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Non-perturbative QCD: renormalization, O(a)-improvement and matching to Heavy Quark Effective Theory [1]

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Abstract

We give an introduction to three topics in lattice gauge theory:

I. The Schrödinger functional and O(a) improvement.

O(a) improvement has been reviewed several times. Here we focus on explaining the basic ideas in detail and then proceed directly to an overview of the literature and our personal assessment of what has been achieved and what is missing.

II. The computation of the running coupling, running quark masses and the extraction of the renormalization group invariants.

We focus on the basic strategy and on the large effort that has been invested in understanding the continuum limit. We point out what remains to be done.

III. Non-perturbative Heavy Quark Effective Theory.

Since the literature on this subject is still rather sparse, we go beyond the basic ideas and discuss in some detail how the theory works in principle and in practice.

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1 Introduction

Lattice QCD, the subject of this school, is our prime tool to make quantitative predictions in the low energy sector of QCD. Also connecting this sector to the perturbative high energy regime requires non-perturbative control over the theory, which can be achieved by lattice gauge theories. In these lectures the emphasis is on a non-perturbative treatment of the theory *including* its renormalization. Connecting the perturbative and the non-perturbative regions is one of the main subjects (II.).

Heavy quarks require special care on a lattice with spacing a, simply because their mass is of the order of the cutoff, a^{-1}, or higher. Effective theories can be used in this situation, in particular Heavy Quark Effective Theory (HQET) is appropriate for hadrons with a single heavy quark. It allows to compute the expansion of their properties in terms of the inverse quark mass (in practice the b-quark mass). The renormalization of this effective theory introduces couplings whose number grows with the order of the expansion. In order to preserve the predictivity of the theory, these couplings ought to be determined from the underlying theory, QCD. Again this step can be seen as the renormalization of the effective theory. As will be explained, non-perturbative precision is required if one wants to be able to take the continuum limit of the lattice effective field theory. Actually it is a general property of the expansion that a $1/m_{\rm b}$ correction is only defined once all parts including the matching are done non-perturbatively.

Renormalization is an ultraviolet phenomenon with relevant momentum scales of order a^{-1}. Since the QCD coupling becomes weak in the ultraviolet, one may expect to be able to perform renormalizations perturbatively, i.e. computed in a power series in the bare coupling g_0^2 as one approaches the continuum limit $a \to 0$.[2] However, one has to care about the following point. In order to keep the numerical effort of a simulation tractable, the number of degrees of freedom in the simulation may not be excessively large. This means that the lattice spacing a can not be taken very much smaller than the relevant physical length scales of the observable that is considered. Consequently the momentum scale a^{-1} that is relevant for the renormalization is not always large enough to justify the truncation of the perturbative series. In particular one has to remember that the bare coupling vanishes only logarithmically as $a \to 0$: $g_0^2 \sim 1/\log(a\Lambda_{\rm QCD})$. In order to obtain a truly non-perturbative answer, the renormalizations have to be performed non-perturbatively.

Depending on the observable, the necessary renormalizations are of different nature. I will use this introduction to point out the different types, and in particular explain the problem that occurs in a non-perturbative treatment of scale dependent renormalization.

[2] For simplicity we ignore here the cases of mixing of a given operator with operators of lower dimension where this statement does not hold.

1.1 Basic renormalization: hadron spectrum

The calculation of the hadron spectrum starts by choosing certain values for the bare coupling, g_0, and the bare masses of the quarks in units of the lattice spacing, $am_{0,i}$. The flavor index i assumes values $i = \mathrm{u}, \mathrm{d}, \mathrm{s}, \mathrm{c}, \mathrm{b}$ for the up, down, charm and bottom quarks that are sufficient to describe hadrons of up to a few GeV masses. We ignore the problem of simulating the b-quark for the moment, neglect isospin breaking and take the light quarks to be degenerate, $m_{0,\mathrm{u}} = m_{0,\mathrm{d}} = m_{0,\mathrm{l}}$.

Next, from MC simulations of suitable correlation functions, one computes masses of five different hadrons H, e.g. $H = \mathrm{p}, \pi, \mathrm{K}, \mathrm{D}, \mathrm{B}$ for the proton, the pion and the K-,D- and B-mesons,

$$am_H = am_H(g_0, am_{0,\mathrm{l}}, am_{0,\mathrm{s}}, am_{0,\mathrm{c}}, am_{0,\mathrm{b}}) \ . \tag{1.1}$$

The theory is renormalized by first setting $m_\mathrm{p} = m_\mathrm{p}^{\mathrm{exp}}$, where $m_\mathrm{p}^{\mathrm{exp}}$ is the experimental value of the proton mass. This determines the lattice spacing via

$$a = (am_\mathrm{p})/m_\mathrm{p}^{\mathrm{exp}} \ . \tag{1.2}$$

Next one must choose the parameters $am_{0,i}$ such that (1.1) is indeed satisfied with the experimental values of the meson masses. Equivalently, one may say that at a given value of g_0 one fixes the bare quark masses from the condition

$$(am_H)/(am_\mathrm{p}) = m_H^{\mathrm{exp}}/m_\mathrm{p}^{\mathrm{exp}}, \quad H = \pi, \mathrm{K}, \mathrm{D}, \mathrm{B} \ . \tag{1.3}$$

and the bare coupling g_0 then determines the value of the lattice spacing through eq. (1.2).

After this *renormalization*, namely *the elimination of the bare parameters in favor of physical observables*, the theory is completely defined and predictions can be made. E.g. the leptonic decay constant, F_π, of the pion can be determined,

$$F_\pi = a^{-1}[aF_\pi][1 + \mathrm{O}(a)] \ . \tag{1.4}$$

For the rest of this section, I assume that the bare parameters have been eliminated and consider the additional renormalizations of more complicated observables.

Note. Renormalization as described here is done without any reference to perturbation theory. One could in principle use the perturbative formula for $(a\Lambda_{\mathrm{QCD}})(g_0)$ for the renormalization of the bare coupling, where Λ_{QCD} denotes the Λ-parameter of the theory (in some scheme). Proceeding in this way, one obtains a further prediction namely $m_\mathrm{p}/\Lambda_{\mathrm{QCD}}$ but at the price of introducing $\mathrm{O}(g_0^2)$ errors in the prediction of the observables. As mentioned before, such errors decrease very slowly as one performs the continuum limit. A better method to compute the Λ-parameter will be discussed later.

1.2 Scale dependent renormalization and fundamental parameters of QCD

As we take the relevant length scales in correlation functions to be small or take the energy scale in scattering processes to be high, QCD is better and better approximated by weakly coupled quarks and gluons. The strength of the interaction may be measured for instance by the ratio of the production rate of three jets to the rate for two jets in high energy $e^+\ e^-$ collisions[3]

$$\alpha(\mu) \quad \propto \quad \frac{\sigma(e^+\ e^- \to q\ \bar{q}\ g)}{\sigma(e^+\ e^- \to q\ \bar{q})}\,, \quad \mu^2 = q^2 = (p_{e^-} + p_{e^+})^2 \gg 10\mathrm{GeV}^2\ . \tag{1.5}$$

We observe the following points.

- The perturbative renormalization group tells us that $\alpha(\mu)$ decreases logarithmically with growing energy μ. In other words the renormalization from the bare coupling to a renormalized one is logarithmically scale dependent.
- Different definitions of α are possible; but with increasing energy, α depends less and less on the definition (or the process).
- In a similar way, one may define running quark masses $\overline{m}$ from combinations of observables at high energies.
- Using a suitable definition (scheme), the μ-dependence of α and $\overline{m}$ can be determined non-perturbatively and at high energies the short distance parameters α and $\overline{m}$ can be converted to the renormalization group invariants using perturbation theory in α. Being defined non-perturbatively, the latter are the natural fundamental parameters of QCD.

Explaining these points in detail is the main objective of the second lecture.

1.3 Irrelevant operators

Another category of renormalization is associated with the removal of lattice discretization errors such as the linear a-term in eq. (1.4). Following Symanzik's improvement program, this can be achieved order by order in the lattice spacing by adding irrelevant operators, i.e. operators of dimension larger than four, to the lattice Lagrangian [1]. The coefficients of these operators are easily determined at tree level of perturbation theory, but in general they need to be renormalized. We will explain the general idea of the non-perturbative determination of the coefficients arising at order a and then briefly review the present status of O(a) improvement.

Note also the alternative approach of removing lattice artifacts order by order in the coupling constant but non-perturbatively in the lattice spacing a described in the

[3] One should really use some rather inclusive process, e.g. one computable directly in the Euclidean theory. For explaining the principle we ignore this issue.

lectures by Peter Hasenfratz. Linear effects in a are automatically absent if the lattice regularization has enough chiral symmetry. Indeed chiral symmetry can be kept exactly in the discretized theory [2–4], but these theories are rather expensive to simulate. On the other hand also the "twisted mass" regularization [5, 6] is automatically[4] O(a)-improved [7] (see the appendix of [8] and Stefan Sint's lectures at this school for a simple argument), but at the price of the violation of isospin symmetry.

1.4 Heavy Quark Effective Theory

This theory is very promising for B-physics. It approximates heavy-light bound state properties systematically in an expansion of $\Lambda_{\rm QCD}/m_{\rm b}$, a small expansion parameter. A non-trivial issue is the renormalization of the theory. Already at the lowest order in $1/m_{\rm b}$, the associated uncertainties are significant if renormalization is treated perturbatively. At that order renormalization can be carried out by the methods discussed in the second lecture [9–11], but when one includes O($1/m_{\rm b}$) corrections one has to deal in addition with the mixing of operators of different dimensions.[5] The continuum limit of the effective theory then exists only if the *power divergent mixing coefficients* are computed non-perturbatively.

In the third lecture we will explain these issues in detail. We will formulate HQET non-perturbatively. The power divergent mixing coefficients can then be determined by matching the theory to QCD. A possible strategy will be explained. As an example we will show the computation of the b-quark mass including $1/m_{\rm b}$ corrections.

[4] "Automatically" still means that the standard mass term has to be tuned to zero, but that can be done by the use of the PCAC relation.

[5] Note that the computation of an order $\Lambda_{\rm QCD}$ term in the renormalized quark mass already constitutes a O($1/m_{\rm b}$) correction to the leading term, although it is done in static approximation.

Lecture I.

The Schrödinger functional and $\mathrm{O}(a)$-improvement of lattice QCD

I.1 The Schrödinger functional (SF)

For various applications, for instance scale dependent renormalization in QCD, $\mathrm{O}(a)$-improvement and Heavy Quark Effective Theory, we need QCD in a finite volume with boundary conditions suitable for (easy) perturbative calculations and MC simulations. These are provided by the SF of QCD, which we introduce below. For a while we restrict the discussion to the pure gauge theory. In this part the presentation follows closely [12]; we refer to this work for further details as well as proofs of the properties described below.

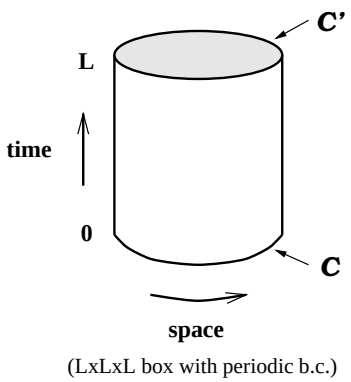


Figure 1: Illustration of the Schrödinger functional.

I.1.1 Definition

Here, we give a formal definition of the SF in the Yang-Mills theory in continuum space-time, noting that a rigorous treatment is possible in the lattice regularized theory.

Space-time is taken to be a cylinder illustrated in Fig. 1. We impose Dirichlet boundary conditions for the vector potentials[6] in time,

$$A_k(x) \;=\; \begin{cases} C_k^{\Lambda}(\mathbf{x}) & \text{at} \quad x_0 = 0 \\ C'_k(\mathbf{x}) & \text{at} \quad x_0 = L \end{cases} \quad , \tag{I.1.1}$$

where C, C' are classical gauge potentials and A^{Λ} denotes the gauge transform of A,

$$A_k^{\Lambda}(\mathbf{x}) \;=\; \Lambda(\mathbf{x})A_k(\mathbf{x})\Lambda(\mathbf{x})^{-1} + \Lambda(\mathbf{x})\partial_k\Lambda(\mathbf{x})^{-1}, \qquad \Lambda \in \mathrm{SU}(N) \ . \tag{I.1.2}$$

[6] We use anti-hermitian vector potentials.

In space, we impose periodic boundary conditions,

$$A_k(x + L\hat{k}) \;=\; A_k(x), \qquad \Lambda(\mathbf{x} + L\hat{k}) = \Lambda(\mathbf{x}) \;\; . \tag{I.1.3}$$

The (Euclidean) partition function with these boundary conditions defines the SF,

$$\begin{aligned} \mathcal{Z}[C', C] &\equiv \int \mathrm{D}[\Lambda] \int \mathrm{D}[A]\, \mathrm{e}^{-S_{\mathrm{G}}[A]} \;\; , \\ S_{\mathrm{G}}[A] &= -\frac{1}{2g_0^2} \int \mathrm{d}^4x \;\mathrm{tr}\; \{F_{\mu\nu} F_{\mu\nu}\} , \\ F_{\mu\nu} &= \partial_\mu A_\nu - \partial_\nu A_\mu + [A_\mu, A_\nu] \;\; , \\ \mathrm{D}[A] &= \prod_{\mathbf{x},\mu,a} \mathrm{d}A^a_\mu(x), \qquad \mathrm{D}[\Lambda] = \prod_{\mathbf{x}} \mathrm{d}\Lambda(\mathbf{x}) \;\; . \end{aligned} \tag{I.1.4}$$

Here $\mathrm{d}\Lambda(\mathbf{x})$ denotes the Haar measure of SU(N). It is easy to show that the SF is a gauge invariant functional of the boundary fields,

$$\mathcal{Z}[C'^{\Omega'}, C^{\Omega}] = \mathcal{Z}[C', C] \;\; , \tag{I.1.5}$$

where also large gauge transformations are permitted. The invariance under the latter is an automatic property of the SF defined on a lattice, while in the continuum formulation it is enforced by the integral over Λ in eq. (I.1.4).

I.1.2 Quantum mechanical interpretation

The SF is the quantum mechanical transition amplitude from a state $|C\rangle$ to a state $|C'\rangle$ after a (Euclidean) time L. To explain the meaning of this statement, we introduce the Schrödinger representation. The Hilbert space consists of wave-functionals $\Psi[A]$ which are functionals of the spatial components of the vector potentials, $A^a_k(\mathbf{x})$. The canonically conjugate field variables are represented by functional derivatives, $E^a_k(\mathbf{x}) = \frac{1}{i}\frac{\delta}{\delta A^a_k(\mathbf{x})}$, and a scalar product is given by

$$\langle \Psi | \Psi' \rangle = \int \mathrm{D}[A]\, \Psi[A]^* \Psi'[A], \qquad \mathrm{D}[A] = \prod_{\mathbf{x},k,a} \mathrm{d}A^a_k(\mathbf{x}) \;\; . \tag{I.1.6}$$

The Hamilton operator,

$$\mathbf{H} = \int_0^L \mathrm{d}^3x \, \left\{ \frac{g_0^2}{2} E^a_k(\mathbf{x}) E^a_k(\mathbf{x}) + \frac{1}{4g_0^2} F^a_{kl}(\mathbf{x}) F^a_{kl}(\mathbf{x}) \right\} \;\; , \tag{I.1.7}$$

commutes with the projector, $\mathbb{P}$, onto the physical subspace of the Hilbert space (i.e. the space of gauge invariant states), where $\mathbb{P}$ acts as

$$\mathbb{P}\psi[A] = \int \mathrm{D}[\Lambda]\, \psi[A^\Lambda] \;\; . \tag{I.1.8}$$

Finally, each classical gauge field defines a state $|C\rangle$ through

$$\langle C|\Psi\rangle = \Psi[C] \ . \tag{I.1.9}$$

After these definitions, the quantum mechanical representation of the SF is given by

$$\begin{aligned} \mathcal{Z}[C', C] &= \langle C'|\mathrm{e}^{-\mathbf{H}T}\mathbb{P}|C\rangle \\ &= \sum_{n=0}^{\infty} \mathrm{e}^{-E_n T}\Psi_n[C']\Psi_n[C]^* \ . \end{aligned} \tag{I.1.10}$$

In Wilson's original lattice formulation, eq. (I.1.10) can be derived rigorously and is valid with real energy eigenvalues E_n.

