(x) = i\epsilon^a (t^a_R)_{jk}\phi^{(R)}_k(x)\,, \tag{4.324}$$

and ϵ^a are x-independent infinitesimal parameters. Since any element of a (connected) Lie group G can be obtained by multiplying elements in a neighbourhood of the identity, the infinitesimal form Eq. (4.324) is as good as the finite form Eq. (4.323). A symmetry is said to be *local* if Eq. (4.323) holds for x-dependent $g = g(x)$, or, in infinitesimal form, if (4.324) holds for x-dependent $\epsilon^a = \epsilon^a(x)$,

$$\delta\phi^{(R)}_j(x) = i\epsilon^a(x) (t^a_R)_{jk}\phi^{(R)}_k(x)\,. \tag{4.325}$$

A transformation of this type is called an infinitesimal *gauge transformation*. Given a globally-invariant Lagrangean, $\mathscr{L} = \mathscr{L}(\phi)$, its upgrading to a locally invariant one is problematic if there

are field derivatives, which is the case for all the interesting Lagrangeans. The problem is that global invariance amounts to

$$\begin{aligned}\delta_{\text{global}}\mathscr{L}(\phi,\partial_\mu\phi) &= \delta\phi_j^{(R)}\frac{\partial\mathscr{L}}{\partial\phi_j^{(R)}(x)} + \delta(\partial_\mu\phi_j^{(R)})\frac{\partial\mathscr{L}}{\partial(\partial_\mu\phi_j^{(R)}(x))}\\ &= \delta\phi_j^{(R)}\frac{\partial\mathscr{L}}{\partial\phi_j^{(R)}(x)} + \partial_\mu(\delta\phi_j^{(R)})\frac{\partial\mathscr{L}}{\partial(\partial_\mu\phi_j^{(R)}(x))}\\ &= i\epsilon^a(t_R^a)_{jk}\left(\phi_k^{(R)}(x)\frac{\partial\mathscr{L}}{\partial\phi_j^{(R)}(x)} + \partial_\mu\phi_k^{(R)}(x)\frac{\partial\mathscr{L}}{\partial(\partial_\mu\phi_j^{(R)}(x))}\right) = 0\,,\end{aligned} \tag{4.326}$$

which implies

$$\begin{aligned}0 &= i(t_R^a)_{jk}\left(\phi_k^{(R)}(x)\frac{\partial\mathscr{L}}{\partial\phi_j^{(R)}(x)} + \partial_\mu\phi_k^{(R)}(x)\frac{\partial\mathscr{L}}{\partial(\partial_\mu\phi_j^{(R)}(x))}\right)\\ &= \frac{\partial}{\partial\eta^a}\mathscr{L}(\phi + i(\eta\cdot t)\phi, \partial_\mu\phi + i(\eta\cdot t)\partial_\mu\phi)\Big|_{\eta=0}\,,\end{aligned} \tag{4.327}$$

where $\eta\cdot t = \eta^a t^a$ and the use of appropriate representation for each of the fields $\phi^{(R)}$ is understood. Since fields and their derivatives are arbitrary, it follows that

$$\frac{\partial}{\partial\eta^a}\mathscr{L}(A + i(\eta\cdot t)A, B + i(\eta\cdot t)B)\Big|_{\eta=0} = 0\,. \tag{4.328}$$

On the other hand, under a local transformation

$$\begin{aligned}\delta_{\text{local}}\mathscr{L}(\phi,\partial_\mu\phi) &= \delta\phi_j^{(R)}\frac{\partial\mathscr{L}}{\partial\phi_j^{(R)}(x)} + \delta(\partial_\mu\phi_j^{(R)})\frac{\partial\mathscr{L}}{\partial(\partial_\mu\phi_j^{(R)}(x))}\\ &= \delta\phi_j^{(R)}\frac{\partial\mathscr{L}}{\partial\phi_j^{(R)}(x)} + \partial_\mu(\delta\phi_j^{(R)})\frac{\partial\mathscr{L}}{\partial(\partial_\mu\phi_j^{(R)}(x))}\\ &= i\epsilon^a(x)(t_R^a)_{jk}\phi_k^{(R)}(x)\frac{\partial\mathscr{L}}{\partial\phi_j^{(R)}(x)} + i(t_R^a)_{jk}\partial_\mu(\epsilon^a(x)\phi_k^{(R)}(x))\frac{\partial\mathscr{L}}{\partial(\partial_\mu\phi_j^{(R)}(x))}\\ &= i\epsilon^a(x)(t_R^a)_{jk}\left(\phi_k^{(R)}(x)\frac{\partial\mathscr{L}}{\partial\phi_j^{(R)}(x)} + \partial_\mu\phi_k^{(R)}(x)\frac{\partial\mathscr{L}}{\partial(\partial_\mu\phi_j^{(R)}(x))}\right)\\ &\quad + i(t_R^a)_{jk}\partial_\mu(\epsilon^a(x))\phi_k^{(R)}(x)\frac{\partial\mathscr{L}}{\partial(\partial_\mu\phi_j^{(R)}(x))}\\ &= (\partial_\mu\epsilon^a(x))\left(i(t_R^a)_{jk}\phi_k^{(R)}(x)\frac{\partial\mathscr{L}}{\partial(\partial_\mu\phi_j^{(R)}(x))}\right) \neq 0\,,\end{aligned} \tag{4.329}$$

i.e., there is an extra term involving $\partial_\mu\epsilon^a$ that does not necessarily vanish – as a matter of fact, for fields satisfying the equations of motion the unwanted term is equal to $(\partial_\mu\epsilon^a)j^{a\mu}_{\text{Noether}}$.

Gauge fields The unwanted term can be compensated if we introduce new fields that couple to the symmetry current and are endowed with a suitable transformation law that involves $\partial_\mu\epsilon^a$.

To achieve this, we introduce the *gauge fields* A^a_μ, $a = 1, \ldots, \mathcal{D}_G$, and couple them to the *matter fields* $\phi^{(R)}$ through the covariant derivatives $D^{(R)}_\mu \phi^{(R)}$,

$$\begin{aligned} D^{(R)}_\mu &\equiv \partial_\mu + i g_R A^a_\mu t^a_R \,, \\ (D^{(R)}_\mu \phi^{(R)})_j &= \partial_\mu \phi^{(R)}_j + i g_R A^a_\mu (t^a_R)_{jk} \phi^{(R)}_k = (\partial_\mu \delta_{jk} + i g_R A^a_\mu (t^a_R)_{jk}) \phi^{(R)}_k \,, \end{aligned} \tag{4.330}$$

for some constant g_R, that may in principle depend on the set of matter fields $\phi^{(R)}$ on which it is applied. If we can make $D^{(R)}_\mu \phi^{(R)}$ transform like $\phi^{(R)}$, i.e.,

$$\delta(D^{(R)}_\mu \phi^{(R)})_j = i\epsilon^a(x)(t^a_R)_{jk}(D^{(R)}_\mu \phi^{(R)})_k \tag{4.331}$$

and replace the ordinary derivatives $\partial_\mu \phi^{(R)}$ in $\mathscr{L}$ with covariant derivatives $D^{(R)}_\mu \phi^{(R)}$, then under the new transformation δ'_{local}

$$\begin{aligned} \delta'_{\text{local}} \mathscr{L}(\phi, D_\mu \phi) &= \delta\phi^{(R)}_j \frac{\partial \mathscr{L}}{\partial \phi^{(R)}_j(x)} + \delta(D_\mu \phi^{(R)}_j) \frac{\partial \mathscr{L}}{\partial (D_\mu \phi^{(R)}_j(x))} \\ &= i\epsilon^a(x)(t^a_R)_{jk} \left(\phi^{(R)}_k(x) \frac{\partial \mathscr{L}}{\partial \phi^{(R)}_j(x)} + D_\mu \phi^{(R)}_k(x) \frac{\partial \mathscr{L}}{\partial (D_\mu \phi^{(R)}_j(x))} \right) \\ &= \epsilon^a(x) \frac{\partial}{\partial \eta^a} \mathscr{L}(\phi + i(\eta \cdot t)\phi, D_\mu \phi + i(\eta \cdot t) D_\mu \phi) \Big|_{\eta=0} = 0 \,, \end{aligned} \tag{4.332}$$

thanks to Eq. (4.328). We still need to find the appropriate transformation law for the gauge fields in order for Eq. (4.331) to hold. To this end, notice that

$$\begin{aligned} \delta(D^{(R)}_\mu \phi^{(R)}) &= \partial_\mu \left(\delta\phi^{(R)} \right) + i g_R A^a_\mu t^a_R \left(\delta\phi^{(R)} \right) + i g_R \left(\delta A^a_\mu \right) t^a_R \phi^{(R)} \\ &= i\epsilon^a(x) t^a_R \partial_\mu \phi^{(R)}(x) + i(\partial_\mu \epsilon^a(x)) t^a_R \phi^{(R)}(x) \\ &\quad + i g_R A^b_\mu t^b_R i\epsilon^a(x) t^a_R \phi^{(R)} + i g_R \left(\delta A^a_\mu \right) t^a_R \phi^{(R)} \\ &= i\epsilon^a(x) t^a_R (\partial_\mu + i g_R A^b_\mu t^b_R) \phi^{(R)}(x) \\ &\quad + i(\partial_\mu \epsilon^a(x)) t^a_R \phi^{(R)}(x) + i\epsilon^a(x) i g_R A^b_\mu [t^b_R, t^a_R] \phi^{(R)} + i g_R \left(\delta A^a_\mu \right) t^a_R \phi^{(R)} \\ &= i\epsilon^a(x) t^a_R D^{(R)}_\mu \phi^{(R)}(x) \\ &\quad + i g_R \left(\frac{1}{g_R} \partial_\mu \epsilon^a(x) t^a_R - \epsilon^a(x) f^c{}_{ba} A^b_\mu t^c_R \right) \phi^{(R)}(x) + i g_R \left(\delta A^a_\mu \right) t^a_R \phi^{(R)} \\ &= i\epsilon^a(x) t^a_R D^{(R)}_\mu \phi^{(R)}(x) \\ &\quad + i g_R t^a_R \left(\frac{1}{g_R} \partial_\mu \epsilon^a(x) - f^a{}_{bc} A^b_\mu \epsilon^c(x) + \delta A^a_\mu \right) \phi^{(R)}(x) \,, \end{aligned} \tag{4.333}$$

so Eq. (4.331) holds if we set

$$\delta A^a_\mu = -\frac{1}{g_R} \partial_\mu \epsilon^a(x) - f^a{}_{bc} \epsilon^b(x) A^c_\mu = -\frac{1}{g_R} \partial_\mu \epsilon^a(x) + f^a{}_{bc} \epsilon^c(x) A^b_\mu \,. \tag{4.334}$$

However, one and the same transformation law applies to A^a_μ, independently of what matter fields it is coupled to, and so we are forced to set $g_R = g$ for all matter fields. Setting $(t^c_A)_{ab} = -i f^a{}_{bc}$, we finally have the transformation law of the gauge fields,

$$\delta A^a_\mu = -\frac{1}{g_R} \partial_\mu \epsilon^a(x) + i\epsilon^c(x)(t^c_A)_{ab} A^b_\mu \,. \tag{4.335}$$

The matrices t^c_A provide the so-called *adjoint representation* of the algebra (this follows from the Jacobi identity $[A,[B,C]]+\text{cyclic permutations}=0$ applied to the group generators).

Finite transformations Collecting the infinitesimal transformation laws found so far, we have

$$\begin{aligned}\delta\phi^{(R)}_j(x) &= i\epsilon^a(t^a_R)_{jk}\phi^{(R)}_k(x)\,,\\ \delta(D^{(R)}_\mu\phi^{(R)})_j &= i\epsilon^a(x)(t^a_R)_{jk}(D^{(R)}_\mu\phi^{(R)})_k\,,\\ \delta A^a_\mu &= -\frac{1}{g_R}\partial_\mu\epsilon^a(x)+i\epsilon^c(x)(t^c_A)_{ab}A^b_\mu\,.\end{aligned} \tag{4.336}$$

The behaviour of matter fields and corresponding covariant derivative under finite transformations is easily found by "exponentiating" the infinitesimal ones. In matrix notation,

$$\begin{aligned}\phi^{(R)\prime}(x) &= D_R(g(x))\phi^{(R)}(x) = U_R(x)\phi^{(R)}(x)\,,\\ (D^{(R)}_\mu\phi^{(R)})'(x) &= D_R(g(x))(D^{(R)}_\mu\phi^{(R)})(x) = U_R(x)(D_\mu\phi^{(R)})(x)\,,\end{aligned} \tag{4.337}$$

where $U_R(x)$ is shorthand for $U_R(x)=D_R(g(x))=e^{i\alpha_a(x)t^a_R}$. To find the behaviour of A^a_μ, notice first from the second equation in Eq. (4.337) that

$$\begin{aligned}(D^{(R)}_\mu\phi^{(R)})'(x) &= (\partial_\mu+igA'^a_\mu(x)t^a_R)\phi^{(R)\prime}(x) = (\partial_\mu+igA'^a_\mu(x)t^a_R)U_R(x)\phi^{(R)}(x)\\ &= U_R(x)(D_\mu\phi^{(R)})(x) = U_R(x)(\partial_\mu+igA^a_\mu(x)t^a_R)\phi^{(R)}(x)\,,\end{aligned} \tag{4.338}$$

which implies

$$\begin{aligned}A'^a_\mu(x)t^a_R &= U_R(x)A^a_\mu(x)t^a_RU_R(x)^{-1}-\frac{1}{ig}(\partial_\mu U_R(x))U_R(x)^{-1}\\ &= U_R(x)A^a_\mu(x)t^a_RU_R(x)^{-1}-\frac{i}{g}U_R(x)\partial_\mu U_R(x)^{-1}\,.\end{aligned} \tag{4.339}$$

The homogeneous part of this equation is seen to correspond to the adjoint group representation acting on A^a_μ, independently of R:

$$\begin{aligned}U_R(x)A^a_\mu(x)t^a_RU_R(x)^{-1} &= A^a_\mu(x)U_R(x)t^a_RU_R(x)^{-1} = A^a_\mu(x)t^b_R(U_A(x))_{ba}\\ &= t^a_R\left((U_A(x))_{ab}A^b_\mu(x)\right)\,.\end{aligned} \tag{4.340}$$

We now show that also $U_R(x)\partial_\mu U_R(x)^{-1}=-(\partial_\mu U_R(x))U_R(x)^{-1}$ is a linear combination of t^a_R, the same independently of R. In fact, recalling that $U_R(x)=D_R(g(x))$, since $g(x+dx)$ is close to $g(x)$ (assuming differentiability), then

$$g(x+dx)=\bar g(dx,g(x))g(x)\,, \tag{4.341}$$

where $\bar g(dx,g)$ is a group element close to the identity e, that depends on $g(x)$ and dx. But then

$$\begin{aligned}U_R(x+dx) &= D_R(g(x+dx)) = D_R(\bar g(dx,g(x))g(x)) = D_R(\bar g(dx,g(x)))D_R(g(x))\,,\\ (\partial_\mu U_R(x))U_R(x)^{-1} &= \frac{U_R(x+dx)-U_R(x)}{dx}U_R(x)^{-1} = \frac{U_R(x+dx)U_R(x)^{-1}-1}{dx}\\ &= \frac{D_R(\bar g(dx,g(x))g(x))D_R(g(x)^{-1})-1}{dx} = \frac{D_R(\bar g(dx,g(x)))-1}{dx}\,.\end{aligned} \tag{4.342}$$

Group elements close to the identity can be written as $\bar{g}(dx, g(x)) = e^{idxM_a(x)L_a}$ in terms of the generators L, for some small $\alpha_a = dxM_a(x)$ that must vanish proportionally to dx. Then, using Eq. (4.321),

$$\begin{aligned}(\partial_\mu U_R(x))U_R(x)^{-1} &= \frac{D_R(e^{idxM_a(x)L_a}) - 1}{dx} = \frac{e^{idxM_a(x)d_R(L_a)} - 1}{dx} = \frac{1 + idxM_a(x)t^a_R - 1}{dx} \\ &= M_a(x)t^a_R\,.\end{aligned} \tag{4.343}$$

For practical purposes, it is convenient to denote $A^a_\mu t^a_R = A_{R\mu}$, which under a finite gauge transformation transforms as $A_{R\mu} \to U_R A_{R\mu} U_R^{-1} - (i/g)U_R \partial_\mu U_R^{-1}$ [see Eq. (4.339)], and keep in mind that the transformation law that this implies for A^a_μ is independent of the R that one is using.

Field strength tensor In order to endow the gauge fields with some dynamics, one needs to include suitable kinetic terms in the Lagrangian. This, however, must be done in such a way as to preserve the local (gauge) symmetry. The simplest way to construct a gauge-invariant object involving derivatives of A^a_μ is to first construct a gauge-covariant object of this type, i.e., an object that transforms homogeneously under gauge transformations, like the fields $\phi^{(R)}$ do, and like the gauge fields do not because of the term $\partial_\mu \epsilon^a$. In turn, a simple way to build such an object is consider the commutator of two covariant derivatives. One has

$$\begin{aligned}[D^{(R)}_\mu, D^{(R)}_\nu] &= [\partial_\mu + igt^b_R A^b_\mu, \partial_\nu + igt^c_R A^c_\nu] \\ &= ig(\partial_\mu t^c_R A^c_\nu - \partial_\nu t^b_R A^b_\mu + igA^b_\mu A^c_\nu [t^b_R, t^c_R]) \\ &= igt^a_R \left(\partial_\mu A^a_\nu - \partial_\nu A^a_\mu - gf^a{}_{bc} A^b_\mu A^c_\nu\right) \equiv igt^a_R F^a_{\mu\nu}\,.\end{aligned} \tag{4.344}$$

Despite being the commutator of two differential operators, this object is not a differential operator anymore. To find its transformation properties, notice that under a finite gauge transformation

$$\begin{aligned}\left([D^{(R)}_\mu, D^{(R)}_\nu]\phi^{(R)}\right)'(x) &= [D^{(R)\prime}_\mu, D^{(R)\prime}_\nu]\phi^{(R)\prime}(x) \\ &= U_R(x)[D^{(R)}_\mu, D^{(R)}_\nu]\phi^{(R)}(x) \\ &= \left(U_R(x)[D^{(R)}_\mu, D^{(R)}_\nu]U_R(x)^{-1}\right)\left(U_R(x)\phi^{(R)}(x)\right) \\ &= \left(U_R(x)[D^{(R)}_\mu, D^{(R)}_\nu]U_R(x)^{-1}\right)\phi^{(R)\prime}(x)\end{aligned} \tag{4.345}$$

and so

$$t^a_R F'^a_{\mu\nu} = U_R(x)t^a_R F^a_{\mu\nu} U_R(x)^{-1} = t^a_R \left(U_A(x)\right)_{ab} F^b_{\mu\nu} \Rightarrow F'^a_{\mu\nu} = \left(U_A(x)\right)_{ab} F^b_{\mu\nu}\,, \tag{4.346}$$

or in infinitesimal form

$$\delta F^a_{\mu\nu} = i\epsilon^c (t^c_A)_{ab} F^b_{\mu\nu}\,. \tag{4.347}$$

This is the same homogeneous transformation law one would find for a matter field in the adjoint representation.

Restrictions on the gauge group The simplest Lorentz and parity-invariant quantity that we can construct from $F^a_{\mu\nu}$ is a quadratic term of the form

$$-\frac{1}{4}g_{ab}F^a_{\mu\nu}F^{b\mu\nu} \tag{4.348}$$

for some matrix g_{ab} that can be taken symmetric without loss of generality. The prefactor is introduced for future convenience. Under a gauge transformation, one finds from Eq. (4.347) that

$$\begin{aligned}\delta\left(g_{ab}F^a_{\mu\nu}F^{b\mu\nu}\right) &= g_{ab}\delta\left(F^a_{\mu\nu}\right)F^{b\mu\nu} + g_{ab}F^a_{\mu\nu}\delta\left(F^{b\mu\nu}\right)\\ &= g_{ab}\left(i\epsilon^c(t^c_A)_{ad}F^d_{\mu\nu}F^{b\mu\nu} + F^a_{\mu\nu}i\epsilon^c(t^c_A)_{be}F^{e\mu\nu}\right)\\ &= i\epsilon^c\left(g_{ae}(t^c_A)_{ad} + g_{db}(t^c_A)_{be}\right)F^d_{\mu\nu}F^{e\mu\nu}\\ &= i\epsilon^c\left(g_{ea}(t^c_A)_{ad} + g_{db}(t^c_A)_{be}\right)F^d_{\mu\nu}F^{e\mu\nu}\,.\end{aligned} \tag{4.349}$$

In order for this to hold for arbitrary ϵ^c and without imposing restrictions on $F^a_{\mu\nu}$, one needs

$$g_{ea}(t^c_A)_{ad} + g_{db}(t^c_A)_{be} = 0 \quad\Longrightarrow\quad g_{ea}f^a{}_{dc} + g_{db}f^b{}_{ec} = 0\,. \tag{4.350}$$

Since we intend to use Eq. (4.348) as the kinetic term in a Lagrangean, there are two more conditions that g_{ab} must satisfy: it must be real, so that after quantisation the Hamiltonian derived from it be Hermitean; and it must be positive-definite, so that a Hilbert space with a positive-definite scalar product can be built for the quantised system. The origin of the second condition can be understood by analogy with the case of a scalar field. Noticing that $\Pi^{ai} = F^{ai0}$ are the canonical momenta conjugate to A^a_i (more on this later), one has

$$-g_{ab}F^a_{\mu\nu}F^{b\mu\nu} = g_{ab}\left(2\sum_i F^{ai0}F^{bi0} - \sum_{ij}F^a_{ij}F^b_{ij}\right) = g_{ab}\left(2\sum_i(\Pi^{ai})^2 - \sum_{ij}F^a_{ij}F^b_{ij}\right)\,, \tag{4.351}$$

similarly to what finds for a real scalar field, for which $\Pi = \mathcal{Z}\partial_0\phi$ if $\mathscr{L} = \mathcal{Z}/2(\partial_\mu\phi)^2 + \ldots$, and

$$\mathcal{Z}\partial_\mu\phi\partial^\mu\phi = \Pi^2/\mathcal{Z} - \mathcal{Z}(\vec{\nabla}\phi)^2\,. \tag{4.352}$$

In this case, a calculation identical to that used to derive the Källén-Lehmann representation of the propagator shows that

$$\langle 0|[\phi(x),\phi(0)]|0\rangle = \int ds\,\rho(s)\int_0^\infty d\Omega^{(s)}_p\,\left(e^{-ip\cdot x} - e^{ip\cdot x}\right)\,,\qquad p^0 = \sqrt{s+\vec{p}^2}\,. \tag{4.353}$$

Multiplying by $\mathcal{Z}$, taking the derivative with respect to x^0 and then setting $x^0 = 0$, one finds

$$\begin{aligned}\mathcal{Z}\langle 0|[\dot{\phi}(0,\vec{x}),\phi(0)]|0\rangle &= -i\delta^{(3)}(\vec{x}) = \mathcal{Z}\int_0^\infty ds\,\rho(s)\int d\Omega^{(s)}_p\,(-ip^0)\left(e^{i\vec{p}\cdot\vec{x}} + e^{-i\vec{p}\cdot\vec{x}}\right)\\ &= -i\delta^{(3)}(\vec{x})\mathcal{Z}\int_0^\infty ds\,\rho(s) \Rightarrow \frac{1}{\mathcal{Z}} = \int_0^\infty ds\,\rho(s) \geq 0\,,\end{aligned} \tag{4.354}$$

with positivity of ρ originating in the positivity of the scalar product. Hence, a negative $\mathcal{Z}$ is incompatible with a positive-definite scalar product in the Hilbert space of the quantised system.

We now have to find a matrix g_{ab} that is (1.) real, symmetric, positive-definite, and (2.) satisfies the invariance condition Eq. (4.350). One has the following theorem:

A matrix g_{ab} that satisfies the conditions (1.) and (2.) exists if and only if the Lie algebra defined by the structure constants $f^a{}_{bc}$ is the direct sum of commuting simple compact and U(1) Lie algebras.

The direct sum of Lie algebras is their direct sum as linear spaces. The U(1) algebra is the Lie algebra of the group U(1) of complex numbers of modulus 1 equipped with the usual multiplication. More than one copy of the same algebra is allowed. For a direct sum of algebras one can choose the generators L_a so that they correspond to the generators of the various component algebras, i.e., $L_a^{(n)}$, where n labels the subalgebra[28] and a the generator within the subalgebra with

$$[L_{(n)a}, L_{(m)b}] = if^{(o)c}{}_{(n)a(m)b} L_{(o)c} = \delta_{mo}\delta_{no} if^{[n]c}{}_{ab} L_{(n)c} \tag{4.355}$$

and $f^{[n]c}{}_{ab}$ the structure constants of the nth component. A direct sum $\oplus_i \mathfrak{g}_i$ of Lie algebras $\mathfrak{g}_i$ corresponding to Lie groups G_i is the Lie algebra of the direct product of the groups $\otimes G_i$.

A simple Lie algebra is the Lie algebra of a simple Lie group,[29] which in turn is a Lie group without any normal subgroup. A normal subgroup H is such that $ghg^{-1} \in H \ \forall h \in H, g \in G$. A compact simple Lie algebra is the algebra of a simple Lie group which is also compact as a manifold (for matrix groups this means a closed and bounded subspace of some space $\mathbb{R}^N$). In terms of the structure constants $f^a{}_{bc}$, a Lie algebra is simple if and only if the bilinear form defined by the symmetric matrix $K_{ab} = -f^c{}_{ad} f^d{}_{bc}$ is non-degenerate, i.e, if $v_a w_b K_{ab} = 0$ $\forall w \in \mathbb{R}^{\mathcal{D}_G}$ then $v = 0$. A Lie algebra is simple and compact if and only if K_{ab} is positive-definite, i.e., $v_a v_b K_{ab} \geq 0$ with equality holding only if $v = 0$. For a simple compact Lie algebra one can choose the basis of generators L_a in such a way that the resulting structure constants are invariant under cyclic permutations of the indices, i.e.,

$$f^a{}_{bc} = f^c{}_{ab} = f^b{}_{ca} \tag{4.356}$$

and as such totally antisymmetric, since they are obviously antisymmetric in the second pair of indices. We can then write them as $f_{abc} = f_{cab} = f_{bca}$ without any ambiguity.

Yang-Mills Lagrangean Having restricted the choice of group as discussed above, and having chosen the generators so that Eq. (4.355) holds, the invariance condition Eq. (4.350) for the matrix g_{ab} can be written as

$$\begin{aligned} 0 &= g_{ea}(t_A^c)_{ad} + g_{db}(t_A^c)_{be} = g_{ea}(-if_{adc}) + g_{db}(-if_{bec}) \\ &= -g_{ea}(-if_{dac}) + g_{db}(-if_{bec}) = -(t_A^c)_{da} g_{ae} + g_{db}(t_A^c)_{be}\,, \end{aligned} \tag{4.357}$$

or in matrix notation

$$[g, t_A^c] = 0\,. \tag{4.358}$$

The representatives t_A^c in the adjoint representation for the choice of generators $L_{(n)a}$ appearing in Eq. (4.355) read

$$\begin{aligned} \left(t_A^{(o)c}\right)_{(n)a(m)b} &= -if^{(o)c}{}_{(n)a(m)b}\delta_{mo}\delta_{no} = \delta_{mo}\delta_{no}(-if^{[o]c}{}_{ab}) \\ &= \delta_{mo}\delta_{no}(-if^{[o]}{}_{cab}) = \delta_{mo}\delta_{no}(t_A^{[o]c})_{ab}\,, \end{aligned} \tag{4.359}$$

[28] A subalgebra $\mathfrak{h}$ of a Lie algebra $\mathfrak{g}$ is a linear subspace of $\mathfrak{g}$ that is invariant under commutators, i.e., schematically, $[\mathfrak{h}, \mathfrak{h}] \subseteq \mathfrak{h}$. Clearly, the various component algebras are subalgebras of their direct sum.

[29] A more direct characterisation of a simple Lie algebra $\mathfrak{g}$ is that it does not contain any ideal, other than the empty set and the whole of $\mathfrak{g}$. An ideal is a linear subspace $\mathfrak{h}$ that is left invariant by commutators with the whole algebra, schematically $[\mathfrak{g}, \mathfrak{h}] \subseteq \mathfrak{h}$.

i.e., they are block-diagonal with non-zero entries only in the diagonal block with $n = m = o$, corresponding to the oth subalgebra. The entries of this block provide the adjoint representation of the oth subalgebra. In particular, blocks corresponding to the U(1) subalgebras are zero. It is known that the adjoint representation of a simple algebra is irreducible,[30] and that a matrix M that commutes with all the representatives of the generators in an irreducible representation is a multiple of the identity (Schur's lemma). Equation reads explicitly (the notation should be clear)

$$\begin{aligned}
\sum_{K,k} g_{Nn,Kk} t^{Oa}_{Kk,Mm} &= \sum_{K,k} t^{Oa}_{Nn,Kk} g_{Kk,Mm} \\
\sum_{K,k} g_{Nn,Kk} \delta_{OK}\delta_{OM} t^{[O]a}_{km} &= \sum_{K,k} \delta_{OK}\delta_{ON} t^{[O]a}_{nk} g_{Kk,Mm} \\
\sum_{K,k} g^{[NK]}_{nk} \delta_{OK}\delta_{OM} t^{[O]a}_{km} &= \sum_{K,k} \delta_{OK}\delta_{ON} t^{[O]a}_{nk} g^{[KM]}_{km} \\
\delta_{OM} \sum_{k} g^{[NO]}_{nk} t^{[O]a}_{km} &= \delta_{ON} \sum_{k} t^{[O]a}_{nk} g^{[OM]}_{km} \\
\delta_{OM} g^{[NO]} t^{[O]a} &= \delta_{ON} t^{[O]a} g^{[OM]} \,.
\end{aligned} \tag{4.360}$$

For $N = O \neq M$

$$t^{[N]a} g^{[NM]} = 0 \,, \tag{4.361}$$

and for $N \neq O = M$

$$g^{[NM]} t^{[M]a} = 0 \,. \tag{4.362}$$

For N corresponding to a U(1) subalgebra and M corresponding to a simple subalgebra, these two equations tell us that $g^{[NM]} = g^{[MN]} = 0$. For $N \neq M$ both corresponding to a U(1) subalgebra, these equations are trivially satisfied and give no information on $g^{[NM]}$. Consider then $N \neq M$ corresponding to simple subalgebras. Exponentiating Eq. (4.361) one finds that the columns of $g^{[NM]}$ are left invariant by all elements of an irreducible representation of the Lie group corresponding to the Nth subalgebra, i.e.,

$$D^{[N]}(\alpha) g^{[NM]} = e^{i \sum_{a=1}^{\mathcal{D}_G} \alpha_a t^{[N]a}} g^{[NM]} = \left(1 + \sum_{n=1}^{\infty} \frac{i^n}{n!} \left(\sum_{a=1}^{\mathcal{D}_G} \alpha_a t^{[N]a} \right)^n \right) g^{[NM]} = g^{[NM]} \,. \tag{4.363}$$

However, no nontrivial subspace is left invariant by an irreducible representation, and so $g^{[NM]} = 0$. Another way to obtain this result is to observe that from Eqs. (4.361) and (4.362) follows that for $N \neq M$ and all a in the Nth subalgebra,

$$0 = t^{[N]a} g^{[NM]} g^{[MN]} = g^{[NM]} g^{[MN]} t^{[N]a} \,, \tag{4.364}$$

so in particular $[t^{[N]a}, g^{[NM]} g^{[MN]}] = 0$, and by Schur's lemma $g^{[NM]} g^{[MN]} = A \mathbf{1}^{[N]}$, but since $0 = t^{[N]a} g^{[NM]} g^{[MN]} = A t^{[N]a}$ it follows $A = 0$. In particular then

$$0 = \operatorname{tr} g^{[NM]} g^{[MN]} = \sum_{nm} g^{[NM]}_{nm} g^{[MN]}_{mn} = \sum_{nm} g_{Nn,Mm} g_{Mm,Nn} = \sum_{nm} g^2_{Nn,Mm} \tag{4.365}$$

[30] An irreducible representation leaves no subspace of the representation space invariant. The adjoint representation represents the Lie algebra $\mathfrak{g}$ on itself (considered as a linear space), i.e., it is provided by the set of linear operators ad_X acting on $\mathfrak{g}$ defined by $\mathrm{ad}_X Y = [X, Y]$. One can show easily that $\mathrm{ad}_{L_a} = t^a_A$. If the adjoint representation were reducible, then a nontrivial invariant subspace of the representation space would exist, meaning $\mathfrak{s} \subseteq \mathfrak{g}$ with $\mathrm{ad}_X \mathfrak{s} \subseteq \mathfrak{s}$. But then $[X, \mathfrak{s}] \subseteq \mathfrak{s}$ $\forall X \in \mathfrak{g}$, and so $\mathfrak{s}$ would be an ideal, which for a simple algebra cannot be nontrivial.

and so $g_{Nn,Mm} = 0$ for $N \neq M$. For $N = M$ instead Eq. (4.360) gives

$$[g^{[NN]}, t^{[N]a}] = 0\,, \tag{4.366}$$

and so by Schur's lemma

$$g^{[NN]} = G^{[N]}\mathbf{1}^{[N]} = g_N^{-2}\mathbf{1}^{[N]} \tag{4.367}$$

where $G^{[N]}$ is necessarily a positive constant due to the positive-definiteness of g, and in the second passage we have made it explicit by setting $G^{[N]} = g_N^{-2}$. While not determined by Eqs. (4.361)–(4.366), the part of $g^{[NM]}$ corresponding to U(1) subalgebras can be diagonalised by a suitable orthogonal transformation, after which one finds

$$g_{Nn,Mm} = g^{[NM]}_{nk} = g_N^{-2}\delta^{NM}\delta_{nk}\,, \tag{4.368}$$

i.e., a diagonal positive-definite matrix of couplings.

