Computation of hadronic two-point functions in Lattice QCD

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Remark for Post-FPCP(added on 20.7.2018): These notes are based on freestyle lectures I gave elsewhere. They have overlap with what I talked about but they are different, in particular the introductory part. What is also missing is the discussion of applications in the context of flavour physics. The notes are, however, more specific about the lattice calculation itself (which I would have covered in a second lecture had I not left). Whoever wants to know more, please feel free to read 1.3.2 etc. Also the signs are correct in the notes. Moreover, I also corrected these old notes a bit today.

1 Introduction

Strongly interacting particles are called hadrons. These are composed of quarks and gluons. Their masses can be determined in Lattice simulations, from so-called two-point functions, where the particle of interest is created at some initial time and destroyed at a later time, on a four dimensional Euclidean spacetime lattice. The ground state mass is then obtained from the exponential decay at large time differences. We provide a very brief introduction into Lattice QCD and the notations used. Subsequently, the standard methods to construct and to compute these two-point functions and hadron masses are introduced and explained for a simple example. This follows on from the previous lecture where so-called quark propagators are obtained by solving a sparse linear system. These are the building blocks of the two-point functions discussed here.
Remark for the attending mathematicians: we employ the notation $As = b$, instead of $Ax = b$, because in physics x often refers to an element of $\mathbb{R}^4$.

1.1 General overview

The standard model of particle physics contains different elementary particles, which, in this theory, have no substructure:

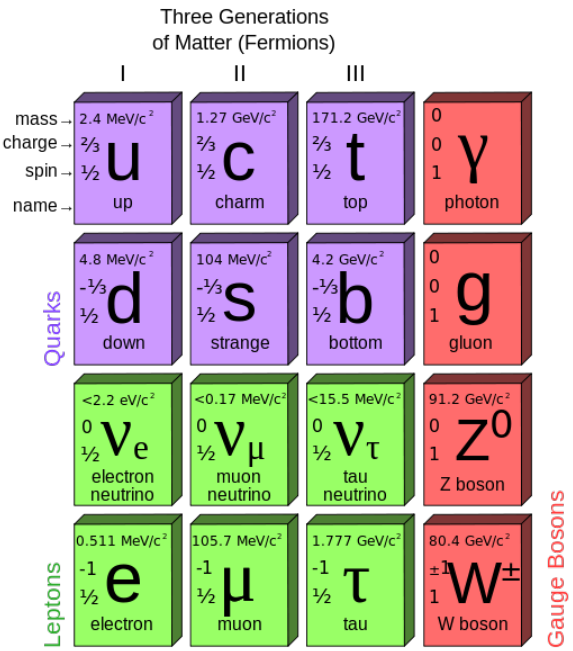

Figure 1: Elementary particle content of the standard model of particle physics (from `http://www.wikipedia.org`).

- Leptons: electron e^-, muon μ^-, tau τ^- with electric charges $-e$ and the electrically neutral neutrinos ν_e, ν_μ, ν_τ.
- Quarks come in 6 flavours: up, down, strange, charm, bottom (or beauty) and top. They carry so-called colour charges and interact via the strong (= colour) interaction. This force is described by Quantum Chromodynamics. In addition, quarks carry electric charges ($u, c, t : +\frac{2}{3}e$, $d, s, b : -\frac{1}{3}e$) and weak charges. They interact with other fermions both electromagnetically and weakly. Each quark has a baryon number 1/3.
- Leptons and quarks are fermions. All known elementary fermions have spin $\frac{1}{2}$.
- The strong force is mediated by gauge bosons (spin 1 particles) called *gluons*. Gluons are massles but, unlike the electrically neutral photon, carry (colour) charges.
- One important property of QCD is confinement: free "coloured" objects like quarks or gluons cannot be observed in Nature. Due to the strong interaction, they are always bound in hadrons. Hadrons can either be mesons (integer spin) or baryons (half-integer spin).

- Mesons have baryon number *zero*, i.e. they contain as many quarks as antiquarks. In the quark model a meson contains one quark and one antiquark ($\bar{q}q$). QCD is more complex and mesons are expected to contain higher "Fock states" like tetraquarks ($\bar{q}q\bar{q}q$) as well. Some mesons may even contain glueball components (with no quarks).

  The pion contains u and d quarks and their anti-particles $\overline{u}$ and $\overline{d}$. In Nature there are two electrically charged and one neutral pion: $\pi^+ : \bar{d}u$, $\pi^- : \bar{u}d$, $\pi^0 : \frac{1}{\sqrt{2}}(\bar{u}u - \bar{d}d)$.

- Baryons have baryon number *one*, i.e. they contain three *valence* quarks. (The number of quarks minus the number of antiquarks equals three.) Within the quark model, baryons contain only valence quarks and no antiquarks. The most prominent examples are the proton (uud, charge $+e$) and the neutron (udd, electrical charge 0). Proton and neutron are also called nucleons since they are the constituents of atomic nuclei.

There is particle-antiparticle creation in quantum field theories. This leads to *sea quark* pairs $\bar{u}u$, $\bar{d}d$ etc. (and gluons), in addition to the valence quarks.
One can compare the electromagnetic coupling constant (fine structure constant) to the strong coupling parameter:

$$\alpha_{em} = \frac{e^2}{4\pi\hbar c} \approx \frac{1}{137} \ll \alpha_{QCD} = \frac{g^2}{4\pi\hbar c} = 0.1 \cdots 1\,,$$

where the range of α_{QCD} indicates that this parameter varies, depending on the process and scales involved. This hierarchy suggests a simplification, the neglection of electromagnetic interactions of the quarks.
The above equation is written out in so-called Heaviside-Lorentz units. We will use *natural units* $\hbar = c = 1$ instead. This means that the units of distance and time and of energy and mass become interchangeable ($c = 1$). Moreover, we do not distinguish between momentum and energy or between momentum and inverse distance units ($\hbar = 1$).