I.1.3 Background field

A complementary aspect of the SF is that it allows a treatment of QCD in a color background field in an unambiguous way. Let us assume that we have a solution B of the equations of motion, which satisfies also the boundary conditions eq. (I.1.1). If, in addition,

$$S[A] > S[B] \tag{I.1.11}$$

for all gauge fields A that are not equal to a gauge transform B^Ω of B, then we call B the background field (induced by the boundary conditions). Here, $\Omega(x)$ is a gauge transformation defined for all x in the cylinder and its boundary and B^Ω is the corresponding generalization of eq. (I.1.2). Background fields B, satisfying these conditions are known; we will describe a particular family of fields, later.

Due to eq. (I.1.11), fields close to B dominate the path integral for weak coupling g_0 and the effective action,

$$\Gamma[B] \equiv -\ln \mathcal{Z}\left[C', C\right] \ , \tag{I.1.12}$$

has a regular perturbative expansion,

$$\begin{aligned} \Gamma[B] &= \frac{1}{g_0^2}\Gamma_0[B] + \Gamma_1[B] + g_0^2\Gamma_2[B] + \dots \ , \\ \Gamma_0[B] &\equiv g_0^2 S[B] \ . \end{aligned} \tag{I.1.13}$$

Above we have used that due to our assumptions, the background field, B, and the boundary values C, C' are in one-to-one correspondence and have taken B as the argument of Γ.

I.1.4 Perturbative expansion

For the construction of the SF as a renormalization scheme, one needs to study the renormalization properties of the functional $\mathcal{Z}$. Lüscher, Narayanan, Weisz and Wolff have performed a one-loop calculation for arbitrary background field [12]. The calculation is done in dimensional regularization with $3-2\varepsilon$ space dimensions and one time dimension. One expands the field A in terms of the background field and a fluctuation field, q, as

$$A_\mu(x) = B_\mu(x) + g_0 q_\mu(x) \ . \tag{I.1.14}$$

Then one adds a gauge fixing term ("background field gauge") and the corresponding Fadeev-Popov term. Of course, care must be taken about the proper boundary conditions in all these expressions. Integration over the quantum field and the ghost fields then gives

$$\Gamma_1[B] = \tfrac{1}{2}\ln\det\hat{\Delta}_1 - \ln\det\hat{\Delta}_0 \ , \tag{I.1.15}$$

where $\hat{\Delta}_1$ is the fluctuation operator and $\hat{\Delta}_0$ the Fadeev-Popov operator defined in [12]. The result can be cast in the form

$$\Gamma_1[B] \underset{\varepsilon\to 0}{=} -\frac{b_0}{\varepsilon}\,\Gamma_0[B] + \mathrm{O}(1) \ , \tag{I.1.16}$$

with the important result that the only (for $\varepsilon \to 0$) singular term is proportional to Γ_0.

After renormalization of the coupling, i.e. the replacement of the bare coupling by $\bar{g}_{\overline{\mathrm{MS}}}$ via

$$g_0^2 = \bar{\mu}^{2\varepsilon}\bar{g}^2_{\overline{\mathrm{MS}}}(\mu)[1 + z_1(\varepsilon)\bar{g}^2_{\overline{\mathrm{MS}}}(\mu)], \quad z_1(\varepsilon) = -\frac{b_0}{\varepsilon} \ , \tag{I.1.17}$$

the effective action is finite,

$$\begin{aligned}
\Gamma[B]_{\varepsilon=0} &= \left\{\frac{1}{\bar{g}^2_{\overline{\mathrm{MS}}}} - b_0\left[\ln\mu^2 - \tfrac{1}{16\pi^2}\right]\right\}\Gamma_0[B] \\
&\quad -\tfrac{1}{2}\zeta'(0|\Delta_1) + \zeta'(0|\Delta_0) + \mathrm{O}(\bar{g}^2_{\overline{\mathrm{MS}}}) \\
\zeta'(0|\Delta) &= \frac{\mathrm{d}}{\mathrm{d}s}\zeta(s|\Delta)\Big|_{s=0}, \qquad \zeta(s|\Delta) = \mathrm{Tr}\,\Delta^{-s} \ .
\end{aligned} \tag{I.1.18}$$

Here, $\zeta'(0|\Delta)$ is a complicated functional of B, which is not known analytically but can be evaluated numerically for specific choices of B.

The important result of this calculation is that (apart from field independent terms that have been dropped everywhere) the SF is finite after eliminating g_0 in favor of $\bar{g}_{\overline{\mathrm{MS}}}$. The presence of the boundaries does *not* introduce any extra divergences. In the following section we argue that this property is correct in general, not just in one-loop approximation.

I.1.5 General renormalization properties

The relevant question here is whether local quantum field theories formulated on space-time manifolds *with boundaries* develop divergences that are not present in the absence of boundaries (periodic boundary conditions or infinite space-time). In general the answer is "yes, such additional divergences exist". In particular, Symanzik studied the ϕ^4-theory with Schrödinger functional boundary conditions [13, 14]. He presented arguments that to all orders of perturbation theory the Schrödinger functional is finite after

- renormalization of the self-coupling, λ, and the mass, m,
- *and* the addition of the boundary counter-terms

$$\int_{x^0=T} \mathrm{d}^3x \, \left\{ Z_1\phi^2 + Z_2\phi\partial_0\phi \right\} + \int_{x^0=0} \mathrm{d}^3x \, \left\{ Z_1\phi^2 - Z_2\phi\partial_0\phi \right\} \quad . \tag{I.1.19}$$

In addition to the standard renormalizations, one has to add counter-terms formed by local composite fields integrated over the boundaries. One expects that in general, all fields with dimension $d \leq 3$ have to be taken into account. Already Symanzik conjectured that counter-terms with this property are sufficient to renormalize the SF of any quantum field theory which is renormalizable when no boundaries are present.

Since this conjecture forms the basis for many applications of the SF, we note a few points concerning its status.

- As mentioned, a proof to all orders of perturbation theory does not exist. An application of power counting in momentum space in order to prove the conjecture is not possible due to the missing translation invariance.
- There is no gauge invariant local field with $d \leq 3$ in the Yang–Mills theory. Consequently no additional counter-term is necessary in accordance with the 1-loop result described in the previous subsection.
- In QCD it has been checked also by explicit 2–loop calculations [15, 16]. MC simulations give further support for its validity beyond perturbation theory; we give examples in the second lecture.

Although a general proof is missing, there is little doubt that Symanzik's conjecture is valid in general. Concerning QCD, this puts us into the position to give an elegant definition of a renormalized coupling in finite volume.

I.1.6 Renormalized coupling

For the definition of a running coupling we need a quantity which depends only on one scale. We choose LB such that it depends only on one dimensionless variable η. In other words, the strength of the field is scaled as $1/L$. The background field is

assumed to fulfill the requirements of Sect. I.1.3. Then, following the above discussion, the derivative

$$\Gamma'[B] = \frac{\partial}{\partial\eta}\Gamma[B] \ , \tag{I.1.20}$$

is finite when it is expressed in terms of a renormalized coupling like $\bar{g}_{\overline{\rm MS}}$ but Γ' is defined non-perturbatively. From eq. (I.1.13) we read off immediately that a properly normalized coupling is given by

$$\bar{g}^2(L) = \Gamma'_0[B] \ / \ \Gamma'[B] \ . \tag{I.1.21}$$

Since there is only one length scale L, it is evident that $\bar{g}$ defined in this way runs with L.

A specific choice for the gauge group SU(3) is the abelian background field induced by the boundary values [17]

$$C_k = \tfrac{i}{L}\begin{pmatrix} \phi_1 & 0 & 0 \\ 0 & \phi_2 & 0 \\ 0 & 0 & \phi_3 \end{pmatrix} , \quad C'_k = \tfrac{i}{L}\begin{pmatrix} \phi'_1 & 0 & 0 \\ 0 & \phi'_2 & 0 \\ 0 & 0 & \phi'_3 \end{pmatrix} , \quad k = 1,2,3, \tag{I.1.22}$$

with

$$\begin{aligned} \phi_1 &= \eta - \tfrac{\pi}{3}, & \phi'_1 &= -\phi_1 - \tfrac{4\pi}{3}, \\ \phi_2 &= -\tfrac{1}{2}\eta, & \phi'_2 &= -\phi_3 + \tfrac{2\pi}{3}, \\ \phi_3 &= -\tfrac{1}{2}\eta + \tfrac{\pi}{3}, & \phi'_3 &= -\phi_2 + \tfrac{2\pi}{3}. \end{aligned} \tag{I.1.23}$$

In this case, the derivatives with respect to η are to be evaluated at $\eta = 0$. The associated background field,

$$B_0 = 0, \qquad B_k = \left[x_0 C'_k + (L - x_0)C_k\right]/L, \quad k = 1,2,3 \ , \tag{I.1.24}$$

has a field tensor with non-vanishing components

$$G_{0k} = \partial_0 B_k = (C'_k - C_k)/L, \quad k = 1,2,3 \ . \tag{I.1.25}$$

It is a constant color-electric field.

I.1.7 Quarks

In the end, the real interest is in the renormalization of QCD and we need to consider the SF with quarks. We restrict our discussion to the original formulation of S. Sint [18].

Special care has to be taken in formulating the Dirichlet boundary conditions for the quark fields; since the Dirac operator is a first order differential operator, the Dirac equation has a unique solution when one half of the components of the fermion fields are

specified on the boundaries. Indeed, a detailed investigation shows that the boundary condition

$$\begin{aligned} P_+\psi|_{x_0=0} &= \rho, \quad P_-\psi|_{x_0=L} = \rho', \qquad P_\pm = \tfrac{1}{2}(1 \pm \gamma_0)\,, & \text{(I.1.26)} \\ \overline{\psi}P_-|_{x_0=0} &= \bar{\rho}, \quad \overline{\psi}P_+|_{x_0=L} = \bar{\rho}'\,, & \text{(I.1.27)} \end{aligned}$$

lead to a quantum mechanical interpretation analogous to eq. (I.1.10). The SF

$$\mathcal{Z}[C', \bar{\rho}', \rho'; C, \bar{\rho}, \rho] = \int \mathrm{D}[A]\mathrm{D}[\,\psi\,]\mathrm{D}[\,\overline{\psi}\,]\,\mathrm{e}^{-S[A,\overline{\psi},\psi\,]} \tag{I.1.28}$$

involves an integration over all fields with the specified boundary values. The full action may be written as

$$\begin{aligned} S[A, \overline{\psi}, \psi\,] &= S_{\mathrm{G}}[\overline{\psi}, \psi\,] + S_{\mathrm{F}}[A, \overline{\psi}, \psi\,] \\ S_{\mathrm{F}} &= \int \mathrm{d}^4x\, \overline{\psi}(x)[\gamma_\mu D_\mu + m]\psi(x) \qquad \text{(I.1.29)} \\ &\quad - \int \mathrm{d}^3\mathbf{x}\,[\overline{\psi}(x)P_-\psi(x)]_{x_0=0} - \int \mathrm{d}^3\mathbf{x}\,[\overline{\psi}(x)P_+\psi(x)]_{x_0=L}\ , \end{aligned}$$

with S_{G} as given in eq. (I.1.4). In eq. (I.1.29) we use standard Euclidean γ-matrices. The covariant derivative, D_μ, acts as $D_\mu\psi(x) = \partial_\mu\psi(x) + A_\mu(x)\psi(x)$.

Let us now discuss the renormalization of the SF with quarks. In contrast to the pure Yang-Mills theory, gauge invariant composite fields of dimension three are present in QCD. Taking into account the boundary conditions one finds [18] that the counter-terms,

$$\overline{\psi}P_-\psi|_{x_0=0} \text{ and } \overline{\psi}P_+\psi|_{x_0=L}\ , \tag{I.1.30}$$

have to be added to the action with weight $1 - Z_{\mathrm{b}}$ to obtain a finite renormalized functional. These counter-terms are equivalent to a multiplicative renormalization of the boundary values,

$$\rho_{\mathrm{R}} = Z_{\mathrm{b}}^{-1/2}\rho,\ \ldots\ , \bar{\rho}'_{\mathrm{R}} = Z_{\mathrm{b}}^{-1/2}\bar{\rho}'\ . \tag{I.1.31}$$

It follows that – apart from the renormalization of the coupling and the quark mass – no additional renormalization of the SF is necessary for *vanishing* boundary values $\rho, \ldots, \bar{\rho}'$. So, after imposing homogeneous boundary conditions for the fermion fields, a renormalized coupling may be defined as in the previous subsection.

As an important aside, we point out that the boundary conditions for the fermions introduce a gap into the spectrum of the Dirac operator (at least for weak couplings). One may hence simulate the lattice SF for vanishing physical quark masses. It is then convenient to supplement the definition of the renormalized coupling by the requirement $m = 0$. In this way, one defines a mass-independent renormalization scheme with simple renormalization group equations. In particular, the β-function remains independent of the quark mass.

I.1.7.1 Correlation functions

are given in terms of the expectation values of any product $\mathcal{O}$ of fields,

$$\langle \mathcal{O} \rangle = \left\{ \frac{1}{\mathcal{Z}} \int \mathrm{D}[A]\mathrm{D}[\,\psi\,]\mathrm{D}[\,\overline{\psi}\,]\,\mathcal{O}\,\mathrm{e}^{-S[A,\overline{\psi},\psi]} \right\}_{\bar{\rho}\,'=\rho\,'=\bar{\rho}=\rho=0} \quad , \tag{I.1.32}$$

evaluated for vanishing boundary values $\rho, \ldots, \bar{\rho}'$. Apart from the gauge field and the quark and anti-quark fields integrated over, $\mathcal{O}$ may involve the "boundary fields" [19]

$$\begin{aligned} \zeta(\mathbf{x}) &= \frac{\delta}{\delta\bar{\rho}(\mathbf{x})}, \qquad \overline{\zeta}(\mathbf{x}) = -\frac{\delta}{\delta\rho(\mathbf{x})}, \\ \zeta'(\mathbf{x}) &= \frac{\delta}{\delta\bar{\rho}'(\mathbf{x})}, \qquad \overline{\zeta}'(\mathbf{x}) = -\frac{\delta}{\delta\rho'(\mathbf{x})} \quad . \end{aligned} \tag{I.1.33}$$

An application of fermionic correlation functions including the boundary fields is the definition of the renormalized quark mass in the SF scheme to be discussed next.

I.1.7.2 Renormalized mass

Just as in the case of the coupling constant, there is a great freedom in defining renormalized quark masses. A natural starting point is the PCAC relation which expresses the divergence of the axial current [7] ,

$$A_\mu^a(x) = \overline{\psi}(x)\gamma_5\gamma_\mu\tfrac{1}{2}\tau^a\psi(x) \quad , \tag{I.1.34}$$

(for simplicity we have chosen just $N_\mathrm{f} = 2$ degenerate flavors and the Pauli matrix τ^a acts in this flavor space), in terms of the associated pseudo-scalar density,

$$P^a(x) = \overline{\psi}(x)\gamma_5\tfrac{1}{2}\tau^a\psi(x) \quad , \tag{I.1.35}$$

via

$$\partial_\mu A_\mu^a(x) = 2mP^a(x) \quad . \tag{I.1.36}$$

This operator identity is easily derived at the classical level (cf. Sect. I.2). After renormalizing the operators,

$$\begin{aligned} (A_\mathrm{R})_\mu^a &= Z_\mathrm{A} A_\mu^a \quad , \\ P_\mathrm{R}^a &= Z_\mathrm{P} P^a \quad , \end{aligned} \tag{I.1.37}$$

a renormalized current quark mass may be defined by

$$m_\mathrm{R} = \overline{m} = \frac{Z_\mathrm{A}}{Z_\mathrm{P}} m \quad . \tag{I.1.38}$$

[7] The reader is not to confuse $A_\mu^a(x)$, with the gauge vector potentials $A_\mu(x)$.

Here, m, is to be taken from eq. (I.1.36) inserted into an arbitrary correlation function and $Z_{\rm A}$ can be determined from a proper chiral Ward identity [20–22]. Note that m does not depend on which correlation function is used because the PCAC relation is an operator identity. The definition of $\overline{m}$ is completed by supplementing eq. (I.1.37) with a specific normalization condition for the pseudo-scalar density. The running mass $\overline{m}$ then inherits its scheme- and scale-dependence (μ) from the corresponding dependence of $P_{\rm R}$. Such a normalization condition may be imposed through infinite volume correlation functions. Since we want to be able to compute $\overline{m}(\mu)$ for large energy scales μ, we do, however, need a finite volume definition (see Sect. II.1.2). This is readily given in terms of correlation functions in the SF.