In conclusion, the most general gauge group that can be used is the direct product of simple compact and U(1) groups, and for such a group the most general Lagrangean of the form Eq. (4.348) can be cast by a suitable redefinition of the fields as

$$\mathscr{L}_{\rm YM} = -\frac{1}{4}\sum_N g_N^{-2} F^{[N]a}_{\mu\nu} F^{[N]a\mu\nu}\,, \tag{4.369}$$

where the sum runs over the subgroups/subalgebras. This is the Yang-Mills Lagrangean (strictly speaking, a generalisation thereof). A simple redefinition of the fields, $A^{[N]a}_\mu = g_N \bar{A}^{[N]a}_\mu$, allows to remove g_N^{-2} from Eq. (4.369), at the price of redefining the field strength tensor and the covariant derivative as

$$\begin{aligned}
\bar{F}^{[N]a}_{\mu\nu} &= \partial_\mu \bar{A}^{[N]a}_\nu - \partial_\mu \bar{A}^{[N]a}_\nu - g g_N f_{abc} \bar{A}^{[N]b}_\mu \bar{A}^{[N]c}_\nu \\
&= \partial_\mu \bar{A}^{[N]a}_\nu - \partial_\mu \bar{A}^{[N]a}_\nu - \bar{g}_N f_{abc} \bar{A}^{[N]b}_\mu \bar{A}^{[N]c}_\nu\,, \\
D^{(R)}_\mu[\bar{A}] &= \partial_\mu + \sum_N i g g_N \bar{A}^{[N]a}_\mu t^{[N]a}_R = \partial_\mu + \sum_N i \bar{g}_N \bar{A}^{[N]a}_\mu t^{[N]a}_R\,, \\
\mathscr{L}_{\rm YM}(\bar{A}) &= -\frac{1}{4}\sum_N \bar{F}^{[N]a}_{\mu\nu} \bar{F}^{[N]a\mu\nu}\,.
\end{aligned} \tag{4.370}$$

The gauge transformation of the gauge fields read

$$\begin{aligned}
\delta \bar{A}^{[N]a}_\mu &= \delta(g_N^{-1} A^{[N]a}_\mu) = -\frac{1}{g g_N}\partial_\mu \epsilon^a(x) + i\epsilon^c(x)(t^c_A)_{ab} g_N^{-1} A^{[N]b}_\mu \\
&= -\frac{1}{\bar{g}_N}\partial_\mu \epsilon^a(x) + i\epsilon^c(x)(t^c_A)_{ab} \bar{A}^{[N]b}_\mu\,.
\end{aligned} \tag{4.371}$$

The simplest locally (gauge) invariant generalisation of a globally invariant Lagrangian $\mathscr{L}(\phi, \partial\phi)$ is then

$$\mathscr{L}(\phi, \partial\phi) \to \mathscr{L}(\phi, D[\bar{A}]\phi) + \mathscr{L}_{\rm YM}(\bar{A})\,. \tag{4.372}$$

Notably, each simple factor of the gauge group is associated with one universal coupling constant, the same for each matter field. The same coupling constant also appears in the self-interaction terms involving the gauge fields only. While apparently the same holds for the U(1) factors, since

any real number gives a possible representative $t_R^{[\mathrm{U}(1)]}$ of the single generator of the algebra, this restriction does not hold.[31] The universality of the coupling and the presence of self-interactions of the gauge fields are distinctive features of non-Abelian gauge fields, as opposed to the Abelina (i.e., U(1)) fields.

Topological term* If one requires Lorentz but not parity invariance, theere is a second quadratic terms that one can build from $F^a_{\mu\nu}$, namely

$$\theta_{ab}\epsilon_{\mu\nu\rho\sigma}F^{a\mu\nu}F^{b\rho\sigma} = \theta_{ab}F^{a\mu\nu}\tilde{F}^b_{\mu\nu}\,, \tag{4.373}$$

with θ_{ab} symmetric without loss of generality. Gauge invariance leads to the same condition Eq. (4.350) found previously for the Yang-Mills term, i.e.,

$$\theta_{ea}f^a{}_{dc} + \theta_{db}f^b{}_{ec} = 0\,. \tag{4.374}$$

For the type of gauge groups discussed above, using the same argument used above for g_{ab}, this condition leads to $\theta_{Aa,Bb} = \delta_{AB}\delta_{ab}\theta_A$. However, restricting our attention to a single simple compact factor, the term

$$q = \frac{1}{32\pi^2}\epsilon_{\mu\nu\rho\sigma}F^{a\mu\nu}F^{a\rho\sigma} = \frac{\bar{g}^2}{32\pi^2}\epsilon_{\mu\nu\rho\sigma}\bar{F}^{a\mu\nu}\bar{F}^{a\rho\sigma} \tag{4.375}$$

is the divergence of a four-vector, $q = \partial_\mu K^\mu$, with

$$K^\mu = \frac{1}{16\pi^2}\epsilon^{\mu\nu\rho\sigma}A^a_\nu\left(F^a_{\rho\sigma} + \frac{g}{3}f_{abc}A^b_\rho A^c_\sigma\right) = \frac{1}{8\pi^2}\epsilon^{\mu\nu\rho\sigma}A^a_\nu\left(\partial_\rho A^a_\sigma - \frac{g}{3}f_{abc}A^b_\rho A^c_\sigma\right)\,. \tag{4.376}$$

It follows that q does not affect the equations of motion, and can be ignored for the moment. To show that $q = \partial_\mu K^\mu$, notice that

$$\begin{aligned}
\partial_\mu(16\pi^2K^\mu) &= 2\epsilon^{\mu\nu\rho\sigma}(\partial_\mu A^a_\nu)\left(\partial_\rho A^a_\sigma - \frac{g}{3}f_{abc}A^b_\rho A^c_\sigma\right) + 2\epsilon^{\mu\nu\rho\sigma}A^a_\nu\left(\partial_\mu\partial_\rho A^a_\sigma - \frac{g}{3}f_{abc}\partial_\mu(A^b_\rho A^c_\sigma)\right)\\
&= 2\epsilon^{\mu\nu\rho\sigma}(\partial_\mu A^a_\nu)\left(\partial_\rho A^a_\sigma - \frac{g}{3}f_{abc}A^b_\rho A^c_\sigma\right) - \frac{4g}{3}\epsilon^{\mu\nu\rho\sigma}A^a_\nu f_{abc}(\partial_\mu A^b_\rho)A^c_\sigma\\
&= 2\epsilon^{\mu\nu\rho\sigma}(\partial_\mu A^a_\nu)\partial_\rho A^a_\sigma - 2g\epsilon^{\mu\nu\rho\sigma}f_{abc}(\partial_\mu A^a_\nu)A^b_\rho A^c_\sigma\\
&= \frac{1}{2}\epsilon^{\mu\nu\rho\sigma}(\partial_\mu A^a_\nu - \partial_\nu A^a_\mu)(\partial_\rho A^a_\sigma - \partial_\sigma A^a_\rho) - g\epsilon^{\mu\nu\rho\sigma}f_{abc}(\partial_\mu A^a_\nu - \partial_\nu A^a_\mu)A^b_\rho A^c_\sigma\\
&= \frac{1}{2}\epsilon^{\mu\nu\rho\sigma}\left(F^a_{\mu\nu}F^a_{\rho\sigma} - g^2f_{abc}f_{ade}A^b_\mu A^c_\nu A^d_\rho A^e_\sigma\right)\,.
\end{aligned} \tag{4.377}$$

[31] Notice, however, that irreducible representations of the *group* $\mathrm{U}(1) = \{e^{i\theta}, \theta \in [0, 2\pi)\}$ are of the form $D_n(e^{i\theta}) = e^{in\theta}$, and so $t_n^{[\mathrm{U}(1)]} = n$, which basically follows from periodicity in θ. This requires that the "electric" charges $\bar{g}_{\mathrm{U}(1)}t_n^{[\mathrm{U}(1)]} = n\bar{g}_{\mathrm{U}(1)}$ be integer multiples of a basic unit charge $\bar{g}_{\mathrm{U}(1)}$, thus indicating quantisation of the electric charge. On the other hand, the restriction found above is on the gauge *algebra*, and since the U(1) algebra is the same as the $\mathbb{R}$ algebra (i.e., real numbers with addition as the group law), one could think of the U(1) factors in the gauge group as $\mathbb{R}$ factors, for which the restriction on the irreducible representations does not apply.

The second term, however, is zero: exploiting the antisymmetry properties of $\epsilon^{\mu\nu\rho\sigma}$ and f_{abc}, one finds

$$\begin{aligned}
&\epsilon^{\mu\nu\rho\sigma} f_{abc} f_{ade} A^b_\mu A^c_\nu A^d_\rho A^e_\sigma = -\epsilon^{\mu\nu\rho\sigma} (t^c_A)_{ab} (t^e_A)_{ad} A^b_\mu A^c_\nu A^d_\rho A^e_\sigma = \epsilon^{\mu\nu\rho\sigma} (t^c_A)_{ba} (t^e_A)_{ad} A^b_\mu A^c_\nu A^d_\rho A^e_\sigma \\
&= \frac{1}{2}\epsilon^{\mu\nu\rho\sigma} \left((t^c_A)_{ba} (t^e_A)_{ad} A^b_\mu A^c_\nu A^d_\rho A^e_\sigma + (t^e_A)_{ba} (t^c_A)_{ad} A^b_\mu A^e_\nu A^d_\rho A^c_\sigma \right) \\
&= \frac{1}{2}\epsilon^{\mu\nu\rho\sigma} \left((t^c_A)_{ba} (t^e_A)_{ad} A^b_\mu A^c_\nu A^d_\rho A^e_\sigma + (t^e_A)_{ba} (t^c_A)_{ad} A^b_\mu A^c_\sigma A^d_\rho A^e_\nu \right) \\
&= \frac{1}{2}\epsilon^{\mu\nu\rho\sigma} \left((t^c_A)_{ba} (t^e_A)_{ad} A^b_\mu A^c_\nu A^d_\rho A^e_\sigma - (t^e_A)_{ba} (t^c_A)_{ad} A^b_\mu A^c_\nu A^d_\rho A^e_\sigma \right) \\
&= \frac{1}{2}\epsilon^{\mu\nu\rho\sigma} \left((t^c_A)_{ba} (t^e_A)_{ad} - (t^e_A)_{ba} (t^c_A)_{ad} \right) A^b_\mu A^c_\nu A^d_\rho A^e_\sigma \\
&= \frac{1}{2}\epsilon^{\mu\nu\rho\sigma} i f_{cea} (t^a_A)_{bd} A^b_\mu A^c_\nu A^d_\rho A^e_\sigma = \frac{1}{2}\epsilon^{\mu\nu\rho\sigma} f_{cea} f_{abd} A^b_\mu A^c_\nu A^d_\rho A^e_\sigma = \frac{1}{2}\epsilon^{\mu\nu\rho\sigma} f_{ace} f_{abd} A^b_\mu A^c_\nu A^d_\rho A^e_\sigma \\
&= \frac{1}{2}\epsilon^{\mu\nu\rho\sigma} f_{acb} f_{aed} A^e_\mu A^c_\nu A^d_\rho A^b_\sigma = -\frac{1}{2}\epsilon^{\sigma\nu\rho\mu} f_{abc} f_{ade} A^b_\sigma A^c_\nu A^d_\rho A^e_\mu = -\frac{1}{2}\epsilon^{\mu\nu\rho\sigma} f_{abc} f_{ade} A^b_\mu A^c_\nu A^d_\rho A^e_\sigma \\
&= 0 \,.
\end{aligned} \tag{4.378}$$

It follows that

$$32\pi^2 \partial_\mu K^\mu = \epsilon^{\mu\nu\rho\sigma} F^a_{\mu\nu} F^a_{\rho\sigma} \,. \tag{4.379}$$

Equations of motion The prototypical non-Abelian gauge theory involves a single simple compact factor for the gauge group, and a single fermionic matter field transforming in some representation R. The corresponding Lagrangean reads

$$\begin{aligned}
\mathscr{L} &= -\frac{1}{4} F^a_{\mu\nu} F^{a\mu\nu} + \bar\psi [i(\partial_\mu + i g A^a_\mu t^a_R)\gamma^\mu - m]\psi = -\frac{1}{4} F^a_{\mu\nu} F^{a\mu\nu} + \bar\psi (i D^{(R)}_\mu \gamma^\mu - m)\psi \\
&= -\frac{1}{4} F^a_{\mu\nu} F^{a\mu\nu} + \bar\psi (i \not{D}^{(R)} - m)\psi \,,
\end{aligned} \tag{4.380}$$

where we have dropped the overbars from the gauge fields for notational clarity. Before quantisation, the complex fermionic fields ψ_α and $\bar\psi_\alpha$, $\alpha = 1, \ldots, 4$, are related via $\bar\psi = \psi^\dagger \gamma^0$, but can be treated as independent fields corresponding to two different combinations of the real and imaginary parts of ψ.

The equations of motion for A^a_μ are obained from Eq. (4.380) in the usual way. One has

$$\begin{aligned}
\frac{\partial \mathscr{L}}{\partial(\partial_\mu A^a_\nu)} &= -\frac{1}{2} F^{b\rho\sigma} \frac{\partial F^{b\rho\sigma}}{\partial(\partial_\mu A^a_\nu)} = -\frac{1}{2} F^{b\rho\sigma} \delta_{ab} \left(\delta^\mu{}_\rho \delta^\nu{}_\sigma - \delta^\mu{}_\sigma \delta^\nu{}_\rho \right) = -F^{a\mu\nu} \,, \\
\frac{\partial \mathscr{L}}{\partial A^a_\nu} &= -\frac{1}{2} F^{b\rho\sigma} \frac{\partial F^{b\rho\sigma}}{\partial A^a_\nu} + i^2 g \bar\psi t^a_R \gamma^\nu \psi \\
&= -\frac{1}{2} F^{b\rho\sigma} (-g f_{bcd}) \left(\delta_{ac} \delta^\nu{}_\rho A^d_\sigma + \delta_{ad} A^c_\rho \delta^\nu{}_\sigma \right) - g \bar\psi t^a_R \gamma^\nu \psi \\
&= g f_{bad} F^{b\nu\sigma} A^d_\sigma - g \bar\psi t^a_R \gamma^\nu \psi \\
&= i g (-i f_{abd}) F^{b\sigma\nu} A^d_\sigma - g \bar\psi t^a_R \gamma^\nu \psi = i g (t^d_A)_{ab} A^d_\sigma F^{b\sigma\nu} - g \bar\psi t^a_R \gamma^\nu \psi \\
&= i g (t^d_A)_{ab} A^d_\mu F^{b\mu\nu} - g \bar\psi t^a_R \gamma^\nu \psi \,.
\end{aligned} \tag{4.381}$$

Setting

$$\begin{aligned} J^{a\nu} &= J^{a\nu}_G + J^{a\nu}_F \,, \\ J^{a\nu}_G &= ig(t^d_A)_{ab} A^d_\mu F^{b\mu\nu} = -g f_{adb} A^d_\mu F^{b\mu\nu} \,, \\ J^{a\nu}_F &= -g\bar\psi t^a_R \gamma^\nu \psi \,, \end{aligned} \tag{4.382}$$

we find the EOM

$$\partial_\mu \frac{\partial \mathscr{L}}{\partial(\partial_\mu A^a_\nu)} = \frac{\partial \mathscr{L}}{\partial A^a_\nu} \quad \Longrightarrow \quad -\partial_\mu F^{a\mu\nu} = J^{a\nu} \,. \tag{4.383}$$

The EOM for the matter fields are obtained by noticing that $\mathscr{L}$ is independent of $\partial_\mu\bar\psi$, so

$$0 = \frac{\partial \mathscr{L}}{\partial \bar\psi} = (i\not{D}^{(R)} - m)\psi \,. \tag{4.384}$$

It follows from Eq. (4.383) that $J^{a\nu}$ are conserved currents, since trivially $\partial_\nu\partial_\mu F^{a\mu\nu} = 0$ due to antisymmetry of the field strength tensor. This equation can also be recast as

$$\begin{aligned} -(\partial_\mu F^{a\mu\nu} + J^{a\nu}_G) &= J^{a\nu}_F \,, \\ -(\partial_\mu \delta_{ab} + ig(t^c_A)_{ab} A^c_\mu) F^{b\mu\nu} &= J^{a\nu}_F \,, \\ -(D^{(A)}_\mu)^a{}_b F^{b\mu\nu} &= J^{a\nu}_F \,. \end{aligned} \tag{4.385}$$

This form shows that the EOM are gauge-covariant, since both sides transform (homogeneously) in the adjoint representation. It also shows that the matter current $J^{a\nu}_F$ is covariantly conserved:

$$\begin{aligned} -(D^{(A)}_\nu)^a{}_b J^{b\nu}_F &= (D^{(A)}_\nu)^a{}_b (D^{(A)}_\mu)^b{}_c F^{c\mu\nu} = \frac{1}{2}([D^{(A)}_\nu, D^{(A)}_\mu]))^a{}_c F^{c\mu\nu} \\ &= \frac{1}{2} ig F^d_{\nu\mu} (t^d_A)^a{}_c F^{c\mu\nu} = \frac{1}{2} g F^d_{\nu\mu} F^{c\mu\nu} f_{dac} = \frac{1}{2} g F^d_{\mu\nu} F^{c\mu\nu} f_{adc} = 0 \,, \end{aligned} \tag{4.386}$$

since $F^d_{\mu\nu} F^{c\mu\nu}$ is symmetric and f_{adc} antisymmetric under $c \leftrightarrow d$.

The field strength tensor satisfies the identities

$$(D^{(A)}_\mu)^a{}_b F^b_{\nu\rho} + (D^{(A)}_\rho)^a{}_b F^b_{\mu\nu} + (D^{(A)}_\nu)^a{}_b F^b_{\rho\mu} = 0 \tag{4.387}$$

known as *Bianchi identities*, independently of it being a solution of the equations of motion. These are proved noticing that

$$\begin{aligned} [D^{(R)}_\mu, [D^{(R)}_\nu, D^{(R)}_\rho]] &= ig[D^{(R)}_\mu, F^a_{\nu\rho} t^a_R] = ig\left(\partial_\mu F^a_{\nu\rho} t^a_R + ig A^b_\mu F^a_{\nu\rho} [t^b_R, t^a_R]\right) \\ &= igt^c_R \left(\partial_\mu F^c_{\nu\rho} + ig A^b_\mu F^a_{\nu\rho} i f_{bac}\right) = igt^c_R \left(\partial_\mu \delta_{ca} + ig A^b_\mu (t^b_A)_{ca}\right) F^a_{\nu\rho} \\ &= igt^c_R (D^{(A)}_\mu)^c{}_a F^a_{\nu\rho} \,, \end{aligned} \tag{4.388}$$

and using the Jacobi identity,

$$[D^{(R)}_\mu, [D^{(R)}_\nu, D^{(R)}_\rho]] + [D^{(R)}_\rho, [D^{(R)}_\mu, D^{(R)}_\nu]] + [D^{(R)}_\nu, [D^{(R)}_\rho, D^{(R)}_\mu]] = 0 \,. \tag{4.389}$$

Equations of motion and gauge invariance Let us now spell Eq. (4.383) out in detail. Denoting with $j,k=1,2,3$ the spatial indices, we have

$$\begin{aligned} -\partial_k F^{ak0} &= J^{a0} = ig(t_A^d)_{ab}A_k^d F^{bk0} + J_F^{a0} = -gf_{adb}A_k^d F^{bk0} + J_F^{a0}\,, \\ -\partial_0 F^{a0k} - \partial_j F^{ajk} &= J^{ak} = ig(t_A^d)_{ab}A_0^d F^{b0k} + ig(t_A^d)_{ab}A_j^d F^{bjk} + J_F^{ak} \\ &= -gf_{adb}A_0^d F^{b0k} - gf_{dab}A_j^d F^{bjk} + J_F^{ak}\,. \end{aligned} \tag{4.390}$$

Clearly, $\ddot{A}^0$ does not appear on the left-hand side of these equations, and not even $\dot{A}^0$ appears on the right-hand side. On the other hand, $\ddot{A}^k$ does appear on the left-hand side, and $\dot{A}^0$ appears in the second set of equations only. We have then a system of equations that are second-order in time for $\vec{A}^a$ and first-order in time for A^{a0}. Explicitly, using the notation $\vec{\nabla}_k = \partial_k$, $\Delta = \vec{\nabla}^2$, $\vec{A}_k^a = A^{ak}$ $\vec{J}_{Fk}^a = J_F^{ak}$, we havefor the left-hand side quantities

$$\begin{aligned} \partial_k F^{ak0} &= \partial_k\left(\partial^k A^{a0} - \partial^0 A^{ak} - gf_{abc}A^{bk}A^{c0}\right) = -\vec{\nabla}\cdot\left(\vec{\nabla}A^{a0} + \dot{\vec{A}}^a + gf_{abc}(\vec{A}^b A^{c0})\right)\,, \\ \partial_0 F^{a0k} &= \partial_0\left(\partial^0 A^{ak} - \partial^k A^{a0} - gf_{abc}A^{b0}A^{ck}\right) = \partial_0\left(\partial_0 A^{ak} + \vec{\nabla}_k A^{a0} + gf_{abc}\vec{A}_k^b A^{c0}\right) \\ \partial_j F^{ajk} &= \partial_j\left(\partial^j A^{ak} - \partial^k A^{aj} - gf_{abc}A^{bj}A^{ck}\right) = \vec{\nabla}_j\left(-\vec{\nabla}_j\vec{A}_k^a + \vec{\nabla}_k\vec{A}_j^a - gf_{abc}\vec{A}_j^b\vec{A}_k^c\right) \\ &= -\left(\Delta\vec{A}_k^a - \vec{\nabla}_k\vec{\nabla}\cdot\vec{A}^a + gf_{abc}(\vec{\nabla}\cdot\vec{A}^b)\vec{A}_k^c + gf_{abc}(\vec{A}^b\cdot\vec{\nabla})\vec{A}_k^c\right)\,. \end{aligned} \tag{4.391}$$

The first equation in Eq. (4.390) reads explicitly

$$\vec{\nabla}\cdot\left(\vec{\nabla}A^{a0} + \dot{\vec{A}}^a + gf_{abc}(\vec{A}^b A^{c0})\right) - J^{a0} = 0\,, \tag{4.392}$$

and is only first-order in time for $\vec{A}^a$ and zero-order for A^{a0}, acting as a constraint rather than a dynamical equation. To deal with this asymmetric setting, we can first solve the second set of equations, that read

$$\partial_0\left(\partial_0 A^{ak} + \vec{\nabla}_k A^{a0} + gf_{abc}\vec{A}_k^b A^{c0}\right) - \vec{\nabla}_j F^{ajk} + J^{ak} = 0\,, \tag{4.393}$$

for a given, arbitrary A^{a0}, and then use Eq. (4.392) to possibly constrain A^{a0}. However, taking the divergence of Eq. (4.393) we find

$$\begin{aligned} 0 &= \vec{\nabla}_k\partial_0\left(\partial_0 A^{ak} + \vec{\nabla}_k A^{a0} + gf_{abc}\vec{A}_k^b A^{c0}\right) - \vec{\nabla}_k\vec{\nabla}_j F^{ajk} + \vec{\nabla}_k J^{ak} \\ &= \partial_0\left(\vec{\nabla}_k\left(\partial_0 A^{ak} + \vec{\nabla}_k A^{a0} + gf_{abc}\vec{A}_k^b A^{c0}\right) - J^{a0}\right)\,, \end{aligned} \tag{4.394}$$

which is just the temporal derivative of Eq. (4.392). Therefore, if $\vec{A}^a$ have been obtained for a given A^{a0} with initial conditions $\vec{A}^a(t=0)$, $\dot{\vec{A}}^a(t=0)$ at $t=0$ that satisfy the constraint Eq. (4.392), then the constraint will be satisfied at all times, no matter what A^{a0} we have chosen. In other words, A^{a0} is completely undetermined, and has to be given as part of the input data to solve the system of differential equations. Alternatively and perhaps more accurately, if $\vec{A}^a$ have been obtained for a given A^{a0} with initial conditions $\vec{A}^a(t=0)$, then the only restriction on A^{a0} is on the initial condition $A^{a0}(t=0)$, that has to obey the constraint Eq. (4.392) at $t=0$, while $\dot{A}^{a0}$ is entirely aribitrary. Moreover, the combination of $\vec{A}^a$ appearing under the

temporal derivative in Eq. (4.394) is not dynamical, but is entirely determined by the request that the constraint be obeyed at all times once that A^{a0} is given. There are therefore only two dynamical degrees of freedom for the gauge field.

This finding is not really surprising: after all we are describing a system of equations that is invariant under gauge transformations, Eqs. (4.337) and (4.339), which leaves an arbitrariness parameterised by the $\mathcal{D}_G$ functions $\alpha_a(x)$ used to define $U_R(x) = D_R(g(\alpha(x)))$. This corresponds to the need to specify the arbitrary functions A^{a0} when setting up the system of differential equations.

A practical way to provide A^{a0} is actually indirect, and is based on imposing a gauge condition $C[\vec{A}] = 0$ on the $\vec{A}^a$ that eliminates the gauge freedom. Such condition must be accessible, i.e., given an arbitrary configuration $A^{a\mu}$ it must be possible by means of a gauge transformation U to obtain a new (but physically equivalent) configuration $A_U^{a\mu}$ that satisfies $C[\vec{A}_U] = 0$. The gauge condition should also have a unique solution, thus removing the gauge arbitrariness completely. Once that the gauge condition is imposed, the value of A^{a0} is determined by imposing the constraint equation Eq. (4.392). Looking at it backwards, one has that using the resulting A^{a0} one obtains $\vec{A}^a$ satisfying the desired gauge conditions by imposing the constraint, up to an initial condition. Either way, at this point both A^{a0} and some combination of the $\vec{A}^a$ has been obtained explicitly in terms of the remaining fields and their derivatives; only these ones still have to be determined by solving the equations of motion.

Recall now that by definition the canonical momenta conjugate to A^a_μ are

$$\Pi^{a\mu} \equiv \frac{\partial \mathscr{L}}{\partial(\partial_0 A^a_\mu)} = -F^{a0\mu} = F^{a\mu 0}\,, \tag{4.395}$$

so in particular

$$\Pi^{a0} = 0\,, \tag{4.396}$$

and

$$\vec{\Pi}^a_k \equiv \Pi^{ak} = \partial^k A^{a0} - \partial^0 A^{ak} - g f_{abc} A^{bk} A^{c0} \Rightarrow \vec{\Pi}^a = -(\dot{\vec{A}}^a + \vec{\nabla} A^{a0} + g f_{abc} \vec{A}^b A^{c0})\,. \tag{4.397}$$

By plugging Eq. (4.395) into the first equation in Eq. (4.390), we find

$$-\partial_k F^{ak0} = J^{a0} \Rightarrow -\vec{\nabla} \cdot \vec{\Pi}^a = J^{a0}\,. \tag{4.398}$$

This shows that only two of the $\vec{\Pi}^a$ are independent (*before* imposing any gauge condition!). Even after specifying the arbitrary functions A^{a0}, so that they can be dropped from the set of dynamical variables, one still has only two sets of independent $\vec{\Pi}^a$ and three sets of $\dot{\vec{A}}^a$, so that one cannot invert $\dot{\vec{A}}^a$ for the $\vec{\Pi}^a$. In order to be able to do so, one needs to impose a gauge condition on the $\vec{A}^a$, so that one set of $\dot{\vec{A}}^a$ will be fixed and the inversion becomes possible. While before A^{0a} was determined by combining the gauge condition with the constraint on $\dot{\vec{A}}^a$, now it is determined by combining the gauge condition with the constraint on $\dot{\vec{\Pi}}^a$ and the definition of $\vec{\Pi}^a$. One can then trade this situation for having the gauge condition on $\vec{A}^a$ plus a condition on A^{0a} and the constraint equation on $\vec{\Pi}^a$ as given, with the defining relation of $\vec{\Pi}^a$ in terms of A^{0a} and $\dot{\vec{A}}^a$ becoming a dynamical equation for $\dot{\vec{A}}^a$ in terms of $\vec{\Pi}^a$ and A^{0a}. In particular, the constraint Eq. (4.398) can be recast as a constraint on the momentum conjugate to the combination of $\vec{A}^a$ determined by the gauge-fixing condition.

Hamiltonian approach At this point, two coordinates are specified, two momenta are constrained, and the remaining pair of coordinates and momenta are actually dynamical. One can then try to set up a Hamiltonian formalism in a standard way. Naively, one would do so but performing a Legendre transform with respect to the remaining dynamical variables only and resolving the constraints in the Lagrangean. This is not generally guaranteed to work, since taking derivatives of the resulting Hamiltonian with resolved constraints with respect to the dynamical variables may not lead to equations equivalent to the original Lagrangean equations plus the gauge condition. This can be seen by the following example:

$$\frac{dF(x,f(x))}{dx} = \frac{\partial F(x,y)}{\partial x}\bigg|_{y=f(x)} + \frac{\partial F(x,y)}{\partial y}\bigg|_{y=f(x)} \frac{df(x)}{dx} \neq \frac{\partial F(x,y)}{\partial x}\bigg|_{y=f(x)} . \tag{4.399}$$

As a matter of fact, a Hamiltonian density $\mathscr{H}$ associated with $\mathscr{L}$ which is a function of $A^{\mu a}$ and $\dot{A}^{\mu a}$ only through $A^{\mu a}$ and $\Pi^{\mu a}(A^{\mu a}, \dot{A}^{\mu a})$ can always be defined. This is obtained in the standard way as

$$\mathscr{H}_{\rm can} = -\vec{\Pi}^a \cdot \dot{\vec{A}}^a + \pi\dot{\psi} - \mathscr{L} \,, \tag{4.400}$$

where "can" stands for "canonical" and only the constraint Π^{a0} has been imposed, and $\pi = i\bar{\psi}\gamma^0$. By considering an arbitrary variation of $A^{\mu a}$ and $\dot{A}^{\mu a}$, one shows that $\mathscr{H}_{\rm can}$ depends on $\dot{A}^{\mu a}$ only through the variations $\delta\Pi^{a\mu}$ of the momenta:

$$\begin{aligned}\delta\mathscr{H}_{\rm can} &= -\delta\vec{\Pi}^a \cdot \dot{\vec{A}}^a - \vec{\Pi}^a \cdot \delta\dot{\vec{A}}^a + \delta\pi\dot{\psi} + \pi\delta\dot{\psi} - \delta A^{a\mu}\frac{\partial\mathscr{L}}{\partial A^{a\mu}} - \delta\dot{A}^{a\mu}\frac{\partial\mathscr{L}}{\partial(\partial_0 A^{a\mu})} - \delta\psi\frac{\partial\mathscr{L}}{\partial\psi} - \delta\dot{\psi}\frac{\partial\mathscr{L}}{\partial\dot{\psi}} \\ &= -\delta\vec{\Pi}^a \cdot \dot{\vec{A}}^a + \delta\pi\dot{\psi} - \delta A^{a\mu}\frac{\partial\mathscr{L}}{\partial A^{a\mu}} - \delta\psi\frac{\partial\mathscr{L}}{\partial\psi}\end{aligned} \tag{4.401}$$

However, one cannot get the Hamilton equations of motion this way since the $\delta\vec{\Pi}^a$ are not independent due to Eq. (4.398). The proper way to deal with this issue is briefly discussed below. Here we attempt a more direct approach.

Recall the relevant equations. The equations of motions are

$$\partial_\mu F^{a\mu\nu} = -J^{a\nu} = -J^{a\nu}_G - J^{a\nu}_F \,, \tag{4.402}$$

where the gauge and fermion currents read

$$\begin{aligned} J^{a\nu}_G &= -g f_{abc} A^b_\mu F^{c\mu\nu} \,, \\ J^{a\nu}_F &= -g\bar{\psi} t^a \gamma^\nu \psi \,. \end{aligned} \tag{4.403}$$

The conjugate momenta are

$$\Pi^{a\mu} = F^{a\mu 0} \,, \tag{4.404}$$

and explicitly

$$\begin{aligned} \Pi^{a0} &= 0 \,, \\ \Pi^{ak} &= \partial^k A^{a0} - \partial^0 A^{ak} - g f_{abc} A^{bk} A^{c0} = -(\partial_k A^{a0} + \dot{A}^{ak} + g f_{abc} A^{bk} A^{c0}) \\ &= -[\dot{A}^{ak} + (\partial_k \delta_{ac} + g f_{bac} A^b_k) A^{c0}] = -[\dot{A}^{ak} + (D^{(A)}_k A^0)^a] \,. \end{aligned} \tag{4.405}$$

The gauge current can be written as

$$\begin{aligned} J^{a0}_G &= -g f_{abc} A^b_k F^{ck0} = -g f_{abc} A^b_k \Pi^{ck} = g f_{abc} A^{bk} \Pi^{ck} = g f_{abc} \vec{A}^b \cdot \vec{\Pi}^c \,, \\ J^{ak}_G &= -g f_{abc} (A^b_0 F^{c0k} + A^b_j F^{cjk}) = g f_{abc} (A^{b0} \Pi^{ck} - A^b_j F^{cjk}) \,. \end{aligned} \tag{4.406}$$

The constraint equation, i.e., Eq. (4.402) for $\nu = 0$, is

$$\partial_\mu F^{a\mu 0} = \partial_k F^{ak0} = -J^{a0}\,, \tag{4.407}$$

and in terms of momenta

$$\vec{\nabla}\cdot\vec{\Pi}^a = -J^{a0}\,. \tag{4.408}$$

More explicitly

$$\begin{aligned}
\vec{\nabla}\cdot\vec{\Pi}^a &= -J^{a0}_F - g f_{abc}\vec{A}^b\cdot\vec{\Pi}^c = -J^{a0}_F + g f_{bac}\vec{A}^b\cdot\vec{\Pi}^c\,,\\
-J^{a0}_F &= (\vec{\nabla}\delta_{ac} - g f_{bac}\vec{A}^b)\cdot\vec{\Pi}^c = (\nabla_k\delta_{ac} + g f_{bac}A^b_k)\Pi^{ck}\\
&= (\nabla_k\delta_{ac} + ig(t^b_A)_{ac}A^b_k)\Pi^{ck} = (D^{(A)}_k)_{ac}\Pi^{ck} = \vec{D}^{(A)}_{ac}\cdot\vec{\Pi}^c\,.
\end{aligned} \tag{4.409}$$

The dynamical equations of motion, i.e., Eq. (4.402) for $\nu = k = 1,2,3$, read

$$\partial_0 F^{a0k} + \partial_j F^{ajk} = -\partial_0 F^{ak0} + \partial_j F^{ajk} = -J^{ak}\,, \tag{4.410}$$

and in terms of momenta

$$\dot{\Pi}^{ak} = \partial_j F^{ajk} + J^{ak}\,. \tag{4.411}$$

The divergence of this equation is

$$\partial_k\dot{\Pi}^{ak} = \partial_k\partial_j F^{ajk} + \partial_k J^{ak} = \partial_k J^{ak} = -\partial_0 J^{a0} \Rightarrow \partial_0(\vec{\nabla}\cdot\vec{\Pi}^a + J^{a0}) = 0\,, \tag{4.412}$$

due to antisymmetry of F^{ajk} and conservation of $J^{a\mu}$, and so it expresses the consistency of the constraint Eq. (4.408) with the temporal evolution.