- We quote momenta, energies and masses in GeV = 1000 MeV = 10^9 eV (units of energy). This is approximately the mass of the proton m_p.

- We measure distance and time in fm = 10^{-15} m. This is approximately the radius of the proton r_p.

- We can convert between GeV and fm:

$$0.197\,\text{fm} \cdot \text{GeV} \approx 1\,.$$

We compare the masses of quarks, the nucleons and the pions:

- $m_u \approx 2$ MeV, $m_d \approx 5$ MeV, $m_s \approx 100$ MeV,

- $m_p \approx 938$ MeV, $m_n \approx 940$ MeV,

- $m_{\pi^\pm} \approx 140$ MeV, $m_{\pi^0} \approx 135$ MeV.

Note that atomic binding energies E_B (i.e. the difference between the mass of an atom and its constituent nucleus and electrons) are related to the radius of a state through the virial theorem for the Coulomb potential as $E_B = -\alpha_{em}\langle r^{-1}\rangle/2$. The fact that $m_p \approx E_B \approx 5\, r_p^{-1}$ (note the sign!) indicates that the QCD coupling is large and that something very different from (Q)ED is going on. Why is the proton stable if its constituents are lighter than the proton itself?
The masses of the hadrons are much bigger than the masses of their valence quarks. Moreover, $m_d - m_u \ll m_s, m_\pi, m_n$. So usually the approximation $m_u \approx m_d \approx m_{ud} = (m_u + m_d)/2$ is employed and electromagnetic interactions are neglected. In this particular limit the so-called isospin symmetry is realized and $m_{\pi^\pm} = m_{\pi^0}$ and $m_p = m_n$. To resolve the $\mathcal{O}(1\,\mathrm{MeV})$ corrections to this approximation, one would have to include the two sources of isospin breaking ($m_d - m_u$ mass difference and the electric charge difference).

1.2 The QCD Lagrangian

The Lagrange density of QCD is given as

$$\mathscr{L}_{QCD}(x) = -\frac{1}{2g^2}\mathrm{tr}\; F_{\mu\nu}(x)F^{\mu\nu}(x) + \sum_{f=1}^{n_f} \bar{\Psi}(x)_f \big(iD_\mu\gamma^\mu - m_f\big)\Psi(x)_f\,. \tag{1}$$

This notation is very compact and we need to explain it in more detail. The second part $\sum_{f=1}^{n_f} \bar{\Psi}(x)_f \big(iD_\mu\gamma^\mu - m_f\big)\Psi(x)_f$ contains the fermions:

- $f \in \{u, d, s, \ldots\}$ is the flavour index and m_f is the mass of a quark of flavour f.
- D_μ is the covariant derivative $D_\mu = \partial_\mu + iA_\mu$ with $\partial_\mu = \partial/\partial x^\mu$. The Lorentz index $\mu = 0, 1, 2, 3$ labels the directions in space-time (0=time, 1,2,3=space)
- $A_\mu(x) = \sum_{a=1}^{N^2-1} A_\mu^a(x)T^a$ is the four-vector potential with $A_\mu^a(x) \in \mathbb{R}$ and T^a are the generators of the SU(N) group ($N = 3$ in QCD). They satisfy

  $$\big[T^a, T^b\big] = i\sum_{c=1}^{N^2-1} f^{abc}T^c\,,$$

  where $f^{abc} \in \mathbb{R}$ are totally anti-symmetric structure constants. In the fundamental representation, these T^a are complex, traceless and hermitian $N \times N$ matrices with components T_{ij}. The indices $i, j = 1, \ldots, N$ are colour indices and the following normalization of the T^a holds: $\mathrm{tr}\; T^aT^b = \delta^{ab}/2$. The T^a are generators of the group since

  $$\forall \quad U \in \mathrm{SU}(N): \quad \exists \quad \omega^a \in [0, 4\pi) \quad \text{so that} \quad U = \exp\left(i\sum_{a=1}^{N^2-1}\omega^a T^a\right)$$

  with $UU^\dagger = \mathbb{1}$, $\det U = 1$

- γ^μ are Dirac matrices (4×4 matrices in four spacetime dimensions) which satisfy

$$\{\gamma^\mu, \gamma^\nu\} = \gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2\eta^{\mu\nu}\mathbb{1}_{4\times 4}\,,$$

  where $\eta = \mathrm{diag}(1,-1,-1,-1)$ is the metric tensor. This metric defines the product of two four-vectors a and b: $a\cdot b = a_\mu b^\mu = a^\mu b^\nu \eta_{\mu\nu} = a^0 b^0 - \sum_{j=1}^3 a^j b^j$. Note that $a^0 = a_0$, $a^j = -a_j$ for $j = 1,2,3$. The components of γ^μ can be written as $\gamma^\mu_{\alpha,\beta}$ with Dirac or spinor indices $\alpha, \beta = 1,2,3,4$.

- The fermion field Ψ_f has $4 \times N$ components (spin $\times$ color). We can write: $\Psi^\alpha_{i\,f}$, where α is the spinor index and i is the color index. In QCD $N = 3$ and $i = 1,2,3$.

The first term on the r.h.s. of (1), $\frac{1}{2g^2}\mathrm{tr}\ F_{\mu\nu}(x)F^{\mu\nu}(x)$, describes the dynamics of the gluons.

- $g^2 = 4\pi\alpha_{QCD}$ is the coupling "constant".