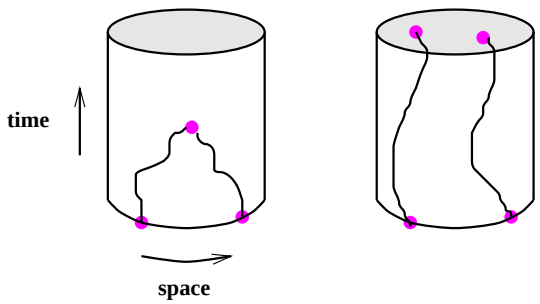


Figure 2: $f_{\rm P}$ (left) and f_1 (right) in terms of quark propagators.

To start with, let us define (iso-vector) pseudo-scalar fields at the boundary of the SF,

$$\begin{aligned} \mathcal{O}^a &= \int {\rm d}^3\mathbf{u} \int {\rm d}^3\mathbf{v}\, \overline{\zeta}(\mathbf{u})\gamma_5 \tfrac{1}{2}\tau^a \zeta(\mathbf{v}), \\ \mathcal{O}'^a &= \int {\rm d}^3\mathbf{u} \int {\rm d}^3\mathbf{v}\, \overline{\zeta}'(\mathbf{u})\gamma_5 \tfrac{1}{2}\tau^a \zeta'(\mathbf{v}) \ , \end{aligned} \tag{I.1.39}$$

to build up the correlation functions

$$\begin{aligned} f_{\rm P}(x_0) &= -\tfrac{1}{3}\langle P^a(x)\mathcal{O}^a\rangle \ , \\ f_1 &= \langle \mathcal{O}'^a \mathcal{O}^a\rangle \ , \end{aligned} \tag{I.1.40}$$

which are illustrated in Fig. 2.

We then form the ratio

$$Z_{\rm P} = {\rm const.}\sqrt{f_1}/f_{\rm P}(x)|_{x_0=L/2} \ , \tag{I.1.41}$$

such that the renormalization of the boundary quark fields, eq. (I.1.31), cancels out. The proportionality constant is to be chosen such that $Z_{\rm P} = 1$ at tree level. To define the scheme completely one needs to further specify the boundary values C, C' and the boundary conditions for the quark fields in space. These details are of no importance, here.

We rather mention some more basic points about this renormalization scheme. Just like in the case of the running coupling, the only physical scale that exists in our definitions eq. (I.1.38), eq. (I.1.41) is the linear dimension of the SF, the length scale, L. So the mass $\overline{m}(\mu)$ runs with $\mu = 1/L$. We have already emphasized that $\bar{g}$ is to be evaluated at zero quark mass. It is advantageous to do the same for $Z_{\rm P}$. In this way we define a mass-independent renormalization scheme, with simple renormalization group equations.

By construction, the SF scheme is non-perturbative and independent of a specific regularization. For a concrete non-perturbative computation, we do, however, need to evaluate the expectation values by a MC-simulation of the corresponding lattice theory. We proceed to introduce the lattice formulation of the SF.

I.1.8 Lattice formulation

A detailed knowledge of the form of the lattice action is not required for an understanding of the following sections. Nevertheless, we give a definition of the SF in lattice regularization. This is done both for completeness and because it allows us to obtain a first impression about the size of discretization errors.

We choose a hyper-cubic Euclidean lattice with spacing a. A gauge field U on the lattice is an assignment of a matrix $U(x,\mu) \in \mathrm{SU}(N)$ to every lattice point x and direction $\mu = 0,1,2,3$. Quark and anti-quark fields, $\psi(x)$ and $\overline{\psi}(x)$, reside on the lattice sites and carry Dirac, color and flavor indices as in the continuum. To be able to write the quark action in an elegant form it is useful to extend the fields, initially defined only inside the SF manifold (cf. Fig. 1) to all times x_0 by "padding" with zeros. In the case of the quark field one sets

$$\psi(x) = 0 \quad \text{if } x_0 < 0 \text{ or } x_0 > L,$$

and

$$P_-\psi(x)|_{x_0=0} = P_+\psi(x)|_{x_0=L} = 0,$$

and similarly for the anti-quark field. Gauge field variables that reside outside the manifold are set to 1.

We may then write the fermionic action as a sum over all space-time points without restrictions for the time-coordinate,

$$S_{\rm F}[U,\bar{\psi},\psi] \;\; = \;\; a^4 \sum_x \bar{\psi}(D+m_0)\psi, \tag{I.1.42}$$

and with the standard Wilson-Dirac operator,

$$D = \tfrac{1}{2}\sum_{\mu=0}^{3}\{\gamma_\mu(\nabla^*_\mu + \nabla_\mu) - a\nabla^*_\mu\nabla_\mu\}\,. \tag{I.1.43}$$

Here, forward and backward covariant derivatives,

$$\nabla_\mu \psi(x) = \tfrac{1}{a}[U(x,\mu)\psi(x+a\hat{\mu}) - \psi(x)], \tag{I.1.44}$$
$$\nabla^*_\mu \psi(x) = \tfrac{1}{a}[\psi(x) - U(x-a\hat{\mu},\mu)^{-1}\psi(x-a\hat{\mu})] \ , \tag{I.1.45}$$

are used and m_0 is to be understood as a diagonal matrix in flavor space with elements m_0^f.

The gauge field action $S_{\rm G}$ is a sum over all oriented plaquettes p on the lattice, with the weight factors $w(p)$, and the parallel transporters $U(p)$ around p,

$$S_{\rm G}[U] = \frac{1}{g_0^2}\sum_p w(p)\ {\rm tr}\,\{1 - U(p)\} \ . \tag{I.1.46}$$

The weights $w(p)$ are 1 for plaquettes in the interior and

$$w(p) = \begin{cases} \frac{1}{2}c_s & \text{if } p \text{ is a spatial plaquette at } x_0 = 0 \text{ or } x_0 = L, \\ c_t & \text{if } p \text{ is time-like and attached to a boundary plane.} \end{cases} \tag{I.1.47}$$

The choice $c_s = c_t = 1$ corresponds to the standard Wilson action. However, these parameters can be tuned in order to reduce lattice artifacts, as will be briefly discussed below.

With these ingredients, the path integral representation of the Schrödinger functional reads [18],

$$\mathcal{Z} = \int {\rm D}[\psi]{\rm D}[\bar{\psi}]{\rm D}[U]\,{\rm e}^{-S}\,, \quad S = S_{\rm F} + S_{\rm G} \ , \tag{I.1.48}$$
$${\rm D}[U] = \prod_{x,\mu} {\rm d}U(x,\mu) \ ,$$

with the Haar measure ${\rm d}U$.

I.1.8.1 Boundary conditions and the background field.

The boundary conditions for the lattice gauge fields may be obtained from the continuum boundary values by forming the appropriate parallel transporters from $x + a\hat{k}$ to x at $x_0 = 0$ and $x_0 = L$. For the constant abelian boundary fields C and C' that we considered before, they are simply

$$U(x,k)|_{x_0=0} = \exp(aC_k), \qquad U(x,k)|_{x_0=L} = \exp(aC'_k), \tag{I.1.49}$$

for $k = 1, 2, 3$. All other boundary conditions are as in the continuum.

For the case of eq. (I.1.22),eq. (I.1.23), the boundary conditions (I.1.49) lead to a unique (up to gauge transformations) minimal action configuration V, the lattice background field. It can be expressed in terms of B (I.1.24),

$$V(x,\mu) = \exp\{aB_\mu(x)\} \ . \tag{I.1.50}$$

I.1.8.2 Lattice artifacts.

Now we want to get a first impression about the dependence of the lattice SF on the value of the lattice spacing. In other words we study lattice artifacts. At lowest order in the bare coupling we have, just like in the continuum,

$$\Gamma = \frac{1}{g_0^2}\Gamma_0[V] + \mathrm{O}((g_0)^0)\,, \quad \Gamma_0[V] \equiv g_0^2 S_{\mathrm{G}}[V] \ . \tag{I.1.51}$$

Furthermore one easily finds the action for small lattice spacings,

$$\begin{aligned} S_{\mathrm{G}}[V] &= \left[1 + (1-c_{\mathrm{t}})\tfrac{2a}{L}\right] \frac{3L^4}{g_0^2} \sum_{\alpha=1}^{N} \left\{ \frac{2}{a^2} \sin\left[\frac{a^2}{2L^2}\left(\phi'_\alpha - \phi_\alpha\right)\right]\right\}^2 \\ &= \frac{3}{g_0^2}\sum_{\alpha=1}^{N}\left(\phi'_\alpha - \phi_\alpha\right)^2 \left[1 + (1-c_{\mathrm{t}})\tfrac{2a}{L} + \mathrm{O}(a^4)\right] \ . \end{aligned} \tag{I.1.52}$$

We observe: at tree-level of perturbation theory, all linear lattice artifacts are removed when one sets $c_{\mathrm{t}} = 1$. Beyond tree-level (and in the theory without quarks), one has to tune the coefficient c_{t} as a function of the bare coupling. We will show the effect, when this is done to first order in g_0^2, below. Note that the existence of linear $\mathrm{O}(a)$ errors in the Yang-Mills theory is special to the SF; they originate from dimension four operators $F_{0k}F_{0k}$ and $F_{kl}F_{kl}$ which are irrelevant terms (i.e. they carry an explicit factor of the lattice spacing) when they are integrated over the surfaces. c_{s}, which can be tuned to cancel the effects of $F_{kl}F_{kl}$, does not appear for the electric field that we discussed above.

Once quark fields are present, there are more irrelevant operators that can generate $\mathrm{O}(a)$ effects as discussed in detail in [19]. Here we emphasize a different feature of eq. (I.1.52): once the $\mathrm{O}(a)$-terms are canceled, the remaining a-effects are tiny. This special feature of the abelian background field is most welcome for the numerical computation of the running coupling; it allows for reliable extrapolations to the continuum limit.

I.1.8.3 Explicit expression for Γ'.

Let us finally explain that Γ' is an observable that can easily be calculated in a MC simulation. From its definition we find immediately

$$\Gamma' = -\frac{\partial}{\partial\eta}\ln\left\{\int \mathrm{D}[\psi]\mathrm{D}[\bar\psi]\mathrm{D}[U]\,\mathrm{e}^{-S}\right\} = \left\langle\frac{\partial S_{\mathrm{G}}}{\partial\eta}\right\rangle + \left\langle\frac{\partial S_{\mathrm{F}}}{\partial\eta}\right\rangle \ . \tag{I.1.53}$$

The derivative $\frac{\partial S_{\mathrm{G}}}{\partial\eta}$ evaluates to the (color 8 component of the) electric field at the boundary,

$$\frac{\partial S_{\mathrm{G}}}{\partial\eta} = -\frac{2}{g_0^2\,L}a^3\sum_{\mathbf{x}}\left\{E_k^8(\mathbf{x}) - (E_k^8)'(\mathbf{x})\right\} \ , \tag{I.1.54}$$

$$E_k^8(\mathbf{x}) = \frac{1}{a^2}\mathrm{Re\ tr}\left\{i\lambda_8 U(x,k)U(x+a\hat{k},0)U(x+a\hat{0},k)^{-1}U(x,0)^{-1}\right\}_{x_0=0} \ ,$$

where $\lambda_8 = \mathrm{diag}(1, -1/2, -1/2)$. (A similar expression holds for $(E^8_k)'(\mathbf{x})$). The second term $\frac{\partial S_\mathrm{F}}{\partial \eta}$, which is only non-zero in the O(a)-improved formulation is numerically less relevant. An explicit expression is given in [23].

The renormalized coupling is related to the expectation value of a local operator; no correlation function is involved. This means that it is easy and fast in computer time to evaluate it. It further turns out that a good statistical precision is reached with a moderate size statistical ensemble.

I.1.9 More literature

We here give some guide for further reading on the SF. Independently of the work of Symanzik, G. C. Rossi and M. Testa discussed different boundary conditions imposed at fixed time [24, 25]. The renormalization properties of that functional have not yet been discussed.

There are also rather recent developments. Different formulations of the lattice Schrödinger functional with overlap fermions satisfying the Ginsparg Wilson relation have been found by Y. Taniguchi using an orbifold construction [26], and by M. Lüscher using a general universality argument concerning QFT's with boundaries [14]; see also [27]. As the Schrödinger functional breaks chiral symmetry by the boundary conditions, it is relevant into which direction in flavor space the mass term is introduced. The Schrödinger functional with a twisted mass term [5, 6] and the boundary conditions specified above differs from the SF with a standard mass term (at finite quark mass). S. Sint found a modification of the boundary conditions, which yields the standard SF as the continuum limit of the lattice theory with a twisted mass [28]. An even number of flavors is required in this formulation. It offers also advantages in the massless limit, where "automatic bulk O(a)-improvement" is achieved *after the tuning of one counter-term*. It is discussed in detail in S. Sint's lectures at this school. Another Schrödinger functional with automatic bulk O(a)-improvement is proposed in [29].

I.2 Chiral symmetry and O(a)-improvement

The main focus of this section is on the O(a) improvement of Wilson's lattice QCD. However, we also mention the finite normalization of isovector currents. Both of these problems have the same origin, namely that chiral symmetry is broken in Wilson's regularization and then also the same solution: chiral Ward identities. The possibility to use these to normalize the currents has first been discussed by Refs. [20,30]. Here, we describe their application in the computation of the O(a)-improved action and currents. A difference to the aforementioned work is that we insist that only on-shell improvable correlation functions are used in the normalization conditions in order to be compatible with on-shell improvement.

Before going into more details, we would like to convey the general idea of the application of chiral Ward identities. For simplicity we assume an isospin doublet of

mass-degenerate quarks. Consider first a regularization of QCD which preserves the full $\mathrm{SU}(2)_\mathrm{V}\times\mathrm{SU}(2)_\mathrm{A}$ flavor symmetry as it is present in the continuum Lagrangian of massless QCD. Indeed, such regularizations exist [2–4], see Peter Hasenfratz' lectures.

We can derive chiral Ward identities in the Euclidean formulation of the theory. These then provide exact relations between different correlation functions. Immediate consequences of these relations are that there are currents V_μ^a, A_μ^a which do not get renormalized ($Z_\mathrm{A} = Z_\mathrm{V} = 1$) and the quark mass does not have an additive renormalization.

In a general discretization, such as the Wilson formulation, lattice QCD does *not* have the $\mathrm{SU}(2)_\mathrm{A}$ flavor symmetry for finite values of the lattice spacing. Then, the Ward identities are not satisfied exactly. From universality, we do, however, expect that the correlation functions may be renormalized such that they obey the same Ward identities as before – up to $\mathrm{O}(a)$ corrections. Therefore we may impose those Ward identities for the renormalized currents, to fix their normalizations.

Furthermore, following Symanzik [1], it suffices to a add a few local irrelevant terms to the action and to the currents in order to obtain an improved lattice theory, where the continuum limit is approached with corrections of order a^2. The coefficients of these terms can be determined by imposing improvement conditions. For example one may require certain chiral Ward identities to be valid at finite lattice spacing a.

I.2.1 Chiral Ward identities

For the moment we do not pay attention to a regularization of the theory and derive the Ward identities in a formal way. As mentioned above these identities are exact in a regularization that preserves chiral symmetry. To derive the Ward identities, one starts from the path integral representation of a correlation function and performs the change of integration variables

$$\begin{aligned}
\psi(x) &\to \mathrm{e}^{i\frac{\tau^a}{2}[\epsilon_\mathrm{A}^a(x)\gamma_5+\epsilon_\mathrm{V}^a(x)]}\psi(x) \\
&= \psi(x) + i\epsilon_\mathrm{A}^a(x)\delta_\mathrm{A}^a\psi(x) + i\epsilon_\mathrm{V}^a(x)\delta_\mathrm{V}^a\psi(x) \ , \\
\overline{\psi}(x) &\to \overline{\psi}(x)\mathrm{e}^{i\frac{\tau^a}{2}[\epsilon_\mathrm{A}^a(x)\gamma_5-\epsilon_\mathrm{V}^a(x)]} \\
&= \overline{\psi}(x) + i\epsilon_\mathrm{A}^a(x)\delta_\mathrm{A}^a\overline{\psi}(x) + i\epsilon_\mathrm{V}^a(x)\delta_\mathrm{V}^a\overline{\psi}(x) \ ,
\end{aligned} \tag{I.2.1}$$

where we have taken $\epsilon_\mathrm{A}^a(x), \epsilon_\mathrm{V}^a(x)$ infinitesimal and introduced the variations

$$\begin{aligned}
\delta_\mathrm{V}^a\psi(x) &= \tfrac{1}{2}\tau^a\psi(x), \qquad & \delta_\mathrm{V}^a\overline{\psi}(x) &= -\overline{\psi}(x)\tfrac{1}{2}\tau^a \ , \\
\delta_\mathrm{A}^a\psi(x) &= \tfrac{1}{2}\tau^a\gamma_5\psi(x), \qquad & \delta_\mathrm{A}^a\overline{\psi}(x) &= \overline{\psi}(x)\gamma_5\tfrac{1}{2}\tau^a \ .
\end{aligned} \tag{I.2.2}$$

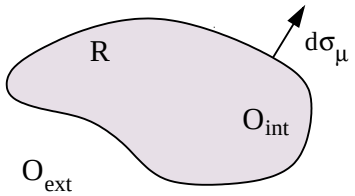
The Ward identities then follow from the invariance of the path integral representation of correlation functions with respect to such changes of integration variables. They obtain contributions from the variation of the action and the variations of the fields in the correlation functions. The variations of the currents

$$V_\mu^a(x) = \overline{\psi}(x)\gamma_\mu\tfrac{1}{2}\tau^a\psi(x) \tag{I.2.3}$$

and A^a_μ, eq. (I.1.34), is given by

$$\begin{aligned} \delta^a_{\rm V} V^b_\mu(x) &= -i\epsilon^{abc} V^c_\mu(x), \qquad \delta^a_{\rm A} V^b_\mu(x) = -i\epsilon^{abc} A^c_\mu(x), \\ \delta^a_{\rm V} A^b_\mu(x) &= -i\epsilon^{abc} A^c_\mu(x), \qquad \delta^a_{\rm A} A^b_\mu(x) = -i\epsilon^{abc} V^c_\mu(x) \ . \end{aligned} \tag{I.2.4}$$

They form a closed algebra under these variations.