To remove the arbitrariness of A^{a0} associated with gauge invariance, we impose the following condition:

$$A^{a3} = 0\,. \tag{4.413}$$

This is called the *axial gauge* condition, and one can show that given any gauge configuration, one can perform a gauge transformation that leads to a new configuration satisfying Eq. (4.413). Since Eq. (4.413) must hold at all times one has that $\dot{A}^{a3} = 0$, and from Eq. (4.405) it follows that

$$\Pi^{a3} = -\partial_3 A^{a0}\,. \tag{4.414}$$

We now solve the constraint equation Eq. (4.408), obtaining

$$\begin{aligned}
\vec{\nabla}_\perp\cdot\vec{\Pi}^a_\perp + \partial_3\Pi^{a3} = \vec{\nabla}_\perp\cdot\vec{\Pi}^a_\perp - \partial_3^2 A^{a0} &= -J^{a0} = -J^{a0}_F - g f_{abc}\vec{A}^b_\perp\cdot\vec{\Pi}^c_\perp\\
\partial_3^2 A^{a0} = \vec{\nabla}_\perp\cdot\vec{\Pi}^a_\perp + J^{a0} &= \vec{\nabla}_\perp\cdot\vec{\Pi}^a_\perp + g f_{abc}\vec{A}^b_\perp\cdot\vec{\Pi}^c_\perp + J^{a0}_F = (\vec{D}^{(A)}_\perp\cdot\vec{\Pi}_\perp)^a + J^{a0}_F\,,
\end{aligned} \tag{4.415}$$

where the subscript $\perp$ indicates that the sum over spatial components is restricted to $k = 1,2$. A solution for A^{a0} is obtained by integrating twice over x^3 with suitable boundary conditions, which we denote as

$$A^{a0} = \frac{1}{\partial_3^2}\left(\vec{\nabla}_\perp\cdot\vec{\Pi}^a_\perp + J^{a0}\right)\,, \tag{4.416}$$

where the right-hand side depends only on $\vec{A}^a_\perp$, $\vec{\Pi}^a_\perp$, and fermionic (matter) fields. Substituting in Eq. (4.414) we find

$$\Pi^{a3} = -\partial_3 A^{a0} = -\frac{1}{\partial_3}\left(\vec{\nabla}_\perp\cdot\vec{\Pi}^a_\perp + J^{a0}\right)\,. \tag{4.417}$$

Since $\Pi^{a0}=0$, we now have that the pairs of variables (A^{a0},Π^{a0}) and (A^{a3},Π^{a3}) are entirely expressed in terms of $(\vec{A}^a_\perp,\vec{\Pi}^a_\perp)=(A^{a1},\Pi^{a1},A^{a2},\Pi^{a2})$ only. In the remaining, dynamical equations Eq. (4.411) for $k=1,2$ there appears the following quantities (here $F^{jk}_\perp$ denotes that one restricts $j,k=1,2$)

$$\begin{aligned}\partial_j F^{ajk}_\perp+\partial_3 F^{a3k}=\partial_j F^{ajk}_\perp+\partial_3\partial^3 A^{ak}_\perp=\partial_j F^{ajk}_\perp-\partial_3^2 A^{ak}_\perp\,,\\ J^{ak}_{G\perp}=gf_{abc}(A^{b0}\Pi^{ck}_\perp-A^b_{\perp j}F^{cjk}_\perp)\,.\end{aligned}\tag{4.418}$$

where the axial gauge condition has been imposed. Equation (4.411) for $k=1,2$ then reads

$$\dot{\Pi}^{ak}_\perp=\nabla_{\perp j}F^{ajk}_\perp-\partial_3^2A^{ak}_\perp+J^{ak}_\perp\,,\tag{4.419}$$

with the right-hand side a function of $(\vec{A}^a_\perp,\vec{\Pi}^a_\perp)$ only [once A^{a0} is expressed through Eq. (4.416)]. Using Eq. (4.405) one has the relation

$$-\dot{A}^{ak}_\perp=\Pi^{ak}_\perp+\nabla_{\perp k}A^{a0}+gf_{abc}A^{bk}_\perp A^{c0}=\Pi^{ak}_\perp+(D^{(A)}_{\perp k}A^0)^a\,,\tag{4.420}$$

which is again entirely determined in terms of $(\vec{A}^a_\perp,\vec{\Pi}^a_\perp)$.

We now tentatively define a Hamiltonian density as

$$\mathscr{H}=-\vec{\Pi}^a_\perp\cdot\dot{\vec{A}}^a_\perp+\pi\dot{\psi}-\mathscr{L}(\vec{A}_\perp,\vec{\Pi}_\perp)\,,\tag{4.421}$$

where $\mathscr{L}$ is expressed in terms of $(\vec{A}^a_\perp,\vec{\Pi}^a_\perp)$ using the gauge condition and Eqs. (4.416), (4.417), and (4.420). Since

$$\begin{aligned}F^{a\mu\nu}F^a_{\mu\nu}&=2F^{ak0}F^a_{k0}+F^{aij}F^a_{ij}=-2\Pi^{ak}\Pi^{ak}+F^{aij}F^a_{ij}\\&\overset{A^{a3}=0}{=}-2\vec{\Pi}^a_\perp\cdot\vec{\Pi}^a_\perp-2(\partial_3A^{a0})^2+2\partial_3\vec{A}^a_\perp\cdot\partial_3\vec{A}^a_\perp+F^{aij}_\perp F^a_{\perp ij}\,,\\-\dot{A}^{ak}_\perp&=\Pi^{ak}_\perp+\nabla_{\perp k}A^{a0}+gf_{abc}A^{bk}_\perp A^{c0}\,,\end{aligned}\tag{4.422}$$

one finds

$$\begin{aligned}\mathscr{H}&=\Pi^{ak}_\perp(\Pi^{ak}_\perp+\nabla_{\perp k}A^{a0}+gf_{abc}A^{bk}_\perp A^{c0})\\&\quad-\frac{1}{2}\vec{\Pi}^a_\perp\vec{\Pi}^a_\perp-\frac{1}{2}(\partial_3A^{a0})^2+\frac{1}{2}\partial_3\vec{A}^a_\perp\cdot\partial_3\vec{A}^a_\perp+\frac{1}{4}F^{aij}_\perp F^a_{\perp ij}\\&\quad+\pi\dot{\psi}-\pi\dot{\psi}-\bar{\psi}i^2gA^{a0}t^a\gamma^0\psi+\bar{\psi}i^2g\vec{A}^{ak}t^a\gamma^k_\perp\psi-\bar{\psi}(i\not{\nabla}-m)\psi\\&=\frac{1}{2}\vec{\Pi}^a_\perp\vec{\Pi}^a_\perp+\vec{\Pi}^a_\perp\cdot\vec{\nabla}_\perp A^{a0}-A^{c0}gf_{cba}A^{bk}_\perp\Pi^{ak}_\perp-\frac{1}{2}(\partial_3A^{a0})^2\\&\quad+\frac{1}{2}\partial_3\vec{A}^a_\perp\cdot\partial_3\vec{A}^a_\perp+\frac{1}{4}F^{aij}_\perp F^a_{\perp ij}-A^{a0}J^{a0}_F+\vec{A}^a_\perp\cdot\vec{J}^a_{F\perp}-\bar{\psi}(i\not{\nabla}-m)\psi\\&=\frac{1}{2}\vec{\Pi}^a_\perp\vec{\Pi}^a_\perp+\vec{\Pi}^a_\perp\cdot\vec{\nabla}_\perp A^{a0}-A^{a0}J^{a0}-\frac{1}{2}(\partial_3A^{a0})^2+\frac{1}{2}\partial_3\vec{A}^a_\perp\cdot\partial_3\vec{A}^a_\perp+\frac{1}{4}F^{aij}_\perp F^a_{\perp ij}\\&\quad+\vec{A}^a_\perp\cdot\vec{J}^a_{F\perp}-\bar{\psi}(i\not{\nabla}-m)\psi\,.\end{aligned}\tag{4.423}$$

Integrating over $\vec{x}$ and using integration by parts and Eq. (4.416) one obtains

$$\begin{aligned} H &= \int d^3x\, \mathscr{H} \\ &= \int d^3x \left\{ \frac{1}{2}\vec{\Pi}^a_\perp \vec{\Pi}^a_\perp - A^{a0}(\vec{\nabla}_\perp \cdot \vec{\Pi}^a_\perp + J^{a0}) - \frac{1}{2}(\partial_3 A^{a0})^2 + \frac{1}{2}\partial_3 \vec{A}^a_\perp \cdot \partial_3 \vec{A}^a_\perp \right. \\ &\qquad \left. + \frac{1}{4}F^{aij}_\perp F^a_{\perp ij} + \vec{A}^a_\perp \cdot \vec{J}^a_{F\perp} - \bar{\psi}(i\not{\nabla} - m)\psi \right\} \\ &= \int d^3x \left\{ \frac{1}{2}\vec{\Pi}^a_\perp \vec{\Pi}^a_\perp + \frac{1}{2}(\partial_3 A^{a0})^2 + \frac{1}{2}\partial_3 \vec{A}^a_\perp \cdot \partial_3 \vec{A}^a_\perp + \frac{1}{4}F^{aij}_\perp F^a_{\perp ij} + \vec{A}^a_\perp \cdot \vec{J}^a_{F\perp} - \bar{\psi}(i\not{\nabla} - m)\psi \right\} . \end{aligned} \tag{4.424}$$

In order for the usual Hamilton equations to describe the temporal evolution of the system, they should match the one described by Eqs. (4.419) and (4.420). To see that this is the case, we compute

$$\begin{aligned} \frac{\delta H}{\delta \Pi^{ak}_\perp(x)} &= \Pi^{ak}_\perp(x) - \int d^3z\, A^{b0}(z) \frac{\delta\left(\partial_3^2 A^{b0}(z)\right)}{\delta \Pi^{ak}_\perp(x)} , \\ \frac{\delta H}{\delta A^{ak}_\perp(x)} &= -\partial_3 A^{ak}_\perp(x) + J^{ak}_{F\perp}(x) + \int d^3z \left(-A^{b0}(z) \frac{\delta\left(\partial_3^2 A^{b0}(z)\right)}{\delta A^{ak}_\perp(x)} + \frac{1}{2}F^{bij}_\perp \frac{\delta F^b_{\perp ij}}{\delta A^{ak}_\perp(x)} \right) . \end{aligned} \tag{4.425}$$

For the first equation we have

$$\begin{aligned} \frac{\delta\left(\partial_3^2 A^{b0}(z)\right)}{\delta \Pi^{ak}_\perp(x)} &= \left(\nabla^z_{\perp k}\delta_{ab} + g f_{bca} A^{ck}_\perp(z) \right) \delta^{(3)}(z-x) \\ &= \left(\nabla^z_{\perp k}\delta_{ab} + g f_{cba} A^c_{\perp k}(z) \right) \delta^{(3)}(z-x) , \end{aligned} \tag{4.426}$$

from which we obtain

$$\begin{aligned} \frac{\delta H}{\delta \Pi^{ak}_\perp(x)} &= \Pi^{ak}_\perp(x) - \int d^3z\, A^{b0}(z) \left(\nabla^z_{\perp k}\delta_{ab} + g f_{cba} A^c_{\perp k}(z) \right) \delta^{(3)}(z-x) \\ &= \Pi^{ak}_\perp(x) + \int d^3z\, \delta^{(3)}(z-x) \left(\nabla^z_{\perp k}\delta_{ab} + g f_{cab} A^c_{\perp k}(z) \right) A^{b0}(z) \\ &= \Pi^{ak}_\perp(x) + \nabla_{\perp k} A^{a0}(x) + g f_{abc} A^{bk}_\perp(x) A^{c0}(x) . \end{aligned} \tag{4.427}$$

For the second equation we have

$$\begin{aligned} \frac{\delta\left(\partial_3^2 A^{b0}(z)\right)}{\delta A^{ak}_\perp(x)} &= \frac{\delta J^{b0}_G(z)}{\delta A^{ak}_\perp(x)} = g f_{bac} \Pi^{ck}_\perp(z) \delta^{(3)}(z-x) , \\ \frac{\delta F^b_{\perp ij}}{\delta A^{ak}_\perp(x)} &= \delta_{ab}(\partial^z_i \eta_{kj} - \partial^z_j \eta_{ki}) \delta^{(3)}(z-x) - g(f_{bac}\eta_{ik} A^c_{\perp j} + f_{bca}\eta_{jk} A^c_{\perp i}) \delta^{(3)}(z-x) , \end{aligned} \tag{4.428}$$

from which it follows

$$\begin{aligned}
\frac{\delta H}{\delta A^{ak}_{\perp}(x)} &= -\partial_3 A^{ak}_{\perp}(x) + J^{ak}_{F\perp}(x) \\
&\quad + \int d^3z \Big(-A^{b0}(z) g f_{bac} \Pi^{ck}_{\perp}(z) \delta^{(3)}(z-x) \\
&\qquad + \frac{1}{2} F^{bij}_{\perp} \delta_{ab} (\partial^z_i \eta_{kj} - \partial^z_j \eta_{ki}) \delta^{(3)}(z-x) \\
&\qquad - g(f_{bac}\eta_{ik} A^c_{\perp j} + f_{bca}\eta_{jk} A^c_{\perp i}) \delta^{(3)}(z-x) \Big) \\
&= -\partial_3 A^{ak}_{\perp}(x) + J^{ak}_{F\perp}(x) + g f_{abc} A^{b0}(x) \Pi^{ck}_{\perp}(x) + \partial_i F^{aik}_{\perp}(x) - g f_{abc} A^b_{\perp j}(x) F^{cjk}_{\perp}(x) \\
&= -\partial_3 A^{ak}_{\perp}(x) + J^{ak}_{F\perp}(x) + g f_{abc} (A^{b0}(x) \Pi^{ck}_{\perp}(x) - A^b_{\perp j}(x) F^{cjk}_{\perp}(x)) + \partial_i F^{aik}_{\perp}(x) \\
&= -\partial_3 A^{ak}_{\perp}(x) + J^{ak}_{F\perp}(x) + J^{ak}_{G\perp}(x) + \partial_i F^{aik}_{\perp}(x) \\
&= -\partial_3 A^{ak}_{\perp}(x) + J^{ak}_{\perp}(x) + \partial_i F^{aik}_{\perp}(x) \,,
\end{aligned} \tag{4.429}$$

having used the gauge condition $A^{a3} = 0$ and Eq. (4.406). According to Hamilton's equations, one should have[32]

$$\begin{aligned}
\frac{\delta H}{\delta \Pi^{ak}_{\perp}(x)} &= -\dot{A}^{ak}_{\perp}(x) \,, \\
\frac{\delta H}{\delta A^{ak}_{\perp}(x)} &= \dot{\Pi}^{ak}_{\perp}(x) \,,
\end{aligned} \tag{4.430}$$

and comparing with Eqs. (4.419) and (4.420) this is exactly what we find.

Canonical quantisation The main result of the lengthy procedure discussed above are the Hamilton equations Eq. (4.430), which allow one to write the temporal evolution of the unconstrained variables $(\vec{A}^a_{\perp}, \vec{\Pi}^a_{\perp})$ in terms of a restricted but otherwise standard Poisson bracket,

$$\dot{A}^a_{\perp k} = \{A^a_{\perp k}, H\} \,, \qquad \dot{\Pi}^{ak}_{\perp} = \{\Pi^{ak}_{\perp}, H\} \,, \tag{4.431}$$

where

$$\{F, G\} = \frac{\partial F}{\partial A^a_{\perp k}} \frac{\partial G}{\partial \Pi^{ak}_{\perp}} - \frac{\partial F}{\partial \Pi^{ak}_{\perp}} \frac{\partial G}{\partial A^a_{\perp k}} \,. \tag{4.432}$$

In order to quantise the system, one can promote $(\vec{A}^a_{\perp}, \vec{\Pi}^a_{\perp})$ to operators and the (equal time) Poisson bracket to a commutator, $\{\cdot,\cdot\} \to -i[\cdot,\cdot]$, i.e.,

$$\{A^a_{\perp k}(x), \Pi^{bl}_{\perp}(y)\}_{\rm ET} = \delta_{ab}\delta^l_k \delta^{(3)}(x-y) \to [A^a_{\perp k}(x), \Pi^{bl}_{\perp}(y)]_{\rm ET} = i\delta_{ab}\delta^l_k \delta^{(3)}(x-y) \,, \tag{4.433}$$

resulting in the temporal evolution of the operators $(\hat{\vec{A}}^a_{\perp}, \hat{\vec{\Pi}}^a_{\perp})$ being given by $(\hat{\vec{A}}^a_{\perp}, \hat{\vec{\Pi}}^a_{\perp}) = (-i[\hat{\vec{A}}^a_{\perp}, \hat{H}], -i[\hat{\vec{\Pi}}^a_{\perp}, \hat{H}])$, with $\hat{H}$ equal to Eq. (4.424) with $(\hat{\vec{A}}^a_{\perp}, \hat{\vec{\Pi}}^a_{\perp})$ set equal to the solution of Eq. (4.430) (up to operator-ordering issues). Since we are imposing quantisation conditions only on a restricted set of variables, we are not incurring into contradictions between the commutation relations of the full set of operators $(A^a_{\mu}, \Pi^{a\mu})$ and the constraints, since these are determined by the expressions of A^{a0}, A^{a3}, Π^{a0}, and Π^{a3} in terms of the restricted set of variables $(\vec{A}^a_{\perp}, \vec{\Pi}^a_{\perp})$

[32] The opposite sign with respect to the usual equation is due to $\Pi^{ak}_{\perp}$ being conjugate to $A^a_{\perp k} = -A^{ak}_{\perp}$.

and by Eq. (4.433), thus resulting in commutation relations, that are automatically compatible with the constraints. This would not have been the case had we directly imposed the standard commutation relations

$$[A^a_{\perp\mu}(x), \Pi^{b\nu}_{\perp}(y)]_{\rm ET} = i\delta_{ab}\delta^\nu_\mu \delta^{(3)}(x-y)\,, \tag{4.434}$$

which instead *would have been incompatible* with the constraints.

Hamiltonian equations of motion - reprise∗ We now briefly return on the Hamiltonian approach. The canonical Hamiltonian density reads explicitly

$$\begin{aligned}
\mathscr{H}_{\rm can} &= -\vec{\Pi}^a \cdot \dot{\vec{A}}^a + i\bar\psi\gamma^0\partial_0\psi - \mathscr{L} \\
&= \vec{\Pi}^a \cdot (\vec{\Pi}^a + \vec\nabla A^{a0} + g f_{abc}\vec{A}^b A^{c0}) + \frac{1}{2}F^{a0k}F^a_{0k} + \frac{1}{4}F^{ajk}F^a_{jk} \\
&\quad - i^2 g\bar\psi A^{a0}\gamma^0 t^a_R\psi - \bar\psi(iD^{(R)}_k - m)\gamma^k\psi \\
&= \vec{\Pi}^a \cdot (\vec{\Pi}^a + \vec\nabla A^{a0} + g f_{abc}\vec{A}^b A^{c0}) - \frac{1}{2}(\vec{\Pi}^a)^2 + \frac{1}{4}F^{ajk}F^a_{jk} \\
&\quad + g\bar\psi A^{a0}\gamma^0 t^a_R\psi - \bar\psi(iD^{(R)}_k - m)\gamma^k\psi \\
&= \frac{1}{2}(\vec{\Pi}^a)^2 + \vec{\Pi}^a\cdot\vec\nabla A^{a0} - (J^{a0}_G + J^{a0}_F)A^{a0} + \frac{1}{4}F^{ajk}F^a_{jk} \\
&\quad - \bar\psi(iD^{(R)}_k - m)\gamma^k\psi \\
&= \frac{1}{2}(\vec{\Pi}^a)^2 + (\vec{\Pi}^a\cdot\vec\nabla A^{a0} - J^{a0}A^{a0}) + \frac{1}{4}F^{ajk}F^a_{jk} - \bar\psi(iD^{(R)}_k - m)\gamma^k\psi\,. \\
&= \frac{1}{2}(\vec{\Pi}^a)^2 - (\vec\nabla\cdot\vec{\Pi}^a + J^{a0})A^{a0} + \frac{1}{4}F^{ajk}F^a_{jk} - \bar\psi(iD^{(R)}_k - m)\gamma^k\psi + \text{total divergence}\,.
\end{aligned} \tag{4.435}$$

At this stage the momenta $\Pi^{a\mu}$ are given functions of $A^{a\mu}$ and $\dot{A}^{a\mu}$, and as such one has that Π^{a0} vanishes. This constraint is then imposed in Eq. (4.435) to drop a term $\Pi^{a0}\dot{A}^{a0}$ from the full Legendre transform $\Pi^{a\mu}\dot{A}^{a\mu} - \mathscr{L}$. This constraint follows directly from the definition of the momenta and so it defines the submanifold in the phase space $(A^{a\mu}, \Pi^{a\mu})$ where any possible trajectory of the system must lie, not only those that solve the equations of motion. In contrast, the constraint on $\vec{\Pi}^a$ follows from the equations of motion and so holds only for a the class of trajectories that obey them, and should not be imposed at this stage. It should be noted that extending $\mathscr{H}_{\rm can}$ beyond the constraint surface $\Pi^{a0} = 0$ involves some arbitrariness, since all that is required is that it agrees with Eq. (4.435) on the constraint surface.

As explained above, although $\mathscr{H}_{\rm can}$ depends on the temporal derivatives of the fields only through the momenta, one cannot get the equations of motion straightforwardly from it, since one cannot get an equation for A^{a0} ($\dot{A}^{a0}$ does not appear anywhere, and so this quantity is arbitrary), and since the Lagrangian equations of motion include a constraint on the $\vec{\Pi}^a$ that depends on A^{a0}. One can nonetheless modify the Hamiltonian density and the Hamiltonian as

follows,

$$\begin{aligned}\mathscr{H}' &= \frac{1}{2}(\vec{\Pi}^a)^2 + (\vec{\Pi}^a\cdot\vec{\nabla}A^{a0} - J^{a0}A^{a0}) + \frac{1}{4}F^{ajk}F^a_{jk} - \bar{\psi}(iD^{(R)}_k - m)\gamma^k\psi + u^a\Pi^{a0}\,,\\ H' &= \int d^3x\left\{\frac{1}{2}(\vec{\Pi}^a)^2 + (\vec{\Pi}^a\cdot\vec{\nabla}A^{a0} - J^{a0}A^{a0}) + \frac{1}{4}F^{ajk}F^a_{jk} - \bar{\psi}(iD^{(R)}_k - m)\gamma^k\psi + u^a\Pi^{a0}\right\}\\ &= \int d^3x\left\{\frac{1}{2}(\vec{\Pi}^a)^2 - A^{a0}(\vec{\nabla}\cdot\vec{\Pi}^a + J^{a0}) + \frac{1}{4}F^{ajk}F^a_{jk} - \bar{\psi}(iD^{(R)}_k - m)\gamma^k\psi + u^a\Pi^{a0}\right\},\end{aligned} \tag{4.436}$$

where the u^a are a new set of variables, and obtain the correct equations of motion as the usual Hamilton's equations, plus the equations obtained by setting $\delta H'/\delta u^a = 0$. Recalling Eq. (4.406), $J^{a0}_G = gf_{abc}\vec{A}^b\cdot\vec{\Pi}^c$, one finds taking functional derivatives with respect to the momenta

$$\begin{aligned}\dot{A}^{a0} &= \frac{\delta H'}{\delta\Pi^{a0}} = u^a\,,\\ \dot{\vec{A}}^a_k &= -\frac{\delta H'}{\delta\vec{\Pi}^a_k} = -\vec{\Pi}^a_k - \vec{\nabla}_k A^{a0} + gf_{cba}A^{c0}\vec{A}^b_k\,,\end{aligned} \tag{4.437}$$

while taking functional derivatives with respect to the fields one obtains

$$\begin{aligned}\dot{\Pi}^{a0} &= -\frac{\delta H'}{\delta A^{a0}} = \vec{\nabla}\cdot\vec{\Pi}^a + J^{a0}\,,\\ \dot{\vec{\Pi}}^a_k &= \frac{\delta H'}{\delta\vec{A}^a_k} = \int d^3x\left\{\frac{1}{2}\frac{\partial F^{bjl}}{\partial A^{ak}}F^b_{jl} - A^{b0}\frac{\partial J^{b0}}{\partial A^{ak}}\right\} - g\bar{\psi}t^a_R\gamma^k\psi\\ &= \left(\vec{\nabla}_j F^{ajk} - gf_{abc}A^{b0}\vec{\Pi}^c_k + \vec{J}^a_{Gk} + gf_{abc}A^{b0}\vec{\Pi}^c_k\right) + \vec{J}^a_{Fk} = \vec{\nabla}_j F^{ajk} + \vec{J}^a_k\end{aligned} \tag{4.438}$$

and finally from functional derivatives with respect to u^a one recovers the constraint on Π^{a0},

$$0 = \frac{\delta H'}{\delta u^a} = \Pi^{a0}\,. \tag{4.439}$$

The first equation in Eq. (4.437) gives $\dot{A}^{a0}$ in terms of an undetermined set of functions u^a, while the second equation can be recast as

$$\vec{\Pi}^a_k = -(\dot{\vec{A}}^a_k + \vec{\nabla}_k A^{a0} + gf_{abc}\vec{A}^b_k A^{c0})\,, \tag{4.440}$$

which is just Eq. (4.397). The constraint equation Eq. (4.439) gives $\Pi^{a0} = 0$, so that substituted on the left-hand side of the first equation in Eq. (4.438) one obtains the constraint on $\vec{\Pi}^a$, Eq. (4.398),

$$0 = \dot{\Pi}^{a0} = \vec{\nabla}\cdot\vec{\Pi}^a + J^{a0}\,. \tag{4.441}$$

Finally, the second equation in Eq. (4.438) is

$$J^{ak} = \vec{J}^a_k = \dot{\vec{\Pi}}^a_k - \vec{\nabla}_j F^{ajk} = \partial_0 F^{ak0} - \vec{\nabla}_j F^{ajk} = -\partial_0 F^{a0k} - \vec{\nabla}_j F^{ajk} = -\partial_\mu F^{\mu k}\,. \tag{4.442}$$

We have then recovered all the original Euler-Lagrange equations, at the price of introducing explicitly the undetermined functions u^a.

Constrained Hamiltonian systems* The reason why the procedure above works is the following.[33] The situation we are dealing with is a special case of a singular Lagrangean $L = L(q, \dot{q})$, a function of $q^a, \dot{q}^a$ with $a = 1, \ldots, m$, where the matrix M_{ab},

$$M_{ab} = \frac{\partial^2 L}{\partial \dot{q}^a \partial \dot{q}^b} \,, \tag{4.443}$$

is not invertible, i.e., $\det M = 0$. Let the rank of M be $m - r$, $0 < r \leq m$ (we assume for simplicity that it is constant), and relabel the variables so that the rank of the restricted matrix M_{AB}, $A, B = 1, \ldots, m - r$, is equal to $m - r$. Let

$$p_a = \frac{\partial L}{\partial \dot{q}^a} \,, \quad a = 1, \ldots, m \,, \tag{4.444}$$

be the canonical momenta. By the inverse function theorem, at least locally one can invert the $m-r$ velocities $v^A = \dot{q}^A$ as a function of the $m-r$ momenta p_A, $A = 1, \ldots, m-r$, of the q^a, and of the remaining velocities $v^i = \dot{q}^i$, $i = m - r + 1, \ldots, m$, i.e., $v^A = f^A(q^a, p_A, v^i)$. Substituted in the equations for the remaining momenta p_i, $i = m - r + 1, \ldots, m$, one must have that the p_i are independent of v^i, or the rank of M would exceed $m - r$. There are then r equations,

$$p_i = \left. \frac{\partial L}{\partial \dot{q}^i} \right|_{v^A = v^A(q^a, p_A, v^i)} = \pi_i(q^a, p_A) \,, \quad i = m - r + 1, \ldots, m \,, \tag{4.445}$$

showing that the momenta p_a are not all independent. The functions $\phi_i(q^a, p_a) = p_i - \pi_i(q^a, p_A)$ then define constraints $\phi_i(q^a, p_a) = 0$ among the canonical variables, called primary constraints. One then defines the primary Hamiltonian as

$$\begin{aligned} H(q^a, p_a, v^i) &= \left[p_a v^a - L(q^a, v^a) \right]_{v^A = f^A(q^a, p_A, v^i)} \\ &= p_A U^A(q^a, p_A, v^i) + p_i v^i - \left[L(q^a, v^a) \right]_{v^A = f^A(q^a, p_A, v^i)} \,. \end{aligned} \tag{4.446}$$

This depends on the canonical variables plus the set of velocities that could not be inverted. One now shows that $H(q^a, p_a, v^i)$ is linear in v^i with coefficients ϕ_i:

$$\begin{aligned} \frac{\partial H(q^a, p_a, v^i)}{\partial v^i} &= \left(p_A - \left. \frac{\partial L(q^a, v^a)}{\partial v^A} \right|_{v^A = f^A(q^a, p_A, v^i)} \right) \frac{\partial f^A(q^a, p_A, v^i)}{\partial v^i} \\ &\quad + \left(p_i - \left. \frac{\partial L(q^a, v^a)}{\partial v^i} \right|_{v^A = f^A(q^a, p_A, v^i)} \right) \\ &= (p_A - p_A) \frac{\partial f^A(q^a, p_A, v^i)}{\partial v^i} + (p_i - \pi_i(q^a, p_A)) = \phi_i(q^a, p_a) \,, \end{aligned} \tag{4.447}$$

and conclude that

$$H(q^a, p_a, v^i) = \tilde{H}(q^a, p_a) + v^i \phi_i(q^a, p_a) \,, \tag{4.448}$$

with v^i-independent $\tilde{H}$. One can now finally show that the Lagrangean equations of motion are equivalent to the Hamilton equations,

$$\dot{q}^a = \frac{\partial H}{\partial p_a} \,, \qquad \dot{p}_a = -\frac{\partial H}{\partial q^a} \,, \qquad 0 = \frac{\partial H}{\partial v^i} \,. \tag{4.449}$$

[33] The following discussion is based on T. Thiemann, "Introduction to Modern Canonical Quantum General Relativity", section III.1 [arXiv:gr-qc/0110034].

In fact,

$$\begin{aligned}
\frac{\partial H(q^a,p_a,v^i)}{\partial p_a} &= \left[v^a + p_a\frac{\partial v^a}{\partial p_a} - \frac{\partial L(q^a,v^a)}{\partial v^a}\frac{\partial v^a}{\partial p_a}\right]_{v^A=f^A(q^a,p_A,v^i)} \\
&= \left[v^a + p_a\frac{\partial v^a}{\partial p_a} - p_a\frac{\partial v^a}{\partial p_a}\right]_{v^A=f^A(q^a,p_A,v^i)} = v^a|_{v^A=f^A(q^a,p_A,v^i)}\,, \\
\frac{\partial H(q^a,p_a,v^i)}{\partial q^a} &= \left[p_a\frac{\partial v^a}{\partial q^a} - \frac{\partial L(q^a,v^a)}{\partial q^a} - \frac{\partial L(q^a,v^a)}{\partial v^a}\frac{\partial v^a}{\partial q^a}\right]_{v^A=f^A(q^a,p_A,v^i)} \\
&= \left[p_a\frac{\partial v^a}{\partial q^a} - \frac{\partial L(q^a,v^a)}{\partial q^a} - p_a\frac{\partial v^a}{\partial q^a}\right]_{v^A=f^A(q^a,p_A,v^i)} \\
&= -\left.\frac{\partial L(q^a,v^a)}{\partial q^a}\right|_{v^A=f^A(q^a,p_A,v^i)}\,, \\
\frac{\partial H(q^a,p_a,v^i)}{\partial v^i} &= \phi_i(q^a,p_a)\,.
\end{aligned} \tag{4.450}$$

The first equation in Eq. (4.449) gives $\dot{q}^a = v^a$, which in particular for $a = A$ gives $\dot{q}^A = f^A(q^a, p_A, v^i)$, while $\dot{q}^i = v^i$ simply assigns the value v^i to the temporal derivative of q^i. Inverting the inverse function f^A, one sees that the p_A are related to $q, \dot{q}$ by $p_A(q,\dot{q}) = \partial L(q,v)/\partial v^A|_{v=\dot{q}}$. The third equation requires $\phi_i(q^a, p_a) = 0$, and so using the definition of the constraint one finds $p_i(q,\dot{q}) = \partial L(q,v)/\partial v^i|_{v=\dot{q}}$. Finally, using this in the second equation, one has

$$\dot{p}_a = \frac{d}{dt}\left(\frac{\partial L(q,v)}{\partial v^a}\right)\Big|_{v=\dot{q}} = \left.\frac{\partial L(q^a,v^a)}{\partial q^a}\right|_{v=\dot{q}}\,, \tag{4.451}$$

which are the Euler-Lagrange equations of motion. The v^i are at this stage arbitrary non-dynamical variables, not obeying any equation of motion and not restricted by the constraints. However, the existence of solutions to the equations of motion compatible with the constraints may impose restrictions on the v^i; whether this happens or not depends on the details of the system.

In our case, $\mathscr{L}$ is independent of $\dot{A}^{a0}$, so it is easy to identify the velocities that can be inverted, namely $\dot{A}^{ak}$, that can be written as functions of Π^{ak} and A^{a0} (which is a particular subset of $A^{a\mu}$ and the remaining velocities $\dot{A}^{a0}$, on which $\dot{A}^{ak}$ depend trivially). The resulting primary constraints are simply $\Pi^{a0} = 0$, and the primary Hamiltonian equals the canonical Hamiltonian plus $\Pi^{a0}v^a$. The primary Hamiltonian then depends on the canonical variables plus the set of v^a, and the Hamilton equation for $\dot{A}^{a0}$, $\dot{A}^{a0} = v^a$, merely expresses the fact that $\dot{A}^{a0}$ is arbitrary at this stage. One can show that now restrictions on $\dot{A}^{a0}$ are required by the equations of motion, and so they are fully arbitrary (see below).