- $F_{\mu\nu}$ is the field strength tensor:

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + i[A_\mu, A_\nu] = -i[D_\mu, D_\nu] = \sum_a F^a_{\mu\nu}T^a\,.$$

  In non-Abelian theories like QCD the commutator $[A_\mu, A_\nu]$ does not vanish. One easily sees that

$$\mathrm{tr}\ F_{\mu\nu}F^{\mu\nu} = \sum_{\mu\nu,ab} F^{\mu\nu a}F^b_{\mu\nu}\mathrm{tr}\ T^aT^b = \frac{1}{2}F^a_{\mu\nu}F^{\mu\nu a}\,,$$

  where the summation over μ, ν and a is implicitly assumed on the r.h.s.

We can now write the Lagrangian in a less compact way (again the summation over repeated indices is assumed):

$$\mathscr{L}_{QCD}(x) = -\frac{1}{4g^2}F^a_{\mu\nu}(x)F^{\mu\nu a}(x) + \sum_{f=1}^{n_f}\bar{\Psi}^\alpha_j(x)_f\left(iD_{\mu,jk}\gamma^\mu_{\alpha\beta} - m_f\delta_{jk}\delta_{\alpha\beta}\right)\Psi^\beta_k(x)_f\,,$$

where

$$(D_\mu)_{jk} = \partial_\mu\delta_{jk} + iA^a_\mu(T^a)_{jk}\,. \tag{2}$$

D_μ is spin-diagonal and γ^μ is colour-diagonal.
It turns out that $g^2 = g^2(q^2), m_f = m_f(q^2)$ where q is a momentum scale. As long as physical observables only depends on processes with momenta $q \ll \mu$, they should be independent of any ultraviolet cut-off μ. The running of the coupling and quark masses is a common feature of quantum field theories: not directly measurable parameters need to be adjusted as functions of the scale at which QCD is evaluated, to keep physical observables (e.g. hadron masses) constant and well defined. This scale may be a momentum or for the coupling and masses appearing in a renormalized Lagrangian it may be the cut-off scale itself. In QCD this procedure possible and no new terms need to be introduced as μ is sent to infinity.

QCD is a *renormalizable* quantum field theory. Instead of explicitly introducing a cut-off on momenta, usually the technique of dimensional regularisation is employed, which has many advantages in perturbative calculations.
Another way of *regularising* QCD is to discretize it on a lattice with spacing $a \sim 1/\mu$. Removing this cut-off ($a \to 0$) then corresponds to taking the continuum limit. QCD is *asymptotically free*: it turns out that at large scales q $g^2(q) \to 0$ and the quarks only weakly interact. Near the *continuum limit* where $\mu \sim a^{-1}$ is large (and $q \ll \mu$ can be taken large), a connection can be made with perturbation theory. At low momenta, i.e. at typical hadronic distance scales, however, the coupling becomes strong and non-perturbative methods are required.

1.3 Lattice QCD

1.3.1 Technical trick: Euclidean time

It is convenient to employ a Euclidean metric with $x_j = x^{j\,\mathrm{M}}$, $x_4 = it = ix^{0\,\mathrm{M}}$ where the superscript "M" denotes the Minkowski spacetime. The integral over x_4 then runs along the imaginary axis but can be rotated to an integration along the real axis if there are no poles in the first and third quadrants of the complex plane. This is the case under certain conditions that are usually met in QCD.
The product of two Euclidean four-vectors reads: $a_\mu b^\mu = a_\mu b_\mu = \sum_{\mu=1}^{4} a_\mu b_\mu$ The Euclidean γ matrices satisfy the anti-commutation relations

$$\{\gamma^\mu, \gamma^\nu\} = 2\delta^{\mu\nu}\mathbb{1}\,, \quad \gamma^\mu = \gamma^{\mu^\dagger}\,,$$

where $(\gamma^{\mu^\dagger})_{\alpha\beta} = (\gamma^\mu_{\beta\alpha})^*$ and $*$ denotes the complex conjugate. The Euclidean action (space-time integral of the Lagrangian) becomes:

$$\begin{aligned} S_{QCD} &= \int d^4x\, \mathscr{L}_{QCD}(x) = \\ &= \int d^4x \left\{ \frac{1}{2g^2}\mathrm{tr}\,[F_{\mu\nu}(x)F_{\mu\nu}(x)] + \sum_{f=1}^{n_f} \bar{\Psi}(x)_f (D_\mu\gamma^\mu + m_f)\Psi(x)_f \right\}, \end{aligned}$$

where we have employed the convention $S_{QCD} = -S^{\mathrm{M}}_{QCD}$. The n point Green functions (see below) contain the same information about the theory as the partition function (see below) that is defined by the action. Green functions can be analytically continued from the Euclidean to the original Minkowski metric. It turns out that many properties are identical in both metrics, for example particle masses. These therefore need not be continued back into Minkowskian spacetime.

1.3.2 Putting QCD on a lattice

- We introduce a Euclidean lattice Λ with $N_S^3 \cdot N_T$ sites (points) and a lattice spacing a. We do not know the physical value of a *a priori*. We first have to "measure" a physical

observable on the lattice and relate it to its experimental value. Therefore, we can only "set the scale" $a(g^2, m_f)$ *a posteriori*. The lattice is a *mass-independent scheme* and so one would usually use the same $a(g^2)$ for all m_f rather than $a(g^2, m_f)$. This requires an interpolation or extrapolation to the quark mass values that are realized in Nature, where the connection to the experimental value can be made. If the computer tells us a proton mass number $M_p \in \mathbb{R}^+$ then we can obtain the lattice spacing from the relation $M_p(g^2)a^{-1}(g^2) = m_p$ where m_p denotes the experimental value.