Since this is convenient for our applications, we write the Ward identities in an integrated form. Let R be a space-time region with smooth boundary ∂R. Suppose $\mathcal{O}_{\rm int}$ and $\mathcal{O}_{\rm ext}$ are polynomials in the basic fields localized in the interior and exterior of R respectively (see left). The general vector current Ward identity then reads

$$\int_{\partial R} {\rm d}\sigma_\mu(x) \, \left\langle V^a_\mu(x) \mathcal{O}_{\rm int} \mathcal{O}_{\rm ext} \right\rangle = - \left\langle (\delta^a_{\rm V} \mathcal{O}_{\rm int}) \, \mathcal{O}_{\rm ext} \right\rangle , \tag{I.2.5}$$

while for the axial current one obtains

$$\begin{aligned} \int_{\partial R} {\rm d}\sigma_\mu(x) \, \left\langle A^a_\mu(x) \mathcal{O}_{\rm int} \mathcal{O}_{\rm ext} \right\rangle &= - \left\langle (\delta^a_{\rm A} \mathcal{O}_{\rm int}) \, \mathcal{O}_{\rm ext} \right\rangle \\ &\quad + 2m \int_R {\rm d}^4x \, \left\langle P^a(x) \mathcal{O}_{\rm int} \mathcal{O}_{\rm ext} \right\rangle \ . \end{aligned} \tag{I.2.6}$$

Here volume integrals over for example $\partial_\mu A^a_\mu(x)$ have been changed to surface integrals. The integration measure ${\rm d}\sigma_\mu(x)$ points along the outward normal to the surface ∂R and $P^a(x)$ was defined in eq. (I.1.35).

We may also write down the precise meaning of the PCAC-relation eq. (I.1.36). It is eq. (I.2.6) in a differential form,

$$\left\langle \left[\partial_\mu A^a_\mu(x) - 2m P^a(x) \right] \mathcal{O}_{\rm ext} \right\rangle = 0 \ , \tag{I.2.7}$$

where now $\mathcal{O}_{\rm ext}$ may have support everywhere except for at the point x.

Going through the same derivation in the lattice regularization, one finds equations of essentially the same form as the ones given above, but with additional terms [20]. At the classical level these terms are of order a. More precisely, in eq. (I.2.7) the important additional term originates from the variation of the Wilson term, $a\,\delta^a_{\rm A}(\overline{\psi}\nabla^*_\mu\nabla_\mu\psi)$, and is a local field of dimension 5. Such O(a)-corrections are present in any observable computed on the lattice and are no reason for concern. However, as is well known in field theory, such operators mix with the ones of lower and equal dimensions when one goes beyond the classical approximation. In the present case, the dimension five operator mixes among others also with $\partial_\mu A^a_\mu(x)$ and $P^a(x)$. This means that part of the classical O(a)-terms turn into O(g_0^2) in the quantum theory. The essential observation is now that this mixing can simply be written in the form of a renormalization of the

terms that are already present in the Ward identities, since all dimension three and four operators with the right quantum number are already there.

We conclude that the identities, which we derived above in a formal manner, are valid in any proper lattice regularization after

- replacing the bare fields A, V, P and quark mass m_0 by renormalized ones, where one must allow for the most general renormalizations,

$$\begin{aligned} (A_{\rm R})^a_\mu &= Z_{\rm A} A^a_\mu \ , \quad (V_{\rm R})^a_\mu = Z_{\rm V} V^a_\mu \ , \\ (P_{\rm R})^a &= Z_{\rm P} P^a \ , \quad m_{\rm R} = Z_{\rm m} m_{\rm q} \, , \quad m_{\rm q} = m_0 - m_c \ , \end{aligned}$$

- allowing for the usual $\mathrm{O}(a)$ lattice artifacts.

Note that the additive quark mass renormalization m_c diverges like $\mathrm{O}(g_0^2/a)$ for dimensional reasons.

As a result of this discussion, the formal Ward identities may be used to determine the normalizations of the currents. We refer the reader to [21,31] for details and explain here the general idea how one can use the Ward identities to determine improvement coefficients.

I.2.2 On-shell $\mathrm{O}(a)$-improvement

I.2.2.1 Motivation

Let us first recall why one wants to remove lattice spacing effects linear in a. The prime reason is as follows. If linear effects are present, one has to vary a in the numerical simulations over a large range in order to be able to get a reasonable estimate of their magnitude.[8] In contrast if the cutoff effects are $\mathrm{O}(a^2)$, a range of $0.05\,\mathrm{fm} \leq a \leq 0.1\,\mathrm{fm}$ typically allows to check well whether they contribute significantly. In fact a reasonably well controlled extrapolation to the continuum can then be done allowing for a term proportional to a^2 and also a smaller range in a may be sufficient. Examples can be found e.g. in [33]. In addition, it does turn out that linear a effects can be quite large. Let us give here just two examples.

The first one is the current quark mass m defined by the PCAC relation. As detailed below, its value is independent of kinematical variables such as the boundary conditions. Dependences on such variables are pure lattice artifacts. We examined the current quark mass in the valence approximation by numerical Monte Carlo simulations and found large lattice artifacts even for quite small lattice spacings [32] (cf. fig. 3).

The second example is the mass of the vector meson, made dimensionless by multiplying with r_0. This quantity has large cutoff effects in the quenched approximation [34]. Depending on the quark mass, a-effects of around 20% and more are seen at $a \approx 0.15\,\mathrm{fm}$; see for example Fig. 1 of [34], Fig. 1 of [35].

[8] Obviously it does not really help to have a large range by considering large values of a. Then one enters the regime where either the higher order terms are significant or – more likely – the whole asymptotic expansion in a breaks down.

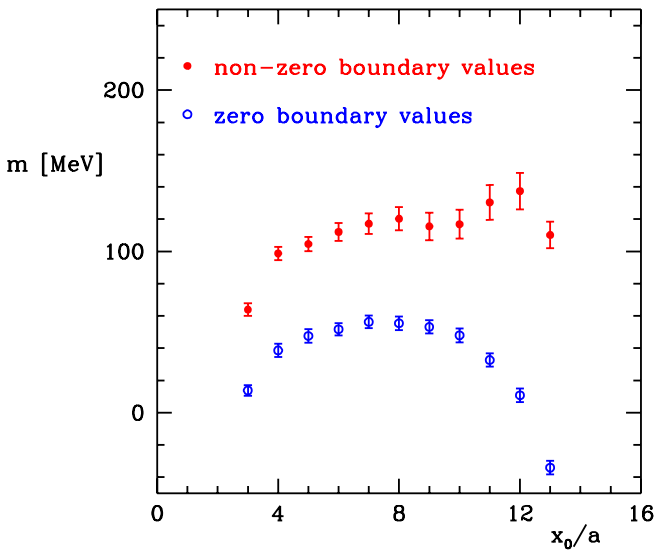


Figure 3: Dependence of current quark mass m on the boundary condition and the time coordinate [32]. The calculation is done in the quenched approximation on a 16×8^3 lattice at $\beta = 6.4$, which corresponds to a lattice spacing of $a \approx 0.05\,\mathrm{fm}$. "Boundary values" refer to the gauge field boundary conditions in the SF. Their values are given in [32].

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I.2.2.2 A warning from two dimensions

Before entering the discussion of the O(a) improvement programme, we mention some unexpected results from thorough examinations of 2-d O(N) sigma models. The theoretical basis for the discussion and removal of a-effects is Symanzik's effective theory, see Sect. I.2.2.3. O(N) sigma models were the second class of models investigated by Symanzik in order to establish this theory. For these models the basic statement is that (up to logarithmic modifications) the cutoff effects are quadratic in a, when a is small enough.

It therefore came as a surprise that Hasenfratz and Niedermayer found in a numerical study of the Lüscher-Weisz-Wolff (LWW) renormalized coupling [37] of the 2-d O(3) sigma model that its step scaling function shows an a-dependence which is roughly linear in a for quite small a (large correlation length) [38]. With a further improved algorithm, a Bern-Berlin collaboration confirmed this behavior with even higher precision and smaller lattice spacing [36]. We show their result in Fig. 4. On the other hand it was known that the cutoff effects of the step scaling function are O(a^2) in the large N limit of the O(N) models [37]. Subsequent numerical studies for $N = 4, 8$ showed no conclusive results: just like in the $N = 3$ case, the cutoff effects look linear when judged by eye, but they can also be fitted with O(a^2) functions, in particular when the

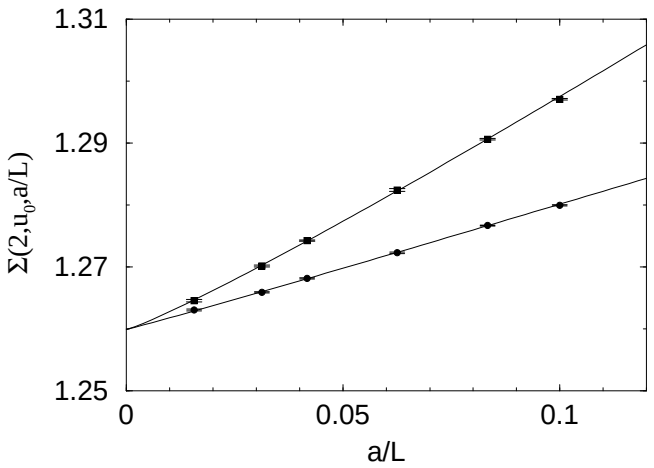


Figure 4: Lattice spacing dependence of the step scaling function of the LWW coupling in the 2-d O(3) sigma model [36] for coupling $u_0 = 1.0595$. The data points with the smaller cutoff effects are for the standard nearest neighbor action.

expected logarithmic modifications are taken into account [39].

Later the $1/N$ correction was worked out at finite lattice spacing [39]. Recall that at order $(1/N)^0$ one has $O(a^2)$ effects. The cutoff effect proportional to $1/N$ is shown in Fig. 5. Over a large range in a it is almost a linear function of a, but close to $a = 0$ it is dominated by an $O(a^2)$ term. Thus our personal conclusion is that there is no conflict with Symanzik's effective theory in the $O(N)$ models. One should also note that all the a-effects discussed here are rather small.

However, there is a clear warning that, depending on model and observable, the lattice spacing may have to be rather small for the leading correction term in the effective theory to dominate. On the more practical side, long continuum extrapolations with significant slopes may be dangerous, since in QCD we do not have much information where the asymptotic expansion in a is accurate [40]. This is one of the reasons why we will spend much time on understanding the cutoff effects in the QCD step scaling function of the coupling in Sect. II.2.2 and Sect. II.2.3.

I.2.2.3 Symanzik's local effective theory (SET)

In the following explanation of the theory we follow quite closely [19]. We consider QCD on an infinitely extended lattice with two degenerate light Wilson quarks of bare mass m_0 [41]. The action is then given as in Sect. I.1.8 except that no boundary conditions or boundary terms are necessary.

Quite some time ago, Symanzik provided arguments that a lattice theory can be described in terms of a local effective theory, when the lattice spacing is small enough [1].

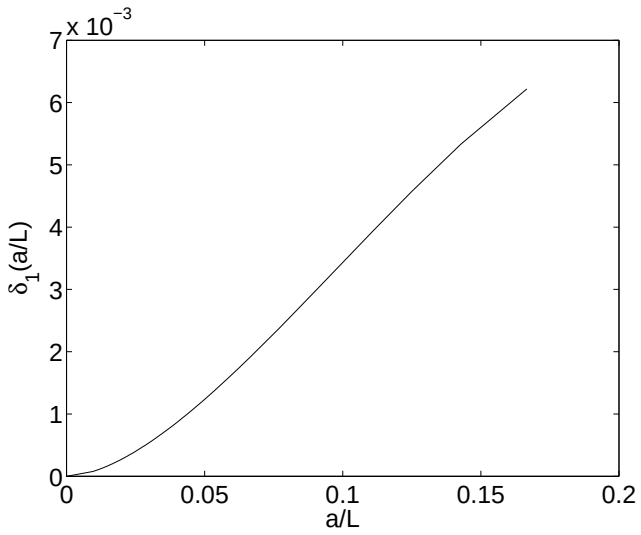


Figure 5: Coefficient of $1/N$ in the $1/N$-expansion of the cutoff effects of the step scaling function of the LWW coupling of 2-d O(N) sigma models. Graph prepare by U. Wolff based on [39].

The effective action,

$$S_{\rm eff} = S_0 + aS_1 + a^2 S_2 + \dots \,, \tag{I.2.8}$$

has as a leading order, S_0, the action of the continuum theory [9]. The terms S_k, $k = 1, 2, \dots$, are space-time integrals of Lagrangians $\mathcal{L}_k(x)$. These are given as general linear combinations of local gauge-invariant composite fields which respect the exact symmetries of the lattice theory and have canonical dimension $4 + k$. We use the convention that explicit (non-negative) powers of the quark mass m are included in the dimension counting. A possible basis of fields for the Lagrangian $\mathcal{L}_1(x)$ reads

$$\begin{aligned}
\mathcal{O}_1 &= \overline{\psi}\,\sigma_{\mu\nu}F_{\mu\nu}\psi, \\
\mathcal{O}_2 &= \overline{\psi}\,D_\mu D_\mu\psi + \overline{\psi}\,\overleftarrow{D}_\mu\overleftarrow{D}_\mu\psi, \\
\mathcal{O}_3 &= m\,\mathrm{tr}\left\{F_{\mu\nu}F_{\mu\nu}\right\}, \\
\mathcal{O}_4 &= m\left\{\overline{\psi}\,\gamma_\mu D_\mu\psi - \overline{\psi}\,\overleftarrow{D}_\mu\gamma_\mu\psi\right\}, \\
\mathcal{O}_5 &= m^2\overline{\psi}\psi,
\end{aligned} \tag{I.2.9}$$

where $F_{\mu\nu}$ is the gluon field tensor and $\sigma_{\mu\nu} = \frac{i}{2}[\gamma_\mu, \gamma_\nu]$.

When considering correlation functions of local gauge invariant fields the action is not the only source of cutoff effects. If $\phi(x)$ denotes such a lattice field (e.g. the axial density or the isospin currents), one expects the connected n-point function

$$G_n(x_1, \dots, x_n) = (Z_\phi)^n \left\langle \phi(x_1) \dots \phi(x_n) \right\rangle_{\rm con} \tag{I.2.10}$$

[9] If more rigor is desired one may define it on a lattice with spacing $\varepsilon \ll a$.

to have a well-defined continuum limit, provided the renormalization constant Z_ϕ is correctly tuned and the space-time arguments $x_1, \ldots, x_n$ are kept at a physical distance from each other.