Going back to Eqs. (4.436)–(4.439), the equations of motion obtained from $\mathscr{H}' = \mathscr{H}_{\rm can} + u^a\Pi^{a0}$ can be summarised as

$$\begin{aligned}
\dot{A}^a_0 &= u^a\,, \\
\dot{A}^a_k &= \frac{\partial \mathscr{H}_{\rm can}}{\partial \Pi^{ak}}\,, \\
\dot{\Pi}^{a\mu} &= -\frac{\partial \mathscr{H}_{\rm can}}{\partial A^{a\mu}}\,.
\end{aligned} \tag{4.452}$$

Using standard (functional) Poisson brackets,

$$\{F,G\} \equiv \frac{\delta F}{\delta A^a_\mu}\frac{\delta G}{\delta \Pi^{a\mu}} - \frac{\delta F}{\delta \Pi^{a\mu}}\frac{\delta G}{\delta A^a_\mu}\,, \tag{4.453}$$

Eq. (4.452) can be written in compact form as

$$\begin{aligned} \dot{A}^{a\mu} &= \{A^{a\mu}, H'\} \approx \{A^{a\mu}, H_{\rm can}\} + u^b\{A^{a\mu}, \Pi^{b0}\}\,, \\ \dot{\Pi}^{a\mu} &= \{\Pi^{a\mu}, H'\} \approx \{\Pi^{a\mu}, H_{\rm can}\} + u^b\{A^{a\mu}, \Pi^{b0}\}\,, \end{aligned} \tag{4.454}$$

where $\approx$ means that equality holds when imposing the constraints (after computing the brackets). This follows since

$$\{F, u^b\Pi^{b0}\} = u^b\{F,\Pi^{b0}\} + \{F,u^b\}\Pi^{b0} \approx u^b\{F,\Pi^{b0}\} \tag{4.455}$$

clearly holds. The u^a are arbitrary. For a general function F,

$$\dot{F} \approx \{F, H'\}\,. \tag{4.456}$$

Gauge-fixing in the constrained Hamiltonian language* To make the system of equations fully determined, one can add a set of gauge conditions $G^a(\vec{A}) = g(\vec{A}^a) = 0$, which act as a further constraints. Consistency of the primary constraints and of the gauge conditions with the equations of motion requires

$$\begin{aligned} 0 &\approx \{\Pi^{a0}, H_{\rm can}\} + u^b\{\Pi^{b0},\Pi^{b0}\} = \{\Pi^{a0}, H_{\rm can}\} = \tilde{\Pi}^a = -\frac{\delta H_{\rm can}}{\delta A^{a0}}\,, \\ 0 &\approx \{G^a, H_{\rm can}\} + u^b\{G^a,\Pi^{b0}\} = \{G^a, H_{\rm can}\} = \tilde{G}^a = -\frac{\delta G^a}{\delta A^{ak}}\frac{\delta H_{\rm can}}{\delta \Pi^{ak}}\,, \end{aligned} \tag{4.457}$$

yielding a set of secondary constraints. This procedure should in principle be repeated, but one can show that no new constraints are generated from $\tilde{\Pi}^a$ (which is nothing but the constraint on $\vec{\Pi}^a$ originating from the equations of motion for A^{a0}, that we repeatedly discussed). One can show that $\{\tilde{\Pi}^a, \Pi^{b0}\} = 0$, so in particular if no gauge condition were imposed, then no restriction on u^b would be found, implying the full arbitrariness of $\dot{A}^{a0}$, as anticipated. Moreover, one clearly has $\{G^a, \Pi^{b0}\} = 0$, and using the Jacobi identity

$$\{\tilde{G}^a, \Pi^{b0}\} = \{\{G^a, H\}, \Pi^{b0}\} = -\{\{\Pi^{b0}, G^a\}, H\} - \{\{H, \Pi^{b0}\}, G^a\} = \{\tilde{\Pi}^b, G^a\}\,. \tag{4.458}$$

At this point one has four constraints, and if indeed one imposed a good gauge fixing condition then the u^a should not be undetermined anymore. This is the case if

$$0 \approx \{\tilde{G}^a, H_{\rm can}\} + u^b\{\tilde{G}^a, \Pi^{b0}\} \tag{4.459}$$

is such that $K^{ab} = \{\tilde{G}^a, \Pi^{b0}\}$ can be inverted to yield a solution for u^b. This means that no new constraints are obtained by requiring consistency of $\tilde{G}^a$ with the equations of motion, but merely a (complete) restriction on the u^b, and the procedure of looking for new constraints stops.

The matrix of Poisson brackets of all the constraints $\Phi_A = \Pi^{a0}, \tilde{\Pi}^a, G^a, \tilde{G}^a$ is of the form

$$C_{AB} = \{\Phi_A, \Phi_B\} = \begin{pmatrix} 0 & 0 & 0 & -K \\ 0 & 0 & K & \tilde{K} \\ 0 & -K & 0 & \hat{K} \\ K & 0 & -\hat{K} & 0 \end{pmatrix} = \begin{pmatrix} \mathbf{0} & \mathbf{c} \\ -\mathbf{c}^T & \mathbf{d} \end{pmatrix}\,, \tag{4.460}$$

for some $\tilde{K}^{ab} = \{\tilde{\Pi}^a, \tilde{G}^b\}$ and $\hat{K}^{ab} = \{G^a, \tilde{G}^b\}$. Clearly, K, $\tilde{K}$, and $\hat{K}$ are diagonal. Since obviously $[\mathbf{c}, \mathbf{0}] = [K, 0] = 0$, it follows by elementary linear algebra that

$$\det C = \det\left(\mathbf{c}\,\mathbf{c}^T\right) = (\det \mathbf{c})^2 = (\det(K^2))^2 = (\det K)^4 \neq 0\,. \tag{4.461}$$

The matrix C is invertible, and one can then construct the Dirac bracket,

$$\{F, G\}_D = \{F, G\} - \{F, \Phi_A\}(C^{-1})^{AB}\{\Phi_B, G\}\,. \tag{4.462}$$

One can show that the Dirac bracket has all the good properties of a Poisson bracket (antisymmetry, derivative property, Jacobi identity), and moreover is such that if G is a function that has vanishing Poisson brackets with all the constraints on the resulting constraint surface $\Phi_A = 0$ (first-class function), then for an arbitrary F,

$$\{F, G\}_D = \{F, G\}\,. \tag{4.463}$$

Moreover, if G is one of the constraints that have at least one non-vanishing Poisson bracket with another constraint, then $\{F, G\}_D = 0$ for arbitrary F. Here all the constraints are of this type, and so $\{F, \Phi_A\}_D = 0$. By construction, $H' = H_{\text{can}} + u^b\Pi^{b0}$ has vanishing Poisson brackets with all the constraints on the constraint surface $\Phi_A = 0$ (the secondary constraints and the u^b were found precisely by requiring this) and so is first class, and therefore

$$\dot{F} \approx \{F, H'\} \approx \{F, H'\}_D\,. \tag{4.464}$$

One can furthermore show that the Dirac bracket is equal to the Poisson bracket computed with a suitable restricted set of variables (Q^α, P_α),

$$\{F, G\}^{\text{restr.}} = \frac{\partial F}{\partial Q^\alpha}\frac{\partial G}{\partial P_\alpha} - \frac{\partial F}{\partial P_\alpha}\frac{\partial G}{\partial Q^\alpha}\,. \tag{4.465}$$

When quantising, one can then promote the Poisson bracket of this restricted set to a commutator of operators, with the resulting operator Hamiltonian H' automatically generating their temporal evolution. One can verify that the restricted set of variables $(\vec{A}^a_\perp, \vec{\Pi}^a_\perp)$ used when quantising in axial gauge is precisely such that $\{F, G\}^{\text{restr.}} = \{F, G\}_D$.

Path-integral quantisation Having performed canonical quantisation of the system, we can now forget about it and use the equivalent path-integral formalism, where vacuum expectation values of observables are obtained by suitable insertions of functions $\mathcal{O}[A, \psi, \bar{\psi}]$ in the path integral

$$\int \mathrm{D}A_\perp \int \mathrm{D}\Pi_\perp \int \mathrm{D}\psi \int \mathrm{D}\pi\, \exp\left\{ i \int d^4x \left[-\vec{\Pi}^a_\perp \cdot \dot{\vec{A}}^a_\perp + \pi\dot{\psi} - \mathscr{H} \right] \right\}, \tag{4.466}$$

where now $\vec{\Pi}^a_\perp$ and $\dot{\vec{A}}^a$ are not related, but are simply integration variables, and $\mathscr{H}$ is given by Eq. (4.423) (or an equivalent expression differing only by a total divergence) where A^{a0} should be expressed as a function of $\vec{\Pi}^a_\perp$ and $\vec{A}^a$ through Eq. (4.416). Here suitable "ϵ" terms are understood. While the exponent in Eq. (4.466) is quadratic in $\vec{\Pi}^a_\perp$ so that the corresponding Gaussian path integral could be evaluated explicitly, the result would involve a field-dependent

functional determinant, and it would be even harder to keep track of the already non-manifest Lorentz invariance.

To make things easier, we proceed as follows. As mentioned above, $\mathscr{H}$ is a function of $\mathscr{H} = \mathscr{H}(\vec{\Pi}^a_\perp, \vec{A}^a, A^{a0})$ where A^{a0} should be replaced by

$$\begin{aligned} A^{a0} &= \mathrm{A}^a(\vec{\Pi}^a_\perp, \vec{A}^a)\,, \\ \mathrm{A}^a(\vec{\Pi}^a_\perp, \vec{A}^a) &= \frac{1}{\partial_3^2}\left(\vec{\nabla}_\perp \cdot \vec{\Pi}^a_\perp + J^{a0}\right) = \frac{1}{\partial_3^2}\mathrm{B}^a(\vec{\Pi}^a_\perp, \vec{A}^a)\,, \\ \mathrm{B}^a(\vec{\Pi}^a_\perp, \vec{A}^a) &= \left(\vec{\nabla}_\perp \cdot \vec{\Pi}^a_\perp + J^{a0}\right) = \partial_3^2 \mathrm{A}^a(\vec{\Pi}^a_\perp, \vec{A}^a)\,. \end{aligned} \tag{4.467}$$

The quantity A^a enters the exponent quadratically, resulting in a factor

$$\exp\left\{-i\int d^4x \frac{1}{2}(\partial_3 \mathrm{A}^a)^2\right\} \tag{4.468}$$

in the integrand. This factor can be expressed as follows exploiting the properties of Gaussian integrals,

$$\begin{aligned} \exp\left\{-i\int d^4x \frac{1}{2}(\partial_3 \mathrm{A}^a)^2\right\} &= \exp\left\{i\int d^4x \frac{1}{2}\mathrm{A}^a\partial_3^2\mathrm{A}^a\right\} = \exp\left\{i\int d^4x \frac{1}{2}\mathrm{B}^a\frac{1}{\partial_3^2}\mathrm{B}^a\right\} \\ &\propto \int \mathrm{D}A^0 \exp\left\{-i\int d^4x \left(\frac{1}{2}A^{a0}\partial_3^2 A^{a0} - \mathrm{B}^a A^{a0}\right)\right\} \\ &= \int \mathrm{D}A^0 \exp\left\{i\int d^4x \left[\frac{1}{2}(\partial_3 A^{a0})^2 + A^{a0}\left(\vec{\nabla}_\perp \cdot \vec{\Pi}^a_\perp + J^{a0}\right)\right]\right\}\,, \end{aligned} \tag{4.469}$$

where now A^{a0} is a new set of integration variables, unrelated to $(\vec{\Pi}^a_\perp, \vec{A}^a)$, and the omitted proportionality factor is field-independent and will drop from any expectation value. Recalling that $J^{a0}_G = J^{a0}_F + g f_{abc}\vec{A}^b_\perp \cdot \vec{\Pi}^c_\perp$, one sees that the exponent is linear in $\vec{\Pi}^a_\perp$.

After rewriting the integrand in this way we have for the integral

$$\int \mathrm{D}A_\perp \int \mathrm{D}A^0 \int \mathrm{D}\Pi_\perp \int \mathrm{D}\psi \int \mathrm{D}\bar{\psi}\, e^{iI}\,, \tag{4.470}$$

where

$$\begin{aligned} I &= \int d^4x \left[-\vec{\Pi}^a_\perp \cdot \dot{\vec{A}}^a_\perp + \bar{\psi} i\partial_0\gamma^0\psi - \frac{1}{2}\vec{\Pi}^a_\perp\vec{\Pi}^a_\perp + \frac{1}{2}(\partial_3 A^{a0})^2 + A^{a0}\left(\vec{\nabla}_\perp \cdot \vec{\Pi}^a_\perp + J^{a0}\right)\right. \\ &\qquad \left. - \frac{1}{2}\partial_3\vec{A}^a_\perp \cdot \partial_3\vec{A}^a_\perp - \frac{1}{4}F^{aij}_\perp F^a_{\perp ij} - \vec{A}^a_\perp \cdot \vec{J}^a_{F\perp} + \bar{\psi}(i\not{\nabla} - m)\psi\right] \\ &= \int d^4x \left[-\vec{\Pi}^a_\perp \cdot \dot{\vec{A}}^a_\perp - \frac{1}{2}\vec{\Pi}^a_\perp\vec{\Pi}^a_\perp + \frac{1}{2}(\partial_3 A^{a0})^2 - \vec{\Pi}^a_\perp \cdot \vec{\nabla}_\perp A^{a0} + A^{a0}(J^{a0}_F + g f_{abc}\vec{A}^b_\perp \cdot \vec{\Pi}^c_\perp)\right. \\ &\qquad \left. - \frac{1}{2}\partial_3\vec{A}^a_\perp \cdot \partial_3\vec{A}^a_\perp - \frac{1}{4}F^{aij}_\perp F^a_{\perp ij} - \vec{A}^a_\perp \cdot \vec{J}^a_{F\perp} + \bar{\psi}(i\not{\partial} - m)\psi\right]\,, \end{aligned} \tag{4.471}$$

having used integration by parts, and we have set $\pi = i\bar{\psi}\gamma^0$ (ignoring field-independent factors in the Jacobian). We can now proceed to perform the Gaussian integral over $\vec{\Pi}^a_\perp$. Collecting all

the relevant terms, we find

$$\begin{aligned}
&\int \mathrm{D}\Pi_\perp \, \exp\left\{-i\int d^4x \left[\frac{1}{2}\vec{\Pi}^a_\perp\vec{\Pi}^a_\perp + \vec{\Pi}^a_\perp\cdot\dot{\vec{A}}^a + \vec{\Pi}^a_\perp\cdot\vec{\nabla}_\perp A^{a0} - g f_{abc}A^{b0}\vec{A}^c_\perp\cdot\vec{\Pi}^a_\perp\right]\right\} \\
&\qquad \propto \exp\left\{\frac{i}{2}\int d^4x \left(\dot{\vec{A}}^a_\perp + \vec{\nabla}_\perp A^{a0} - g f_{abc}A^{b0}\vec{A}^c_\perp\right)^2\right\} \\
&\qquad = \exp\left\{\frac{i}{2}\int d^4x \left(\partial^0 A^{ak}_\perp - \partial^k A^{a0} - g f_{abc}A^{b0}A^{ck}_\perp\right)^2\right\} = \exp\left\{\frac{i}{2}\int d^4x \left(F^{a0k}_\perp\right)^2\right\} \\
&\qquad = \exp\left\{-\frac{i}{2}\int d^4x \, F^{a0k}_\perp F^a_{\perp 0k}\right\} ,
\end{aligned} \tag{4.472}$$

again with an irrelevant, field-independent proportionality factor that can be ignored. The path integral of interest reads now

$$\int \mathrm{D}A_\perp \int \mathrm{D}A^0 \int \mathrm{D}\psi \int \mathrm{D}\bar{\psi}\, e^{i\bar{I}} , \tag{4.473}$$

with

$$\begin{aligned}
\bar{I} &= \int d^4x \left[-\frac{1}{2}F^{a0k}_\perp F^a_{\perp 0k} - \frac{1}{2}\partial^3 A^{a0}\partial_3 A^a_0 - \frac{1}{2}\partial^3 A^{ak}_\perp \partial_3 A^a_{\perp k} - \frac{1}{4}F^{aij}_\perp F^a_{\perp ij}\right. \\
&\qquad \left. + \bar{\psi}(i\not{\partial} - m)\psi + A^a_0 J^{a0}_F + A^a_{\perp k}J^{ak}_{F\perp}\right] \\
&= \int d^4x \left[-\frac{1}{2}F^{a0k}_\perp F^a_{\perp 0k} - \frac{1}{2}\partial^3 A^{a0}\partial_3 A^a_0 - \frac{1}{2}\partial^3 A^{ak}_\perp \partial_3 A^a_{\perp k} - \frac{1}{4}F^{aij}_\perp F^a_{\perp ij}\right. \\
&\qquad \left. + \bar{\psi}(i\not{\partial} - m)\psi + i^2 g A^a_0\bar{\psi}t^a\gamma^0\psi + i^2 g A^a_{\perp k}\bar{\psi}t^a\gamma^k_\perp\psi\right] \\
&= \int d^4x \left[-\frac{1}{4}F^{a\mu\nu}F^a_{\mu\nu} + \bar{\psi}(i\not{D} - m)\psi\right]_{A^{a3}=0} = \int d^4x \, \mathscr{L}|_{A^{a3}=0} ,
\end{aligned} \tag{4.474}$$

with $\mathscr{L}$ the original classical Lagrangian from which we started [see Eq. (4.380)], and the notation $\mathscr{L}|_{A^{a3}=0}$ indicates that it has to be evaluated at $A^{a3} = 0$. The path integral of interest can now be written simply as

$$\int \mathrm{D}A^0 \int \mathrm{D}A_\perp \int \mathrm{D}\psi \int \mathrm{D}\bar{\psi}\, e^{i\int d^4x\,\mathscr{L}|_{A^{a3}=0}} = \int \mathrm{D}A \int \mathrm{D}\psi \int \mathrm{D}\bar{\psi} \prod_{a,x}\delta(A^{a3}(x))\, e^{i\int d^4x\,\mathscr{L}} , \tag{4.475}$$

where $\mathrm{D}A = \prod_\mu \mathrm{D}A^\mu$ is the integration measure over all four spacetime components of $A^{a\mu}$, and the axial gauge condition is enforced by a product of delta functions. Expression Eq. (4.475) is particularly nice since it is Lorentz invariance except for the enforcement of the gauge condition, and since it looks exactly like what we would have naively guessed for the path integral formulation of a gauge theory, with the usual phase factor e^{iS} with S the classical action, and a constraint on the integration variables enforcing the gauge condition.

Unfortunately, things are not so straightforward, and the simplicity of Eq. (4.475) is a consequence of the gauge choice: if one were to repeat the quantisation procedure in another gauge $f^a[A;x] = 0$, one would not find the same expression with $\prod_{a,x}\delta(A^{a3}(x))$ replaced by the corresponding gauge-fixing quantity $\prod_{a,x}\delta(f^a[A;x])$ (beside encountering other complications along

the way). On the other hand, the explicit breaking of Lorentz invariance in axial gauge is undesirable, and one would prefer to use other gauges where Lorentz invariance is manifest. We will see below how one should modify the formalism in order to be able to do so.

Gauge fixing In the meantime, one word about what kind of gauge fixing we are generally interested in, also to explain some notation that will be extensively used below. We have already used above the notation $f^a[A;x]$. These are meant to be non-gauge-invariant gauge-fixing functionals of the $A^b_\mu(y)$ that depend on a and x. The simplest possibilities are $f^a[A;x]$ that are functions of the $A^b_\mu(x)$ and their derivatives at x, such as the axial gauge condition $f^a = A^{a3}$ used above, or the well-known Lorenz gauge condition $f^a = \partial_\mu A^{a\mu}$. On the other hand, one could also use non-local functionals, such as $\exp\{t^a f^a[A;x]\} = \mathrm{Pexp}\{ig\int_{\mathcal{C}_{x_0,x}} dx^\mu A^b_\mu t^b\}$, with $\mathcal{C}_{x_0,x}$ specified paths from a reference point x_0 to x and Pexp the path-ordered exponential,

$$\begin{aligned}
&\mathrm{Pexp}\left\{ig\int_{\mathcal{C}_{x_0,x}} dx^\mu A^b_\mu t^b\right\} = \sum_{n=0}^{\infty}\frac{(ig)^n}{n!}\int_0^1 ds_1\ldots\int_0^1 ds_n\,\dot{x}^{\mu_1}(s_1)\ldots\dot{x}^{\mu_n}(s_n)\mathrm{P}(A_{\mu_1}(s_1)\ldots A_{\mu_n}(s_n))\,,\\
&\qquad\qquad x(0)=x_0\,,\qquad x(1)=x\,,\qquad \dot{x}^\mu(s)=\frac{dx^\mu(s)}{ds}\,,\\
&\mathrm{P}(A_{\mu_1}(s_1)\ldots A_{\mu_n}(s_n)) = \theta(s_n-s_{n-1})\ldots\theta(s_2-s_1)A^{b_1}_{\mu_1}t^{b_1}\ldots A^{b_n}_{\mu_n}t^{b_n}\,.
\end{aligned} \tag{4.476}$$

Besides the choice of gauge fixing functionals, there is also the question of how these are used, i.e., how the gauge condition is enforced. The most straightforward way is simply to impose them strictly at all space-time points.[34] On the other hand, one may want to impose the gauge condition more "softly", by disfavouring gauge configurations that violate it without entirely forbidding them in the path integral. In general, one wants to use a numerical functional $B[f]$, that depends on the $f^a[A;x]$ for all values of a and x, to weigh the gauge configurations. Examples are the strictly-enforcing delta-functions,

$$B[f] = \prod_{x,a}\delta(f^a[A;x]) \tag{4.477}$$

or the "softer" Gaussian functional

$$B[f] = \exp\left\{-\frac{i}{2}\int d^4x\, f^a[A;x]f^a[A;x]\right\}\,. \tag{4.478}$$

Gauge-invariance of the integration measure As a preliminary result to extend the path-integral formalism to a more general setting, we now show that the integration measure is gauge invariant. To this end it is sufficient to consider infinitesimal gauge transformations,

$$A^a_{\epsilon\,\mu} = A^a_\mu - \frac{1}{g}\partial_\mu\epsilon^a + f_{abc}A^b_\mu\epsilon^c\,. \tag{4.479}$$

[34] Notice that one has to be cautious when using nonlocal choices such as the one discussed above and in Eq. (4.476). Requiring $f^a = 0$ is equivalent to imposing $W(x_0,x) = \mathrm{Pexp}\{ig\int_{\mathcal{C}_{x_0,x}} dx^\mu A^b_\mu t^b\} = \mathbf{1}$, and in doing so one should be careful in choosing paths so that no closed paths is formed. In fact, this quantity is gauge-invariant for closed paths, i.e., for $x = x_0$, so that in this case it cannot be modified by a gauge transformation; and it obeys the semigroup property $W(x_0,x_1)W(x_1,x_2) = W(x_0,x_2)$.

One has for the integration measure the relation

$$\mathrm{D}A_\epsilon = \mathrm{Det}\,\mathcal{N}\,\mathrm{D}A\,, \tag{4.480}$$

where $\mathrm{Det}\,\mathcal{N}$ is the functional determinant of the Jacobian matrix

$$\begin{aligned}\mathcal{N}_{ab\,\mu\nu\,xy} &= \frac{\delta A^a_{\epsilon\,\mu}(x)}{\delta A^b_\nu(y)} = \delta_{ab}\delta_\mu{}^\nu\delta^{(4)}(x-y) + f_{abc}\epsilon^c(x)\delta_\mu{}^\nu\delta^{(4)}(x-y) \\ &= \delta_\mu{}^\nu\delta^{(4)}(x-y)\left[\delta_{ab} + i\epsilon^c(x)(t^c_A)_{ab}\right]\,.\end{aligned} \tag{4.481}$$

One finds, since ϵ^c are infinitesimal,

$$\begin{aligned}\mathrm{Det}\,\mathcal{N} &= \det_{\mu\nu}(\delta_\mu{}^\nu)\,\mathrm{Det}_{xy}(\delta^{(4)}(x-y))\,\det_{ab}(\delta_{ab} + i\epsilon^c(x)(t^c_A)_{ab}) \\ &= 1 + i\epsilon^c(x)\mathrm{tr}\,t^c_A = 1\,,\end{aligned} \tag{4.482}$$

where we use the fact that the functional determinant $\mathrm{Det}_{xy}(\delta^{(4)}(x-y))$ of the functional identity $\delta^{(4)}(x-y)$ is 1.[35]

Gauge-group measure A second preliminary result to be discussed is that of the invariant measure on the gauge group. In general, we are interested in gauge transformations that map our fields, collectively denoted by ϕ, into new fields ϕ_Λ, where $\Lambda = \Lambda^a(x)$ are the parameters entering the (finite) gauge transformation matrices $U(\Lambda) = e^{i\Lambda^a(x)t^a}$. Due to the group composition law, if we first transform $\phi \to \phi' = \phi_{\Lambda_2}$ and then $\phi' \to \phi_{\Lambda_1}\phi'$, the full transformation is implemented by the matrix $U(\Lambda_1)U(\Lambda_2) = U(K(\Lambda_2,\Lambda_1))$, and so is equivalent to the transformation $\phi \to \phi_{K(\Lambda_2,\Lambda_1)}$, for some functions $K^a(\Lambda_2(x),\Lambda_1(x)) = K(\Lambda_2,\Lambda_1)^a(x)$ entirely determined by the group composition law. Set now

$$\mathcal{R}_{ab\,xy}(\Lambda) = \left.\frac{\delta K(\Lambda,\epsilon)^a(x)}{\delta\epsilon^b(y)}\right|_{\epsilon=0} = \delta^{(4)}(x-y)\left.\frac{\partial K^a(\Lambda(x),\epsilon)}{\partial\epsilon^b}\right|_{\epsilon=0} = \delta^{(4)}(x-y)R_{ab}(\Lambda(x))\,. \tag{4.483}$$

We want to show that the measure

$$\mathrm{D}\Lambda\,\frac{1}{\mathrm{Det}\,\mathcal{R}} \tag{4.484}$$

is left invariant by the change of variables $\Lambda = K(\lambda,\tilde\Lambda)$, corresponding to setting $U(\Lambda) = U(\tilde\Lambda)U(\lambda)$. As a first step, notice that

$$\mathrm{D}\Lambda = \mathrm{D}\tilde\Lambda\,\mathrm{Det}\,\mathcal{M}(\tilde\Lambda)\,, \qquad \mathcal{M}_{ab\,xy}(\tilde\Lambda) = \frac{\delta K(\lambda,\tilde\Lambda)^a(x)}{\delta\tilde\Lambda^b(y)}\,. \tag{4.485}$$

Next, changing variables in $\mathcal{R}(\Lambda)$, we find

$$\mathcal{R}_{ab\,xy}(\Lambda(\tilde\Lambda)) = \left.\frac{\delta K(\Lambda(\tilde\Lambda),\epsilon)^a(x)}{\delta\epsilon^b(y)}\right|_{\epsilon=0} = \left.\frac{\delta K(K(\lambda,\tilde\Lambda),\epsilon)^a(x)}{\delta\epsilon^b(y)}\right|_{\epsilon=0}\,. \tag{4.486}$$

[35] While this statement is a bit shaky from the mathematical point of view, what matters is that $\mathrm{Det}\,\mathcal{N}$ is a numerical factor that does not depend on the fields, and therefore drops from any expectation value.

The parameters $K(K(\tilde{\Lambda},\lambda),\epsilon)$ correspond to the a composition of gauge transformations, and exploiting associativity of the group composition law we find

$$\begin{aligned} U(K(K(\lambda,\tilde{\Lambda}),\epsilon)) &= U(\epsilon)U(K(\lambda,\tilde{\Lambda})) = U(\epsilon)U(\tilde{\Lambda})U(\lambda) \\ &= U(K(\tilde{\Lambda},\epsilon))U(\lambda) = U(K(\lambda,K(\tilde{\Lambda},\epsilon)))\,, \end{aligned} \tag{4.487}$$

i.e.,

$$K(K(\lambda,\tilde{\Lambda}),\epsilon) = K(\lambda,K(\tilde{\Lambda},\epsilon))\,. \tag{4.488}$$

Using this in Eq. (4.486) we find

$$\begin{aligned} \mathcal{R}_{ab\,xy}(\Lambda(\tilde{\Lambda})) &= \frac{\delta K(\lambda,K(\tilde{\Lambda},\epsilon))^a(x)}{\delta\epsilon^b(y)}\bigg|_{\epsilon=0} = \int d^4z\,\frac{\delta K(\lambda,\Lambda)^a(x)}{\delta\Lambda^c(z)}\bigg|_{\Lambda=K(\tilde{\Lambda},\epsilon)}\frac{\delta K(\tilde{\Lambda},\epsilon)^c(z)}{\delta\epsilon^b(y)}\bigg|_{\epsilon=0} \\ &= \int d^4z\,\frac{\delta K(\lambda,\bar{\Lambda})^a(x)}{\delta\bar{\Lambda}^c(z)}\bigg|_{\bar{\Lambda}=\tilde{\Lambda}}\mathcal{R}_{cb\,zy}(\tilde{\Lambda}) = \int d^4z\,\mathcal{M}_{ac\,xz}(\tilde{\Lambda})\mathcal{R}_{cb\,zy}(\tilde{\Lambda})\,. \end{aligned} \tag{4.489}$$

But then

$$\begin{aligned} \mathrm{D}\Lambda\,\frac{1}{\mathrm{Det}\,\mathcal{R}(\Lambda)} &= \mathrm{D}\tilde{\Lambda}\,\mathrm{Det}\,\mathcal{M}(\tilde{\Lambda})\frac{1}{\mathrm{Det}\,\mathcal{R}(\Lambda(\tilde{\Lambda}))} = \mathrm{D}\tilde{\Lambda}\,\mathrm{Det}\,\mathcal{M}(\tilde{\Lambda})\frac{1}{\mathrm{Det}\,\mathcal{R}(\tilde{\Lambda})\mathrm{Det}\,\mathcal{M}(\tilde{\Lambda})} \\ &= \mathrm{D}\tilde{\Lambda}\,\frac{1}{\mathrm{Det}\,\mathcal{R}(\tilde{\Lambda})}\,, \end{aligned} \tag{4.490}$$

as it was to prove. Notice that since $\mathcal{R}$ is diagonal in space [see Eq. (4.483)], the gauge group volume equals

$$\mathcal{V}_G = \int \mathrm{D}\Lambda\,\frac{1}{\mathrm{Det}\,\mathcal{R}(\Lambda)} = \prod_x \int d\Lambda(x)\,\frac{1}{\det R(\Lambda(x))} = \prod_x V_G\,, \tag{4.491}$$

where V_G is the volume of the group (in the sense of the Haar measure). This is yet another mathematically not well defined quantity, that is fully regularised by discretising spacetime on a finite lattice, but diverges in the continuum limit.

Gauge-invariant path-integral formulation What we did so far was to canonically quantise the theory in axial gauge and then represent the result as a path integral. In principle, one could do without canonical quantisation entirely and formulate the theory directly in terms of a path integral. This is done by identifying the expectation values of field products defined from the path integral with the vacuum expectation of (time-ordered) product of field operators, which implicitly defines the vacuum state and the action of the field operators on it. One then identifies the states of the system with what one obtains by acting on the vacuum with products of field operators, and gives them a Hilbert space structure by using the vacuum expectation values to define scalar products (linearity is trivial). Apart form technical issues, the trickiest point is showing that the scalar product defined in this way is positive-definite. This is particularly tricky for gauge theories because the states that one would like to have in the physical Hilbert space are only a subset of all those that can be built acting on the vacuum with the field operators, namely the subset which is left invariant by gauge transformations. The initial construction produces in general a pre-Hilbert space structure where states with zero or negative norm may be present, from which one has to build a proper Hilbert structure by somehow

isolating the physical states. This can be done, but it requires us to have a gauge-invariant path-integral formulation to begin with, so that gauge-invariant combinations of fields can be identified and used to build gauge-invariant, physical states.

The most straightforward way is to give a precise meaning to the following path integral,

$$\int \mathrm{D}\phi\, e^{iS[\phi]}\mathcal{O}[\phi]\,, \tag{4.492}$$

where ϕ denotes collectively the gauge and matter fields and $\mathcal{O}$ is a generic observable. Modulo renormalisability issues, this object is in fact formally gauge invariant if $\mathcal{O}$ is, since S and the measure are. However, precisely because of this reason, each point on a gauge orbit (i.e., the set of configurations that are connected by gauge transformations) will give the same contribution to the integral, that will contain a gauge-group volume factor $\mathcal{V}_G$, that as we saw above is divergent. At the very least, then, we need to use

$$\frac{1}{\mathcal{V}_G}\int \mathrm{D}\phi\, e^{iS[\phi]}\mathcal{O}[\phi]\,, \tag{4.493}$$

where formally the divergent gauge-group-volume factors cancel in the numerator and denominator. This expression becomes mathematically well defined if one regularises the integral by replacing the infinite spacetime continuum with a finite, discrete lattice of points (this takes care of regularising UV divergences as well). This can be done in a manifestly gauge-invariant way, which can then be used to define the desired theory in the limit in which the discretisation is removed. This is the lattice approach to gauge theories.