- Notation:

$$x = (x_\mu) \in \Lambda\,, \quad x_\mu = an_\mu$$

with space-components $n_1, n_2, n_3 \in \{0, \ldots, N_S - 1\}$ and a time component $n_4 \in \{0, \ldots, N_T - 1\}$. We define vectors $\hat{\mu}$ in the direction $\mu \in \{1, 2, 3, 4\}$ of modulus $|\hat{\mu}| = a$. Λ usually has toroidal boundary conditions: the neighbouring point in the direction j of a point with coordinate $n_j = N_S - 1$ has $n_j = 0$. The same convention is realized in the Euclidean time (4-)direction.

- The transporter between two neighbouring lattice sites

$$U_{x,\mu} = P \exp\left\{ i \int_x^{x+\hat{\mu}} dx'_\mu \, A_\mu(x') \right\} \approx e^{iA_\mu\left(x+\frac{\hat{\mu}}{2}\right))} \in \mathrm{SU}(3) \tag{3}$$

is called a *gauge link*, link variable or link. $U_{x,\mu} = U^\dagger_{x+\hat{\mu},-\mu}$ is the link connecting the site x with its neighbour (distance a) in the direction μ.

- Quarks reside on the lattice sites: $\Psi_x = \Psi(x)$.

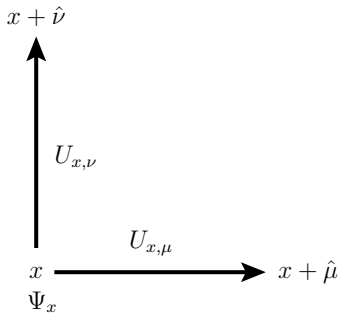

Figure 2: Quarks and gluons on the lattice

- We have to discretize derivatives:

$$\begin{aligned}(\bar{\Psi}\partial_\mu\Psi)(x) &= \frac{1}{2a}\bar{\Psi}_x\big(\Psi_{x+\hat{\mu}} - \Psi_{x-\hat{\mu}}\big)\big(1 + \mathcal{O}(a^2)\big) \\ (\bar{\Psi}D_\mu\Psi)(x) &= \frac{1}{2a}\bar{\Psi}_x\big(U_{x,\mu}\Psi_{x+\hat{\mu}} - U^\dagger_{x-\hat{\mu},\mu}\Psi_{x-\hat{\mu}}\big)\big(1 + \mathcal{O}(a^2)\big)\end{aligned} \tag{4}$$

- This lattice discretization enables a simple realization of local gauge transformations. For $g_x \in \mathrm{SU}(3)$:

$$\begin{aligned} U_{x,\mu} &\to U^g_{x,\mu} = g_x U_{x,\mu} g^\dagger_{x+\hat{\mu}}, \\ \Psi_x &\to \Psi^g_x = g_x \Psi_x, \\ \bar{\Psi}_x &\to \bar{\Psi}^g_x = \bar{\Psi}_x g^\dagger_x. \end{aligned}$$

- We find that $\bar{\Psi} D_\mu \Psi$ is gauge invariant:

$$\begin{aligned} \bar{\Psi}^g D^g_\mu \Psi^g &= \frac{1}{2a} \bar{\Psi}^g_x \big(U^g_{x,\mu} \Psi^g_{x+\hat{\mu}} - U^{g\dagger}_{x-\hat{\mu},\mu} \Psi^g_{x-\hat{\mu}} \big) \\ &= \frac{1}{2a} \Bigg(\bar{\Psi}_x \underbrace{g^\dagger_x g_x}_{=\mathbb{1}} U_{x,\mu} \underbrace{g^\dagger_{x+\hat{\mu}} g_{x+\hat{\mu}}}_{=\mathbb{1}} \Psi_{x+\hat{\mu}} - \bar{\Psi}_x \underbrace{g^\dagger_x g_x}_{=\mathbb{1}} U^\dagger_{x-\hat{\mu},\mu} \underbrace{g^\dagger_{x-\hat{\mu}} g_{x-\hat{\mu}}}_{=\mathbb{1}} \Psi_{x-\hat{\mu}} \Bigg) \\ &= \bar{\Psi} D_\mu \Psi \,. \end{aligned}$$

  Lattice discretizations are not unique but in the continuum limit different discretizations should give the same results (*universality*).

- It is easy to see that traces over products of links along closed loops, so-called Wilson loops, are gauge invariant too. The "minimal" Wilson loop is the plaquette (closed loop of links along a square):

$$U_{x,\mu\nu} = U_{x,\mu} U_{x+\hat{\mu},\nu} U^\dagger_{x+\hat{\nu},\mu} U^\dagger_{x,\nu} = e^{ia^2 \left[\mathcal{F}_{\mu\nu}\left(x + \frac{\hat{\mu}}{2} + \frac{\hat{\nu}}{2}\right)\right]} \quad \text{with} \quad \mathcal{F}_{\mu\nu}(x) = F_{\mu\nu}(x) + \mathcal{O}(a) \,,$$

  where we used the definition (3) as well as the Taylor expansion and the simplified Baker-Campbell-Hausdorff (=Glauber) relation

$$A_{x+\hat{\mu},\nu} = A_{x,\nu} + \hat{\mu} \partial_\mu A_{x,\nu} + \mathcal{O}(a^2) \,, \quad e^A e^B \approx e^{A+B+\frac{1}{2}[A,B]} \,.$$

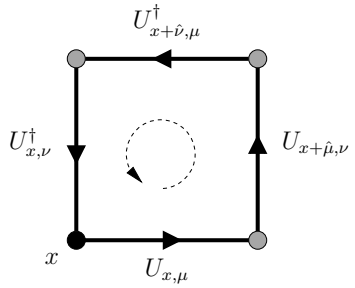

Figure 3: A sketch of the plaquette.