In the effective theory the renormalized lattice field $Z_\phi \phi(x)$ is represented by an effective field,

$$\phi_{\text{eff}}(x) = \phi_0(x) + a\phi_1(x) + a^2\phi_2(x) + \ldots, \tag{I.2.11}$$

where the $\phi_k(x)$ are linear combinations of composite, local fields with the appropriate dimension and symmetries. For example, in the case of the axial current (I.1.34), ϕ_1 is given as a linear combination of the terms

$$\begin{aligned} (\mathcal{O}_6)^a_\mu &= \overline{\psi}\,\gamma_5 \tfrac{1}{2}\tau^a \sigma_{\mu\nu}[D_\nu - \overleftarrow{D}_\nu]\psi, \\ (\mathcal{O}_7)^a_\mu &= \overline{\psi}\,\tfrac{1}{2}\tau^a \gamma_5 [D_\mu + \overleftarrow{D}_\mu]\psi, \\ (\mathcal{O}_8)^a_\mu &= m\overline{\psi}\,\gamma_\mu\gamma_5 \tfrac{1}{2}\tau^a \psi. \end{aligned} \tag{I.2.12}$$

The convergence of $G_n(x_1, \ldots, x_n)$ to its continuum limit can now be studied in the effective theory,

$$\begin{aligned} G_n(x_1, \ldots, x_n) &= \langle \phi_0(x_1) \ldots \phi_0(x_n) \rangle_{\text{con}} \\ &\quad - a \int \mathrm{d}^4 y \, \langle \phi_0(x_1) \ldots \phi_0(x_n) \mathcal{L}_1(y) \rangle_{\text{con}} \\ &\quad + a \sum_{k=1}^{n} \langle \phi_0(x_1) \ldots \phi_1(x_k) \ldots \phi_0(x_n) \rangle_{\text{con}} \, + \, \mathrm{O}(a^2), \end{aligned} \tag{I.2.13}$$

where the expectation values on the right-hand side are to be taken in the continuum theory with action S_0.

Using the field equations

For most applications, it is sufficient to compute on-shell quantities such as particle masses, S-matrix elements and correlation functions at space-time arguments, which are separated by a physical distance. It is then possible to make use of the field equations to reduce first the number of basis fields in the effective Lagrangian $\mathcal{L}_1$ and, in a second step, also in the $\mathrm{O}(a)$ counter-term ϕ_1 of the effective composite fields.

Of course, in the quantum theory, the field equations have to be used with care. Performing changes in the integration variables of the path integral shows immediately that the field equations are only valid up to additional terms. In particular, if one uses the field equations in the Lagrangian $\mathcal{L}_1$ under the space-time integral in eq. (I.2.13), the errors made are contact terms that arise when y comes close to one of the arguments $x_1, \ldots, x_n$. Using the operator product expansion and the dimensions and symmetries, one easily verifies that these contact terms must have the same structure as the insertions of ϕ_1 in the last term of eq. (I.2.13). The use of the field equations in $\mathcal{L}_1$ therefore just means a redefinition of the coefficients in the counter-term ϕ_1 (apart from contributions

that are absorbed in the renormalization factor Z_ϕ, which originate from the mixing of ϕ_1 with ϕ).

It turns out that one may eliminate two of the terms in eq. (I.2.9) by using the field equations. A possible choice is to stay with the terms $\mathcal{O}_1$, $\mathcal{O}_3$ and $\mathcal{O}_5$, which yields the effective continuum action for on-shell quantities to order a. Having made this choice one may apply the field equations once again to simplify the term ϕ_1 in the effective field as well. In the example of the axial current it is then possible to eliminate the term $\mathcal{O}_6$ in eq. (I.2.12).

I.2.2.4 Improved lattice action and fields

The on-shell O(a) improved lattice action is obtained by adding a counter-term to the unimproved lattice action such that the effects of the action S_1 in the effective theory are canceled in on-shell amplitudes. This can be achieved by adding lattice representatives of the terms $\mathcal{O}_1$, $\mathcal{O}_3$ and $\mathcal{O}_5$ to the unimproved lattice Lagrangian, with coefficients that are functions of the bare coupling g_0 only. Leaving the discussion of suitable improvement conditions for later, we here note that the fields $\mathcal{O}_3$ and $\mathcal{O}_5$ already appear in the unimproved theory and thus merely lead to a re-parametrization of the bare parameters g_0 and m_0. In the following, we will not consider these terms any further. Their relevance in connection with massless renormalization schemes is discussed in detail in Ref. [19].

We choose the standard discretization $\widehat{F}_{\mu\nu}$ of the field tensor [19] and add the improvement term to the Wilson-Dirac operator, eq. (I.1.43),

$$D_{\rm impr} = D + c_{\rm sw}\,\frac{ia}{4}\sigma_{\mu\nu}\widehat{F}_{\mu\nu}. \tag{I.2.14}$$

With a properly chosen coefficient $c_{\rm sw}(g_0)$, this yields the on-shell O(a) improved lattice action which has first been proposed by Sheikholeslami and Wohlert [42].

The perturbative expansion of $c_{\rm sw}$ reads $c_{\rm sw} = 1 + c_{\rm sw}^{(1)} g_0^2 + \mathrm{O}(g_0^4)$, with [43, 44] $c_{\rm sw}^{(1)} = 0.26590(7)$ where the Wilson plaquette gauge action is assumed.

The O(a) improved isospin currents and the axial density can be parametrized as follows,

$$\begin{aligned}
(A_{\rm R})^a_\mu &= Z_{\rm A}(1 + b_{\rm A} a m_{\rm q})\{A^a_\mu + a c_{\rm A}\tilde{\partial}_\mu P^a\},\\
(V_{\rm R})^a_\mu &= Z_{\rm V}(1 + b_{\rm V} a m_{\rm q})\{V^a_\mu + a c_{\rm V}\tilde{\partial}_\nu T^a_{\mu\nu}\},\\
(P_{\rm R})^a &= Z_{\rm P}(1 + b_{\rm P} a m_{\rm q})P^a\,,
\end{aligned} \tag{I.2.15}$$

where

$$T^a_{\mu\nu} = i\overline{\psi}\sigma_{\mu\nu}\tfrac{1}{2}\tau^a\psi\,.$$

We have included the normalization constants $Z_{\rm A,V,P}$, which have to be fixed by appropriate normalization conditions. Again, the improvement coefficients $b_{\rm A,V,P}$ and $c_{\rm A,V}$ are functions of g_0 only. At tree level of perturbation theory, they are given by

$b_{\rm A} = b_{\rm P} = b_{\rm V} = 1$ and $c_{\rm A} = c_{\rm V} = 0$ [19, 45] and to 1-loop accuracy and with the plaquette gauge action we have [43, 46]

$$\begin{aligned} c_{\rm A} &= -0.005680(2) \times g_0^2 C_{\rm F} + {\rm O}(g_0^4), \\ c_{\rm V} &= -0.01225(1) \times g_0^2 C_{\rm F} + {\rm O}(g_0^4), \\ b_{\rm A} &= 1 + 0.11414(4) \times g_0^2 C_{\rm F} + {\rm O}(g_0^4), \\ b_{\rm V} &= 1 + 0.11492(4) \times g_0^2 C_{\rm F} + {\rm O}(g_0^4), \\ b_{\rm P} &= 1 + 0.11484(2) \times g_0^2 C_{\rm F} + {\rm O}(g_0^4). \end{aligned} \tag{I.2.16}$$

Here $C_{\rm F} = 4/3$. Non-perturbative determinations will be mentioned below.

I.2.3 The PCAC relation

We assume for the moment that on-shell ${\rm O}(a)$ improvement has been fully implemented, i.e. the improvement coefficients are assigned their correct values. If $\mathcal{O}$ denotes a renormalized on-shell ${\rm O}(a)$ improved field localized in a region not containing x, we thus expect that the PCAC relation,

$$\tilde{\partial}_\mu \langle (A_{\rm R})^a_\mu(x)\, \mathcal{O} \rangle = 2m_{\rm R} \langle (P_{\rm R})^a(x)\, \mathcal{O} \rangle \tag{I.2.17}$$

$$\tilde{\partial}_\mu = \tfrac{1}{2}(\partial^*_\mu + \partial_\mu) \tag{I.2.18}$$

holds up to corrections of order a^2. At this point we note that the field $\mathcal{O}$ need not be improved for this statement to be true. To see this we use again Symanzik's local effective theory and denote the ${\rm O}(a)$ correction term in $\mathcal{O}_{\rm eff}$ by ϕ_1. Eq. (I.2.17) then receives an order a contribution

$$a \langle \Big\{ \partial_\mu (A_{\rm R})^a_\mu(x) - 2m_{\rm R} (P_{\rm R})^a(x) \Big\}\, \phi_1 \rangle, \tag{I.2.19}$$

which is to be evaluated in the continuum theory. The PCAC relation holds exactly in the continuum and the extra term (I.2.19) thus vanishes, a conclusion that holds also in the Schrödinger functional.

I.2.4 Non-perturbative improvement

The coefficients of the different improvement terms need to be fixed by suitable improvement conditions. One considers pure lattice artifacts, i.e. combinations of observables that are known to vanish in the continuum limit of the theory. Improvement conditions require these lattice artifacts to vanish, thus defining the values of the improvement coefficients as a function of the lattice spacing.

In perturbation theory, lattice artifacts can be obtained from any (renormalized) quantity by subtracting its value in the continuum limit. The improvement coefficients are unique and some of them have been cited above.

Beyond perturbation theory, one wants to determine the improvement coefficients by MC calculations and it requires significant effort to take the continuum limit. It

is therefore advantageous to use lattice artifacts that derive from a symmetry of the continuum field theory that is not respected by the lattice regularization. One may require rotational invariance of the static potential $V(\mathbf{r})$, e.g.

$$V(\mathbf{r} = (2,2,1)r/3) - V(\mathbf{r} = (r,0,0)) = 0\,,$$

or Lorentz invariance,

$$[E(\mathbf{p})]^2 - [E(\mathbf{0})]^2 - \mathbf{p}^2 = 0\,,$$

for the momentum dependence of a one-particle energy E.

For $\mathrm{O}(a)$ improvement of QCD it is advantageous to use violations of the PCAC relation (I.2.7), instead. PCAC can be used in the context of the Schrödinger functional (SF), where one has a large flexibility to choose appropriate improvement conditions and can compute the improvement coefficients also for small values of the bare coupling g_0, making contact with their perturbative expansions. A further – and maybe the most significant – advantage of the SF in this context is the following. As we have seen earlier, in the SF we may choose boundary conditions such that the induced background field, has non-vanishing components $F_{\mu\nu}$. Remembering eq. (I.2.14), we observe that correlation functions are then sensitive to the improvement coefficient c_{sw} already at tree level of perturbation theory. With a vanishing background field this would be the case at higher orders only. Also in the non-perturbative regime this is the basis for a good sensitivity of the improvement conditions to c_{sw}.

As a consequence of the freedom to choose improvement conditions, the resulting values of improvement coefficients such as c_{sw}, c_{A} depend on the exact choices made. The corresponding variation of c_{sw}, c_{A} is of order a. It changes the effects of order a^2 in physical observables computed after improvement. We will come back to this point, but first we proceed to sketch the non-perturbative calculation of the coefficient c_{sw} [19, 43].

We define a bare current quark mass, m, viz.

$$m \equiv \frac{\left\langle \left[\partial_\mu (A_{\mathrm{I}})^a_\mu(x)\right] \mathcal{O}^a \right\rangle}{2\left\langle P^a(x)\mathcal{O}^a\right\rangle}\,, \quad (A_{\mathrm{I}})^a_\mu = A^a_\mu + a c_{\mathrm{A}} \tfrac{1}{2}(\partial_\mu + \partial^*_\mu) P^a \tag{I.2.20}$$

with the pseudo scalar boundary operator $\mathcal{O}^a$ from eq. (I.1.39). When all improvement coefficients have their proper values, the renormalized quark mass, defined by the renormalized PCAC-relation, is related to m by

$$m_{\mathrm{R}} = \frac{Z_{\mathrm{A}}(1 + b_{\mathrm{A}} a m_{\mathrm{q}})}{Z_{\mathrm{P}}(1 + b_{\mathrm{P}} a m_{\mathrm{q}})} m + \mathrm{O}(a^2)\ . \tag{I.2.21}$$

It now suffices to choose 3 different versions of eq. (I.2.20) by different choices of the time coordinate x_0 and/or boundary conditions and obtain 3 different values of m, denoted by m_1, m_2, m_3. Since the prefactor in front of m in eq. (I.2.21) is just a numerical factor, we may conclude that all m_i have to be equal in the improved theory up to errors of

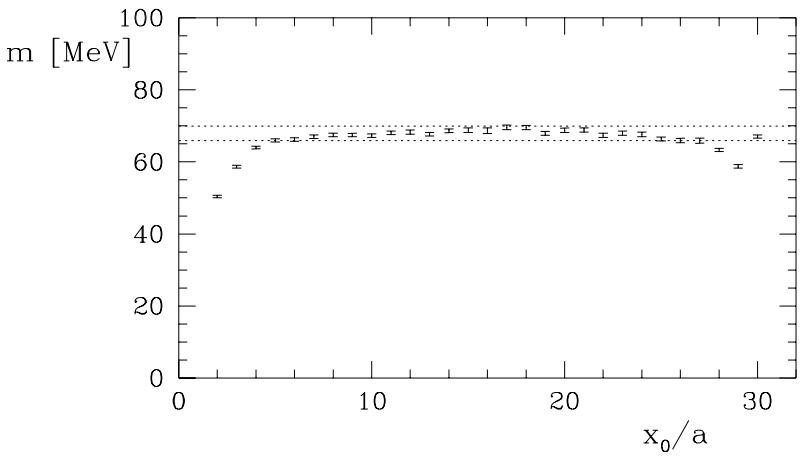


Figure 6: Unrenormalized current quark mass m in the improved theory, with non-perturbatively determined $c_{\rm sw}$ and $c_{\rm A}$, as a function of the time x_0 on a 32×16^3 lattice at $\beta = 6.2$ ($a \approx 0.07\,$fm)and $\kappa = 0.1350$. The width of the corridor bounded by the dotted horizontal lines is 4 MeV.

order a^2. $c_{\rm sw}$ and $c_{\rm A}$ may therefore be computed by requiring [10]

$$m_1 = m_2 = m_3 \ . \tag{I.2.22}$$

This simple idea has first been used to compute $c_{\rm sw}$ and $c_{\rm A}$ as a function of g_0 in the quenched approximation [19]. A good accuracy has been reached in these determinations for $a \leq 0.1\,$fm. We comment on more recent determinations below, after showing some tests of the effectiveness of O(a)-improvement, namely the test whether cutoff effects are indeed significantly reduced in practical calculations.

Verification of O(a)*-improvement*

The first test of the size of residual O(a^2) effects is provided again by the PCAC relation. To set the scale, remember that the cutoff effects in the PCAC mass m were as large as several tens of MeV before improvement (cf. fig. 3). The situation after improvement, and for a somewhat larger value of the lattice spacing, is illustrated in fig. 6. Away from the boundaries, where the effect of states with energies of the order of the cutoff induces noticeable effects, m is independent of time to within $\pm 2\,$MeV. Compared to the situation before O(a) improvement, this is a change by more than an order of magnitude.

The second test is in the scaling of the vector meson mass, which is improved dramatically in the quenched approximation. In the range $0.01 \leq a^2/r_0^2 \leq 0.035$ ($a \leq$

[10] In the practical calculations actually four different masses m_i were used to compute $c_{\rm sw}$ and two more to extract $c_{\rm A}$.

0.1 fm)[11] and with statistical errors of 1-3%, no a effect was found (see Fig. 3, Ref. [33]). This is a significant test because i) the a-effects were large before improvement, ii) the statistical precision is good and iii) a^2 varies by more than a factor 3.

In the quenched approximation several other tests of cutoff effects in the improved theory have been carried out [33, 48] revealing that O(a)-improvement works. More precisely we mean by this that for $a \leq 0.1$ fm cutoff effects found after improvement are generally reasonably small (O(5 %)) and well compatible with an O(a^2) behavior. Still, no miracles have been achieved: at $a \approx 0.1$ fm also cutoff effects of about 15% have been found [33].

We now proceed to discuss a rather relevant detail in the non-perturbative determination of improvement coefficients.

I.2.4.1 The constant physics condition

We have mentioned before that beyond perturbation theory the improvement coefficients are not unique; they depend on the improvement condition. This ambiguity is of O(a) in the coefficients and then of O(a^2) in the physical observables after improvement. So everything is correct, but if these ambiguities are large, one has to take extra care.