The lattice approach is, however, quite inconvenient for perturbative calculations, since it breaks Lorentz invariance. Instead, we would prefer a formulation that works directly in the continuum and in infinite volume, so that Lorentz invariance can be preserved. In doing this we have to take into accoount that perturbation theory requires to define a propagator, and this cannot be done starting from the gauge invariant Lagrangian. In fact, the part quadratic in the gauge fields reads

$$\begin{aligned}\mathscr{L}^{(2)} &= -\frac{1}{4}\left(\partial^\mu A^{a\nu} - \partial^\nu A^{a\mu}\right)\left(\partial_\mu A^a_\nu - \partial_\nu A^a_\mu\right)\\ &= -\frac{1}{2}A^{a\mu}\delta^{ab}\left(-\Box\eta_{\mu\nu} + \partial_\mu\partial_\nu\right)A^{b\nu} + \text{total divergence.}\end{aligned} \tag{4.494}$$

The kernel $\mathcal{K}^{ab}_{\mu\nu}(x-y) = \delta^{ab}(-\Box\eta_{\mu\nu}+\partial_\mu\partial_\nu)\delta^{(4)}(x-y)$ has zero modes, and so cannot be inverted. Indeed, the longitudinal component of $A^{a\mu}$, $A^{a\mu}_{\parallel} = \partial^\mu\partial_\nu A^{a\nu}$, is clearly a zero mode of $\mathcal{K}_{\mu\nu}(x-y)$. Even more simply, going over to momentum space one finds

$$\tilde{\mathcal{K}}^{ab}_{\mu\nu}(p) = \delta^{ab}\left(p^2\eta_{\mu\nu} - p_\mu p_\nu\right)\,, \tag{4.495}$$

and clearly $\tilde{\mathcal{K}}^{ab}_{\mu\nu}(p)p^\nu = 0$. The longitudinal component of $A^{a\mu}$ is precisely the component corresponding to the gauge directions (i.e., only $A^{a\mu}_{\parallel}$ changes under a gauge transformation), and unsurprisingly it does not appear in $\mathscr{L}^{(2)}$. In order to make the path integral finite and be able to define a propagator we need to remove these zero modes from the path integral, either by imposing a gauge condition that just picks out one representative from each gauge orbit; or at least by including some non-gauge-invariant factor that dampens out the integrand as one

moves on the gauge orbits, and in doing so lifts the zero modes of $\mathcal{K}_{\mu\nu}$ to nonzero modes. One would then naively consider path integrals of the form

$$\int \mathrm{D}\phi\, e^{iS[\phi]}\mathcal{O}[\phi]B[f[\phi]]\,, \tag{4.496}$$

where, as already explained above, $f_a[\phi;x]$ are non-gauge-invariant functionals of ϕ that depend on a and x, and $B[f]$ a numerical functional of the $f_a[\phi;x]$ for all a and x. Such a functional should be chosen so to make the integral convergent (and at the very least not invariant) along the gauge orbits. The path integral obtained after canonical quantisation in axial gauge is of this form, so one may hope to connect that to more general gauge-fixing approaches, in particular ones that do not spoil Lorentz invariance. It turns out, however, that (4.496) is not a gauge-invariant quantity even for gauge-invariant observable $\mathcal{O}$, and so is not good enough for our purposes.

To obtain a gauge-invariant object, we define the matrix

$$\mathcal{F}_{ab\,xy}[\phi] = \left.\frac{\partial f_a[\phi_\epsilon;x]}{\delta\epsilon^b(y)}\right|_{\epsilon=0}, \tag{4.497}$$

and its functional determinant $\mathrm{Det}\,\mathcal{F}[\phi]$, the *Faddeev-Popov determinant*. Here ϕ_ϵ denotes the transformed of ϕ under an infinitesimal gauge transformation with parameters $\epsilon^a(x)$. Explicitly,

$$\begin{aligned}
\psi_\epsilon(x) &= \psi(x) + ig\epsilon^a(x)t^a\psi(x)\,,\\
\bar\psi_\epsilon(x) &= \bar\psi(x) - ig\epsilon^a(x)\bar\psi(x)t^a\,,\\
A^a_{\epsilon\,\mu}(x) &= A^a_\mu(x) - \tfrac{1}{g}\partial_\mu\epsilon^a(x) + f_{abc}A^b_\mu(x)\epsilon^c(x)\,.
\end{aligned} \tag{4.498}$$

The quantity we are going to study is the integral

$$\mathcal{I}_\mathcal{O} = \int \mathrm{D}\phi\, e^{iS[\phi]}\mathcal{O}[\phi]B[f[\phi]]\mathrm{Det}\,\mathcal{F}[\phi]\,. \tag{4.499}$$

We will show that for gauge-invariant observables $\mathcal{O}$, $\mathcal{I}_\mathcal{O}$ is independent of f_a and depends on B only through a constant, field-independent factor that drops out of ratios of $\mathcal{I}_\mathcal{O}$, so in particular out of the expectation values $\langle\mathcal{O}\rangle = \mathcal{I}_\mathcal{O}/\mathcal{I}_1$. Equation (4.499) can then be used as the starting point for a gauge-invariant path integral formulation of gauge theories in the continuum that allows for a perturbative treatment. Notice that $\mathcal{I}_\mathcal{O}$ is well defined also for non-gauge-invariant $\mathcal{O}$: it simply gives results that do depend on f_a and B.

To connect this with our previous result and to have a feeling of how $\mathcal{F}$ is computed, notice that for the axial gauge choice $f_a = A^{a3}$ and $B = \prod_{a,x}\delta(f_a[\phi;x])$ one has

$$\begin{aligned}
f_a[\phi_\epsilon;x] &= A^a_3(x) - \tfrac{1}{g}\partial_3\epsilon^a(x) + f_{acb}A^c_3(x)\epsilon^b(x)\,,\\
\left.\frac{\partial f_a[\phi_\epsilon;x]}{\delta\epsilon^b(y)}\right|_{\epsilon=0} &= -\tfrac{1}{g}\delta_{ab}\partial_3\delta^{(4)}(x-y) + f_{acb}A^c_3(x)\delta^{(4)}(x-y)\,,\\
B[f[\phi]]\mathrm{Det}\,\mathcal{F}[\phi] &= \prod_{a,x}\delta(A^{a3}(x))\mathrm{Det}\left(-\tfrac{1}{g}\delta_{ab}\partial_3\delta^{(4)}(x-y)\right)\,,
\end{aligned} \tag{4.500}$$

and so after imposing the axial gauge-fixing condition $\mathrm{Det}\,\mathcal{F}$ is a field-independent, constant quantity that factors out of the path integral, and so drops in expectation values. In other

words, up to an irrelevant factor the path integral of interest in axial gauge, Eq. (4.475), is a quantity of the form Eq. (4.499), and the same applies to Eq. (4.475) with the insertion of gauge invariant observables. According to our statement about $\mathcal{I}_{\mathcal{O}}$, results obtained through canonical in axial gauge and through $\mathcal{I}_{\mathcal{O}}$ with more general gauge-fixing functionals do coincide.

We now prove the statement. First simply relabel the integration variables as ϕ_Λ, and then change variables to ϕ so that $\phi_\Lambda[\phi]$ are the fields obtained from ϕ through a finite gauge transformation with parameters Λ:

$$\begin{aligned}\mathcal{I}_{\mathcal{O}} &= \int \mathrm{D}\phi_\Lambda \, e^{iS[\phi_\Lambda]} \mathcal{O}[\phi_\Lambda] B[f[\phi_\Lambda]] \mathrm{Det}\, \mathcal{F}[\phi_\Lambda] \\ &= \int \mathrm{D}\phi \mathrm{Det}\, \frac{\delta \phi_\Lambda}{\delta \phi} \, e^{iS[\phi_\Lambda[\phi]]} \mathcal{O}[\phi_\Lambda[\phi]] B[f[\phi_\Lambda[\phi]]] \mathrm{Det}\, \mathcal{F}[\phi_\Lambda[\phi]] \\ &= \int \mathrm{D}\phi \, e^{iS[\phi]} \mathcal{O}[\phi] B[f[\phi_\Lambda[\phi]]] \mathrm{Det}\, \mathcal{F}[\phi_\Lambda[\phi]] \,,\end{aligned} \tag{4.501}$$

wheere in the last passage we used gauge invariance of the measure, of S, and of $\mathcal{O}$. The left-hand side is Λ-independent, so we can integrate it over the gauge group with some factor $\rho[\Lambda]$ and divide by the integral of ρ and obtain the same quantity. Then

$$\mathcal{I}_{\mathcal{O}} \frac{1}{\mathcal{V}_G} \int \mathrm{D}\Lambda \, \rho[\Lambda] = \frac{1}{\mathcal{V}_G} \int \mathrm{D}\Lambda \, \rho[\Lambda] \int \mathrm{D}\phi \, e^{iS[\phi]} \mathcal{O}[\phi] B[f[\phi_\Lambda[\phi]]] \mathrm{Det}\, \mathcal{F}[\phi_\Lambda[\phi]] \,, \tag{4.502}$$

where we also included a gauge-group volume factor. The key point is now that

$$\begin{aligned}\mathcal{F}[\phi_\Lambda[\phi]] &= \left. \frac{\partial f_a[(\phi_\Lambda[\phi])_\epsilon; x]}{\delta \epsilon^b(y)} \right|_{\epsilon=0} = \left. \frac{\partial f_a[(\phi_{K(\Lambda,\epsilon)}[\phi]); x]}{\delta \epsilon^b(y)} \right|_{\epsilon=0} \\ &= \int d^4 z \left. \frac{\partial f_a[(\phi_{\tilde{\Lambda}}[\phi]); x]}{\delta \tilde{\Lambda}^c(z)} \right|_{\tilde{\Lambda}=K(\Lambda,\epsilon)} \left. \frac{\partial K(\Lambda,\epsilon)^c(z)}{\delta \epsilon^b(y)} \right|_{\epsilon=0} \\ &= \int d^4 z \, \mathcal{J}_{ac\, xz}[\phi_\Lambda[\phi]] \mathcal{R}_{cb\, zy}[\Lambda] \,,\end{aligned} \tag{4.503}$$

so that $\mathrm{Det}\, \mathcal{F} = \mathrm{Det}\, \mathcal{J} \mathrm{Det}\, \mathcal{R}$. This suggests we choose $\rho = 1/\mathrm{Det}\, \mathcal{R}$. Furthermore, $\mathrm{Det}\, \mathcal{J}$ is the Jacobian factor for the change of variables from $\Lambda^a(x)$ to $f_a[\phi_\Lambda[\phi; x]]$ and so[36]

$$\begin{aligned}\mathcal{I}_{\mathcal{O}} = \mathcal{I}_{\mathcal{O}} \frac{1}{\mathcal{V}_G} \int \mathrm{D}\Lambda \, \frac{1}{\mathrm{Det}\, \mathcal{R}} &= \frac{1}{\mathcal{V}_G} \int \mathrm{D}\phi \, e^{iS[\phi]} \mathcal{O}[\phi] \int \mathrm{D}\Lambda \, B[f[\phi_\Lambda[\phi]]] \, \frac{\mathrm{Det}\, \mathcal{J}\, \mathrm{Det}\, \mathcal{R}}{\mathrm{Det}\, \mathcal{R}} \,, \\ = \frac{1}{\mathcal{V}_G} \int \mathrm{D}\phi \, e^{iS[\phi]} \mathcal{O}[\phi] \int \mathrm{D}f \, B[f] &= \mathcal{C}_B \frac{1}{\mathcal{V}_G} \int \mathrm{D}\phi \, e^{iS[\phi]} \mathcal{O}[\phi] \,.\end{aligned} \tag{4.504}$$

All the dependence on B is contained in the numerical prefactor $\mathcal{C}_B$, which does not affect expectation values, as was to be proved. The formalism developed above is known as the *De Witt-Faddeev-Popov formalism*.

[36] It is implicitly assumed that $\mathrm{Det}\, \mathcal{J}$ never vanishes, so that $|\mathrm{Det}\, \mathcal{J}| = \pm \mathrm{Det}\, \mathcal{J}$ with the same sign everywhere, which also means that the change of variables is invertible at all x, and there are no multiple Λs solving $f_a[\phi_\Lambda[\phi; x]] = \bar{f}_a$. This turns out not to be the case due to the existence of Gribov copies. Nonetheless, for perturbative calculations where one is interested only in fluctuations around vanishing guage fields, this does not constitute a problem

In order to set up perturbation theory, it is convenient to use a B that makes calculations simple. Such a B is for example the Gaussian functional of Eq. (4.478), that we slightly generalise to

$$B[f] = \exp\left\{-\frac{i}{2\xi}\int d^4x\, f^a[A;x] f^a[A;x]\right\}\,, \tag{4.505}$$

where ξ is a new gauge parameter. Moreover, it is convenient to use Lorentz-invariant gauge fixing functionals f_a to keep Lorentz invariance manifest, such as the Lorenz gauge gauge-fixing functional,

$$f_a = \partial_\mu A^{a\mu}\,, \tag{4.506}$$

which yields

$$B[f] = \exp\left\{-\frac{i}{2\xi}\int d^4x \sum_a (\partial_\mu A^{a\mu})^2\right\} = \exp\left\{-\frac{i}{2\xi}\int d^4x\, \mathscr{L}_{\rm gf}^{\rm Lorenz}\right\}\,. \tag{4.507}$$

For this choice one has

$$\begin{aligned}
\mathcal{F}_{ab\,xy} &= \frac{\delta}{\delta\epsilon^b(y)}\partial_{x\mu}\left(A^{a\mu}(x) - \tfrac{1}{g}\partial_x^\mu\epsilon^a(x) + f_{acb}A^{c\mu}(x)\epsilon^b(x)\right)\\
&= \partial_{x\mu}\left(-\tfrac{1}{g}\partial_x^\mu\delta_{ab}\delta^{(4)}(x-y) + f_{acb}A^{c\mu}(x)\delta^{(4)}(x-y)\right)\\
&= -\tfrac{1}{g}\partial_{x\mu}\left(\partial_x^\mu\delta_{ab}\delta^{(4)}(x-y) + ig(-if_{cab})A^{c\mu}(x)\delta^{(4)}(x-y)\right)\\
&= -\tfrac{1}{g}\partial_{x\mu}\left(\partial_x^\mu\delta_{ab}\delta^{(4)}(x-y) + ig(t_A^c)_{ab}A^{c\mu}(x)\delta^{(4)}(x-y)\right)\\
&= -\tfrac{1}{g}\partial_{x\mu}(D_x^{(A)\mu})_{ab}\delta^{(4)}(x-y)\,,
\end{aligned} \tag{4.508}$$

where it has been made explicit that the derivative $\partial_{x\mu}$ and the covariant derivative in the adjoint representation $D_{x\mu}^{(A)}$ act here on x. Including the contribution from Eq. (4.507), the quadratic part of the gauge-fixed Lagrangian $\mathscr{L}' = \mathscr{L} + \mathscr{L}_{\rm gf}^{\rm Lorenz}$ reads

$$\begin{aligned}
\mathscr{L}'^{\,(2)} &= -\frac{1}{2}A^{a\mu}\left(-\Box\eta_{\mu\nu} + \partial_\mu\partial_\nu\right)A^{a\nu} + \frac{1}{2\xi}A^{a\mu}\partial_\mu\partial_\nu A^{a\nu} + \text{total divergence}\\
&= -\frac{1}{2}A^{a\mu}\delta^{ab}\left(-\Box\eta_{\mu\nu} + \left(1-\frac{1}{\xi}\right)\partial_\mu\partial_\nu\right)A^{b\nu} + \text{total divergence}.
\end{aligned} \tag{4.509}$$

The modified kernel is now invertible, as it is evident going over to momentum space:

$$\begin{aligned}
\mathcal{K}'^{ab}_{\mu\nu}(p) &= \delta^{ab}\left[p^2\eta_{\mu\nu} - \left(1-\frac{1}{\xi}\right)p_\mu p_\nu\right] = \delta^{ab}p^2\left[\left(\eta_{\mu\nu} - \frac{p_\mu p_\nu}{p^2}\right) + \frac{1}{\xi}\frac{p_\mu p_\nu}{p^2}\right]\,,\\
\mathcal{K}'^{-1\,ab}_{\mu\nu}(p) &= \delta^{ab}\frac{1}{p^2}\left[\left(\eta_{\mu\nu} - \frac{p_\mu p_\nu}{p^2}\right) + \xi\frac{p_\mu p_\nu}{p^2}\right] = \delta^{ab}\frac{1}{p^2}\left(\eta_{\mu\nu} - (1-\xi)\frac{p_\mu p_\nu}{p^2}\right)\,.
\end{aligned} \tag{4.510}$$

Now that a gauge-field propagator is defined, one can read off the interaction vertices from the cubic and quartic terms of the gauge-field Lagrangian, as well as off the matter Lagrangian, and derive the Feynman rules of the theory. Notice that since the propagator is the lowest-order contribution to the two-point function $\langle A_\mu^a A_\nu^b\rangle = \mathcal{K}'^{-1\,ab}_{\mu\nu}(p) + \ldots$, it is a gauge-dependent quantity. Nonetheless, the perturbative series is gauge independent.

Ghost fields The Faddeev-Popov determinant in the calculation is most easily dealt with by representing it as a Grassmann path integral,

$$\begin{aligned}\operatorname{Det}\mathcal{F} &= \int \mathrm{D}\omega \int \mathrm{D}\omega^* \, \exp\left\{ i \int d^4x \int d^4y \; \omega_a^*(x)\, \mathcal{F}_{ab\,xy}\, \omega_b(y) \right\} \\ &= \int \mathrm{D}\omega \int \mathrm{D}\omega^* \, \exp\left\{ i \int d^4x \, \mathscr{L}_{\mathrm{ghost}} \right\} ,\end{aligned} \tag{4.511}$$

where ω_a and ω_a^* are two sets of independent Grassmann (anticommuting) variables collectively called *ghost fields*, or simply ghosts, with a running over as many values as there are generators in the gauge group. To distinguish them, ω_a are referred to as ghost fields and ω_a^* as antighost fields. A new quantum number, the ghost number, is introduced, taking value $+1$ for ω_a, -1 for ω_a^*, and 0 for any other field. In this way one has an ordinary path integral with an extended set of integration variables and a total Lagrangian that reads $\mathscr{L}_{\mathrm{tot}} = \mathscr{L}' + \mathscr{L}_{\mathrm{ghost}} = \mathscr{L} + \mathscr{L}_{\mathrm{gf}} + \mathscr{L}_{\mathrm{ghost}}$.

The ghost fields are fermionic scalar fields, and as such they violate the spin-statistics connection. The corresponding excitations then represent unphysical states that should not be part of the physical Hilbert space. We already now that there exist gauges where ghosts are absent, e.g., the axial gauge, using which a physical Hilbert space, i.e., including only positive-norm states, can be reconstructed straightforwardly. Since the expectation values of gauge-invariant operators in the De Witt-Faddeev-Popov formalism is independent of the gauge choice, the corresponding states in the reconstructed pre-Hilbert space will automatically have positive norms independently of the gauge that one uses. One can then construct a physical Hilbert space also using gauges other than the axial gauge, where in general one finds also zero or negative-norm states in the pre-Hilbert space obtained from the path integral. These states, however, do not affect the observable physics.

Nonetheless, the contribution of ghost fields to $\mathcal{I}_{\mathcal{O}}$ is essential to achieve the desired gauge invariance, and cures what otherwise would be problems with unitarity of the perturbative series. In practical calculations, Feynman diagrams with external ghost or antighost lines can simply be ignored, while those with ghost lines appear only in internal loops must be included. The corresponding Feynman rules are derived from $\mathscr{L}_{\mathrm{ghost}}$ in the standard way. For example, in Lorenz gauge one finds from Eq. (4.508) (using integration by parts)

$$\begin{aligned}\int d^4x \, \mathscr{L}_{\mathrm{ghost}} &= -\frac{1}{g} \int d^4x \int d^4y \, \omega_a^*(x) \partial_{x\mu} (D_x^{(A)\mu})_{ab} \delta^{(4)}(x-y) \omega_b(y) \\ &= -\frac{1}{g} \int d^4x \int d^4y \, \left[(D_x^{(A)\mu})_{ba} \partial_{x\mu} \omega_a^*(x) \right] \delta^{(4)}(x-y) \omega_b(y) \\ &= -\frac{1}{g} \int d^4x \, \left[(D_x^{(A)\mu})_{ba} \partial_{x\mu} \omega_a^*(x) \right] \omega_b(x) \\ &= \frac{1}{g} \int d^4x \, \partial_\mu \omega_a^*(x) (D^{(A)\mu})_{ab} \, \omega_b(x) \\ &= \frac{1}{g} \int d^4x \, \left[\partial_\mu \omega_a^*(x) \partial^\mu \omega_a(x) + ig (t_A^c)_{ab} (\partial_\mu \omega_a^*(x)) \omega_b(x) A^{c\mu}(x) \right] .\end{aligned} \tag{4.512}$$

The factor $1/g$ can be dropped since it can be reabsorbed in a redefinition of the ghost fields producing only a constant prefactor for the path integral. The ghost propagator is the same as that of a massless scalar field, and the only interaction term yields a three-point gauge field-ghost-antighost vertex. As appropriate for a fermionic variable, ghost loops carry an extra

minus sign with respect to analogous gauge-field loops, which are present in a non-Abelian gauge theory due to the self coupling of gauge fields. This can be interpreted as ghost fields compensating the inclusion of the unphysical degrees of freedom of the gauge fields, i.e., those that are modified by a gauge transformation, when using gauge fixing procedures that do not remove them completely. Notice that there are indeed as many ghost-antighost pairs of fields (ω_a, ω_a^*) as there are independent parameters Λ_a in a gauge transformation.

As a final remark, we notice that when building up an operator formalism for the ghost fields, one requires that ω_a and ω_a^* be sets of respectively Hermitean and anti-Hermitean scalar field operators, $\omega_a^\dagger = \omega_a$ and $\omega_a^{*\dagger} = -\omega_a^*$ obeying canonical *anti*commutation relations. However, the momenta conjugate to ω_a and ω_a^* are proportional respectively to $\dot{\omega}_a^*$ and $\dot{\omega}_a$. For free fields, this means that nontrivial anticommutation relations are obeyed by the ghost annihilation and antighost creation operators, and viceversa.

BRST invariance While the formalism developed above is gauge-invariant, the total action $\mathscr{L}_{\rm tot}$ is not. Surprisingly, despite the presence of gauge-non-invariant terms, $\mathscr{L}_{\rm tot}$ still displays invariance under a certain transformation, which is sort of a remnant of the initial gauge invariance. In order to exhibit this symmetry, it is convenient first to recast $\mathcal{I}_{\mathcal{O}}$ as follows,

$$\begin{aligned}
\mathcal{I}_{\mathcal{O}} &= \int \mathrm{D}A \int \mathrm{D}\psi \int \mathrm{D}\bar{\psi} \int \mathrm{D}\omega \int \mathrm{D}\omega^* \, e^{i\int d^4x\, \mathscr{L}_{\rm tot}} \\
&= \int \mathrm{D}A \int \mathrm{D}\psi \int \mathrm{D}\bar{\psi} \int \mathrm{D}\omega \int \mathrm{D}\omega^* \, e^{i\int d^4x\, (\mathscr{L}+\mathscr{L}_{\rm ghost})} e^{-\frac{i}{2\xi}\int d^4x\, f_a f_a} \\
&\propto \int \mathrm{D}A \int \mathrm{D}\psi \int \mathrm{D}\bar{\psi} \int \mathrm{D}\omega \int \mathrm{D}\omega^* \int \mathrm{D}h \, e^{i\int d^4x\, (\mathscr{L}+\mathscr{L}_{\rm ghost})} e^{\frac{i\xi}{2}\int d^4x\, h_a h_a} e^{i\int d^4x\, h_a f_a} \\
&= \int \mathrm{D}A \int \mathrm{D}\psi \int \mathrm{D}\bar{\psi} \int \mathrm{D}\omega \int \mathrm{D}\omega^* \int \mathrm{D}h \, e^{i\int d^4x\, \mathscr{L}_{\rm new}} \,,
\end{aligned} \tag{4.513}$$

where we have used a Gaussian path integral to re-express the gauge-fixing Lagrangian in terms of a new set of fields h_a (the *Nakanishi-Lautrup* fields), with again as many fields as group generators, and where

$$\begin{aligned}
\mathscr{L}_{\rm new} &= \mathscr{L} + \omega_a^* \Delta_a + h_a f_a + \frac{\xi}{2} h_a h_a \,, \\
\Delta_a(x) &= \int d^4y\, \mathcal{F}_{ab\,xy}\, \omega_b(y) \,.
\end{aligned} \tag{4.514}$$

We now show that $\mathscr{L}_{\rm new}$ is invariant under the infinitesimal transformation δ_θ, defined as follows:

$$\begin{aligned}
\delta_\theta \psi &= -igt^a \theta \omega_a \psi \,, \\
\delta_\theta \bar{\psi} &= -ig\theta(-t^a)^* \omega_a \bar{\psi} \,, \\
\delta_\theta A_\mu^a &= \theta (D_\mu^{(A)} \omega)^a = \theta(\partial_\mu \omega_a - g f_{abc} A_\mu^b \omega_c) \,, \\
\delta_\theta \omega_a &= \theta \tfrac{1}{2} g f_{abc} \omega_b \omega_c \,, \\
\delta_\theta \omega_a^* &= \theta g h_a \,, \\
\delta_\theta h_a &= 0 \,.
\end{aligned} \tag{4.515}$$

Here θ is an infinitesimal Grassmann variable, which therefore anticommutes with all fermionic fields and commutes with all bosonic fields. This transformation is extended to more general

functionals of fields by treating it as the infinitesimal version of a finite linear transformation. In particular, it extends trivially by linearity to

$$\delta_\theta(A+B) = (\delta_\theta A) + (\delta_\theta B)\,, \tag{4.516}$$

while for the product of fields

$$\delta_\theta(AB) = (\delta_\theta A)B + A(\delta_\theta B)\,. \tag{4.517}$$

This extends straighforwardly by induction to the product of any number of fields. Then, for a general functional,

$$F[\phi] = \sum_{n=0}^{\infty} \sum_{\{A_i\}_n} \int d^4x_1 \ldots \int d^4x_n\, F_{A_1\ldots A_n} \phi_{A_1}(x_1)\ldots\phi_{A_n}(x_n)\,, \tag{4.518}$$

with $\{A_i\}_n = (A_1, \ldots A_n)$ and each A_i running over the basic fields ($\phi_A = \psi, \bar\psi, A, \omega, \omega^*, h$), the transformation $\delta_\theta F$ is obtained using Eqs. (4.516) and (4.517) together with the basic transformation laws Eq. (4.515), and is equal to[37]

$$\delta_\theta F[\phi] = (F[\phi+\delta_\theta\phi] - F[\phi])|_{\mathcal{O}(\theta)} = \int d^4x\, \frac{\delta F[\phi]}{\delta\phi_A(x)} \delta_\theta\phi_A(x)\,. \tag{4.519}$$

For future purpose it is useful to define the operator s via

$$\delta_\theta F[\phi] = \theta s F[\phi]\,. \tag{4.520}$$

The transformation Eq. (4.515) is known as the Becchi-Rouet-Stora-Tyutin transformation, or *BRST transformation*. The transformation law of the gauge and matter fields is easily recognised as an ordinary gauge transformation with not quite ordinary infinitesimal parameters $\epsilon_a = -g\theta\omega_a$. It is then obvious that $\delta_\theta\mathscr{L} = 0$ since $\mathscr{L}$ is gauge invariant. To prove invariance of the rest, it is convenient to prove first that the operator s is *nilpotent*, i.e., $s^2 = 0$. This in turn is proved in steps, starting from the following observations.

1. For the basic fields one shows by direct calculation that $s^2\phi_A = 0$. This is done below in detail.

2. For the product $\Phi_1\Phi_2$ of two monomials (i.e., products) of basic fields $\Phi_{1,2}$, one has from Eq. (4.517)
$$\begin{aligned} \delta_\theta(\Phi_1\Phi_2) &= (\delta_\theta\Phi_1)\Phi_2 + \Phi_1(\delta_\theta\Phi_2) = (\theta s\Phi_1)\Phi_2 + \Phi_1(\theta s\Phi_2) \\ &= \theta\big((s\Phi_1)\Phi_2 + (-1)^{\mathscr{F}(\Phi_1)}\Phi_1(s\Phi_2)\big) \end{aligned} \tag{4.521}$$
where $\mathscr{F}(\Phi)$ is the fermion number of Φ (1 for fermionic fields, 0 for bosonic fields), and so
$$s(\Phi_1\Phi_2) = (s\Phi_1)\Phi_2 + (-1)^{\mathscr{F}(\Phi_1)}\Phi_1(s\Phi_2)\,. \tag{4.522}$$

[37] The functional derivative with respect to fermionic fields is also an anticommuting object and one should be careful in specifying if it acts on the left or on the right of the functional. We will ignore this issue here.

3. By direct inspection, one has for fundamental fields that the s operator transforms bosons into fermions and viceversa, and so $\mathscr{F}(s\phi_A) = 1 - \mathscr{F}(\phi_A)$, and so also for a general monomial Φ one has

$$\mathscr{F}(s\Phi) = 1 - \mathscr{F}(\Phi) \tag{4.523}$$

which can be seen by using Eq. (4.517) and its generalisation to any number of fields.

By definition, $\delta_\theta s\Phi = \theta s^2\Phi$. Combining Eqs. (4.522) and Eq. (4.523) one finds

$$\begin{aligned}
\theta s^2(\Phi_1\Phi_2) &= \delta_\theta s(\Phi_1\Phi_2) = \delta_\theta\left((s\Phi_1)\Phi_2 + (-1)^{\mathscr{F}(\Phi_1)}\Phi_1(s\Phi_2)\right) \\
&= \left(\delta_\theta\left(s\Phi_1\right)\right)\Phi_2 + \left(s\Phi_1\right)\left(\delta_\theta\Phi_2\right) + (-1)^{\mathscr{F}(\Phi_1)}[\left(\delta_\theta\Phi_1\right)\left(s\Phi_2\right) + \Phi_1\left(\delta_\theta\left(s\Phi_2\right)\right)] \\
&= \theta\left(s^2\Phi_1\right)\Phi_2 + \left(s\Phi_1\right)\theta\left(s\Phi_2\right) + (-1)^{\mathscr{F}(\Phi_1)}[\theta\left(s\Phi_1\right)\left(s\Phi_2\right) + \Phi_1\theta\left(s^2\Phi_2\right)] \\
&= \theta\Big[\left(s^2\Phi_1\right)\Phi_2 + (-1)^{\mathscr{F}(s\Phi_1)}\left(s\Phi_1\right)\left(s\Phi_2\right) \\
&\qquad + (-1)^{\mathscr{F}(\Phi_1)}[\left(s\Phi_1\right)\left(s\Phi_2\right) + (-1)^{\mathscr{F}(\Phi_1)}\Phi_1\left(s^2\Phi_2\right)]\Big] \\
&= \theta\left[\left(s^2\Phi_1\right)\Phi_2 + \left((-1)^{\mathscr{F}(s\Phi_1)} + (-1)^{\mathscr{F}(\Phi_1)}\right)\left(s\Phi_1\right)\left(s\Phi_2\right) + \Phi_1\left(s^2\Phi_2\right)\right] \\
&= \theta\left[\left(s^2\Phi_1\right)\Phi_2 + \Phi_1\left(s^2\Phi_2\right)\right] ,
\end{aligned} \tag{4.524}$$

and so $s^2(\Phi_1\Phi_2) = 0$ if $s^2\Phi_{1,2}$ are. Since this is true for the basic fields, it follows for any monomial by induction, and to any polynomial of any order by linearity, hence to any functional of the fields.

It remains to show that $s^2\phi_A = 0$. For $\phi_A = \psi$,

$$\begin{aligned}
\theta s^2\psi = \delta_\theta s\psi &= -igt^a\left[\left(\theta\tfrac{1}{2}gf_{abc}\omega_b\omega_c\right)\psi - \omega_a\theta igt^b\omega_b\psi\right] \\
&= -\theta ig^2t^a\left[\tfrac{1}{2}f_{abc}\omega_b\omega_c\psi + it^b\omega_a\omega_b\psi\right] \\
&= -\theta ig^2\left[\tfrac{1}{2}f_{abc}t^a + it^bt^c\right]\omega_b\omega_c\psi = \theta\frac{g^2}{2}\left[-if_{bca}t^a + [t^b,t^c]\right]\omega_b\omega_c\psi \\
&= \theta\frac{g^2}{2}\left[-if_{bca}t^a + if_{bca}t^a\right]\omega_b\omega_c\psi = 0 ,
\end{aligned} \tag{4.525}$$

having used $\omega_b\omega_c = -\omega_c\omega_a$ to replace t^bt^c with the commutator. The proof for $\bar\psi$ is identical, replacing the generators $t^a = t^a_R$ in representation R with the generators $(-t^a)^* = (-t^a_R)^*$ in the complex conjugate representation $\bar R$. For $\phi_A = A^a_\mu$,

$$\begin{aligned}
\theta s^2A^a_\mu = \delta_\theta sA^a_\mu &= \partial_\mu(\theta\tfrac{1}{2}gf_{abc}\omega_b\omega_c) - gf_{abc}\left[\theta\left(\partial_\mu\omega_b - gf_{bde}A^d_\mu\omega_e\right)\omega_c + A^b_\mu(\theta\tfrac{1}{2}gf_{cde}\omega_d\omega_e)\right] \\
&= \theta\left\{\tfrac{1}{2}gf_{abc}\partial_\mu(\omega_b\omega_c) - gf_{abc}\left(\partial_\mu\omega_b\right)\omega_c\right. \\
&\qquad \left. + g^2f_{abc}f_{bde}A^d_\mu\omega_e\omega_c - \tfrac{1}{2}g^2f_{abc}f_{cde}A^b_\mu\omega_d\omega_e\right\} \\
&= \theta\left\{gf_{abc}(\partial_\mu\omega_b)\omega_c - gf_{abc}\left(\partial_\mu\omega_b\right)\omega_c + g^2A^d_\mu\omega_e\omega_c\left(f_{abc}f_{bde} - \tfrac{1}{2}f_{adb}f_{bec}\right)\right\} \\
&= \theta g^2A^d_\mu\omega_e\omega_c\left(i(t^c_A)_{ab}i(t^e_A)_{bd} + \tfrac{1}{2}i(t^b_A)_{ad}f_{ceb}\right) \\
&= \theta\frac{g^2}{2}A^d_\mu\omega_e\omega_c\left(-[t^c_A,t^e_A] + if_{ceb}t^b_A\right)_{ad} = 0 ,
\end{aligned} \tag{4.526}$$

having used the anticommuting nature of the ghost fields to show

$$f_{abc}\partial_\mu(\omega_b\omega_c) = f_{abc}[(\partial_\mu\omega_b)\omega_c + \omega_b(\partial_\mu\omega_c)] = f_{abc}[(\partial_\mu\omega_b)\omega_c - (\partial_\mu\omega_c)\omega_b] = 2f_{abc}(\partial_\mu\omega_b)\omega_c\,, \quad (4.527)$$

and to replace $t^c_A t^e_A$ with the commutator in the last passage. For $\phi_A = \omega_a$,

$$\begin{aligned}\theta s^2\omega_a = \delta_\theta s\omega_a &= \frac{1}{2}f_{abc}[(\theta s\omega_b)\omega_c + \omega_b(\theta s\omega_c)] = \theta\frac{g}{2}f_{abc}[(s\omega_b)\omega_c - \omega_b(s\omega_c)] \\ &= \theta g f_{abc}(s\omega_b)\omega_c = \theta\frac{g^2}{2}f_{abc}f_{bde}\omega_d\omega_e\omega_c = -\theta\frac{g^2}{2}\omega_c\omega_d\omega_e f_{acb}f_{deb} = 0\,,\end{aligned} \quad (4.528)$$

where we used the fact that $f_{abc}\omega_b(s\omega_c) = f_{abc}(s\omega_c)\omega_b = -f_{acb}(s\omega_c)\omega_b = -f_{abc}(s\omega_b)\omega_c$ since $s\omega_c$ is bosonic, and where the vanishing of the last quantity follows from the fact that $\omega_c\omega_d\omega_e$ is invariant under cyclic permutations of the indices, and that the structure constants satisfy the identity

$$f_{a\underline{c}b}f_{d\underline{e}\underline{b}} + \text{cyclic permutations of the underlined indices} = 0\,, \quad (4.529)$$

as a consequence of the Jacobi identity. For $\phi_A = \omega^*_a$,

$$\theta s^2\omega^*_a = \delta_\theta s\omega^*_a = \delta_\theta h_a = 0\,. \quad (4.530)$$

Finally, for $\phi_A = h_a$ one has trivially

$$\theta s^2 h_a = \delta_\theta s h_a = 0\,. \quad (4.531)$$

Nilpotency of s is then proved.