Note that the leading lattice corrections to $\mathcal{F}^b_{\mu\nu} = 2\,\mathrm{Re}\,\mathrm{tr}\,\mathcal{F}_{\mu\nu} T^b$ must be of order a^2, due to the invariance of the real part of the trace of the plaquette under $a \to -a$ ($\Rightarrow \hat{\mu} \to -\hat{\mu}$). Moreover, $\mathcal{F}_{\mu\nu} = -\mathcal{F}_{\nu\mu}$.

- With this definition of the plaquette one finds:

$$\frac{2N}{g^2}\sum_x\sum_{\mu>\nu}\frac{1}{N}\mathrm{Re\,tr}\ (\mathbb{1}-U_{x,\mu\nu}) = \sum_x\ \frac{1}{g^2}\sum_{\mu,\nu}\mathrm{tr}\ \Big(\mathbb{1}-\cos(a^2\mathcal{F}_{\mu\nu}(x))\Big) =$$
$$= \sum_x a^4\ \frac{1}{2g^2}\sum_{\mu,\nu}\mathrm{tr}\ \Big(F_{\mu\nu}(x)F_{\mu\nu}(x)(1+\mathcal{O}(a^2))\Big) \overset{a\to 0}{\longrightarrow} \int d^4x\ \frac{1}{2g^2}\sum_{\mu,\nu}\mathrm{tr}\ F_{\mu\nu}(x)F_{\mu\nu}(x)\,,$$

  which is the gluonic part of the Euclidean continuum action.

- We define:

$$S_{x,\mu\nu} \equiv \frac{1}{N}\mathrm{Retr}\ (\mathbb{1}-U_{x,\mu\nu}) \equiv S_\Box \equiv 1-U_\Box\,,$$

  which is real and bounded from above.

1.3.3 The QCD action

We can now write down a lattice version of the QCD action

$$S_{QCD} = \underbrace{\frac{2N}{g^2(a)}}_{\equiv\beta}\sum_\Box S_\Box + \sum_f\sum_{x,y\in\Lambda}\bar\Psi_{x\,f}A_f[U]_{x,y}\Psi_{y\,f}$$
$$= -\beta\sum_\Box U_\Box + \text{const.} + S_f[U]\,.$$

The inverse coupling β controls the lattice spacing $a(\beta)$. Asymptotic freedom means that the continuum limit is reached for $\beta\to\infty$. The constant term can be dropped as it cancels from expectation values (see below).
$A_f[U]_{x,y}$ (colour and spin indices are suppressed) is a sparse diagonally dominant lattice discretization of the Dirac operator. For Wilson-like discretizations this matrix depends on a parameter κ_f that is related to the quark mass m_f via

$$m_f = \frac{1}{2a}\left(\frac{1}{\kappa_f}-\frac{1}{\kappa_c}\right)\,.$$

κ_f is called a hopping parameter, κ_c is the critical hopping parameter. The quark mass vanishes at $\kappa_f=\kappa_c=\frac{1}{8}+\underbrace{\mathcal{O}(g^2)}_{>0}$. For $\kappa_f<\kappa_c$, $m_f>0$.
Remark: $m_f a$ is proportional to the inverse condition number of A_f.
We will keep the discussion general and therefore there is no need to specify the matrix A.

1.3.4 Expectation values

We omit sums and products over flavours. All formulae are written for the case of one quark flavour of mass m. This can trivially be generalized to n_f mass degenerate or non-degenerate quarks.

The expectation value of an observable O, e.g. an n-point Green- (or correlation-) function, can be evaluated via the path integral:

$$\langle O \rangle = \frac{1}{Z} \int \underbrace{[dU]}_{\prod_{x,\mu} dU_{x,\mu}} [d\bar{\Psi}][d\Psi]\, O[U,\Psi,\bar{\Psi}]\, e^{-S[U,\Psi,\bar{\Psi}]}$$

$$S[U,\Psi,\bar{\Psi}] = S_g[U] + S_f[U,\Psi,\bar{\Psi}] = \beta \sum_{\square} S_{\square} + \bar{\Psi} A[U] \Psi \,.$$

$[dU]$ is the so-called Haar measure and Z is the partition function. The normalization condition $\langle \mathbb{1} \rangle = 1$ implies

$$Z = \int [dU][d\bar{\Psi}][d\Psi]\, e^{-S[U,\Psi,\bar{\Psi}]} \,.$$

Quarks follow the so-called Fermi-statistics. This means that the temporal boundary conditions for these fields should be antisymmetric (which can be implemented within A). It also implies that a state cannot be occupied by more than one quark. To realize the latter requirement, the quark field components need to be represented by Grassmann numbers.

Excursion: some facts on Grassmann numbers

- Two Grassmann numbers θ_i anti-commute:

  $$\theta_i \theta_j = -\theta_j \theta_i$$

  In particular: $(\theta_i)^2 = 0$. This means that the Taylor expansion of a function of Grassmann numbers $f(\{\theta_i\}) = a + \beta_i \theta_i + c_{ij} \theta_i \theta_j + \cdots + c \theta_1 \theta_2 \ldots \theta_N$ (where $i = 1, \ldots, N$, N even, $a, c_{ij} = -c_{ji} \in \mathbb{R}$, β_i Grassmann numbers) does not contain any terms that are quadratic in any of the variables θ_i. For quark fields, i will run over spacetime position, colour and flavour.