To give an explicit example, consider the quenched approximation but with non-degenerate quark masses, $m_{\mathrm{R},i} \neq m_{\mathrm{R},j}$. In this theory the renormalized, improved currents and axial densities are given by a straight forward generalization of what we wrote down earlier [49],

$$\begin{aligned}(A_{\mathrm{R}})^{ij}_{\mu} &= Z_{\mathrm{A}}(1+b_{\mathrm{A}}\tfrac{1}{2}(am_{\mathrm{q},i}+am_{\mathrm{q},j}))\{A^{ij}_{\mu}+ac_{\mathrm{A}}\tilde{\partial}_{\mu}P^{ij}\},\\ (P_{\mathrm{R}})^{ij} &= Z_{\mathrm{P}}(1+b_{\mathrm{P}}\tfrac{1}{2}(am_{\mathrm{q},i}+am_{\mathrm{q},j}))P^{ij}\,, \qquad \text{(I.2.23)}\\ A^{ij}_{\mu} &= \overline{\psi}_i\gamma_{\mu}\gamma_5\psi_j\,, \quad P^{ij}=\overline{\psi}_i\gamma_5\psi_j\,,\end{aligned}$$

and the bare quark masses, $m_{0,i}$, of the Lagrangian are related to the renormalized ones via [12]

$$m_{\mathrm{R},i} = \frac{Z_{\mathrm{A}}}{Z_{\mathrm{P}}}\,Z\,m_{\mathrm{q},i}(1+a\,b_{\mathrm{m}}m_{\mathrm{q},i})\,, \quad m_{\mathrm{q},i}=m_{0,i}-m_{\mathrm{c}}\,. \qquad \text{(I.2.24)}$$

One then derives the (unrenormalized) PCAC relation [49]

$$\begin{aligned}&\frac{\partial_{\mu}A^{ij}_{\mu}+a\partial^{*}_{\mu}\partial_{\mu}P^{ij}}{P^{ij}}[1+a\tfrac{1}{2}(b_{\mathrm{A}}-b_{\mathrm{P}})\,(m_{\mathrm{q},i}+m_{\mathrm{q},j})]\\ &= Z\,[m_{\mathrm{q},i}+m_{\mathrm{q},j}+a\,b_{\mathrm{m}}(m^2_{\mathrm{q},i}+m^2_{\mathrm{q},j})]+\mathrm{O}(a^2)\,. \qquad \text{(I.2.25)}\end{aligned}$$

This operator identity has to be understood as in eq. (I.2.17). Applying it with a few external operators/kinematical conditions, one can extract $b_{\mathrm{A}}-b_{\mathrm{P}}$, b_{m} and Z [49, 50].

[11] We use the reference scale r_0 defined in terms of the static quark potential. [47] It has a phenomenological value of $r_0 \approx 0.5$ fm.

[12] In the improved action, b_{m} is the coefficient of the field $\mathcal{O}_5$.

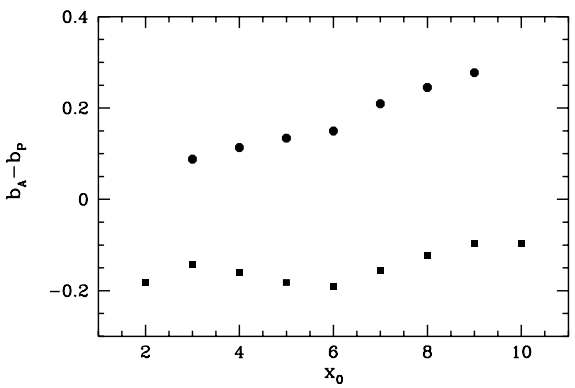


Figure 7: The improvement coefficient $b_{\rm A} - b_{\rm P}$ extracted on a 12×8^3 lattice and a lattice spacing of $a \approx 0.1\,$fm. Axial current and density are inserted at distance x_0. Squares are obtained with standard lattice representatives of the derivatives ∂_μ and $\partial^*_\mu \partial_\mu$, while circles come from improved (and therefore less local) derivatives [51].

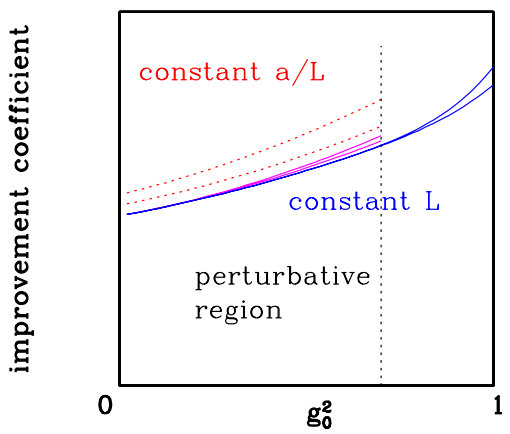
Suitable correlation functions have been implemented in the Schrödinger functional . As shown in Fig. 7, the result for $b_{\rm A} - b_{\rm P}$ at $a \approx 0.1\,$fm does depend a lot on the details, namely here x_0 and the exact lattice representation of derivatives. This is an extreme example of an improvement coefficient that is difficult to determine. The reasons are surely that the $\mathrm{O}(a)$-effects are not dominating over the $\mathrm{O}(a^2)$ effects in the considered correlation functions. Presumably the $\mathrm{O}(a)$-effects are just not very large. We proceed to discuss what one should do in these cases.

When the improvement conditions are formulated through Schrödinger functional correlation functions, we can also study them in perturbation theory. One chooses kinematical variables such as $T/L\,, x_0/L$ exactly as in the non-perturbative set up. One then computes the expansion of an improvement coefficient, here denoted generically by b, as a series

$$b(g_0, a/L) \sim b^{(0)}(a/L) + g_0^2\, b^{(1)}(a/L) + \mathrm{O}(g_0^4)\,. \tag{I.2.26}$$

Taking the case of $b_{\rm A} - b_{\rm P}$ and $L/a = 8, T/a = 12$ as in Fig. 7, the perturbative coefficients $b^{(0)}$, $b^{(1)}$ show a similar dependence on the kinematics as the non-perturbative results [51].

While generically the functions $b^{(0)}(a/L)$, $b^{(1)}(a/L)$ depend on the kinematical choices made in the improvement coefficients, the values $b^{(0)}(0)$, $b^{(1)}(0)$ are unique. This is the precise meaning of our earlier statement that improvement coefficients are unique in perturbation theory.



Generic behavior of improvement coefficients. Dotted lines correspond to two different improvement conditions at fixed a/L, while the full lines are for fixed L in physical units.

On the left we illustrates what happens generically. The continuous lines correspond to two different improvement conditions at *constant physics*. By this we mean that all length scales in the correlation functions which define the improvement condition are kept fixed in physical units, for example in units of r_0. When g_0 is varied, only the lattice spacing a changes and this is the situation to which the SET can be applied. The two different improvement coefficients then very rapidly go to an almost unique function of g_0 as $g_0 \to 0$.

On the other hand, one may want to set improvement conditions at fixed L/a for practical reasons[13]. In this setting, the $\mathrm{O}(a)$ ambiguity in the improvement coefficients does not go to zero as $g_0 \to 0$ (and $a \to 0$) (dotted lines).

If the dependence of $b^{(i)}(a/L)$ on a/L is rather weak, say

$$|b^{(i)}(a/L) - b^{(i)}(0)| \ll 10^{-1}\,, \tag{I.2.27}$$

for the relevant a/L, one may also choose fixed a/L. Still it is clear from our discussion that fixed L/r_0 is to be preferred whenever possible. In cases where it is advantageous to work at finite quark masses, also the combination $r_0\, m_{\mathrm{R},i}$ should be kept constant. Note that these *constant physics* conditions do not have to be satisfied very precisely since we are talking about a correction to an $\mathrm{O}(a)$ term.

Such conditions have first been imposed in Ref. [51] – exactly because of Fig. 7. We show the result for $b_{\mathrm{A}} - b_{\mathrm{P}}$, with the constant physics condition implemented, in Fig. 8. In this extreme case the ambiguity is of the same order as the improvement coefficient itself. In such a situation it is rather tempting to just put the coefficient to zero. However, it should be obvious that it is then not guaranteed that linear a-effects are absent after improvement. An extrapolation to the continuum using an $\mathrm{O}(a^2)$ model function for the cutoff effects might then give significantly wrong results. We repeat this relevant fact in different words. While an unfortunately chosen improvement condition, but implemented at constant physics, may even enlarge the cutoff effects for intermediate a, it guarantees[14] that linear a-effects are absent. Putting the improvement coefficient

[13] In fact this was done originally for c_{sw}, c_{A} [52]. Note, however, that the small tree-level a-effect was subtracted from the non-perturbative ones to insure the improvement coefficients go to their tree-level values exactly and further the conditions were chosen such that also $|b^{(1)}(a/L) - b^{(1)}(0)|$ is very small.

[14] Here we use a strong wording. Remember of course that everything is based on the SET, which has not been proved. Remember also Sect. I.2.2.2.

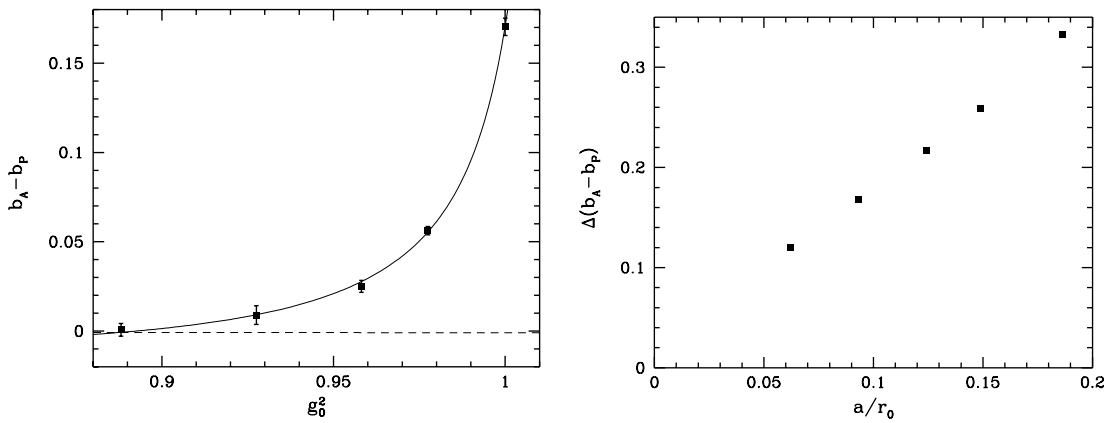


Figure 8: Non-perturbative $b_{\rm A} - b_{\rm P}$ for $N_{\rm f} = 0$ and plaquette gauge action (left) as well as its ambiguity $\Delta(b_{\rm A} - b_{\rm P})$. The latter is the difference of $b_{\rm A} - b_{\rm P}$ for one improvement condition and $b_{\rm A} - b_{\rm P}$ for another one.

to zero or some perturbative approximation does not guarantee the latter and the linear effects should at least be estimated in some way.

Before we review what is known in O(a)-improvement, we return once more to the improvement coefficients $c_{\rm sw}, c_{\rm A}$. With plaquette gauge action, $a/L = 1/8$ and the chosen improvement condition, eq. (I.2.27) is very well satisfied for $i = 0, 1$ [43]. It appears justified to subtract these effects perturbatively as it was done in [52, 53]. For $c_{\rm A}$ there is evidence for a significant O(a) ambiguity [50, 54, 55]. As a consequence, the computation with $N_{\rm f} = 2$ has been carried out with an improvement condition at constant physics [56].

I.2.4.2 Summary of results

A summary of the available results for O(a) improvement coefficients is listed in Table 1. Many investigations have been carried out accumulating a quite advanced knowledge. It is impossible for me to review it all, rather I add only a few comments.

- In the quenched approximation there is a rather complete knowledge for the Wilson gauge action, but $c_{\rm A}$ has not been determined with a constant physics condition. Conservative continuum extrapolations in the improved theory usually start only with values of a which are a bit below 0.1 fm.
  The problem with "exceptional configurations" [64], which is specific to the quenched approximation, is enhanced by $c_{\rm sw} > 0$ [65]. Thus small quark masses can only be reached near the continuum limit.

- For $N_{\rm f} = 2$ and Wilson gauge action, the determination of improvement coefficients is quite advanced. Interesting computations of physical observables can be done in the improved theory.

improvement coefficient or improved fields	order in PT	$N_{\rm f}$	gauge action	reference
$c_{\rm sw}, c_{\rm A}$	1-loop	–	Wilson	[43, 44]
$b_{\rm g}$	1-loop	–	Wilson	[19, 57]
$b_{\rm m}, b_{\rm A}, b_{\rm P}, b_{\rm V}, c_{\rm V}$				
V_μ^a, A_μ^a	1-loop	–	Wilson	[46, 58]
$c_{\rm sw}$	1-loop	–	various	[59]
$c_{\rm sw}, c_{\rm A}$	NP	0	Wilson	[52]
$b_{\rm m}, b_{\rm A} - b_{\rm P}, b_{\rm V}, c_{\rm A}, c_{\rm V}$				
V_μ^a, A_μ^a	NP	0	Wilson	[50]
$c_{\rm A}$	NP	0	Wilson	[54]
$b_{\rm A} - b_{\rm P}, b_{\rm V} - b_{\rm S}, b_{\rm m}$	NP	0	Wilson	[49]
$b_{\rm A} - b_{\rm P}, b_{\rm m}$	NP at CP	0	Wilson	[51]
$b_{\rm A} - b_{\rm P}, b_{\rm m}$	NP at CP	0	Wilson	[60]
$c_{\rm sw}$	NP	2	Wilson	[53]
$c_{\rm sw}$	NP	3	Wilson	[61]
$c_{\rm A}$	NP at CP	2	Wilson	[56]
$b_{\rm m}, b_{\rm A}, b_{\rm P}, b_{\rm V}, c_{\rm V}, b_{\rm T}$				
$V_\mu^a, A_\mu^a, T_{\mu\nu}^a$	1-loop	–	1×1 & 1×2	[58]
$c_{\rm sw}$	1-loop	–	1×1 & 1×2	[62]
$c_{\rm sw}$	NP at CP	0,2,3	Iwasaki	[63]
$c_{\rm A}$	NP at CP	3	Iwasaki	CP-PACS & JLQCD

Table 1: Literature on O(a) improvement coefficients. NP stands for non-perturbative, CP for constant physics condition, Wilson for the Wilson plaquette action, "1×1 & 1×2" for the gauge action including a 1×2 loop and Iwasaki for the action where the coefficient of that term is set to the value proposed by Y. Iwasaki.

- For $N_{\rm f} = 3$ and Wilson gauge action, evidence for the existence of a first order phase transition in the (β, κ)-plane has been reported [66]. The value of $c_{\rm sw}$ was fixed to typical values found for $N_{\rm f} = 0, 2$. The authors conclude that one has to remain with lattice spacings significantly below $a = 0.1\,$fm for this action. Recent investigations [67] have shown that simulations with Wilson fermions at small quark masses are only algorithmically stable when the physical volume is sufficiently large. [15] It is possible that the simulations that lead to the evidence for a phase transition [66] suffer from this problem. We therefore consider the existence (and even more its position) of this phase transition *not* as settled. Unfortunately it appears that only large volume simulations with good statistics can tell. Note that this statement may be controversial.

- With Iwasaki gauge action, $c_{\rm sw}$ is now known [63] non-perturbatively for $N_{\rm f} =$

[15] The lattice spacing should also be sufficiently small, but this is less relevant here. See also [68].

$0, 2, 3$. Non-perturbative computations of $c_{\rm A}$ are in progress and the relevant other improvement coefficients are known to 1-loop order [58]. A small grain of salt is the following. The perturbative expansion seems less trustworthy for this action, since the bare coupling is significantly larger than for the Wilson gauge action at the same lattice spacing, while the perturbative coefficients are of a similar size.

- In Sect. I.2.4.4 we will come to the question whether more information is needed to do interesting computations in QCD.

I.2.4.3 $\mathrm{O}(a^2)$ effects after improvement for $N_{\rm f} = 2$

The ALPHA collaboration has performed a large series of simulations with the Schrödinger functional in small volumes of a linear extent of at most $L \approx 0.5\,\mathrm{fm}$ [23, 69, 70]. The purpose of these simulations was the non-perturbative determination of the running of scale dependent quantities (see Sect. II.1). Extracting the continuum limit of the step scaling functions would have been impossible without $\mathrm{O}(a)$-improvement. It is fair to say that $\mathrm{O}(a)$-improvement worked marvelously well in this situation. The interested reader may in particular study the discussion in [69]. The emerging picture for QCD in the Wilson formulation is that the Symanzik expansion and improvement works very well for lattice spacings around 0.05 fm and below.

At larger lattice spacings, the situation is unclear at present. In particular indirect evidence has been shown that $\mathrm{O}(a^2)$ effects are rather large at $a \approx 0.1\,\mathrm{fm}$ [22, 71]. Large scale simulations in large volume will tell, whether the remaining $\mathrm{O}(a^2)$ effects are a problem in practice. We emphasize that there is no evidence anywhere that the Symanzik theory of a-effects is invalid. The remaining issue is how small a has to be made for it to be precise when truncated to the first one or two correction terms. It is also expected that smaller lattice spacings are needed for smaller quark masses. This issue is discussed in Steve Sharpe's lectures. [72]

I.2.4.4 Do we need more?