To prove BRST invariance of $\mathscr{L}_{\rm new}$ we now study the transformation properties of f_a. To this end, we use Eq. (4.519) to show that

$$\begin{aligned}\delta_\theta f[\phi;x] &= (f_a[\phi+\delta_\theta\phi;x] - f_a[\phi;x])\,|_{\mathcal{O}(\theta)} = (f_a[\phi_\epsilon;x] - f_a[\phi;x])\,|_{\epsilon=-g\theta\omega} \\ &= \int d^4y\,\frac{\delta f_a[\phi_\epsilon;x]}{\delta\epsilon_b(y)}\bigg|_{\epsilon=0}(-g\theta\omega_b(y)) = \int d^4y\,\mathcal{F}_{ab\,xy}(-g\theta\omega_b(y)) \\ &= -g\theta\int d^4y\,\mathcal{F}_{ab\,xy}\omega_b(y) = -g\theta\Delta_a(x)\,,\end{aligned} \quad (4.532)$$

having used the fact that $\mathcal{F}_{ab\,xy}$ is a bosonic quantity, and so

$$s f_a[\phi;x] = -g\Delta_a(x)\,. \quad (4.533)$$

Then

$$g(\omega^*_a\Delta_a + h_a f_a) = (s\omega^*_a)f_a - \omega^*_a(sf_a) = s(\omega^*_a f_a)\,, \quad (4.534)$$

and since also

$$g h_a h_a = (s\omega^*_a)h_a = s(\omega^*_a h_a)\,, \quad (4.535)$$

we find

$$\omega^*_a\Delta_a + h_a f_a + \frac{\xi}{2}h_a h_a = s\left(\tfrac{1}{g}(\omega^*_a f_a + \tfrac{1}{2}\xi\omega^*_a h_a)\right) = s\left(\tfrac{1}{g}\omega^*_a(f_a + \tfrac{1}{2}\xi h_a)\right) = s\Psi\,. \quad (4.536)$$

In conclusion,

$$\mathscr{L}_{\rm new} = \mathscr{L} + s\Psi\,. \quad (4.537)$$

A quantity of the form $s\Psi$, i.e., in the image of s, is called BRST-exact. A quantity Ψ' such that $s\Psi' = 0$ is instead called BRST-closed. We have already mentioned that $s\mathscr{L} = 0$, and since the second term is BRST-exact one finds

$$s\mathscr{L}_{\rm new} = s^2\Psi = 0\,, \quad (4.538)$$

since s is nilpotent.

BRST charge, BRST cohomology, and BRST quantisation As for any other continuous symmetry, there is a Hermitean conserved charge Q associated with the BRST transformation. Due to the peculiar nature of the BRST transformation, that involves a Grassmann parameter rather than an ordinary c-number one, this charge is a fermionic charge, in a sense to be explained shortly. The charge Q generates the BRST transformation, and so for a generic field operator $\hat{\Phi}$ with definite fermion number

$$\delta_\theta \hat{\Phi} = \theta s \hat{\Phi} = i[\theta Q, \hat{\Phi}]_- = i(\theta Q \hat{\Phi} - \hat{\Phi}\theta Q) = i\theta(Q\hat{\Phi} \mp \hat{\Phi}Q) = i\theta[Q, \hat{\Phi}]_\mp \,, \tag{4.539}$$

where the signs $-$ and $+$ correspond to the commutator and anticommutator, respectively, and have to be chosen according to whether $\hat{\Phi}$ is bosonic or fermionic, respectively. Then,

$$[Q, \hat{\Phi}]_\mp = -is\hat{\Phi} \,. \tag{4.540}$$

As a consequence of nilpotency and of the fact that $s\hat{\Phi}$ has fermion number opposite to that of $\hat{\Phi}$, one has

$$0 = -s^2\hat{\Phi} = [Q, [Q, \hat{\Phi}]_\mp]_\pm = [Q, Q\hat{\Phi} \mp \hat{\Phi}Q]_\pm = Q^2\hat{\Phi} \mp Q\hat{\Phi}Q \pm (Q\hat{\Phi}Q \mp \hat{\Phi}Q^2) = [Q^2, \hat{\Phi}]_- \,. \tag{4.541}$$

In order for this to vanish for all $\hat{\Phi}$, Q^2 must be proportional to the identity operator. But from Eq. (4.515) we see that Q^2 has a nonzero ghost number, since its commutator with a basic field of ghost number g yields a field with ghost number $g+1$ (except for the Nakanishi-Lautrup fields h_a), and so the only possibility is for the proportionality factor to be zero, i.e., $Q^2 = 0$.

We now show that $Q|\text{phys}\rangle = 0$ for any physical state $|\text{phys}\rangle = \hat{\mathcal{O}}|0\rangle$ obtained by applying a gauge-invariant operator $\hat{\mathcal{O}}$ built out of gauge and matter fields on the vacuum $|0\rangle$. Such states clearly have vanishing ghost number. We know that a BRST transformation of the gauge and matter fields is a gauge transformation with parameters $-g\theta\omega_a$, and so $[Q, \hat{\mathcal{O}}]_\mp = 0$. The charge Q is a spatial integral of field operators, and as such it commutes with spatial translations, i.e., $[\vec{P}, Q]_- = 0$. Then $0 = [\vec{P}, Q]_-|0\rangle = \vec{P}Q|0\rangle$, i.e., $Q|0\rangle$ is translation invariant and so $Q|0\rangle = c|0\rangle$ due to the vacuum being the unique translation-invariant state. But $c^2 = \langle 0|Q^2|0\rangle = 0$, so $Q|0\rangle = 0$. Then $Q|\text{phys}\rangle = Q\hat{\mathcal{O}}|0\rangle = [Q, \hat{\mathcal{O}}]_-|0\rangle = 0$, i.e., they are BRST-closed. If we now add an arbitrary BRST-exact vector $Q|a\rangle$ to a physical state, we find for the scalar products

$$\begin{aligned}\big(\langle\text{phys}'| + \langle a'|Q\big)\,(|\text{phys}\rangle + Q|a\rangle) &= \langle\text{phys}'|\text{phys}\rangle + \langle a'|Q|\text{phys}\rangle + \langle\text{phys}'|Q|a\rangle + \langle a'|Q^2|a\rangle \\ &= \langle\text{phys}'|\text{phys}\rangle \,.\end{aligned} \tag{4.542}$$

Since such scalar products entirely encode the physics of the system, we have found that vectors in the pre-Hilbert space that differ only by a BRST-exact vector represent the same physical state. The physical Hilbert space is then obtained from the pre-Hilbert space by identifying vectors differing only by a BRST-exact vector $Q|a\rangle$. In mathematical terms, this amounts to associate physical states with equivalence classes with respect to the equivalence relation $\sim$ defined by

$$|v\rangle \sim |w\rangle \quad \text{if} \quad |v\rangle - |w\rangle = Q|a\rangle \quad \text{for some} \quad |a\rangle \,. \tag{4.543}$$

In particular, vectors corresponding to physical states belong to the kernel of Q, $\operatorname{Ker} Q = \{|v\rangle \mid Q|v\rangle = 0\}$, with vectors differing by an element of the image of Q, $\operatorname{Im} Q = \{|v\rangle \mid |v\rangle = Q|w\rangle\}$, representing the same state. Physical states are then the equivalence classes with respect to $\sim$ that contain elements of $\operatorname{Ker} Q$, which form the quotient space $\operatorname{Ker} Q / \operatorname{Im} Q$, or in other

words they are the BRST-closed vectors modulo the BRST-exact ones. For nilpotent operators Q, the quotient space $\mathrm{Ker}\, Q/\mathrm{Im}\, Q$ is called the cohomology of Q.

The discussion above suggests a different way to quantise a gauge theory, known as BRST quantisation, that departs completely from the route followed above (i.e., generalising from canonical quantisation in axial gauge). One starts from a path integral

$$\int \mathrm{D}\phi\, e^{iS_{\mathrm{BRST}}[\phi]}\,, \tag{4.544}$$

where ϕ now denotes collectively gauge, matter, ghost, and Nakanishi-Lautrup fields, with S_{BRST} the most general action of ghost number zero that is invariant under BRST transformations, as well as under Poincaré and all other desired symmetry, and that satisfies the criteria for renormalisability by power counting. We will show in a moment that such an action must be of the form

$$S_{\mathrm{BRST}}[\phi] = S[\phi_{\mathrm{phys}}] + s\Psi[\phi]\,, \tag{4.545}$$

with S a gauge-invariant functional of the gauge and matter fields ϕ_{phys} only, and Ψ an arbitrary functional of ghost number -1. One then identifies the BRST charge Q and the ghost charge Q_g and defines the physical states as the vectors of ghost number zero, i.e., $Q_g|\mathrm{phys}\rangle = 0$, that are unaffected by any change $\delta\Psi$ of Ψ. This means that a generic scalar product $\langle \mathrm{phys}'|\mathrm{phys}\rangle$ between two physical states must be left unchanged, i.e.,

$$0 = \delta\langle \mathrm{phys}'|\mathrm{phys}\rangle = \langle \mathrm{phys}'|is\delta\Psi|\mathrm{phys}\rangle = -\langle \mathrm{phys}'|[Q,\delta\Psi]|\mathrm{phys}\rangle\,, \tag{4.546}$$

which is true for arbitrary $\delta\Psi$ only if $Q|\mathrm{phys}\rangle = 0$. We then require that physical states belong to the kernel of Q, with vectors differing by an element of the image of Q being identified. One can show that the space of physical states selected in this way is a proper, physical Hilbert space with a positive-definite scalar product, and free of ghosts and antighosts. This is expected since we already know that quantisation in axial gauge yields a proper Hilbert space of states, free of ghosts and antighosts that are trivially decoupled. Since scalar products of physical states, that are annihilated by Q, are independent of the choice of Ψ, and since there is at least one Ψ for which ghost and antighost states decouple from the rest, this decoupling will take place for an arbitrary choice of Ψ.[38]

We finally show that Eq. (4.545) provides the most general BRST invariant functional of fields. To do this, notice that except when acting on a functional of the h_a fields only, the BRST transformation Eq. (4.515) leaves the total number of ω_a^* and h_a fields unchanged. In general, we can write a generic functional uniquely as

$$F[\phi] = F_h[h] + \sum_{N=0}^{\infty} F_N[\phi]\,, \tag{4.547}$$

where $F_N[\phi]$ are in general sums of functionals containing N fields ω_a^* and h_a, and at least one basic field different from the h_a. Since h_a is BRST-exact, it is easy to see that so is $F_h[h]$, and so automatically BRST-closed (i.e., BRST-invariant). Moreover, sF_N contains exactly as many ω_a^*

[38] BRST quantisation (in the canonical formalism) is discussed in T. Kugo and I. Ojima, "Local covariant operator formalism of nonabelian gauge theories and quark confinement problem", Prog. Theor. Phys. Suppl. **66** (1979), 1–130.

and h_a fields as F_N, and so $(sF)_N = sF_N$. The most general BRST-invariant functional $S_{\rm BRST}$ is then of the form

$$S_{\rm BRST}[\phi] = S_h[h] + \sum_{N=0}^{\infty} S_N[\phi]\,, \tag{4.548}$$

with S_h arbitrary but automatically BRST-exact, and $sS_N = 0$. Next, introduce an operator t defined by

$$\begin{aligned} th_a &= \tfrac{1}{g}\omega_a^*\,, \\ t\phi_A &= 0\,, \qquad \phi_A \neq h_a\,, \end{aligned} \tag{4.549}$$

on the basic fields, and extended by linearity to act on a generic functional.[39] Clearly $t^2 = 0$. It is easy to see that

$$\begin{aligned} sth_a &= h_a\,, \qquad st\phi_A = 0\,, \qquad \phi_A \neq h_a\,, \\ ts\omega_a^* &= \omega_a^*\,, \qquad ts\phi_A = 0\,, \qquad \phi_A \neq \omega_a\,, \end{aligned} \tag{4.550}$$

resulting in

$$\{s,t\}\phi_A = \begin{cases} \phi_A\,, & \phi_A = \omega_a^*, h_a\,, \\ 0\,, & \phi_A \neq \omega_a^*, h_a\,. \end{cases} \tag{4.551}$$

Applied on S_N, the operator $\{s,t\}$ then simply counts how many fields ω_a^* and h_a are there. To see this in detail, notice that a generic monomial Φ can be written as $h_{a_1}\ldots h_{a_{n_h}}\omega^*_{b_1}\ldots\omega^*_{b_{n^*_\omega}}\bar\Phi$, with $\bar\Phi$ independent of h_a and ω_b^*, and so

$$\begin{aligned} &st\,h_{a_1}\ldots h_{a_{n_h}}\omega^*_{b_1}\ldots\omega^*_{b_{n^*_\omega}}\bar\Phi \\ &= \Big(st\,h_{a_1}\ldots h_{a_{n_h}}\Big)\,\omega^*_{b_1}\ldots\omega^*_{b_{n^*_\omega}}\bar\Phi - (t\,h_{a_1}\ldots h_{a_{n_h}})\,\Big(s\,\omega^*_{b_1}\ldots\omega^*_{b_{n^*_\omega}}\Big)\bar\Phi \\ &\quad - (-1)^{n_{\omega^*}}(t\,h_{a_1}\ldots h_{a_{n_h}})\omega^*_{b_1}\ldots\omega_{b_{n^*_\omega}}(s\,\bar\Phi)\,, \\ &ts\,h_{a_1}\ldots h_{a_{n_h}}\omega^*_{b_1}\ldots\omega^*_{b_{n^*_\omega}}\bar\Phi \\ &= \Big(t\,h_{a_1}\ldots h_{a_{n_h}}\Big)\,\Big(s\,\omega^*_{b_1}\ldots\omega^*_{b_{n^*_\omega}}\bar\Phi\Big) + h_{a_1}\ldots h_{a_{n_h}}\,\Big(ts\,\omega^*_{b_1}\ldots\omega^*_{b_{n^*_\omega}}\Big)\bar\Phi \\ &= \Big(t\,h_{a_1}\ldots h_{a_{n_h}}\Big)\,\Big(s\,\omega^*_{b_1}\ldots\omega^*_{b_{n^*_\omega}}\Big)\bar\Phi + h_{a_1}\ldots h_{a_{n_h}}\,\Big(ts\,\omega^*_{b_1}\ldots\omega^*_{b_{n^*_\omega}}\Big)\bar\Phi \\ &\quad + (-1)^{n_{\omega^*}}\,\Big(t\,h_{a_1}\ldots h_{a_{n_h}}\Big)\,\omega^*_{b_1}\ldots\omega^*_{b_{n^*_\omega}}\,\Big(s\,\bar\Phi\Big)\,, \\ &\{s,t\}h_{a_1}\ldots h_{a_{n_h}}\omega^*_{b_1}\ldots\omega^*_{b_{n^*_\omega}}\bar\Phi \\ &= \Big(st\,h_{a_1}\ldots h_{a_{n_h}}\Big)\,\omega^*_{b_1}\ldots\omega^*_{b_{n^*_\omega}}\bar\Phi + h_{a_1}\ldots h_{a_{n_h}}\,\Big(ts\,\omega^*_{b_1}\ldots\omega^*_{b_{n^*_\omega}}\Big)\bar\Phi \\ &= (n_h + n_{\omega^*})h_{a_1}\ldots h_{a_{n_h}}\omega^*_{b_1}\ldots\omega^*_{b_{n^*_\omega}}\bar\Phi\,. \end{aligned} \tag{4.552}$$

Using this result we now have for a BRST-invariant functional S_N with N antighost and h fields,

$$\{s,t\}S_N = NS_N = stS_N + tsS_N = stS_N\,, \tag{4.553}$$

[39] Since h_a is a bosonic variable, one can write a generic functional F with all hs on the left as (schematically) $h^N\bar F$, with $\bar F$ independent of h, without having to keep track of signs. Since $t\bar F = 0$, there are no problems in choosing the sign when defining $tF = (th^N)\bar F \pm h^N(t\bar F) = (th^N)\bar F = (\sum \omega^* h^{N-1})\bar F$, where the sum runs over the h_a, that t replaces with ω_a^*.

so for $N \neq 0$

$$S_N = s\left(\tfrac{1}{N} t S_N\right) , \tag{4.554}$$

i.e., S_N is BRST-exact. We then have

$$S_{\rm BRST}[\phi] = S_0[\phi] + s\Psi[\phi] , \tag{4.555}$$

where we collected into $s\Psi$ all the BRST-exact terms. As for S_0, it does not contain any h or antighost field, and since we required that $S_{\rm BRST}$ has total ghost number zero it also does not contain any ghost field. Then $S_0 = S_0[\phi_{\rm phys}]$ is a functional of gauge and matter fields only, and Eq. (4.545) follows.

BRST quantisation of U(1) pure gauge theory As an example of how BRST quantisation works, consider U(1) pure gauge theory in Lorenz gauge. As this is an Abelian group, the structure constants vanish. One starts from the Lagrangian Eq. (4.514), setting $f = \partial_\mu A^\mu$. There are a single gauge field, i.e., the photon field A_μ, and a single pair of ghost and antighost fields, ω and ω^*. The ghost action is given by Eq. (4.512), and shows that ghost and antighost do not interact with the photon field. The auxiliary Nakanishi-Lautrup field h can be integrated out without problems, in practice by setting $h = -f/\xi$, as long as one takes that into account in the BRST transformation. The resulting Lagrangian reads

$$\mathscr{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} - \frac{1}{2\xi} (\partial_\mu A^\mu)^2 + \partial_\mu \omega^* \partial^\mu \omega , \tag{4.556}$$

and the BRST transformation $i[Q, \phi]_\pm = s\phi$ becomes

$$sA_\mu = \partial_\mu \omega , \qquad s\omega = 0 , \qquad s\omega^* = -\frac{g}{\xi} \partial_\mu A^\mu . \tag{4.557}$$

Following the canonical procedure, one solves the equations of motion for the massless fields A_μ, ω and ω^*, all required to be Hermitean, and finds

$$\begin{aligned} A_\mu(x) &= \int d\Omega_p \left(a_\mu(p) e^{-ip\cdot x} + a_\mu(p)^\dagger e^{ip\cdot x} \right) , \\ \omega(x) &= \int d\Omega_p \left(c(p) e^{-ip\cdot x} + c(p)^\dagger e^{ip\cdot x} \right) , \\ \omega^*(x) &= \int d\Omega_p \left(b(p) e^{-ip\cdot x} + b(p)^\dagger e^{ip\cdot x} \right) , \end{aligned} \tag{4.558}$$

where $d\Omega_p$ is the usual invariant measure on phase space and $p^0 = |\vec{p}|$. One then imposes canonical (anti)commutation relations on fields and conjugate momenta, that are

$$\Pi^\mu = \frac{\partial \mathscr{L}}{\partial(\partial_0 A_\mu)} = -F^{0\mu} - \frac{1}{\xi} \delta^\mu{}_0 \partial_\alpha A^\alpha , \tag{4.559}$$

for the gauge fields, and[40]

$$\pi = \frac{\partial_R \mathscr{L}}{\partial(\partial_0 \omega)} = \partial^0 \omega^* \qquad \pi^* = \frac{\partial_R \mathscr{L}}{\partial(\partial_0 \omega^*)} = -\partial^0 \omega , \tag{4.560}$$

[40]Here $\partial_R/\partial\theta_i$ denotes the right derivative with respect to the Grassmann variable θ_i of a function $F(\theta)$ of Grassmann variables $\theta_1, \dots \theta_n$, defined as follows. One can always write the most general F as

$$F(\theta) = \sum_{k=0}^{n} \sum_{\substack{\{a_1,\dots,a_k\} \\ a_1<a_2<\dots<a_k}} F_{a_1\dots a_k} \theta_{a_1} \dots \theta_{a_k} ,$$

for the ghost and antighost fields. In particular, for the photon field one has

$$[A_\mu(x),\Pi^\nu(y)]_{\rm ET}=i\delta_\mu{}^\nu\delta^{(3)}(\vec{x}-\vec{y})\,,\qquad [A_\mu(x),A^\nu(y)]_{\rm ET}=[\Pi_\mu(x),\Pi^\nu(y)]_{\rm ET}=0\,, \tag{4.561}$$

which are equivalent to

$$[A_\mu(x),\dot{A}_\nu(y)]_{\rm ET}=-i\eta^{(\xi)}_{\mu\nu}\delta^{(3)}(\vec{x}-\vec{y})\,,\qquad [A_\mu(x),A_\nu(y)]_{\rm ET}=[\dot{A}_\mu(x),\dot{A}_\nu(y)]_{\rm ET}=0\,, \tag{4.562}$$

where $\eta^{(\xi)}_{\mu\nu}=\mathrm{diag}(\xi^{-1},-1,-1,-1)$. These imply

$$[a_\mu(p),a_\nu(q)^\dagger]=-2p^0(2\pi)^3\eta^{(\xi)}_{\mu\nu}\delta^{(3)}(\vec{p}-\vec{q})\,,\qquad [a_\mu(p),a_\nu(q)]=[a_\mu(p)^\dagger,a_\nu(q)^\dagger]=0\,. \tag{4.563}$$

The nontrivial anticommutation relations for the b and c operators are instead

$$\{c(p),b(q)^\dagger\}=-2p^0(2\pi)^3\delta^{(3)}(\vec{p}-\vec{q})\,,\qquad \{b(p),c(q)^\dagger\}=-2p^0(2\pi)^3\delta^{(3)}(\vec{p}-\vec{q})\,. \tag{4.564}$$

Then $c^\dagger$ and $b^\dagger$ create a ghost and an antighost particle, respectively, and b and c annihilate a ghost and an antighost particle, respectively. Defining the vacuum state $|0\rangle$ as the state annihilated by all the $a(p)$, $b(p)$, and $c(p)$, and building the Fock space out of it by means of creation operators, we see from Eqs. (4.563) and (4.564) that this contains states of negative norm. For example, for the states with one temporal photon $|{\rm t}(p)\rangle=a_0(p)^\dagger|0\rangle$ one has

$$\langle{\rm t}(p)|{\rm t}(q)\rangle=\langle0|a_0(p)a_0(q)^\dagger|0\rangle=\langle0|[a_0(p),a_0(q)^\dagger]|0\rangle=-\frac{1}{\xi}2p^0(2\pi)^3\delta^{(3)}(\vec{p}-\vec{q})\,. \tag{4.565}$$

Using now Eq. (4.557), we find

$$\begin{aligned}
&i\int d\Omega_p\left([Q,a_\mu(p)]e^{-ip\cdot x}+[Q,a_\mu(p)^\dagger]e^{ip\cdot x}\right)=-i\int d\Omega_p\left(p_\mu c(p)e^{-ip\cdot x}-p_\mu c(p)^\dagger e^{ip\cdot x}\right)\,,\\
&i\int d\Omega_p\left(\{Q,b(p)\}e^{-ip\cdot x}+\{Q,b(p)^\dagger\}e^{ip\cdot x}\right)=i\frac{g}{\xi}\int d\Omega_p\left(p^\mu a_\mu(p)e^{-ip\cdot x}-p^\mu a_\mu(p)^\dagger e^{ip\cdot x}\right)\,,\\
&i\int d\Omega_p\left(\{Q,c(p)\}e^{-ip\cdot x}+\{Q,c(p)^\dagger\}e^{ip\cdot x}\right)=0\,,
\end{aligned} \tag{4.566}$$

and matching coefficients we obtain

$$\begin{aligned}
&[Q,a_\mu(p)]=-p_\mu c(p)\,, && [Q,a_\mu(p)^\dagger]=p_\mu c(p)^\dagger\,,\\
&\{Q,b(p)\}=\frac{g}{\xi}p^\mu a_\mu(p)\,, && \{Q,b(p)^\dagger\}=\frac{g}{\xi}p^\mu a_\mu(p)^\dagger\,,\\
&\{Q,c(p)\}=0\,, && \{Q,c(p)^\dagger\}=0\,.
\end{aligned} \tag{4.567}$$

It follows from the (anti)commutation relations with annihiliation operators that $Q|0\rangle=0$: in fact, acting on the vacuum with both sides of the relations one finds $a_\mu(p)Q|0\rangle=b(p)Q|0\rangle=c(p)Q|0\rangle=0$, so that $Q|0\rangle\propto|0\rangle$, but since $Q^2=0$ the proportionality constant must be zero.

so it suffices to define $\partial_R/\partial\theta_i$ for ordered monomials $M=\theta_{a_1}\dots\theta_{a_k}$ with $a_1<a_2<\ldots<a_k$, and then extend it by linearity. If a monomial contains θ_i, then it can also be written as $M=(-1)^{\tilde{n}}\theta_{\tilde{a}_1}\dots\theta_{\tilde{a}_{k-1}}\theta_i=\tilde{M}\theta_i$ for a suitable integer $\tilde{n}$ and indices $\tilde{a}_1,\dots,\tilde{a}_{k-1}$. Then $\partial_R M/\partial\theta_i=\tilde{M}$. If instead M does not contain θ_i, then $\partial_R M/\partial\theta_i=0$. One analogously defines the left derivative by writing $M=(-1)^{\hat{n}}\theta_i\theta_{\hat{a}_1}\dots\theta_{\hat{a}_{k-1}}=\theta_i\hat{M}$ and setting $\partial_L M/\partial\theta_i=\hat{M}$, if M contains θ_i, and zero otherwise.

Consider now a generic vector $|\psi\rangle$ corresponding to a physical state, i.e., obeying $Q|\psi\rangle = 0$. If we add a photon with polarisation e^μ, i.e., we apply $e^\mu a_\mu(p)^\dagger = e \cdot a(p)^\dagger$ on $|\psi\rangle$, then

$$Qe \cdot a(p)^\dagger|\psi\rangle = (e \cdot p)c(p)^\dagger|\psi\rangle\,, \tag{4.568}$$

which still obeys the physicality condition if $e \cdot p = 0$, i.e., if e is transverse, $e^\mu = (0, \vec{n}_\perp)$ with $\vec{n}_\perp \cdot \vec{p} = 0$, or if e is longitudinal, $e^\mu = p^\mu$, but not if $e^\mu = (|\vec{p}|, -\vec{p})$. However, since

$$Qb(p)^\dagger|\psi\rangle = \frac{g}{\xi} p^\mu a_\mu(p)^\dagger|\psi\rangle\,, \tag{4.569}$$

adding a longitudinal photon gives a BRST-exact state, which is equivalent to the zero vector, so in particular has norm zero. This equation also tells us that adding an antighost to a physical state makes it an unphysical state. Finally,

$$Qc(p)^\dagger|\psi\rangle = 0\,, \tag{4.570}$$

so that adding a ghost one still finds a physical vector, but since for any e^μ such that $e \cdot p \neq 0$ one has

$$c(p)^\dagger|\psi\rangle = Q(e \cdot p)^{-1}\, e \cdot a(p)^\dagger|\psi\rangle\,, \tag{4.571}$$

such a state is BRST-exact and so equivalent to the zero vector. One then concludes that the physical states contain only transverse photons, modulo BRST-exact vectors containing ghosts and longitudinal photons. Restricted to physical states the scalar product is positive-definite, and a proper Hilbert space is then obtained.

5 Chiral anomaly

Quantisation of a field theory requires the introduction of suitable regulator, in order to deal with the infinite number of degrees of freedom of the system. Such a regulator generally breaks one or more of the symmetries of the classical action, and it is generally not guaranteed that the classical symmetry is recovered after renormalisation and removal of the regulator. In particular, finite symmetry breaking effects may ensue from naively vanishingly small symmetry-breaking terms in the regulated action if they get multiplied by some UV-divergent renormalisation factor. In this case the classical symmetry is lost at the quantum level, and an anomaly is said to be present.

An elegant way to understand anomalies is in terms of the non-invariance of the path integral measure under a transformation of the fields that otherwise leaves the action invariant. To be mathematically sound, this requires to put path integrals on a more solid ground by formulating them in Euclidean rather than Minkowskian metric.

Euclidean field theory Recall that in the quantum field theory of a real scalar field the basic object is the following path integral,

$$Z = \int [\mathrm{D}\phi]\, e^{i\int d^4x \left(\frac{1}{2}(\partial_\mu\phi\partial^\mu\phi - m^2\phi^2) - \frac{g_3}{3!}\phi^3 - \frac{g_4}{4!}\phi^4\right)} = \int [\mathrm{D}\phi]\, e^{iS[\phi]}\,. \tag{5.572}$$

This object is the integral of a wildly oscillating function, and so has very bad convergence properties, which are a bit improved by the inclusion of suitable "$i\epsilon$" terms that damp the exponential when the field and/or its derivatives are large.

The convergence properties of Eq. (5.572) would be drastically improved if we could turn the oscillating factor into a damped exponential altogether. This can be achieved by means of the so-called *Wick rotation*, which consists in the analytic continuation of the time variable x^0 from real to imaginary values. More precisely, one replaces

$$x^0 \to -ix_{E4}\,, \qquad x^i = x_{Ei}\,, \tag{5.573}$$

everywhere, and in turn one defines the Euclidean field $\phi_E(x_E)$ depending on the Euclidean coordinates $x_E = (\vec{x}_E, x_{E4})$,

$$\begin{aligned}
\phi(x) = \phi(x^0,\vec{x}) &\to \phi(-ix_{E4},\vec{x}) \equiv \phi_E(\vec{x}_E, x_{E4}) = \phi_E(x_E)\,,\\
\partial_0\phi(x) = \frac{\partial}{\partial x^0}\phi(x^0,\vec{x}) &\to i\frac{\partial}{\partial x_{E4}}\phi(-ix_{E4},\vec{x}) = i\partial_{E4}\phi_E(x_E)\,,\\
\partial_j\phi(x) = \frac{\partial}{\partial x^j}\phi(x^0,\vec{x}) &\to \frac{\partial}{\partial x_{Ej}}\phi(-ix_{E4},\vec{x}) = \frac{\partial}{\partial x_{Ej}}\phi_E(x_E)\,.
\end{aligned} \tag{5.574}$$

Under the replacement Eq. (5.574) the action becomes ($(\vec{\nabla}_E)_j = \partial_{Ej}$)

$$\begin{aligned}
iS[\phi] &\to i(-i)\int d^4x_E\,\left[\frac{1}{2}\left(i^2(\partial_{E4}\phi_E(x_E))^2 - (\vec{\nabla}_E\phi_E(x_E))^2 - m^2\phi_E^2\right) - \frac{g_3}{3!}\phi_E^3 - \frac{g_4}{4!}\phi_E^4\right]\\
&= -\int d^4x_E\,\left[\frac{1}{2}\left((\partial_{E4}\phi_E(x_E))^2 + (\vec{\nabla}_E\phi_E(x_E))^2 + m^2\phi_E^2\right) + \frac{g_3}{3!}\phi_E^3 + \frac{g_4}{4!}\phi_E^4\right]\\
&= -\int d^4x_E\,\left[\frac{1}{2}\left(\partial_{E\mu}\phi_E(x_E)\partial_{E\mu}\phi_E(x_E) + m^2\phi_E^2\right) + \frac{g_3}{3!}\phi_E^3 + \frac{g_4}{4!}\phi_E^4\right] \equiv S_E[\phi_E]\,.
\end{aligned} \tag{5.575}$$

The action S_E is invariant under translations and under the four-dimensional rotation group SO(4), which are the symmetries of four-dimensional Euclidean space, i.e., $\mathbb{R}^4$ endowed with the Euclidean metric[41] $X_E \cdot Y_E = X_{E\mu}Y_{E\mu} = \delta_{\mu\nu}X_{E\mu}Y_{E\nu}$. This is to be contrasted with the symmetry under translation of the original action $S[\phi]$ under translations and under the (proper orthocronous) Lorentz group SO(3,1), which are the symmetries of Minkowski space, i.e., $\mathbb{R}^4$ endowed with the Minkowski metric $X \cdot Y = X^\mu Y^\nu \eta_{\mu\nu}$. For this reason, Eq. (5.575) is said to define a quantum field theory in Euclidean signature, or briefly a Euclidean quantum field theory. The basic integral Eq. (5.572) is replaced by

$$Z \to Z_E = \int [\mathrm{D}\phi_E]\, e^{-S_E[\phi_E]}\,, \tag{5.576}$$

which (for positive g_4) is the integral of a damped exponential, and so properly convergent (after suitable regularisation). In fact, Eq. (5.576) is just the canonical partition function of a spatially four-dimensional statistical mechanics system with Hamiltonian S_E and corresponding Boltzmann weight e^{-S_E},[42] and for this reason is commonly referred to as the partition function of the system. Correlation functions with respect to the Boltzmann weight e^{-S_E}, denoted by $\langle\ldots\rangle_E$, are the result of Wick rotation of the Minkowskian Green's function. For example,

$$G^{(2)}(x) = \langle\phi(0)\phi(x^0,\vec{x})\rangle \to \langle\phi(0)\phi(-ix_{E4},\vec{x})\rangle_E = \langle\phi_E(0)\phi_E(x_E)\rangle_E = G_E^{(2)}(x_E)\,. \tag{5.577}$$

[41] There is no need here to distinguish between covariant and contravariant indices since $X_{E\mu} = \delta_{\mu\nu}X_E^\nu = X_E^\mu$.