- Grassmann numbers commute with regular numbers $a \in \mathbb{R}$:

  $$\theta_i a = a \theta_i$$

- They have rather simple integration rules:

  $$\begin{aligned} d^N\theta &= d\theta_N d\theta_{N-1} \ldots d\theta_1 \,, \\ d\theta_i d\theta_j &= -d\theta_j d\theta_i \,, \\ d\theta_i \theta_j &= -\theta_j d\theta_i \end{aligned}$$

  $$\int d\theta\, 1 = 0 \qquad \int d\theta\, \theta = 1$$

- These rules, for complex Grassmann numbers $\eta_j = (\theta_j + i\phi_j)/\sqrt{2}$, lead to:

$$\int [d\eta^*][d\eta] \, \exp\left[-\sum_{i,j}^{N} \eta_i^* M_{ij} \eta_j\right] = \det M$$

and

$$\int [d\eta^*][d\eta] \, \eta_m \eta_n^* \, \exp\left[-\eta^\dagger M \eta\right] = M^{-1}_{mn} \, \det M$$

For our purpose we substitute

$$\begin{aligned} \eta_m &\to \Psi_{x,\alpha,i} \\ \eta_n^* &\to \bar{\Psi}_{y,\beta,j} \\ M_{mn} &\to A[U]_{x,y,\alpha,\beta,i,j} \, . \end{aligned}$$

Then on a fixed gauge field background $U = \{U_{x,\mu}\}$:

$$\int [d\bar{\Psi}][d\Psi] \, e^{-\bar{\Psi} A[U] \Psi} \propto \det A[U] \, ,$$

$$\langle \Psi_X \bar{\Psi}_Y \rangle_{|U} = \frac{\int [d\bar{\Psi}][d\Psi] \, \Psi_X \bar{\Psi}_Y \, e^{-\bar{\Psi} A[U] \Psi}}{\int [d\bar{\Psi}][d\Psi] \, e^{-\bar{\Psi} A[U] \Psi}} = A^{-1}_{XY}[U] \, ,$$

where $X = (x, \alpha, i), Y = (y, \beta, j)$ are multi-indices: we can obtain a quark two-point function on a fixed gauge field background (= *quark propagator*) by inverting the Dirac matrix.
On the lattice there are $N_S^3 N_T$ distinct sites, e.g., $32^3 64 = 2^{21} \approx 2 \cdot 10^6$. The fermion matrix A has $(12 N_S^3 N_T)^2$ components. Most of these vanish, due to the next-neighbour nature of discretized derivatives. However, A^{-1} is not sparse anymore. Fortunately, as we have seen above, the Fermions can be integrated out analytically since they only appear as bilinears. Afterwards we are left with the gluonic degrees of freedom only. The gluonic action is highly non-linear and cannot be integrated out analytically. The lattice contains $4 N_S^3 N_T$ links, each of which are complex 3×3 matrices, with 8 independent real components. High dimensional integrals are best solved employing importance sampling (Markov) Monte Carlo techniques. The method is as follows. A gauge ensemble $\{U_i\} = \{U^{(i)}_{x,\mu}\}, i = 1, \ldots, n$ (= set of configurations U_i) is generated. The standard way of doing this at present is the so-called hybrid Monte Carlo algorithm. Each of the configurations is generated with a probability $[dU_i] \frac{e^{-S_{\text{eff}}[U_i]}}{Z}$, where

$$\begin{aligned} e^{-S_{\text{eff}}[U]} &= e^{-S_g[U]} \int [d\Psi][d\bar{\Psi}] e^{-S_f[U,\Psi,\bar{\Psi}]} \\ &= e^{-S_g[U]} \det A \, . \end{aligned}$$

If the number of independent gauge configurations n is sufficiently large for the central limit theorem to hold, we can approximate the expectation value

$$\langle O \rangle = \frac{1}{n} \sum_{i=1}^{n} O[U_i] + \mathcal{O}\left(\frac{1}{\sqrt{n}}\right) \, ,$$

up to a statistical error that can be reduced like $1/\sqrt{n}$, as n is increased. This intrinsic (unbiased) statistical error is the origin of the term "measurement". On n gauge configuration n *measurements* are *taken* and the average is calculated. Any Ψ-dependence of $O[U_i]$ can be integrated out since all bilinears $\Psi_X \bar{\Psi}_Y$ within O can be replaced by $A^{-1}[U_i]_{XY}$, as we have seen above. We also remark that the above statistical interpretation requires a real, bounded action and this is the main reason for our transformation to Euclidean spacetime.

2 Computation of a hadronic two-point function

2.1 Two-point Green function

The expectation value

$$C(t) = \langle 0|O(t+t_0)O^\dagger(t_0)|0\rangle = \langle O(t+t_0)O^\dagger(t_0)\rangle \tag{5}$$

is an example of a two-point Green or correlation function. $O^\dagger(t_0)$ creates a state (e.g. a pion) at time t_0 out of the vacuum $|0\rangle$ and $O(t+t_0)$ destroys it at later time $t+t_0$. The translational invariance of expectation values

$$\langle O(x)\rangle = \langle O(0)\rangle = \frac{1}{N_S^3 N_T}\sum_{x\in\Lambda}\langle O(x)\rangle$$

allows us to choose $t_0 = 0$. We could also average over different t_0-values, thereby reducing the statistical error of the expectation value. However, this would also be more expensive, computationally.
The evolution of a quantum mechanical state in Euclidean time is given by

$$|\psi(t)\rangle = e^{-Ht}|\psi(0)\rangle\,,$$

with a Hamiltonian H (that we do not need to know explicitly). For energy eigenstates $|n\rangle$ this reads, $e^{-Ht}|n\rangle = e^{-E_n t}|n\rangle$, where E_n is the energy of the state $|n\rangle$. Inserting a complete set $\sum_n \frac{|n\rangle\langle n|}{2E_n V_3} = \mathbb{1}$, where $V_3 = N_S^3 a^3$ denotes the three-volume, into (5) results in

$$\begin{aligned} C(t) &= \sum_n \langle 0|\hat{O}|n\rangle \frac{e^{-E_n t}}{2E_n V_3}\langle n|\hat{O}^\dagger|0\rangle = \\ &= \sum_n \frac{|\langle 0|\hat{O}|n\rangle|^2}{2E_n V_3} e^{-E_n t} = \sum_n |C_n|^2 e^{-E_n t}\ : \end{aligned}$$

the correlation function is a sum of exponentials. The factor $E_n V_3$ is due to the usual relativistic normalization convention of states in a volume V_3. Ordering $E_1 < E_2 < \cdots$, we can write for large enough times t:

$$C(t) = \sum_n |C_n|^2 e^{-E_n t} \approx |C_1|^2 e^{-E_1 t}\left(1 + \frac{|C_2|^2}{|C_1|^2} e^{-(E_2-E_1)t}\right)\,.$$