The question arises, whether the knowledge described above is sufficient to do QCD computations.

First, we recall that we assumed that one is interested in on-shell quantities. In the popular MOM-scheme [73] used for the renormalization of composite operators, one does, however, consider off-shell correlation functions. While improvement in that situation has been investigated, too [74–76], we continue under the assumption that off-shell correlation functions are avoided. So far we have restricted our discussion to the case of QCD with mass-degenerate quarks. This does of course not correspond to real QCD. General quark masses are no complication for quenched quarks; we already referred to that situation in Sect. I.2.4.1. However, dynamical quarks of different masses allow for a whole series of new $\mathrm{O}(a)$ counter-terms which are proportional to the difference

of quark masses [77]. Determining them non-perturbatively would be a considerable challenge. However, let us look at their influence in practice[16]. For $N_{\rm f} = 3$, the biggest mass difference is of order $m_{\rm s}$. For $a \leq 0.1\,\mathrm{fm}$, we have

$$am_{\rm q,s} \leq 1/30\,. \tag{I.2.28}$$

Thus we are talking about very small effects even at the largest typical lattice spacing. It is then sufficient to know the coefficient with, an accuracy of 0.25 or so which is surely possible by perturbation theory. The same argument applies to $b_{\rm g}$ [19]. Note, however, that for non-degenerate masses, eq. (I.2.24) is modified already at the level a^0 and this has to be taken into account [77], or better it is avoided by relying on the PCAC masses only.

Obviously, for a dynamical charm quark, the question should be reconsidered carefully.

Another issue is the improvement of more complicated composite operators, such as 4-fermion operators. Many improvement terms may be necessary. For these difficult cases one may consider a mixed action approach, where (some part) of chiral symmetry forbids the O(a) terms [78]. Also twisted mass lattice QCD offers an interesting strategy for these problems. We refer to Stefan Sint's lectures.

In conclusion, a very large class of interesting problems do not seem to need more beyond what is presently known or is being determined. One may therefore take advantage of the simplicity of the formulation and work on the algorithms [79–84] to be able to work at small lattice spacings and quark masses; see also the lectures of Tony Kennedy [85].

[16] We thank M. Lüscher for emphasizing this point.

Lecture II.

Fundamental parameters of QCD from the lattice

II.1 The problem of scale dependent renormalization

Let us investigate the extraction of short distance parameters (Sect. 1.2a) in some detail. After some brief comments on the conventional way of obtaining α from experiments we explain how one can compute it at large energy scales using lattice QCD. This paves the road for a computation of the Λ-parameter and then also for the renormalization group invariant quark masses. We will finally comment briefly on other scale-dependent renormalization.

II.1.1 The extraction of α from experiments

One considers experimental observables O_i depending on an overall energy scale q and possibly some additional kinematical variables denoted by y. The observables can be computed in a perturbative series which is usually written in terms of the $\overline{\rm MS}$ coupling $\alpha_{\overline{\rm MS}}$, [17]

$$O_i(q,y) \;=\; \alpha_{\overline{\rm MS}}(\mu) + A_i(y)\alpha^2_{\overline{\rm MS}}(\mu) + \ldots\,, \quad \mu = q\ . \tag{II.1.1}$$

For example O_i may be constructed from jet cross sections and y may be related to the details of the definition of a jet.

The renormalization group describes the energy dependence of α in a general scheme ($\alpha \equiv \bar{g}^2/(4\pi)$),

$$\mu\frac{\partial\bar{g}}{\partial\mu} \;=\; \beta(\bar{g})\ , \tag{II.1.2}$$

where the β-function has an asymptotic expansion

$$\begin{aligned}\beta(\bar{g}) \;&\overset{\bar{g}\to 0}{\sim}\; -\bar{g}^3\left\{b_0 + \bar{g}^2 b_1 + \ldots\right\}\ , \\ &b_0 = \tfrac{1}{(4\pi)^2}(11 - \tfrac{2}{3}N_{\rm f})\ , \quad b_1 = \tfrac{1}{(4\pi)^4}(102 - \tfrac{38}{3}N_{\rm f})\ ,\end{aligned} \tag{II.1.3}$$

with higher order coefficients b_i, $i > 1$ that depend on the scheme. Eq. (II.1.3) entails asymptotic freedom: at energies that are high enough for eq. (II.1.3) to be applicable and for a number of quark flavors, $N_{\rm f}$, that is not too large, α decreases with increasing energy as indicated in Fig. 9. The solution of eq. (II.1.2) contains an integration constant, the renormalization group invariant parameter Λ. It is (exactly) given by

$$\Lambda = \mu\left(b_0\bar{g}^2\right)^{-b1/(2b_0^2)}\,{\rm e}^{-1/(2b_0\bar{g}^2)}\exp\left\{-\int_0^{\bar{g}}{\rm d}x\left[\tfrac{1}{\beta(x)} + \tfrac{1}{b_0x^3} - \tfrac{b_1}{b_0^2x}\right]\right\}\ , \tag{II.1.4}$$

[17] We can always arrange the definition of the observables such that they start with a term α. For simplicity we neglect all quark mass dependences; they are irrelevant for the main points of the present discussion.

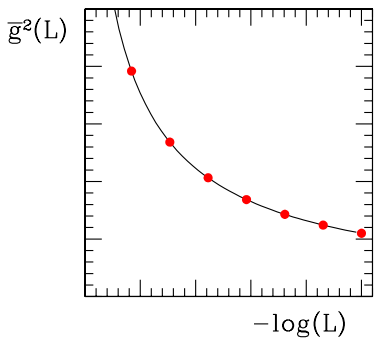


Figure 9: Running of $\bar{g}^2$ and its reconstruction from the step scaling function (points).

where $\bar{g} \equiv \bar{g}(\mu)$ Note that Λ is different in each scheme. If a coupling α_X is related to another one α_Y at the same energy scale via

$$\alpha_Y(\mu) = \alpha_X(\mu) + c_1^{XY}\,[\alpha_X(\mu)]^2 + c_2^{XY}\,[\alpha_X(\mu)]^3 + \dots \quad , \tag{II.1.5}$$

their Λ-parameters are converted via

$$\Lambda_X/\Lambda_Y = \exp\{-c_1^{XY}/(8\pi b_0)\}\,. \tag{II.1.6}$$

From the above equations it is easy to show that eq. (II.1.6) is exact. For large μ one reads off the asymptotics

$$\bar{g}^2 \overset{\mu\to\infty}{\sim} \frac{1}{b_0 \ln(\mu^2/\Lambda^2)} - \frac{b_1 \ln[\ln(\mu^2/\Lambda^2)]}{b_0^3[\ln(\mu^2/\Lambda^2)]^2} + \mathrm{O}\left(\frac{\{\ln[\ln(\mu^2/\Lambda^2)]\}^2}{[\ln(\mu^2/\Lambda^2)]^3}\right)\,. \tag{II.1.7}$$

We note that – neglecting experimental uncertainties – $\alpha_{\overline{\mathrm{MS}}}$ extracted in this way is obtained with a precision given by the terms that are left out in eq. (II.1.1). In addition to α^3-terms, there are non-perturbative contributions which may originate from "renormalons", "condensates" (the two possibly being related), "instantons" or – most importantly – may have an origin that no physicist has yet uncovered. Empirically, one observes that values of $\alpha_{\overline{\mathrm{MS}}}$ determined at different energies and evolved to a common reference point using the renormalization group equation eq. (II.1.2) including b_2 agree rather well with each other; the aforementioned uncertainties are apparently not very large (Fig. 10). Nevertheless, determinations of α are limited in precision because of these uncertainties and in particular if there was a significant discrepancy between α determined at different energies it would be difficult to say whether this was due to the terms left out in eq. (II.1.1) or was due to terms missing in the Standard Model Lagrangian.

It is an obvious possibility and at the same time a challenge for lattice QCD to achieve a determination of α in one (non-perturbatively) well defined scheme and evolve

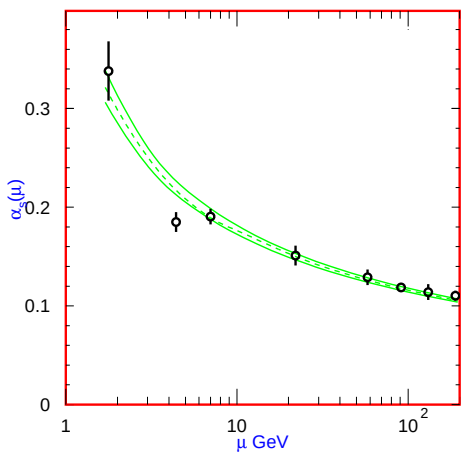


Figure 10: The running coupling in the $\overline{\rm MS}$ scheme extracted from various scattering experiments compared to the perturbative scale dependence. Graph of the particle data group [86].

this coupling to high energies. There one may use eq. (II.1.4) with a perturbative approximation for $\beta(\bar{g})$. For a good precision b_2 should be known.

The Λ-parameter can then serve as an input for perturbative predictions of jet cross sections or the hadronic width of the Z-boson and compare to high energy experiments to test the agreement between theory and experiment. Since in the lattice regularization, QCD is naturally renormalized through the hadron spectrum, such a calculation provides the connection between low energies and high energies, verifying that one and the same theory describes both the hadron spectrum and the properties of jets.

Note. A dis-satisfying property of $\alpha_{\overline{\rm MS}}$ is that it is *only* defined in a perturbative framework; strictly speaking there is no meaning of phrases like "non-perturbative corrections" in the extraction of $\alpha_{\overline{\rm MS}}$ from experiments. The way that I have written eq. (II.1.1) suggests immediately what should be done instead. An observable O_i itself may be taken as a definition of α – of course with due care. Such schemes called *physical schemes* are defined without ambiguities. This is what will be done below for observables that are easily handled in MC-simulations of QCD. For an additional example see [87, 88].

II.1.2 Reaching large scales in lattice QCD

Let us simplify the discussion and restrict ourselves to the pure Yang-Mills theory without matter fields in this section. A natural candidate for a non-perturbative definition of α is the following. Consider a quark and an anti-quark separated by a distance r and

in the limit of infinite mass. They feel a force $F(r)$, the derivative of the static potential $V(r)$, which can be computed from Wilson loops (see e.g. [89]). A physical coupling is defined as

$$\alpha_{\mathrm{q\bar{q}}}(\mu) \equiv \tfrac{1}{C_F} r^2 F(r)\,, \quad \mu = 1/r, \quad C_F = 4/3 \ . \tag{II.1.8}$$

It is related to the $\overline{\mathrm{MS}}$ coupling by eq. (II.1.5) with a certain constant $c_1^{\overline{\mathrm{MS}}\,\mathrm{q\bar{q}}}$, which also determines the ratio of the Λ-parameters (eq. (II.1.6)). Note that $\alpha_{\mathrm{q\bar{q}}}$ is a renormalized coupling defined in continuum QCD.

Problem. If we want to achieve what was proposed in the previous subsection, the following criteria must be met.

- Compute $\alpha_{\mathrm{q\bar{q}}}(\mu)$ at energy scales of $\mu \sim 10\,\mathrm{GeV}$ or higher in order to be able to make the connection to other schemes with controlled perturbative errors.
- Keep the energy scale μ removed from the cutoff a^{-1} to avoid large discretization effects and to be able to extrapolate to the continuum limit.
- Of course, only a finite system can be simulated by MC. To avoid finite size effects one must keep the box size L large compared to both the mass of the lightest physical state (the pion) as well as to a typical QCD scale, say the potential scale r_0 [47].

These conditions are summarized by

$$L \gg r_0, \frac{1}{m_\pi} \sim \frac{1}{0.14\mathrm{GeV}} \gg \frac{1}{\mu} \sim \frac{1}{10\mathrm{GeV}} \gg a \ , \tag{II.1.9}$$

which means that one must perform a MC-computation of an N^4 lattice with $N \equiv L/a \gg 70$. In the near future it is impossible to perform such a computation. The origin of this problem is simply that the extraction of short distance parameters requires that one has control over physical scales that are quite disparate. To cover these scales in one simulation requires a very fine resolution, which is too demanding for a MC-calculation.

Of course, one may attempt to compromise in various ways. E.g. one may perform phenomenological corrections for lattice artifacts, keep $1/\mu \sim a$ and at the same time reduce the value of μ compared to what I quoted in eq. (II.1.9). Calculations of $\alpha_{\mathrm{q\bar{q}}}$ along these lines have been performed in the Yang-Mills theory [90–92]. It is difficult to estimate the uncertainties due to the approximations that are necessary in this approach. More recently, results in the continuum limit could be obtained up to $\mu = 4\,\mathrm{GeV}$ by simulating very large lattices [93, 94], and still it is not obvious that one has reached the perturbative region. We will come back to this.

Solution. Fortunately these compromises can be avoided altogether [37]. The solution is to identify the two physical scales, above,

$$\mu = 1/L \ . \tag{II.1.10}$$

In other words, one takes a finite size effect as the physical observable. The evolution of the coupling with μ can then be computed in several steps, changing μ by factors of order 2 in each step. In this way, no large scale ratios appear and discretization errors are small for $L/a \gg 1$.

The complete strategy to compute short distance parameters is summarized in Fig. 11. One first renormalizes QCD replacing the bare parameters by hadronic observ-

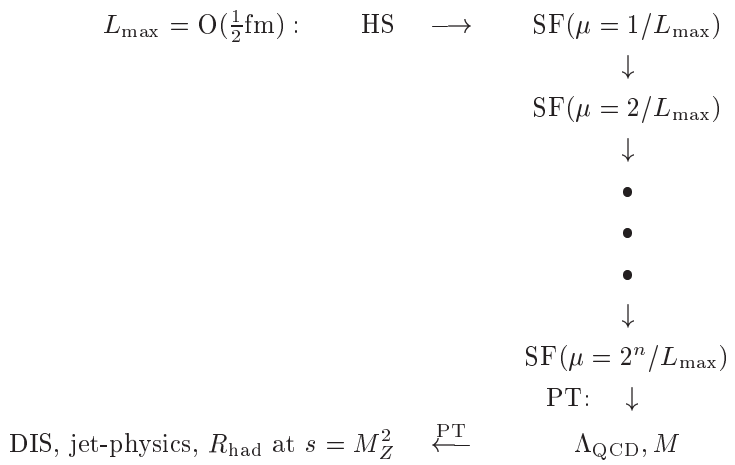


Figure 11: The strategy for a non-perturbative computation of short distance parameters. SF refers to the Schrödinger functional scheme introduced in Sect. I.1.6

ables. This defines the hadronic scheme (HS) as explained in Sect. 1.1. At a low energy scale $\mu = 1/L_{\rm max}$ this scheme can be related to the finite volume scheme denoted by SF in the graph. Within this scheme one then computes the scale evolution up to a desired energy $\mu = 2^n/L_{\rm max}$. As we will see it is no problem to choose the number of steps n large enough to be sure that one is in the perturbative regime. There perturbation theory (PT) is used to evolve further to infinite energy and compute the Λ-parameter and the renormalization group invariant quark masses. Inserted into perturbative expressions these provide predictions for jet cross sections or other high energy observables. In the graph all arrows correspond to relations in the continuum; the whole strategy is designed such that lattice calculations for these relations can be extrapolated to the continuum limit.

For the practical success of the approach, the finite volume coupling (as well as the corresponding quark mass) must satisfy a number of criteria.

- They should have an easy perturbative expansion, such that the β-function (and τ-function, which describes the evolution of the running masses) can be computed to sufficient order.
- They should be easy to calculate in MC (small variance!).
- Discretization errors must be small to allow for safe extrapolations to the continuum limit.

Careful consideration of the above points led to the introduction of renormalized coupling and quark mass through the Schrödinger functional (SF) of QCD [12,17,18,32,95], introduced in Sect. I.1. In the Yang-Mills theory, an alternative finite volume coupling was studied in detail in [96, 97].

The criteria eq. (II.1.9) apply quite generally to any scale dependent renormalization, e.g. the one of 4-fermion operators of the effective weak Hamiltonian at scales $\mu \ll M_{\rm W}$. Indeed, details have been worked out for several cases [9–11, 98–101].

A frequently applied alternative is to search for a "window" where μ is high enough to apply PT but not too close to a^{-1}, the cutoff [102]. An essential advantage of the details of the approach of Ref. [102] as applied to the renormalization of composite quark operators is its simplicity: formulating the renormalization conditions in a *MOM*-scheme [18], one may use results from perturbation theory in infinite volume in the perturbative part of the matching. Since, however, it is difficult to reach high energies μ in this approach, we will not discuss it further and refer to [102–105] for an idea of the present status and further references, instead.