[42] Here one formally has $k_BT = 1$.

Here Euclidean correlation functions are defined as

$$\langle \phi_E(x_{E1}) \dots \phi_E(x_{En}) \rangle_E = \frac{1}{Z_E} \int [\mathrm{D}\phi_E]\, e^{-S_E[\phi_E]}\, \phi_E(x_{E1}) \dots \phi_E(x_{En})\,. \tag{5.578}$$

In operator language, the procedure described above corresponds to analytically continuing the field operators to imaginary time,

$$\hat{\phi}(t) = e^{iHt} \hat{\phi}(0) e^{-iHt} \to \hat{\phi}(-i\tau) = e^{H\tau} \hat{\phi}(0) e^{-H\tau} \equiv \hat{\phi}_E(\tau)\,, \tag{5.579}$$

and represent the Green's functions for imaginary time argument in terms of a path integral. The result are the Euclidean correlation functions, in the statistical mechanics sense, of the fields ϕ_E computed using the Boltzmann weight e^{-S_E}, which are obtained as in Eq. (5.578).[43] As already pointed out above, Euclidean (imaginary time) correlation functions look better than their Minkowskian (real time) counterparts in terms of convergence properties of the path integral. As a matter of fact, they can be even studied in a nonperturbative way by discretising the path integral on a lattice and computing it numerically.

The procedure to get the physically relevant, Minkowskian Green's function is then to start from the Euclidean correlation functions, and then analytically continue back in the temporal variable via $x_{E4} \to ix^0$. For example, for the 2-point function one first computes $G_E^{(2)}(\vec{x}, \tau)$, and then analytically continues from $\tau \in \mathbb{R}^+$ (resp. $\tau \in \mathbb{R}^-$) to it, $t \in \mathbb{R}^+$ (resp. $t \in \mathbb{R}^-$), i.e., counterclockwise in the complex plane, to get

$$G^{(2)}(t, \vec{x}) = G_E^{(2)}(\vec{x}, it)\,. \tag{5.580}$$

The case of general n-point functions is analogous.[44]

The extension of Wick rotation to gauge fields requires only a minor modification. Since A_μ transforms like ∂_μ, the temporal component must acquire a factor of i in order for the Wick-rotated action to display SO(4) invariance. One then performs the following Wick rotation of the gauge fields,

$$A_0^a(x^0, \vec{x}) \to i A_{E4}^a(-ix_{E4}, \vec{x}_E)\,, \qquad A_j^a(x^0, \vec{x}) \to A_{Ej}^a(-ix_{E4}, \vec{x}_E)\,, \tag{5.581}$$

with $\vec{x}_E = \vec{x}$, resulting in

$$F_{0j}^a(x^0, \vec{x}) \to i F_{E4j}^a(-ix_{E4}, \vec{x}_E)\,, \qquad F_{jk}^a(x^0, \vec{x}) \to F_{Ejk}^a(-ix_{E4}, \vec{x}_E)\,, \tag{5.582}$$

[43] It should be clear that the replacement Eq. (5.574) is not simply a change of integration variables in the path integral. Recall that the formal path integral is obtained as the limit $T \to \infty$ of the matrix element $\langle \Phi(\vec{x}) | U(2T) | \Phi(\vec{x}) \rangle$ of the temporal evolution operator $U(t) = e^{-iHt}$, integrated over $\Phi(\vec{x})$. One then writes $U(2T) = e^{iN\epsilon H}$ with $T = N\epsilon$ and with large N (eventually infinite) and small (eventually infinitesimal) ϵ, and inserts complete sets of "coordinate" eigenstates $|\phi(t, \vec{x})\rangle$ after each $e^{i\epsilon H}$. The result is an integral over the discrete "trajectory" $\phi(t_i, \vec{x})$, with identical initial and final points, i.e., $\phi(T = t_N, \vec{x}) = \phi(-T = t_0, \vec{x}) = \Phi(\vec{x})$. The only meaningful external parameter is T, with t_i being merely an index for the integration variables $\phi(t_i, \vec{x})$. The analytic continuation $T \to -iT$ is a nontrivial operation, resulting in e^{i2TH} being replaced by e^{-2TH}, which is a completely different type of operator. In terms of the continuous trajectory $\phi(t, \vec{x})$ and its derivatives, which are shorthand notations for $\phi(t_i, \vec{x})$ and $[\phi(t_{i+1}, \vec{x}) - \phi(t_i, \vec{x})]/\epsilon$, and of the temporal integral $\int dt\, f(t)$ in the action, which is a shortand notation for $\epsilon \sum_i f(t_i)$, the analytic continuation $T \to -iT$ corresponds precisely to the replacement Eq. (5.574).

[44] Conditions under which one can reconstruct a proper (Minkowskian) quantum field theory starting from Euclidean correlation functions (or Schwinger functions) are discussed in K. Osterwalder and R. Schrader, "Axioms for Euclidean Green's functions", Commun. Math. Phys. **31** (1973), 83–112; "Axioms for Euclidean Green's functions. 2", Commun. Math. Phys. **42** (1975), 281.

with $F^a_{E\mu\nu}$ identical in form to $F^a_{\mu\nu}$ except for replecing Minkowskian with Euclidean fields. The Yang-Mills action is then replaced by

$$\begin{aligned} iS_{\rm YM} &= -\frac{1}{4}i\int d^4x\, F^a_{\mu\nu}F^{a\mu\nu} = -\frac{1}{4}i\int d^4x\, \left(-2F^a_{0j}F^a_{0j} + F^a_{jk}F^a_{jk}\right) \\ &\to -\frac{1}{4}i(-i)\int d^4x_E\, \left(2F^a_{E4j}F^a_{E4j} + F^a_{Ejk}F^a_{Ejk}\right) = -\frac{1}{4}\int d^4x_E\, F^a_{E\mu\nu}F^a_{E\mu\nu}\,. \end{aligned} \tag{5.583}$$

Correlation functions are obtained starting from the partition function

$$Z_E = \int [{\rm D}A_E]\, e^{-\int d^4x_E\, \frac{1}{4}F^a_{E\mu\nu}F^a_{E\mu\nu}}\,, \tag{5.584}$$

either suitably discretised on a spacetime lattice, or including a suitable gauge-fixing functional and the corresponding Faddeev-Popov determinant if one is interested in perturbative calculations. Minkowskian Green's functions are then obtained from the Euclidean correlation functions by reversing the analytic continuation Eq. (5.581).

For fermionic fields the Wick rotation reads

$$\psi(x^0,\vec{x}) \to \psi_E(-ix_{E4},\vec{x}_E)\,, \qquad \bar\psi(x^0,\vec{x}) \to \bar\psi_E(-ix_{E4},\vec{x}_E)\,. \tag{5.585}$$

Rotation invariance of the resulting Euclidean action is made explicit by introducing the Euclidean gamma matrices. In fact, the derivative term of the Dirac action is replaced by

$$\begin{aligned} &\not{D} = D_\mu\gamma^\mu = (\partial_\mu + igA^a_\mu(x)t^a)\gamma^\mu \to i(\partial_{E4} + igA^a_{E4}(x_E)t^a)\gamma^0 + (\partial_{Ej} + igA^a_{Ej}(x_E)t^a)\gamma^j \\ &= i\left[(\partial_{E4} + igA^a_{E4}(x_E)t^a)\gamma^0 + (\partial_{Ej} + igA^a_{Ej}(x_E)t^a)(-i\gamma^j)\right] = iD_{E\mu}\gamma_{E\mu} = i\not{D}_E\,, \end{aligned} \tag{5.586}$$

where

$$D_{E\mu} = \partial_{E\mu} + igA^a_{E\mu}(x_E)t^a\,, \tag{5.587}$$

and where the Euclidean gamma matrices

$$\gamma_{E4} = \gamma^0\,, \qquad \gamma_{Ej} = -i\gamma^j \tag{5.588}$$

are Hermitean and obey the anticommutation relations

$$\{\gamma_{E\mu},\gamma_{E\nu}\} = 2\delta_{\mu\nu}\,. \tag{5.589}$$

The fifth gamma matrix is

$$\gamma_{E5} = -\gamma_{E1}\gamma_{E2}\gamma_{E3}\gamma_{E4} = i\gamma^0\gamma^1\gamma^2\gamma^3 = \gamma^5\,, \tag{5.590}$$

which anticommutes with all $\gamma_{E\mu}$,

$$\{\gamma_{E5},\gamma_{E\mu}\} = 0\,. \tag{5.591}$$

The Dirac action is then replaced by

$$iS_{\rm D} = i\int d^4x\, \bar\psi(i\not{D} - m)\psi \to i(-i)\int d^4x_E\, \bar\psi_E(i^2\not{D}_E - m)\psi_E = -\int d^4x_E\, \bar\psi_E(\not{D}_E + m)\psi_E\,. \tag{5.592}$$

Putting together the gauge and fermionic parts of the action, the relevant Euclidean partition function is then

$$\begin{aligned} Z_E &= \int [\mathrm{D}A_E] \int [\mathrm{D}\psi_E] \int [\mathrm{D}\bar{\psi}_E]\, e^{-S_E}\,, \\ S_E &= \int d^4x \left(\frac{1}{4} F^a_{E\mu\nu} F^a_{E\mu\nu} + \bar{\psi}_E (\not{D}_E + m) \psi_E \right). \end{aligned} \tag{5.593}$$

In the following we will be concerned with the Euclidean theory, and so we will drop the subscript E for notational simplicity.

Chiral symmetry For a single massless fermion, the fermionic action in Eq. (5.593) is invariant under independent phase transformations of the two chiral components of the fields. Indeed, since $\bar{\psi}\gamma_5 \not{D}\psi = -\bar{\psi}\not{D}\gamma_5\psi$, setting $\psi = \psi_L + \psi_R$ and $\bar{\psi} = \bar{\psi}_L + \bar{\psi}_R$ with

$$\psi_{L,R} = \frac{1 \mp \gamma_5}{2}\psi\,, \qquad \bar{\psi}_{L,R} = \bar{\psi}\frac{1 \pm \gamma_5}{2}\,, \tag{5.594}$$

one finds

$$\bar{\psi}_{L,R} \not{D} \psi_{R,L} = \bar{\psi}\frac{1 \pm \gamma_5}{2}\not{D}\frac{1 \pm \gamma_5}{2}\psi = \bar{\psi}\not{D}\frac{1 \mp \gamma_5}{2}\frac{1 \pm \gamma_5}{2}\psi = 0\,, \tag{5.595}$$

and so

$$\bar{\psi}\not{D}\psi = \bar{\psi}_L \not{D}\psi_L + \bar{\psi}_R \not{D}\psi_R. \tag{5.596}$$

The "left-handed" and "right-handed" component are then decoupled, and their phases can be changed independently. The most general $\mathrm{U}(1)_L \times \mathrm{U}(1)_R$ chiral transformation can also be written as

$$\begin{aligned} \psi &= e^{i\alpha_L \frac{1-\gamma_5}{2}} e^{i\alpha_R \frac{1+\gamma_5}{2}} \psi' & \bar{\psi} &= \bar{\psi}' e^{-i\alpha_L \frac{1+\gamma_5}{2}} e^{-i\alpha_R \frac{1-\gamma_5}{2}} \\ &= e^{i\frac{\alpha_R+\alpha_L}{2}} e^{i\frac{\alpha_R-\alpha_L}{2}\gamma_5} \psi' & &= \bar{\psi}' e^{-i\frac{\alpha_R+\alpha_L}{2}} e^{i\frac{\alpha_R-\alpha_L}{2}\gamma_5} \\ &= e^{i\alpha} e^{i\beta\gamma_5} \psi'\,, & &= \bar{\psi}' e^{-i\alpha} e^{i\beta\gamma_5}\,. \end{aligned} \tag{5.597}$$

The chiral symmetry group is then also written as $\mathrm{U}(1)_L \times \mathrm{U}(1)_R \sim \mathrm{U}(1)_V \times \mathrm{U}(1)_A$, with the common change of phase $e^{i\alpha}$ of the two chiralities being the "vector" part of the transformation, while the opposite change of phase effected by $e^{i\beta\gamma_5}$ is the "axial" part of the transformation. Invariance under $\mathrm{U}(1)_V$ is recognised as the usual invariance under a phase transformation, corresponding, e.g., to electric charge or baryon number conservation. This symmetry can be preserved without problems when regulating the theory, and so it will survive the renormalisation procedure.[45] The situation is, however, more complicated for the axial part of the symmetry. In general, under the transformation Eq. (5.597) one finds for the integration measure in the path integral

$$\mathrm{D}\psi\mathrm{D}\bar{\psi} = \mathrm{D}\psi'\mathrm{D}\bar{\psi}' \left(\mathrm{Det} \begin{pmatrix} e^{i\alpha} & 0 \\ 0 & e^{-i\alpha} \end{pmatrix} \mathrm{Det} \begin{pmatrix} e^{i\beta\gamma_5} & 0 \\ 0 & e^{i\beta\gamma_5} \end{pmatrix} \right)^{-1} = \mathrm{D}\psi'\mathrm{D}\bar{\psi}' e^{-2i\beta \mathrm{Tr}\gamma_5}\,. \tag{5.598}$$

Naively, one expects $\mathrm{Tr}\gamma_5 = 0$ since $\mathrm{tr}\,\gamma_5 = 0$. On the other hand, Tr formally represents the trace over x, as well as over the discrete indices of the fermion fields, of an x-independent quantity, and it is not warranted that the sum over the discrete indices has to be taken before that over x. One has formally a $0 \times \infty$ kind of indeterminacy with the result depending on how the summation is performed, and only after introducing a suitable regularisation to make the whole expression meaningful one can determine the result.

[45] While it could still possibly break down spontaneously, the Vafa-Witten theorem forbids it. See C. Vafa and E. Witten, "Restrictions on symmetry breaking in vector-like gauge theories", Nucl. Phys. B **234** (1984), 173–188.

Regularisation of the path integral Formally, the fermionic path integral consists of continuously infinitely many Grassmann integrations. To make the number of integrations countable one regulates the theory by putting the system in a finite box with periodic boundary conditions, which makes the spectrum of the Dirac operator $\not{D}$ discrete. One then expands ψ on the complete orthonormal basis of eigenmodes $u_k = u_k(x)_{\alpha a}$ of the anti-Hermitean operator $\not{D}$, $\not{D}u_k = i\lambda_k u_k$, with λ_k real. Here $\alpha = 1, \dots 4$ is the Dirac index and $a = 1, \dots, N_c$ is the index associated with the gauge group representation. Similarly, one expands $\bar{\psi}$ on the basis $u_k^\dagger$ (the difference being due to the different transformation properties under SO(4) transformations). In both cases, the expansion coefficients are Grassmann variables, and one defines the path integral as the integration over such expansion coefficients, i.e.,

$$\psi = \sum_k a_k u_k \,, \quad \bar{\psi} = \sum_k \bar{a}_k u_k^\dagger \,, \quad \mathrm{D}\psi \mathrm{D}\bar{\psi} = \prod_k da_k d\bar{a}_k = \mathrm{D}a\mathrm{D}\bar{a} \,. \tag{5.599}$$

The fermionic action reads now

$$S_{\mathrm{F}} = \int d^4x\, \bar{\psi} \not{D} \psi = \sum_{k,k'} \bar{a}_{k'} a_k \int d^4x\, u_{k'}^\dagger \not{D} u_k = \sum_{k,k'} \bar{a}_{k'} a_k (u_{k'}, \not{D} u_k) = \sum_k i\lambda_k \bar{a}_{k'} a_k \,, \tag{5.600}$$

where

$$\begin{aligned} (u_k, u_{k'}) &= \sum_{\alpha a} \int d^4x\, u_k(x)^*_{a\alpha} u_{k'}(y)_{\alpha a} \,, \\ (u_k, M u_{k'}) &= \sum_{\alpha a, \beta b} \int d^4x \int d^4y\, u_k(x)^*_{\alpha a} M_{\alpha a, \beta b}(x,y) u_{k'}(y)_{\beta b} \,. \end{aligned} \tag{5.601}$$

To see what is the effect of an axial transformation on Eq. (5.600), notice that if $\not{D}\psi = i\lambda\psi$ then

$$\not{D}\gamma_5\psi = -\gamma_5 \not{D}\psi = -i\lambda\gamma_5\psi \,. \tag{5.602}$$

For nonzero modes, $\lambda_k \neq 0$, we can then organise the modes into pairs u_k and $u_{-k} = \gamma_5 u_k$ with opposite eigenvalues. For zero modes, Eq. (5.602) tells us that $\not{D}$ commutes with γ_5 when restricted to the zero sector, and so one can diagonalise them together. One can then choose zero modes ψ_0 with definite chirality, i.e., $\not{D}\psi_0 = 0$ and $\gamma_5\psi_0 = \xi\psi_0$, $\xi = \pm 1$. Under an axial transformation then (ignoring zero modes that do not appear in Eq. (5.600))

$$\begin{aligned} \psi &= \sum_k a_k u_k = e^{i\beta\gamma_5}\psi' = \sum_k a'_k e^{i\beta\gamma_5} u_k = \sum_k a'_k \left(\cos\beta u_k + i \sin\beta u_{-k}\right) \\ &= \sum_k \left(\cos\beta a'_k + i\sin\beta a'_{-k}\right) u_k \,, \\ \bar{\psi} &= \sum_k \bar{a}_k u_k^\dagger = \bar{\psi}' e^{i\beta\gamma_5} = \sum_k \bar{a}'_k u_k^\dagger e^{i\beta\gamma_5} = \sum_k \bar{a}'_k \left(\cos\beta u_k^\dagger + i\sin\beta u_{-k}^\dagger\right) \\ &= \sum_k \left(\cos\beta \bar{a}'_k + i\sin\beta \bar{a}'_{-k}\right) u_k^\dagger \,, \end{aligned} \tag{5.603}$$

from which one reads off the transformation properties of a_k and $\bar{a}_k$ thanks to completeness of the basis,

$$\begin{aligned} a_k &= \cos\beta a'_k + i\sin\beta a'_{-k} \,, \\ \bar{a}_k &= \cos\beta \bar{a}'_k + i\sin\beta \bar{a}'_{-k} \,. \end{aligned} \tag{5.604}$$

For zero modes one has simply

$$\begin{aligned}\psi|_{\text{zero modes}} &= \sum_{k_0,\lambda_{k_0}=0} a_{k_0}u_{k_0} = e^{i\beta\gamma_5}\psi'|_{\text{zero modes}} = \sum_{k_0,\lambda_{k_0}=0} a'_{k_0}e^{i\beta\xi_{k_0}}u_{k_0}\,,\\ \bar\psi|_{\text{zero modes}} &= \sum_{k_0,\lambda_{k_0}=0} \bar a_{k_0}u^\dagger_{k_0} = \bar\psi'|_{\text{zero modes}}e^{i\beta\gamma_5} = \sum_{k_0,\lambda_{k_0}=0} \bar a'_{k_0}e^{i\beta\xi_{k_0}}u^\dagger_{k_0}\,,\end{aligned} \tag{5.605}$$

and so

$$a_{k_0} = a'_{k_0}e^{i\beta\xi_{k_0}}\,,\qquad \bar a_{k_0} = \bar a'_{k_0}e^{i\beta\xi_{k_0}}\,. \tag{5.606}$$

One can verify explicitly that Eq. (5.600) is left invariant by this transformation, since

$$\begin{aligned}\bar a_k a_k - \bar a_{-k}a_{-k} &= (\cos\beta\bar a'_k + i\sin\beta\bar a'_{-k})(\cos\beta a'_k + i\sin\beta a'_{-k})\\ &\quad - (\cos\beta\bar a'_{-k} + i\sin\beta\bar a'_k)(\cos\beta a'_{-k} + i\sin\beta a'_k)\\ &= [(\cos\beta)^2 + (\sin\beta)^2](\bar a'_k a'_k - \bar a'_{-k}a'_{-k})\\ &\quad + i(\sin\beta\cos\beta - \sin\beta\cos\beta)(\bar a'_{-k}a'_k + \bar a'_k a'_{-k})\\ &= a'_k\bar a'_k - a'_{-k}\bar a'_{-k}\,.\end{aligned} \tag{5.607}$$

Organising the Grassmann variables in vectors, schematically of the form $a = (a_k, a_0, a_{-k})$ and $\bar a = (\bar a_k, \bar a_0, \bar a_{-k})$ with $k > 0$ and the subscript 0 denoting the zero modes, the transformation Eqs. (5.604) and (5.605) can be written as

$$a = e^{i\beta\Gamma}a'\,,\qquad \bar a = e^{i\beta\Gamma}\bar a'\,,\qquad \Gamma = \begin{pmatrix}0 & 0 & 1\\ 0 & \xi & 0\\ 1 & 0 & 0\end{pmatrix}\,, \tag{5.608}$$

i.e., Γ is simply γ_5 in the basis $\{u_k\}$, $\Gamma_{kk'} = (u_k, \gamma_5 u_{k'})$. In fact, Eqs. (5.604) and (5.605) can be obtained more directly as[46]

$$a_k = (u_k, e^{i\beta\gamma_5}\psi') = \sum_{k'}(u_k, e^{i\beta\gamma_5}u_{k'})a'_{k'}\,,\qquad \bar a_k = (e^{-i\beta\gamma_5}\bar\psi', u_k) = \sum_{k'}(u_k, e^{i\beta\gamma_5}u_{k'})\bar a'_{k'}\,. \tag{5.609}$$

The Jacobian of the change of variables is then

$$\mathrm{D}a\mathrm{D}\bar a = \mathrm{D}a'\mathrm{D}\bar a'\, e^{-2i\beta\mathrm{Tr}\,\Gamma} = \mathrm{D}a'\mathrm{D}\bar a'\, e^{-2i\beta\mathrm{Tr}\,\gamma_5}\,,\quad \mathrm{Tr}\,\gamma_5 = \sum_k (u_k, \gamma_5 u_k)\,. \tag{5.610}$$

Sums like that in Eq. (5.610) generally appear when evaluating the Grassmann path integral to compute correlation functions of fermionic fields. In fact, these turn out to be given by the functional determinant of the Dirac operator times several copies of the fermion propagator, which is the inverse of the Dirac operator. These can be written respectively as (for a massive fermion)

$$\mathrm{Det}\,(\not D + m) = \prod_k (i\lambda_k + m) = \sum_k e^{\log(i\lambda_k + m)}\,,\qquad \frac{1}{\not D + m} = \sum_k u_k u_k^\dagger \frac{1}{i\lambda_k + m}\,. \tag{5.611}$$

[46] Here $(v, A\psi) = v_\alpha A_{\alpha\beta}\psi_\beta$ and $(A\bar\psi, v) = \bar\psi_\beta A^*_{\alpha\beta}v_\alpha = \bar\psi_\beta A^\dagger_{\beta\alpha}v_\alpha$ when Grassmann variables appear in the scalar product.

The infinite sums over eigenmodes in Eqs. (5.610) and (5.611) are generally divergent and require regularisation. Since we want to preserve gauge invariance, we need a gauge-invariant regulator, which will be removed at the end of the calculation. We will then take care of the large modes by inserting a factor $f(\not{D}^2/M^2)$ whenever needed, where f is some smooth function with $f(0) = 1$ and $f(\infty) = 0$, and M is a mass scale that will eventually be sent to infinity. Any choice of f would do; we will take $e^{\not{D}^2/M^2}$ for simplicity. Then, for example,

$$\frac{1}{\not{D} + m} \to \sum_k e^{\frac{\not{D}^2}{M^2}} u_k u_k^\dagger \frac{1}{i\lambda_k + m} = \sum_k e^{-\frac{\lambda_k^2}{M^2}} u_k u_k^\dagger \frac{1}{i\lambda_k + m} = \sum_k u_k u_k^\dagger e^{\frac{\not{D}^2}{M^2}} \frac{1}{i\lambda_k + m} \,. \quad (5.612)$$

Choosing f as a function of $\not{D}$ guarantees that gauge invariance is preserved in the regulated theory, and that the contributions of large eigenvalues are suppressed in the sum over eigenmodes.

Transformation of the integration measure Consider now the effect of an axial transformation on the path integral measure. For the integration measure of pairs of opposite nonzero modes we have

$$da_k da_{-k} d\bar{a}_k d\bar{a}_{-k} = da'_k da'_{-k} d\bar{a}'_k d\bar{a}'_{-k} \left[\det \begin{pmatrix} \cos\beta & i\sin\beta \\ i\sin\beta & \cos\beta \end{pmatrix}\right]^{-2} = da'_k da'_{-k} d\bar{a}'_k d\bar{a}'_{-k} \,, \quad (5.613)$$

while for the zero modes one finds

$$da_{k_0} d\bar{a}_{k_0} = da'_{k_0} d\bar{a}'_{k_0} e^{-2i\beta\xi_{k_0}} \,, \quad (5.614)$$

and so

$$\mathrm{D}\psi\mathrm{D}\bar{\psi} = e^{-2i\beta\sum_{k_0,\lambda_{k_0}=0}\xi_{k_0}} \mathrm{D}\psi'\mathrm{D}\bar{\psi}' = e^{-2i\beta(n_+ - n_-)} \mathrm{D}\psi'\mathrm{D}\bar{\psi}' \,, \quad (5.615)$$

where $n_\pm$ is the number of zero modes of chirality ± 1. Apparently there is no need for the regulator here, but this is only because we paired opposite nonzero eigenvalues before doing the sum. This is just one specific way of computing the sum $\mathrm{Tr}\,\gamma_5$ in Eq. (5.610). As already pointed out, this sum is only conditionally convergent, meaning that its result depends on how we organise the terms, and gives Eq. (5.615) only if we sum over pairs of opposite nonzero eigenvalues first. Summing over positive modes first we would instead get infinity, form which we should then subtract infinity obtained from the sum over negative modes. To get rid of this ambiguity, we regulate the sum as explained above to get

$$\begin{aligned} \mathrm{Tr}\,\gamma_5 &\to \lim_{M\to\infty} \mathrm{Tr}\,\gamma_5 e^{\frac{\not{D}^2}{M^2}} = \lim_{M\to\infty} \sum_k (u_k, \gamma_5 e^{\frac{\not{D}^2}{M^2}} u_k) = \lim_{M\to\infty} \sum_k e^{-\frac{\lambda_k^2}{M^2}} (u_k, \gamma_5 u_k) \\ &= \lim_{M\to\infty} \sum_{\lambda_{k_0}=0} \xi_{k_0} = n_+ - n_- \,, \end{aligned} \quad (5.616)$$

having used the fact that for nonzero modes u_k and u_{-k} are orthogonal, since they correspond to different eigenvalues. Here $n_\pm$ is the number of zero modes of chirality ± 1.

For a generic gauge configuration there is in general no reason to expect $n_+ - n_-$ to vanish, and so the integration measure has no reason to be invariant under an axial transformation. The $\mathrm{U}(1)_A$ symmetry is the generally anomalous. To convince ourselves of this, and also to

understand when there really is an anomaly, we need to recast this quantity in terms of properties of the gauge configuration. Since the trace does not depend on the basis used to evaluate it, we can as well estimate Eq. (5.616) by employing the plane wave basis,

$$\varphi_p^{(j)} = u^{(j)} e^{ip\cdot x}\,, \tag{5.617}$$

where $u^{(j)}$ is a complete orthonormal basis of Dirac and colour space, i.e.,

$$\sum_j (u^{(j)})_{\alpha a} (u^{(j)\dagger})_{\beta b} = \delta_{\alpha\beta}\delta_{ab}\,. \tag{5.618}$$

To evaluate the trace, we write

$$\begin{aligned} \not{D}^2 &= D_\mu D_\nu \gamma_\mu \gamma_\nu = D_\mu D_\nu \left(\tfrac{1}{2}\{\gamma_\mu,\gamma_\nu\} + \tfrac{1}{2}[\gamma_\mu,\gamma_\nu]\right) = D^2 + \tfrac{i}{2}[D_\mu, D_\nu]\tfrac{1}{2i}[\gamma_\mu,\gamma_\nu] \\ &= D^2 - \tfrac{1}{2}F_{\mu\nu}\sigma_{\mu\nu} = [\partial_\mu\partial_\mu + 2igA_\mu\partial_\mu + ig(\partial_\mu A_\mu) - g^2 A_\mu A_\mu] - \tfrac{g}{2}F_{\mu\nu}\sigma_{\mu\nu}\,, \end{aligned} \tag{5.619}$$

where

$$\sigma_{\mu\nu} = \tfrac{1}{2i}[\gamma_\mu,\gamma_\nu]\,, \quad F_{\mu\nu} = t^a F^a_{\mu\nu}\,, \quad A_\mu = t^a A^a_\mu\,. \tag{5.620}$$

In general, the results of acting with a differential operator $F(\partial) = \sum_n F_n(x)\partial_x^n$ on the functions $g(x)$ and $e^{ikx}g(x)$ differ in a simple way,

$$F(\partial)e^{ikx}g(x) = e^{ikx}F(\partial + ik)g(x)\,. \tag{5.621}$$

Acting with $e^{\frac{\not{D}^2}{M^2}}$ on a plane wave we find then

$$\begin{aligned} e^{\frac{\not{D}^2}{M^2}}\varphi_p^{(j)} &= e^{ip\cdot x}\exp\left\{\frac{1}{M^2}\left[(D+ip)^2 - \frac{g}{2}F_{\mu\nu}\sigma_{\mu\nu}\right]\right\}u^{(j)} \\ &= e^{ip\cdot x}\exp\left\{-\frac{1}{M^2}\left[p^2 - 2ip\cdot D - D^2 + \frac{g}{2}F_{\mu\nu}\sigma_{\mu\nu}\right]\right\}u^{(j)}\,. \end{aligned} \tag{5.622}$$

The trace therefore reads

$$\begin{aligned} \mathrm{Tr}\,\gamma_5 e^{\frac{\not{D}^2}{M^2}} &= \sum_j \int \frac{d^4p}{(2\pi)^4}\int d^4x\, u^{(j)\dagger} e^{-ip\cdot x} e^{ip\cdot x}\gamma_5 e^{-\frac{1}{M^2}\left(p^2 - 2ip\cdot D - D^2 + \frac{g}{2}F_{\mu\nu}\sigma_{\mu\nu}\right)}u^{(j)} \\ &= \int \frac{d^4p}{(2\pi)^4}\int d^4x\, e^{-\frac{p^2}{M^2}}\mathrm{tr}_{D,c}\,\gamma_5 e^{\frac{1}{M^2}\left(2ip\cdot D + D^2 - \frac{g}{2}F_{\mu\nu}\sigma_{\mu\nu}\right)} \\ &= \int \frac{d^4p}{(2\pi)^4}\int d^4x\, M^4\, e^{-p^2}\mathrm{tr}_D\mathrm{tr}_c\,\gamma_5 e^{\frac{1}{M^2}\left(2iMp\cdot D + D^2 - \frac{g}{2}F_{\mu\nu}\sigma_{\mu\nu}\right)}\,, \end{aligned} \tag{5.623}$$

where $\mathrm{tr}_{D,c}$ denote the traces over Dirac and colour indices only. In the large-M limit, only terms of order $O(M^{-4})$ or higher from the expansion of the exponential can survive. On the other hand, due to the trace over Dirac indices, only terms containing at least four Dirac gamma matrices give a nonzero contribution, and so at least two powers of $F_{\mu\nu}\sigma_{\mu\nu}$, which already come

with a factor M^{-4}. Then

$$\begin{aligned}\lim_{M\to\infty}\mathrm{Tr}\,\gamma_5 e^{\frac{\not{D}^2}{M^2}} &= \int\frac{d^4p}{(2\pi)^4}\,e^{-p^2}\int d^4x\,\frac{g^2}{8}\mathrm{tr}_c\,F_{\mu\nu}F_{\rho\sigma}\mathrm{tr}_D\,\gamma_5\sigma_{\mu\nu}\sigma_{\rho\sigma}\\ &= -\frac{g^2}{8}\left(\frac{1}{2\sqrt{\pi}}\right)^4\mathrm{tr}_c\,t^at^b\,\mathrm{tr}_D\,\gamma_5\gamma_\mu\gamma_\nu\gamma_\rho\gamma_\sigma\int d^4x\,F^a_{\mu\nu}F^b_{\rho\sigma}\\ &= -\frac{g^2}{8}\frac{d_R}{16\pi^2}\delta^{ab}(-4)\epsilon_{\mu\nu\rho\sigma}\int d^4x\,F^a_{\mu\nu}F^b_{\rho\sigma}\\ &= \frac{g^2d_R}{32\pi^2}\int d^4x\,\epsilon_{\mu\nu\rho\sigma}F^a_{\mu\nu}F^a_{\rho\sigma} = \frac{g^2d_R}{16\pi^2}\int d^4x\,F^a_{\mu\nu}\tilde{F}^a_{\mu\nu}\,,\end{aligned} \tag{5.624}$$

where $F^a_{\mu\nu}\tilde{F}^a_{\mu\nu} = \frac{1}{2}\epsilon_{\mu\nu\rho\sigma}F^a_{\mu\nu}F^a_{\rho\sigma}$, having used the identity

$$\mathrm{tr}_D\,\gamma_5\gamma_\mu\gamma_\nu\gamma_\rho\gamma_\sigma = -4\epsilon_{\mu\nu\rho\sigma}\,, \tag{5.625}$$

and having chosen the normalisation

$$\mathrm{tr}_c\,t^at^b = d_R\delta^{ab} \tag{5.626}$$

for the generators in representation R. For the fundamental representation one usually chooses $d_R = \frac{1}{2}$. We then find

$$n_+ - n_- = \frac{g^2d_R}{16\pi^2}\int d^4x\,F^a_{\mu\nu}\tilde{F}^a_{\mu\nu}\,, \tag{5.627}$$

and

$$\mathrm{D}\psi\mathrm{D}\bar{\psi} = \mathrm{D}\psi'\mathrm{D}\bar{\psi}'\,e^{-i\beta\frac{g^2d_R}{8\pi^2}\int d^4x\,F^a_{\mu\nu}\tilde{F}^a_{\mu\nu}} = \mathrm{D}\psi'\mathrm{D}\bar{\psi}'\,e^{i\beta\int d^4x\,\mathscr{A}(x)}\,. \tag{5.628}$$

for the transformation of the integration measure.