E_1 is the ground state energy. The combination $E_1 t = (E_1 a)(t/a) = a E_1\, n_4$ is dimensionless. On the computer we will obtain a dimensionless number $aE_1 \in \mathbb{R}^+$.
We define the *effective mass* as

$$\begin{aligned} E_{\text{eff}}(t) &= \frac{1}{a} \ln\left(\frac{C(t)}{C(t+a)}\right) \approx -\frac{d}{dt} \ln C(t) \\ &= E_1 + \underbrace{(E_2 - E_1) \frac{|C_2|^2}{|C_1|^2} e^{-(E_2 - E_1)t}}_{>0} . \end{aligned}$$

At large times t E_{eff} will approach E_1, up to exponential corrections. If the same operator is used at the *source* ($t_0 = 0$) and the *sink* (t) then $E_{\text{eff}}(t)$ will monotonously decrease towards E_1 (within statistical errors). The "speed" of this convergence is determined by the overlap coefficients C_i. If O is chosen such that $|C_1| \gg |C_i|$ for $i > 1$ then the convergence will be fast.

2.2 Technical tricks for computing hadron masses

Trick 1 (Wick contractions): B_{XY} is some arbitrary function of the spacetime-spin-colour multi-indices $X = (x, \alpha, i)$ and $Y = (y, \beta, j)$ that may also depend on the gauge configuration U. We can cast the fermionic average (at fixed U) of a quark bilinear into a trace of the product of ordinary matrices:

$$\begin{aligned} \sum_{x,y} \langle \bar{\Psi}_x B_{xy} \Psi_y \rangle_{|U} &= \sum_{x,y} -\langle \text{tr } B_{xy} \underbrace{\Psi_y \bar{\Psi}_x}_{A^{-1}_{yx}} \rangle_{|U} \\ &= -\sum_{x,y} \text{tr } B_{xy} A^{-1}_{yx}[U] . \end{aligned}$$

The trace is over spin and colour and we have kept spin and colour explicit: A_{xy} and B_{xy} are 12×12 matrices and Ψ_x is a twelve-component vector. Note the minus sign that originates from interchanging the two Grassmann fields. This trick can easily be generalized to more complicated expectation values, where all combinations of quark-antiquark pairs (of the same flavour) need to be contracted into A^{-1} factors.

Trick 2 (Dirac algebra):

$$\gamma_5 \equiv \gamma_1\gamma_2\gamma_3\gamma_4 = (\gamma_4\gamma_3\gamma_2\gamma_1)^\dagger = \gamma_5^\dagger , \quad \gamma_5\gamma_\mu = -\gamma_\mu\gamma_5 , \quad \gamma_5^2 = \mathbb{1} , \quad \gamma_5\gamma_\mu\gamma_5 = -\gamma_\mu$$

$$\Rightarrow \gamma_5 D_\mu \gamma_\mu \gamma_5 = -D_\mu\gamma_\mu = D_\mu^\dagger \gamma_\mu = (D_\mu\gamma_\mu)^\dagger$$

$$\Rightarrow \gamma_5 A \gamma_5 = A^\dagger , \quad \gamma_5 A^{-1} \gamma_5 = A^{\dagger -1} .$$

This last property is known as γ_5-Hermiticity. Also notice that $\gamma_5 A$ is Hermitian.

2.3 The pion two-point function

A pion π with spatial momentum $\mathbf{p}$ can be destroyed by the operator

$$\sum_{\mathbf{x},\alpha\beta,j} e^{-i\mathbf{px}} \bar{\Psi}^{(1)}_{x,\alpha,j} \gamma^5_{\alpha,\beta} \Psi^{(2)}_{x,\beta,j} \,,$$

where the superscripts (1) and (2) denote the flavour, in this case up and down quark. The continuum dispersion relation reads $E_1^2 = m_\pi^2 + \mathbf{p}^2$, where E_1 is the ground state energy and m_π the ground state mass. Up to $\mathcal{O}(a)$ (or $\mathcal{O}(a^2)$, depending on the fermionic action) corrections this also holds on the lattice. For notational simplicity, we restrict ourselves to the rest frame, with momentum $\mathbf{p} = \mathbf{0} \Rightarrow E_1 = m_\pi$.
A general mesonic destruction operator (or interpolator) of quark-antiquark type can be written as

$$\sum_{\mathbf{x}} e^{-i\mathbf{px}} \left(\bar{\Psi}^{(f_1)} \Gamma D[U] \Psi^{(f_2)} \right)_{\mathbf{x}} \,,$$

where we have dropped the colour and spin indices. Γ denotes a product of Γ-matrices and $D[U]$ a gauge covariant spin-diagonal matrix that may contain discretized covariant derivatives (to realize angular momentum) and/or a *smearing* function, to enhance the projection onto the ground state.
We define $\bar{\Psi} \equiv \Psi^\dagger \gamma_4$. This is the Minkowski definition. In Euclidean spacetime the substitution $\bar{\Psi} \to \Psi^\dagger$ in all definitions would be more consistent. However, this allows us to copy all operators one-to-one from the literature that mostly employs Minkowski conventions. As a warm up we perform a manipulation needed to obtain the creation operator:

$$\begin{aligned} \left(\bar{\Psi}^{(1)} \Gamma \Psi^{(2)}\right)^\dagger &= \left(\Psi^{(1)\,\dagger} \gamma_4 \Gamma \Psi^{(2)}\right)^\dagger = -\Psi^{(2)\,\dagger} \Gamma^\dagger \gamma_4 \Psi^{(1)} \\ &= -\Psi^{(2)\,\dagger} \gamma_4 \gamma_4 \Gamma^\dagger \gamma_4 \Psi^{(1)} = \mp \bar{\Psi}^{(2)} \Gamma \Psi^{(1)} \,, \end{aligned}$$

depending on $\gamma_4 \Gamma^\dagger \gamma_4 = \pm \Gamma$. (For $\Gamma = \gamma_5$: $\gamma_4 \gamma_5 \gamma_4 = -\gamma_5$ the + sign is correct.)
Now we can write down an expression for the pion two-point function.

$$\begin{aligned} C_\pi(t) &= \sum_{\mathbf{x},\mathbf{y}} \left\langle \left(\bar{\Psi}^{(1)}_x \gamma_5 \Psi^{(2)}_x\right) \left(\bar{\Psi}^{(2)}_y \gamma_5 \Psi^{(1)}_y\right) \right\rangle \,, \quad x_4 = t \,,\, y_4 = 0 \\ &= -N_S^3 \sum_{\mathbf{x}} \left\langle \mathrm{tr} \, \left[\gamma_5 \left(\Psi^{(2)}_x \bar{\Psi}^{(2)}_0 \right) \gamma_5 \left(\Psi^{(1)}_0 \bar{\Psi}^{(1)}_x \right) \right] \right\rangle \\ &\overset{\text{Trick 1}}{=} -N_S^3 \sum_{\mathbf{x}} \left\langle \mathrm{tr} \, \left(\gamma_5 A^{-1}_{x0} \gamma_5 A^{-1}_{0x} \right) \right\rangle \\ &\overset{\text{Trick 2}}{=} -N_S^3 \sum_{\mathbf{x}} \left\langle \mathrm{tr} \, \left((A^{-1})^\dagger_{0x} A^{-1}_{0x} \right) \right\rangle \,, \end{aligned}$$

where we assume flavours 1 and 2 to be mass-degenerate and, therefore, do not distinguish between $A^{(1)}$ and $A^{(2)}$. Going from the first to the second line, the translational invariance of expectation values was exploited and the minus sign stems from commuting the Grassmann

numbers. We remark that in the case of equal flavours (so-called flavour singlets), a second pairing, with a relative minus-sign would have appeared, applying the Wick contraction (trick 1). This additional term contains A^{-1}_{00} and A^{-1}_{xx}, that are harder to compute. In the non-flavour singlet case above, only 12 rows of A^{-1} are required.
The A^{-1}_{0x} are so-called point-to-all propagators. These are sets of 12 Dirac-vectors (one for each source spin-colour combination), with $12N_S^3N_T$ elements each. Now imagine we would have needed A^{-1}_{yx} for all spacetime positions y! How do we compute A^{-1}_{0x}? We define point-sources:

$$b^{(\beta,j)}_{z,\gamma,\kappa} = \delta^0_z \delta^\beta_\gamma \delta^j_\kappa$$

and solve the 12 sparse linear systems

$$As^{(\beta,j)} = b^{(\beta,j)} \,.$$

This gives the point-to-all propagator:

$$s^{(\beta,j)}_{x,\alpha,i} = A^{-1}_{x,\alpha,i,z,\gamma,\kappa} b^{(\beta,j)}_{z,\gamma,\kappa} = A^{-1}_{x,\alpha,i,0,\beta,j} \,.$$

Remark: A is not Hermitian. It is also possible to solve the system $A^\dagger As = A^\dagger b$, instead, where $A^\dagger A = (\gamma_5 A)(\gamma_5 A)$ is Hermitian. In general, this will require additional multiplications but it may be possible to exploit the fact that the Wilson Dirac operator includes only hops from even to odd sites and vice versa (even-odd preconditioning).
Once the 12 solutions are computed, we can obtain the correlation function

$$C_\pi(t) = -N_S^3 \sum_{\vec{x},\alpha,i,\beta,j} \langle |s^{(\beta,j)}_{x,\alpha,i}|^2 \rangle \tag{6}$$

and extract the mass from its large t behaviour. Smearing may be implemented in the operator too, to enhance the overlap with the physical ground state. In this case, instead of the point sources above one would use *smeared sources*. We have claimed that the correlation function should be positive. This is not the case above. This can be traced back to the fact that we have not consistently implemented Euclidean conventions ($\bar{\Psi}$ instead of $\Psi^\dagger$). Some software packages like Chroma drop in an extra minus sign that leads to positive pion and rho correlation functions but then for instance the scalar becomes negative and this overall sign needs to be corrected by hand.
Finally, it is easy to see that the result for a meson with general Γ ($\bar{\Psi}^{(1)}\Gamma\Psi^{(2)}$) reads

$$C(t) = \pm \sum_{\mathbf{x},\alpha,\beta,\gamma,\delta,i,j} s^{(1)(\beta,j)^*}_{x,\alpha,i} \left(\gamma_5\Gamma\right)_{\alpha\gamma} s^{(2)(\delta,j)}_{x,\gamma,i} \left(\Gamma\gamma_5\right)_{\delta\beta} \,.$$

Since in any standard notation each $\gamma_5\Gamma$ has only four non-vanishing components, computer time can be saved by tabulating the relevant spin bilinears.