The nontrivial anomaly function $\mathscr{A}(x)$ results from the compensation of a factor M^4, originating from the divergent sum over modes, with a factor $1/M^4$, appearing only as a consequence of regularising the theory. One can show directly that using any function $f(\not{D}/M)$ with the properties $f(0) = 1$ and $f(\infty) = 0$ leads to the same result for $\mathscr{A}(x)$. The use of a function of this type is forced on us by the request of preserving gauge invariance, and so while it is possible to get $\mathscr{A} = 0$ if one uses gauge-non-invariant regulators, there is no way of finding a vanishing anomaly if gauge invariance is to be preserved. While being a consequence of the need to regularise the theory, though, the nontrivial anomaly is at the same type independent of the specific choice of gauge-invariant regulator, and so it is not simply an artefact of the regularisation procedure.

Anomaly and topology More insight on the anomaly is obtained by realising that one has $\mathscr{A}(x) = -4d_Rq(x)$, with

$$q(x) = \frac{g^2}{32\pi^2}F^a_{\mu\nu}\tilde{F}^a_{\mu\nu} = \frac{g^2}{32\pi^2}\epsilon_{\mu\nu\rho\sigma}F^a_{\mu\nu}F^a_{\rho\sigma} \tag{5.629}$$

the topological charge density. Equation (5.627) then reads

$$n_+ - n_- = 2d_RQ\,, \tag{5.630}$$

a result is known as the *Atiyah-Singer index theorem*, where Q is the topological charge,

$$Q = \int d^4x\, q(x) = \frac{g^2}{32\pi^2} \int d^4x\, \epsilon_{\mu\nu\rho\sigma} F^a_{\mu\nu} F^a_{\rho\sigma}\,. \tag{5.631}$$

This quantity is a topological invariant, i.e., it is left unchanged by continuous deformations of the gauge configuration, that moreover takes only integer values. The presence of a nontrivial integrated anomaly is then related to nontrivial topological properties of the gauge group, that allow the existence of configurations with $Q \neq 0$.[47]

The change of the integration measure under an axial transformation can then be seen also as a change in the action, $S \to S - 2i\beta d_R Q$. A term $i\theta Q$ could be added to the action without breaking gauge invariance, while P and C invariance would be lost.[48] An axial transformation would then correspond to $\theta \to \theta - 2\beta d_R$. If one considers a massive rather than massless fermion, the result obtained above for the anomaly does not change. On the other hand, the mass term in the fermionic Lagrangian is not left invariant by an axial transformation. This can be used to make the mass coefficients in the Dirac Lagrangian always real, sweeping any nontrivial phase into the coefficient θ of the topological term. The experimental value of θ (defined as the coefficient of Q when all fermion masses are real) is tightly bounded, $|\theta| < 10^{-10}$. Explaining why it is so is the so-called "strong CP problem".

It is worth noticing that $q(x)$, and so $\mathscr{A}(x)$, is the total divergence of a current. Indeed, understanding that t^a are in the fundamental representation with $d_F = \frac{1}{2}$, we have $2\mathrm{tr}\, F_{\mu\nu}F_{\rho\sigma} = F^a_{\mu\nu}F^a_{\rho\sigma}$ and

$$\begin{aligned}
\epsilon_{\mu\nu\rho\sigma}\mathrm{tr}\, F_{\mu\nu}F_{\rho\sigma} &= 4\epsilon_{\mu\nu\rho\sigma}\mathrm{tr}\, \left[(\partial_\mu A_\nu)(\partial_\rho A_\sigma) + 2ig(\partial_\mu A_\nu)A_\rho A_\sigma - g^2 A_\mu A_\nu A_\rho A_\sigma\right] \\
&= 4\epsilon_{\mu\nu\rho\sigma}\mathrm{tr}\, \left[\partial_\mu(A_\nu\partial_\rho A_\sigma) + 2ig(\partial_\mu A_\nu)A_\rho A_\sigma\right] \\
&= 4\partial_\mu\epsilon_{\mu\nu\rho\sigma}\mathrm{tr}\, \left[A_\nu\partial_\rho A_\sigma + \frac{2ig}{3}A_\nu A_\rho A_\sigma\right],
\end{aligned} \tag{5.632}$$

and so

$$q(x) = \partial_\mu K_\mu\,, \qquad K_\mu = \frac{g^2}{8\pi}\epsilon_{\mu\nu\rho\sigma}\mathrm{tr}\, \left[A_\nu\partial_\rho A_\sigma + \frac{2ig}{3}A_\nu A_\rho A_\sigma\right], \tag{5.633}$$

with K_μ known as the Chern-Simons current. The topological term therefore would not affect the equations of motion even for $\theta \neq 0$. On the other hand, it would lead to nontrivial nonperturbative effects.

[47] The topological charge classifies gauge configurations that tend to pure gauge at infinity, $A_\mu(x) \to U(\hat{x})\partial_\mu U(\hat{x})^\dagger$, where $\hat{x} = x/|x|$ is the direction in which infinity is approached. Since $\hat{x} \in S^3$ is a point on the sphere $x^2 = 1$ in four dimensions, configurations of this type provide a mapping from S^3 to the gauge group G. More generally, in dimension $n+1$ one ends up considering mappings from S^n to G. Such mappings can be classified in equivalence classes, each class corresponding to configurations that can be continuously deformed into each other, i.e., $A^{(1)}(x)$ and $A^{(2)}(x)$ are equivalent if $A^{(1)}_\mu(x) = \mathrm{A}_\mu(x,0)$ and $A^{(2)}_\mu(x) = \mathrm{A}_\mu(x,1)$ for some continuous function $\mathrm{A}_\mu(x,t)$, $t \in [0,1]$. Each class is called a homotopy class, and the set of all these classes form the homotopy group $\pi_n(G)$. Configurations with different Q belong to different classes, and $Q \neq 0$ is possible only if $\pi_n(G)$ is a nontrivial group, i.e., $\pi_n(G) \neq \{0\}$. For example, $\pi_1(U(1)) = \mathbb{Z}$, which means that U(1) gauge theory in two dimensions has topologically nontrivial configurations. The same is true for SU(N) theory in four dimensions, since $\pi_3(SU(N)) = \mathbb{Z}$. On the other hand, $\pi_3(U(1)) = \pi_1(SU(N)) = \{0\}$, so topology is trivial for four-dimensional U(1) theory and two-dimensional SU(N) theory. For details see, e.g., M. Nakahara, "Geometry, topology and physics".

[48] When Wick-rotating back to Minkowski spacetime, $\epsilon_{\mu\nu\rho\sigma}F_{\mu\nu}F_{\rho\sigma}$ is analytically continued to a real quantity, hence a factor of i is required in $i\theta Q$ to obtain a term iS_{top} in the Minkowskian path integral.

Ward identities The consequences of the anomaly for correlation functions are summarised in the Ward identities, obtained by working out the effect of an infinitesimal x-dependent axial transformation,

$$\psi(x) = (1 + i\beta(x)\gamma_5)\psi'(x)\,, \qquad \bar\psi(x) = \bar\psi'(x)(1 + i\beta(x)\gamma_5)\,. \tag{5.634}$$

A straighforward calculation shows that

$$\bar\psi(x)\not{D}\psi(x) = \bar\psi'(x)(1+i\beta(x)\gamma_5)\not{D}(1+i\beta(x)\gamma_5)\psi'(x) = \bar\psi'(x)\not{D}\psi'(x)+i(\partial_\mu\beta(x))\bar\psi'(x)\gamma_\mu\gamma_5\psi'(x)\,, \tag{5.635}$$

and so

$$\begin{aligned} S[\psi,\bar\psi] &= S[\psi',\bar\psi'] - i\int d^4x\,\beta(x)\partial_\mu\bar\psi'(x)\gamma_\mu\gamma_5\psi'(x) \\ &= S[\psi',\bar\psi'] - i\int d^4x\,\beta(x)\partial_\mu\left(\bar\psi'(x)\gamma_\mu\gamma_5\psi'(x)\right) \\ &= S[\psi',\bar\psi'] - i\int d^4x\,\beta(x)\partial_\mu j_{5\mu}\,. \end{aligned} \tag{5.636}$$

The Jacobian of the transformation can be obtained by adapting the calculation of the anomaly to an x-dependent β, which amounts to replace[49]

$$\beta\mathrm{Tr}\,\gamma_5 e^{\frac{\not{D}^2}{M^2}} \to \mathrm{Tr}\,\beta\gamma_5 e^{\frac{\not{D}^2}{M^2}} = \sum_k(\beta u_k, \gamma_5 e^{\frac{\not{D}^2}{M^2}}u_k) = \sum_k e^{-\frac{\lambda_k^2}{M^2}}\int d^4x\,\beta(x)u_k(x)^\dagger\gamma_5 u_k(x)\,. \tag{5.637}$$

Evaluating the trace on the plane wave basis as above, one finds simply

$$\mathrm{D}\psi\mathrm{D}\bar\psi = e^{i\int d^4x\,\beta(x)\mathscr{A}(x)}\mathrm{D}\psi'\mathrm{D}\bar\psi' = e^{-2d_R i\int d^4x\,\beta(x)q(x)}\mathrm{D}\psi'\mathrm{D}\bar\psi'\,. \tag{5.638}$$

For the expectation value of an observable $\mathcal{O}[\psi,\bar\psi]$ that under Eq. (5.634) transforms as

$$\mathcal{O}[\psi,\bar\psi] = \mathcal{O}[\psi',\bar\psi'] + i\int d^4x\,\beta(x)\Delta[\psi',\bar\psi';x]\,, \tag{5.639}$$

we find

$$\begin{aligned} \langle\mathcal{O}\rangle &= Z^{-1}\int\mathrm{DA}\int\mathrm{D}\psi\int\mathrm{D}\bar\psi\,e^{-S[\psi,\bar\psi]}\mathcal{O}[\psi,\bar\psi] \\ &= Z^{-1}\int\mathrm{DA}\int\mathrm{D}\psi\int\mathrm{D}\bar\psi\,e^{-S[\psi,\bar\psi]-i\int d^4x\,\beta(x)(-\partial_\mu j_{5\mu}+2d_R q(x))} \\ &\qquad\qquad\times\left(\mathcal{O}[\psi,\bar\psi] + i\int d^4x\,\beta(x)\Delta[\psi,\bar\psi;x]\right) \\ &= \left\langle\left[1 - i\int d^4x\,\beta(x)[-\partial_\mu j_{5\mu}(x) + 2d_R q(x)]\right]\left(\mathcal{O} + i\int d^4x\,\beta(x)\Delta(x)\right)\right\rangle\,, \end{aligned} \tag{5.640}$$

[49] For an x-dependent infinitesimal transformation [see Eq. (5.609)],

$$a_k \simeq (u_k, (1+i\beta\gamma_5)u_{k'})a'_{k'} = a'_k + i(u_k,\beta\gamma_5 u_{k'})a'_{k'}\,,$$

and

$$\mathrm{D}\psi\mathrm{D}\bar\psi = \mathrm{D}\psi'\mathrm{D}\bar\psi'\mathrm{Det}\,[(1+i\beta\gamma_5)]^{-2} = \mathrm{D}\psi'\mathrm{D}\bar\psi' e^{-2i\mathrm{Tr}\,\beta\gamma_5}\,.$$

and so

$$-\partial_\mu \langle j_{5\mu}(x)\mathcal{O}\rangle + 2d_R\langle q(x)\mathcal{O}\rangle = \langle \Delta(x)\rangle\,. \tag{5.641}$$

The second term on the left-hand side shows that $j_{5\mu}$ is not a conserved quantity.[50] Independently of the global topological properties of the gauge group, the topological charge density $q(x) \propto \epsilon_{\mu\nu\rho\sigma}F^a_{\mu\nu}F^a_{\rho\sigma}$ is a non-vanishing local operator, and contributes a nontrivial term to the Ward identities (even in the Abelian case). We stress again that this term originates from the non-invariance of the path-integral measure under axial transformations.

On the other hand, $q = \partial_\mu K_\mu$, and so we can write Eq. (5.641) as

$$-\partial_\mu \langle (j_{5\mu}(x) - 2d_R K_\mu)\mathcal{O}\rangle = -\partial_\mu \langle J_{5\mu}(x)\mathcal{O}\rangle = \langle \Delta(x)\rangle\,. \tag{5.642}$$

The current $J_{5\mu}$ is now a conserved, but non-gauge-invariant current. After analytic continuation back to Minkowski space, a careful study shows that J_{50}, and not j_{50}, is formally the local generator of axial transformations; and that the gauge-invariant vacuum is not invariant under axial transformations. On the other hand, one cannot define the expectation values on a gauge-invariant state of J_{50} times a gauge-invariant order parameter. This means that while axial symmetry is spontaneously broken, in the sense that the vacuum is not invariant, there is no need for the appearance of massless bosons, since the relevant expectation values of the order parameters of the symmetry are not defined, and so Goldstone's theorem does not apply.[51]

The Schwinger model The anomalous behaviour of a gauge theory under axial symmetry transformations has physical consequences. In the case of the physically relevant theories in four dimensions, these have been confirmed experimentally. An example is the width of the process $\pi^0 \to \gamma\gamma$, which due to the axial anomaly is much larger than one would expect. A model in which the axial anomaly has dramatic consequences is the two-dimensional U(1) gauge theory of a single massless Dirac fermion, known as the *Schwinger model*. This is an exactly solvable model which displays confinement, with fermions and antifermions bound together into a massive vector particle, which replaces the massless photon, and is the only particle in the spectrum of the theory. As we will see below, these phenomena (confinement and dynamical mass generation) can be understood in terms of the axial anomaly.

There are several ways to solve the Schwinger model. Here we follow the method of Roskies and Schaposnik based on Fujikawa's treatment of the path integral. The starting point is the Euclidean partition function

$$\begin{aligned} Z &= \int \mathrm{D}A \int \mathrm{D}\psi \int \mathrm{D}\bar\psi\, e^{-S_{\text{Schwinger}}}\, B[f]\,, \\ S_{\text{Schwinger}} &= \int d^2x \left(\frac{1}{4}F_{\mu\nu}F_{\mu\nu} + \bar\psi \not{D}\psi\right) = S_g + S_f\,, \end{aligned} \tag{5.643}$$

[50] If $\mathcal{O} = \mathcal{O}(y_1, \dots y_n)$ is a multilocal observable, depending only on the fields at isolated points $y_1, \dots y_n$, then $\Delta(x)$ is a contact term, given by a sum of Dirac delta functions $\delta(x - y_i)$ multiplied by regular coefficients that depend on $y_1, \dots y_n$. When writing the left-hand side in the operator language one find the vacuum expectation value of the time-ordered product of fields. When taking the ∂_0 derivative, this acts either on j_{50}, or on θ functions of the form $\theta(y_i - x)\theta(x - y_{i+1})$, leading to the appearance of delta functions of the temporal coordinates times an equal time commutator. On the right-hand side of Eq. (5.641) one has precisely the contact terms generated this way. If the current were conserved, $\partial_\mu\langle j_{5\mu}\mathcal{O}\rangle$ would vanish up to these contact terms; the presence of the second term on the left-hand side means that $\partial_\mu\langle j_{5\mu}\mathcal{O}\rangle = 2d_R\langle q(x)\mathcal{O}\rangle + \text{contact terms}$.

[51] For a detailed discussion of these issues, see F. Strocchi, "An introduction to the non-perturbative foundations of quantum field theory".

where $\not{D} = D_\mu \gamma_\mu$, $\mu = 1, 2$, with $D_\mu = \partial_\mu + ieA_\mu$, $\gamma_1 = \sigma^1$ and $\gamma_2 = \sigma^2$, the Abelian field strength tensor is $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$.[52] The role of γ_5 is played here by $\gamma_5 = -i\gamma_1\gamma_2 = \sigma^3$. The two-dimensional Levi-Civita symbol $\epsilon_{\mu\nu}$ reads explicitly $\epsilon_{12} = -\epsilon_{21} = 1$, $\epsilon_{11} = \epsilon_{22} = 0$. Finally, $B[f]$ is a suitable numerical functional of a gauge non-invariant functional $f[A; x]$, used to impose a gauge condition. Since the gauge field is Abelian, there is no need for the Faddeev-Popov determinant. For our purposes it is convenient to use $B[f] = e^{-\frac{1}{2\xi}\int d^2x\, f[A;x]^2}$ and the Lorenz gauge functional, $f = \partial_\mu A_\mu$, and eventually send $\xi \to 0$, which practically imposes $\partial_\mu A_\mu = 0$ in the correlation functions. This choice is called *Landau gauge*.

The fermionic action is manifestly invariant under the axial transformation $\psi = e^{i\beta\gamma_5}\psi'$, $\bar\psi = \bar\psi' e^{i\beta\gamma_5}$, as well as under the vector transformation $\psi = e^{i\alpha\gamma_5}\psi'$, $\bar\psi = \bar\psi' e^{-i\alpha\gamma_5}$. A calculation almost identical to the one done above in four dimensions shows though that the measure is not invariant under axial transformations, and so axial symmetry is anomalous. To see this we start directly with the infinitesimal but x-dependent generalisation of the axial transformation,

$$\psi(x) = (1 + i\delta\beta(x)\gamma_5)\psi'(x)\,, \qquad \bar\psi(x) = \bar\psi'(x)(1 + i\delta\beta(x)\gamma_5)\,, \tag{5.644}$$

which will allow us both to see the appearance of the anomaly, and to solve the model exactly. Adopting the same regularisation for the path integral as above, we expand the fermion fields in the basis of eigenvectors of $\not{D}$, and include a factor $e^{\frac{\not{D}^2}{M^2}}$ in the sums over modes. For the integration measure we find

$$\mathrm{D}\psi\mathrm{D}\bar\psi = \mathrm{D}\psi'\mathrm{D}\bar\psi' e^{-2i\mathrm{Tr}\left(\delta\beta\,\gamma_5 e^{\frac{\not{D}^2}{M^2}}\right)}\,, \tag{5.645}$$

while the fermionic action changes to

$$S_f[\psi,\bar\psi] = S_f[\psi',\bar\psi'] - i\int d^2x\,\delta\beta(x)\partial_\mu\left(\bar\psi'\gamma_\mu\gamma_5\psi'\right) = S_f[\psi',\bar\psi'] - i\int d^2x\,\delta\beta(x)\partial_\mu j_{5\mu}(x)\,. \tag{5.646}$$

Evaluated on the plane wave basis, the trace in Eq. (5.645) gives

$$\begin{aligned}
\mathrm{Tr}\left(\delta\beta\,\gamma_5 e^{\frac{\not{D}^2}{M^2}}\right) &= \int\frac{d^2p}{(2\pi)^2}\int d^2x\,\delta\beta(x)e^{-ip\cdot x}\mathrm{tr}_D\left(\gamma_5 e^{\frac{\not{D}^2}{M^2}}\right)e^{ip\cdot x} \\
&= \int\frac{d^2p}{(2\pi)^2}\int d^2x\,\delta\beta(x)\mathrm{tr}_D\left(\gamma_5 e^{\frac{(\not{D}+i\not{p})^2}{M^2}}\right) \\
&= \int\frac{d^2p}{(2\pi)^2}\int d^2x\,\delta\beta(x)\mathrm{tr}_D\left(\gamma_5 e^{\frac{-p^2+\not{D}^2+2ip\cdot D}{M^2}}\right) \\
&= \int\frac{d^2p}{(2\pi)^2}\,e^{-p^2}\int d^2x\,\delta\beta(x)M^2\mathrm{tr}_D\left(\gamma_5 e^{\frac{D^2-\frac{e}{2}F_{\mu\nu}\sigma_{\mu\nu}+2iMp\cdot D}{M^2}}\right).
\end{aligned} \tag{5.647}$$

In two dimensions

$$F_{\mu\nu}\sigma_{\mu\nu} = 2F_{12}\sigma_{12} = -2iF_{12}\gamma_1\gamma_2 = 2\gamma_5 F_{12} = \gamma_5\epsilon_{\mu\nu}F_{\mu\nu}\,, \tag{5.648}$$

[52] Instead of $x^0 \to -ix_{E2}$, here we are performing the Wick rotation as $x^0 \to -ix_{E1}$, and treating the gauge field and the gamma matrices accordingly. This is immaterial since the Euclidean theory is SO(2) invariant.

so in the limit $M \to \infty$

$$\begin{aligned}
&\lim_{M\to\infty} M^2 \mathrm{tr}_D \left(\gamma_5 e^{\frac{D^2 - \frac{e}{2}F_{\mu\nu}\sigma_{\mu\nu} + 2iMp\cdot D}{M^2}}\right) = \lim_{M\to\infty} M^2 \mathrm{tr}_D \left(\gamma_5 e^{\frac{D^2 - \frac{e}{2}\gamma_5\epsilon_{\mu\nu}F_{\mu\nu} + 2iMp\cdot D}{M^2}}\right) \\
&= \lim_{M\to\infty} M^2 \mathrm{tr}_D \left[\gamma_5 \left(1 + \frac{D^2 - \frac{e}{2}\gamma_5\epsilon_{\mu\nu}F_{\mu\nu} + 2iMp\cdot D}{M^2} - \frac{2}{M^2}(p\cdot D)^2 + \mathcal{O}(M^{-3})\right)\right] \\
&= -e\epsilon_{\mu\nu}F_{\mu\nu}\,.
\end{aligned} \tag{5.649}$$

Momentum integration becomes trivial, and we conclude

$$\lim_{M\to\infty} \mathrm{Tr}\left(\delta\beta\,\gamma_5 e^{\frac{\not{D}^2}{M^2}}\right) = -\frac{e}{4\pi}\int d^2x\,\delta\beta(x)\epsilon_{\mu\nu}F_{\mu\nu}(x)\,. \tag{5.650}$$

In the limit of constant $\delta\beta$, only exact zero modes contribute to the trace and we recover the two-dimensional Atiyah-Singer index theorem,

$$n_+ - n_- = -\frac{e}{4\pi}\int d^2x\,\epsilon_{\mu\nu}F_{\mu\nu}(x)\,. \tag{5.651}$$

For our purposes, instead, we write the net effect of the infinitesimal transformation as

$$\begin{aligned}
\mathrm{D}\psi\mathrm{D}\bar\psi e^{-S_f[\psi,\bar\psi,A]} &= \mathrm{D}\psi'\mathrm{D}\bar\psi' e^{-S_f[\psi',\bar\psi',A]} e^{i\int d^2x\,\delta\beta(x)\left(\partial_\mu j_{5\mu} + \frac{e}{2\pi}\epsilon_{\mu\nu}F_{\mu\nu}\right)} \\
&= \mathrm{D}\psi'\mathrm{D}\bar\psi' e^{-S_f[\psi',\bar\psi',A_\mu]} e^{i\int d^2x\left(-j_{5\mu}\partial_\mu\delta\beta(x) + \delta\beta(x)\frac{e}{2\pi}\epsilon_{\mu\nu}F_{\mu\nu}\right)}\,.
\end{aligned} \tag{5.652}$$

Since $\gamma_\mu\gamma_5 = -i\epsilon_{\mu\nu}\gamma_\nu$, we have

$$j_{5\mu}\partial_\mu\delta\beta = -i\bar\psi\epsilon_{\mu\nu}\gamma_\nu\psi\partial_\mu\delta\beta = e\bar\psi\gamma_\mu\psi\left(\frac{i}{e}\epsilon_{\mu\nu}\partial_\nu\delta\beta\right)\,, \tag{5.653}$$

and so

$$\begin{aligned}
\mathrm{D}\psi\mathrm{D}\bar\psi e^{-S_f[\psi,\bar\psi,A]} &= \mathrm{D}\psi'\mathrm{D}\bar\psi' e^{-\left[S_f[\psi',\bar\psi',A_\mu] + \int d^2x\, ie\bar\psi\gamma_\mu\psi\left(\frac{i}{e}\epsilon_{\mu\nu}\partial_\nu\delta\beta\right)\right] + i\frac{e}{2\pi}\int d^2x\,\delta\beta(x)\epsilon_{\mu\nu}F_{\mu\nu}} \\
&= \mathrm{D}\psi'\mathrm{D}\bar\psi' e^{-S_f[\psi',\bar\psi',A_\mu + \frac{i}{e}\epsilon_{\mu\nu}\partial_\nu\delta\beta] + i\frac{e}{2\pi}\int d^2x\,\delta\beta(x)\epsilon_{\mu\nu}F_{\mu\nu}[A_\alpha]}\,.
\end{aligned} \tag{5.654}$$

The non-invariance of the action under local axial transformation boils down effectively to a redefinition of the gauge field. We can then decouple the fermion fields from the gauge field by means of a suitable finite x-dependent axial transformation, i.e., by iterating the infinitesimal transformation until the sum $\beta(x)$ of the infinitesimal transformation parameters satisfies

$$\tfrac{i}{e}\epsilon_{\mu\nu}\partial_\nu\beta = -A_\mu\,. \tag{5.655}$$

For this to be possible, A_μ must satisfy the Lorenz gauge condition, which is the case here.[53] To solve Eq. (5.655), contract with $\epsilon_{\rho\mu}$ to get

$$ie\epsilon_{\rho\mu}A_\mu = \epsilon_{\rho\mu}\epsilon_{\mu\nu}\partial_\nu\beta = -\epsilon_{\mu\rho}\epsilon_{\mu\nu}\partial_\nu\beta = -\delta_{\rho\nu}\partial_\nu\beta = -\partial_\rho\beta\,. \tag{5.656}$$

[53] Had we worked in a different gauge, it would still be possible to perform an x-dependent vector transformation on the fermion fields, that effectively changes $A_\mu \to A_\mu + \partial_\mu\alpha_\mu = A'_\mu$, and one can choose α so that $\partial_\mu A'_\mu = 0$.

Taking the divergence we find

$$\Box\beta = ie\epsilon_{\rho\mu}\partial_\rho A_\mu = \frac{ie}{2}\epsilon_{\rho\mu}F_{\rho\mu} = ieF_{12}\,, \tag{5.657}$$

and so[54]

$$\beta(x) = ie\left(\frac{1}{\Box}F_{12}\right)(x) \equiv \int d^2y\, G_0^{(2)}(x-y)F_{12}(y)\,, \qquad \Box G_0^{(2)}(x) = \delta(x)\,. \tag{5.658}$$

However, in order for the path integral to be properly regularised after we have effectively changed the value of the field coupled to the vector current in the fermionic action to $A_\mu + \frac{i}{e}\epsilon_{\mu\nu}\partial_\nu\delta\beta$, it is this quantity that has to be used in the factor $e^{\not{D}^2/M^2}$. This is true at each stage of the process, and so the effect of the infinitesimal axial transformations builds up nonlinearly in the anomalous contribution. Let us set $\beta(x) = N\delta\beta(x)$ with N large, and suppose we have made n infinitesimal transformations already, so that $A_\mu \to A_\mu^{(n)} = A_\mu + n\frac{i}{e}\epsilon_{\mu\nu}\partial_\nu\delta\beta(x)$ in the fermion action. Let us denote by $e^{\mathrm{A}[A^{(n)}]}$ the cumulative effect of the non-invariance of the measure at stage n. At the stage $n+1$, it is $A_\mu^{(n)}$ that enters the calculation of the anomaly, which changes by

$$\begin{aligned}
\delta\mathrm{A}[A^{(n)}] &= \mathrm{A}[A^{(n+1)}] - \mathrm{A}[A^{(n)}] = i\frac{e}{2\pi}\int d^2x\,\delta\beta(x)\epsilon_{\mu\nu}F_{\mu\nu}[A_\alpha^{(n)}] \\
&= i\frac{e}{2\pi}\int d^2x\,\delta\beta(x)\,2\epsilon_{\mu\nu}\partial_\mu A_\nu^{(n)} = i\frac{e}{2\pi}\int d^2x\,2A_\mu^{(n)}\,\epsilon_{\mu\nu}\partial_\nu\delta\beta(x) \\
&= \frac{e^2}{2\pi}\int d^2x\,2A_\mu^{(n)}\,\delta A_\mu^{(n)} = \frac{e^2}{2\pi}\int d^2x\,\delta\left(A_\mu^{(n)}A_\mu^{(n)}\right)\,.
\end{aligned} \tag{5.659}$$

Adding up the variations

$$\mathrm{A}[A^{(N)}] - \mathrm{A}[A^{(0)}] = \frac{e^2}{2\pi}\int d^2x\,\left(A_\mu^{(N)}A_\mu^{(N)} - A_\mu^{(0)}A_\mu^{(0)}\right) = -\frac{e^2}{2\pi}\int d^2x\,A_\mu A_\mu\,, \tag{5.660}$$

since by construction $A_\mu^{(N)} = 0$. The net effect is then

$$\mathrm{D}\psi\mathrm{D}\bar\psi e^{-S_f[\psi,\bar\psi,A]} = \mathrm{D}\psi'\mathrm{D}\bar\psi' e^{-S_f[\psi',\bar\psi',0]-\frac{e^2}{2\pi}\int d^2x\,A_\mu A_\mu}\,, \tag{5.661}$$

i.e., fermions and gauge fields are decoupled, but the gauge field has acquired a mass term. Including the gauge-fixing term, the full action reads now

$$S = \int d^2x\,\frac{1}{2}A_\mu\left[\left(-\Box + m^2\right)\delta_{\mu\nu} + \left(1-\frac{1}{\xi}\right)\partial_\mu\partial_\nu\right]A_\nu + S_f[\psi',\bar\psi',0]\,, \tag{5.662}$$

with $m = \frac{e}{\sqrt{\pi}}$ (in two-dimensions the electric charge e has dimensions of mass). The particle spectrum of the theory can be read off the poles of the gauge field propagator after analytic continuation back to Minkowski space. In momentum space, the kernel to be inverted reads

$$K_{\mu\nu} = (p^2+m^2)\delta_{\mu\nu} - \left(1-\frac{1}{\xi}\right)p_\mu p_\nu = (p^2+m^2)\left(\delta_{\mu\nu} - \frac{p_\mu p_\nu}{p^2}\right) + \left(\frac{p^2}{\xi}+m^2\right)\frac{p_\mu p_\nu}{p^2}\,, \tag{5.663}$$

[54] We further impose the boundary condition that $G_0^{(2)}$ vanishes at infinity. This removes the remaining gauge invariance under $A_\mu \to A_\mu + \partial_\mu\Lambda$ with $\Box\Lambda = 0$, not fixed by the Lorenz condition, which should have been done anyway.

and so the momentum-space propagator is

$$\tilde{K}_{\mu\nu}(p)^{-1} = \frac{1}{p^2+m^2}\left(\delta_{\mu\nu} - \frac{p_\mu p_\nu}{p^2}\right) + \frac{1}{m^2+\frac{p^2}{\xi}}\frac{p_\mu p_\nu}{p^2} \underset{\xi\to 0}{\to} \frac{1}{p^2+m^2}\left(\delta_{\mu\nu} - \frac{p_\mu p_\nu}{p^2}\right). \tag{5.664}$$

and in coordinate space

$$D^{(2)}_{E\mu\nu}(x) = \int \frac{d^2p}{(2\pi)^2}\, e^{-ip\cdot x}\frac{1}{p^2+m^2}\left(\delta_{\mu\nu} - \frac{p_\mu p_\nu}{p^2}\right). \tag{5.665}$$

Changing the coordinate labeling so that 0 and 1 correspond to time and space both in Euclidean and Minkowski space, rotating $x_{E0} = e^{i\theta}x^0$ and $p_{E0} = e^{-i\theta}p_0$ in opposite directions, with $\theta \in [0, \pi/2]$, setting $x_{E1} = x^1$ and $p_{E1} = p_1$, and taking into account that for the temporal component of the gauge field the Wick rotation requires $iA_{E0}(x_{E0}) = A_0(-ix_{E0})$, we find

$$\begin{aligned}
&e^{i(\delta_{\mu 0}+\delta_{\nu 0})\theta} D^{(2)}_{E\mu\nu}(e^{i\theta}x^0, x^1) \\
&= \int \frac{d^2p}{(2\pi)^2}\, e^{-i(p_0x^0+p_1x^1)}\frac{e^{i(\delta_{\mu 0}+\delta_{\nu 0})\theta}e^{-i\theta}}{e^{-2i\theta}p_0^2+p_1^2+m^2}\left(\delta_{\mu\nu} - \frac{e^{-i(\delta_{\mu 0}+\delta_{\nu 0})\theta}p_\mu p_\nu}{e^{-2i\theta}p_0^2+p_1^2}\right) \\
&\underset{\theta\to\frac{\pi}{2}}{\to} -i\int \frac{d^2p}{(2\pi)^2}\, e^{-i(p_0x^0+p_1x^1)}\frac{1}{-p_0^2+p_1^2+m^2-i\epsilon}\left(i^{\delta_{\mu 0}+\delta_{\nu 0}}\delta_{\mu\nu} - \frac{p_\mu p_\nu}{-p_0^2+p_1^2-i\epsilon}\right) \\
&= \int \frac{d^2p}{(2\pi)^2}\, e^{-i(p_0x^0+p_1x^1)}\frac{i}{p_0^2-p_1^2-m^2+i\epsilon}\left(\eta_{\mu\nu} - \frac{p_\mu p_\nu}{p_0^2-p_1^2+i\epsilon}\right) = D^{(2)}_{M\mu\nu}(x^0, x^1),
\end{aligned} \tag{5.666}$$

which we can write as

$$\begin{aligned}
D^{(2)}_{M\mu\nu}(x^0, x^1) = \langle 0|\mathrm{T}\{\hat{A}_\mu(x)\hat{A}_\nu(0)\}|0\rangle &= \int \frac{d^2p}{(2\pi)^2}\, e^{-ip\cdot x}\frac{i}{p^2-m^2+i\epsilon}\left(\eta_{\mu\nu} - \frac{p_\mu p_\nu}{p^2+i\epsilon}\right) \\
&= \left(\eta_{\mu\nu} - \frac{\partial_\mu\partial_\nu}{\Box}\right)\int \frac{d^2p}{(2\pi)^2}\, e^{-ip\cdot x}\frac{i}{p^2-m^2+i\epsilon},
\end{aligned} \tag{5.667}$$

where now all scalar products are understood to be in the Minkowski metric, and $\Box^{-1}$ denotes convolution with the free Minkowskian two-point function. Clearly, the only pole in the integrand is at $p^2 = m^2$.

Via the equations of motion, one shows that the gauge field propagator and the correlation function of vector currents $\langle 0|\mathrm{T}\{\bar{\psi}\gamma_\mu\psi(x)\bar{\psi}\gamma_\mu\psi(0)\}|0\rangle$ are proportional, meaning that $\{\bar{\psi}\gamma_\mu\psi(x)$ only excites massive photons out of the vacuum, while fermionic states do not appear in the spectrum of the theory. This can be interpreted as fermions and antifermions being bound into a "vector meson", i.e., the massive photon.

References

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