II.2 The computation of $\alpha(\mu)$ and Λ

We are now in the position to explain the details of Fig. 11 [37,98]. The problem has been solved "completely" in the SU(N) Yang-Mills theories for $N = 2, 3$ [17,93,95,97,98,106]. In QCD with only two dynamical quarks the strategy has been carried out well [69, 70], except for the last line in the graph, which needs more work. In the present context, the Yang-Mills theory is of course equivalent to the quenched approximation of QCD or the limit of zero flavors. We will therefore also refer to results in quenched QCD.

Our central observable is the step scaling function that describes the scale-evolution of the coupling, i.e. moving vertically in Fig. 11. The analogous function for the running quark mass will be discussed in the following section.

II.2.1 The step scaling function

We start from a given value of the coupling, $u = \bar{g}^2(L)$. When we change the length scale by a factor s, the coupling has a value $\bar{g}^2(sL) = u'$.[19] The step scaling function,

[18] We do not use the prefix *RI* (regularization independent), since also the SF-scheme is regularization independent.

[19] Figure 11 is for the most frequently used case $s = 2$.

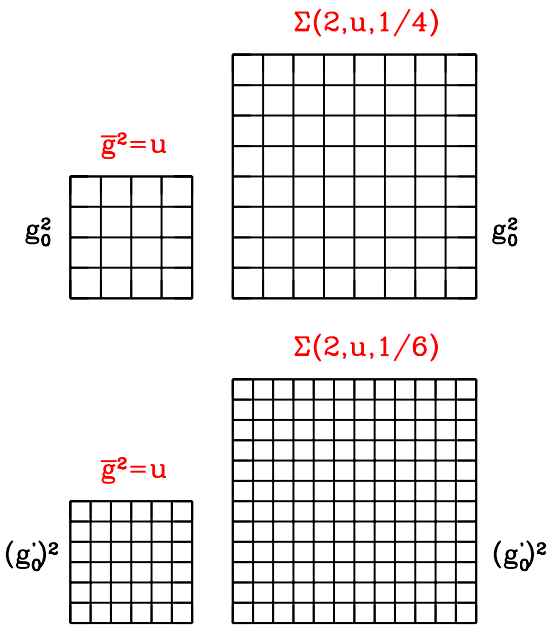


Figure 12: The computation of a lattice step scaling function.

σ is then defined as

$$\sigma(s,u) \quad = \quad u' \quad . \tag{II.2.1}$$

The interpretation is obvious. $\sigma(s,u)$ is a discrete β-function. Its knowledge allows for the recursive construction of the running coupling at discrete values of the length scale,

$$u_k = \bar{g}^2(s^{-k}L) \quad , \tag{II.2.2}$$

once a starting value $u_0 = \bar{g}^2(L)$ is specified (cf. the points in Fig. 9). The step scaling function, σ, which is readily expressed as an integral of the β-function, has a perturbative expansion

$$\sigma(s,u) \quad = \quad u + 2b_0 \ln(s) u^2 + \ldots \quad . \tag{II.2.3}$$

On a lattice with finite spacing, a, the step scaling function will have an additional dependence on the resolution a/L. We define

$$\Sigma(s,u,a/L) \quad = \quad u' \quad , \tag{II.2.4}$$

with

$$\bar{g}^2(L) \quad = \quad u, \quad \bar{g}^2(sL) = u' , \quad g_0 \text{ fixed, } L/a \text{ fixed} \quad . \tag{II.2.5}$$

The continuum limit $\sigma(s,u) = \Sigma(s,u,0)$ is then reached by performing calculations for several different resolutions and extrapolation $a/L \to 0$. The computation of $\sigma(2,u)$ is illustrated in Fig. 12. In detail, one performs the following steps:

1. Choose a lattice with L/a points in each direction.

2. Tune the bare coupling g_0 such that the renormalized coupling $\bar{g}^2(L)$ has the value u and tune the bare quark mass, m_0, such that the PCAC-mass, defined at fixed physical kinematics [69], vanishes.[20]

3. At the same value of g_0, simulate a lattice with twice the linear size; compute $u' = \bar{g}^2(2L)$. This determines the lattice step scaling function $\Sigma(2,u,a/L)$.

4. Repeat steps 1.–3. with different resolutions L/a and extrapolate $a/L \to 0$.

Note that step 2. takes care of the renormalization and 3. determines the evolution of the *renormalized* coupling.

The presently most advanced numerical results are displayed in Fig. 13. The coupling used is exactly the one defined in Sect. I.1.6 and the calculation is done in the theory with $N_{\rm f} = 2$ flavors of O(a)-improved fermions. One observes that the dependence on the resolution is very weak, in fact it is not observable within the precision of the data in Fig. 13. We now investigate in more detail how the continuum limit of Σ is reached. As a first step, we turn to perturbation theory.

II.2.2 Lattice spacing effects in perturbation theory

Symanzik has investigated the cutoff dependence of field theories in perturbation theory [107]. Generalizing his discussion to the present case, one concludes that the lattice spacing effects have the expansion

$$\begin{aligned} \frac{\Sigma(2,u,a/L) - \sigma(2,u)}{\sigma(2,u)} &= \delta_1(a/L)\,u + \delta_2(a/L)\,u^2 + \ldots \qquad \text{(II.2.6)} \\ \delta_n(a/L) &\overset{a/L\to 0}{\sim} \sum_{k=0}^{n} e_{k,n}[\ln(\tfrac{a}{L})]^k(\tfrac{a}{L}) + d_{k,n}[\ln(\tfrac{a}{L})]^k(\tfrac{a}{L})^2 + \ldots \ . \end{aligned}$$

We expect that the continuum limit is reached with corrections O(a/L) also beyond perturbation theory. In this context O(a/L) summarizes terms that contain at least one power of a/L and may be modified by logarithmic corrections as it is the case in eq. (II.2.6). To motivate this expectation recall Sect. 1.3, where we explained that lattice artifacts correspond to irrelevant operators which carry explicit factors of the lattice spacing. Of course, an additional a-dependence comes from their anomalous dimension, but in an asymptotically free theory such as QCD, this just is a logarithmic (in a) modification.

[20] The details of the definition of the kinematics affects only the cutoff effects, see Sect. I.2.2.

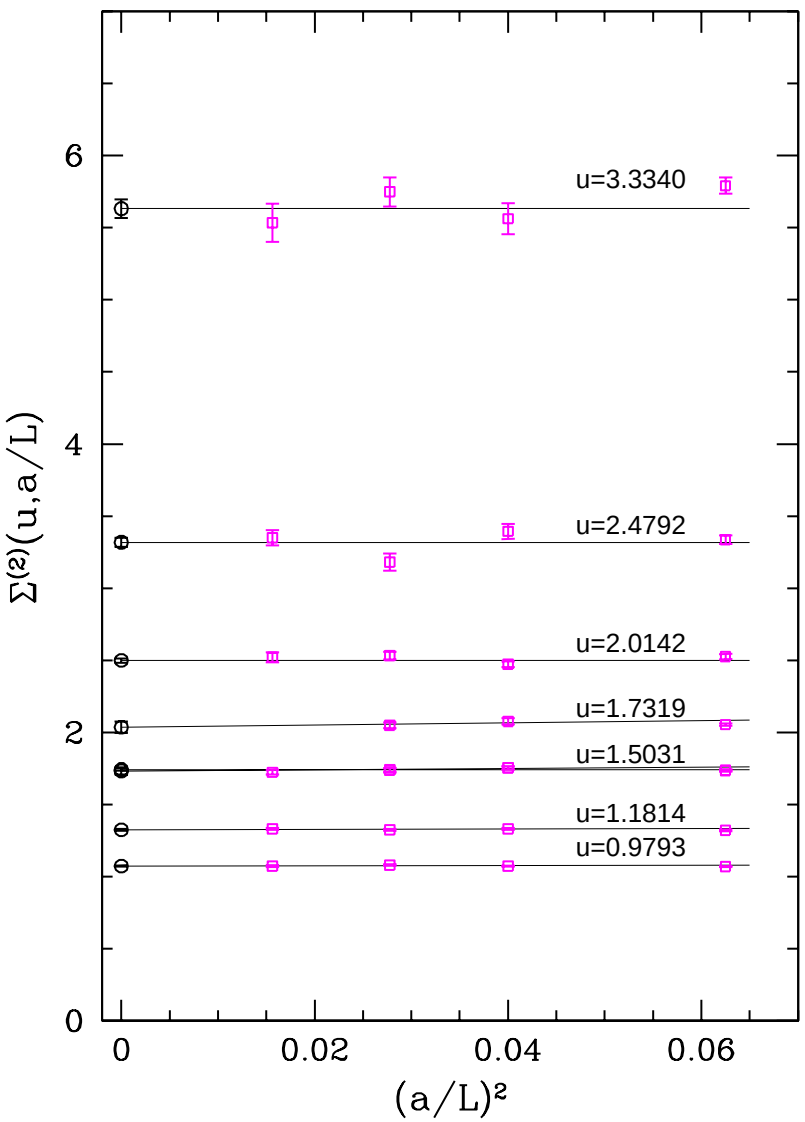


Figure 13: The lattice step scaling function after 2-loop observable improvement for $N_{\rm f} = 2$.

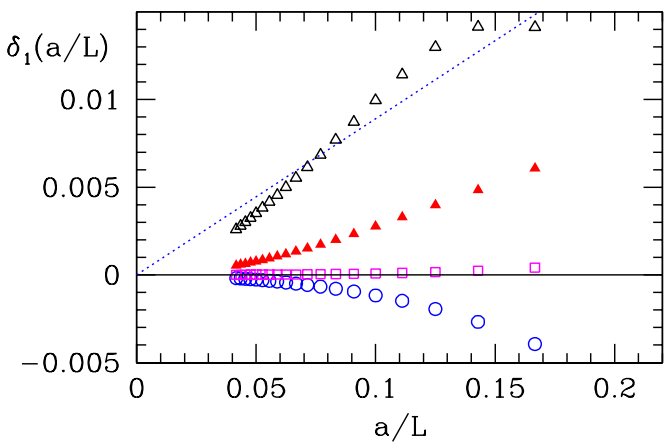


Figure 14: Lattice artifacts at 1-loop order. Points show $\delta_1(a/L)$ for the SU(3) Yang-Mills theory with 1-loop improvement. Wilson (circles), Symanzik (squares), Iwasaki (filled triangles) and DBW2 (empty triangles) are shown. The dotted line corresponds to the linear piece in a, when only tree-level improvement is used, instead (only for Wilson).

As mentioned in Sect. I.1.8, the lattice artifacts may be reduced to $\mathrm{O}((a/L)^2)$ by canceling the leading irrelevant operators. In the case at hand, this is achieved by a proper choice of $c_{\mathrm{t}}(g_0)$. It is interesting to note, that by using the perturbative approximation

$$c_{\mathrm{t}}(g_0) = 1 + c_{\mathrm{t}}^{(1)} g_0^2 \tag{II.2.7}$$

one does not only eliminate $e_{k,n}$ for $n = 0, 1$ but also the logarithmic terms generated at higher orders ($n > 1$)are reduced,

$$e_{n,n} = 0, \quad e_{n-1,n} = 0 \ . \tag{II.2.8}$$

For tree-level improvement, $c_{\mathrm{t}}(g_0) = 1$, the corresponding statement is $e_{n,n} = 0$. Heuristically, the latter is easy to understand. Tree-level improvement means that the propagators and vertexes agree with the continuum ones up to corrections of order $\mathrm{O}(a^2)$. Terms proportional to a can then arise only through a linear divergence of the loop integrals. Once this happens, one cannot have the maximum number of logarithmic divergences any more; consequently $e_{n,n}$ vanishes.

To demonstrate further that the abelian field introduced in the previous section induces small lattice artifacts, we show $\delta_1(a/L)$ for the one loop improved case in Fig. 14 (circles). The term that is canceled by the proper choice $c_{\mathrm{t}}^{(1)} = -0.089$ is shown as a dashed line. The left over $\mathrm{O}((a/L)^2)$-terms are below the 1% level for couplings $u \leq 2$ and lattice sizes $L/a \geq 6$. For not too large coefficient of the 1×2 loop in the action, they are close to quadratic in a/L in the range of interest. Also the fermion contribution

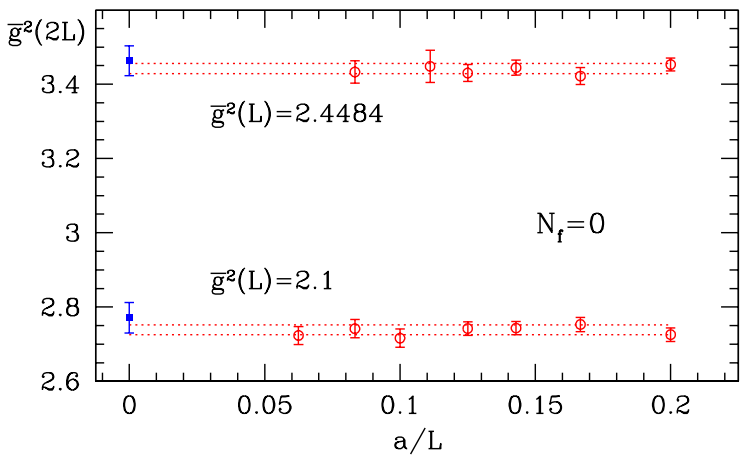


Figure 15: The lattice step scaling function after 2-loop observable improvement for $N_\mathrm{f} = 0$. Data from [98, 113]. The point at $a = 0$ is the continuum limit of [98] taken with a subset of the data.

and the 2-loop cutoff effects are known [16, 57]. When the O(a)-improved theory is used (and the coupling has reasonable values), they turn out to be smaller than the 1-loop terms discussed here.

Of course the cutoff effects also depend on the gauge action. In one class of such actions, one adds a 1×2 rectangular loop. Its coefficient has originally been determined to have tree-level Symanzik O(a^2) improvement in the pure gauge theory [108]. Later other choices have been proposed by Y. Iwasaki [109] and the QCD-TARO collaboration [110], based on renormalization group considerations. We refer to these as "Symanzik,Iwasaki,DBW2". The choice of the action close to the Schrödinger functional boundaries does of course involve an additional freedom discussed in [111, 112]. For the choice favored in [112], we included the corresponding $\delta_1(a/L)$ in Fig. 14. For the tree-level Symanzik improved theory the cutoff effects are remarkably small. One might think that this is so by construction, but note that here we are discussing 1-loop effects and in addition also boundary operators contribute to the SET expansion of the cutoff effects.

Altogether, we now understand better why the a/L-dependence is so small in Fig. 13. Still, because the continuum limit is so important, and we have seen that unexpected difficulties may be present (Sect. I.2.2.2), we continue its discussion in the pure gauge theory. There, numerical simulations with better resolutions have been carried out.

II.2.3 The continuum limit – universality

In fact, it is not only of interest to investigate how exactly the continuum limit is approached. Its very existence and its universality, i.e. the independence of the renor-

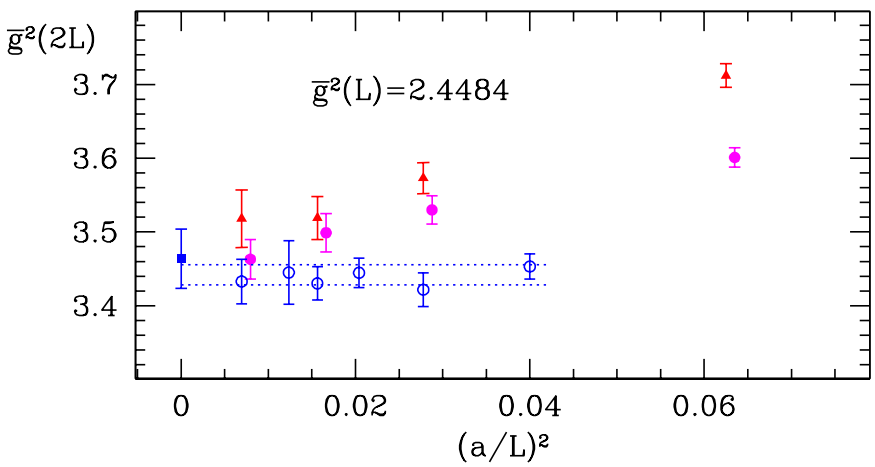


Figure 16: Universality test in the SU(3) Yang Mills theory. The data from top (triangles) to bottom (open circles) are for the Iwasaki, Symanzik and Wilson gauge action. Both the boundary improvement of the action and the improvement of the observables are carried out. At present this is possible at the 2-loop level for the Wilson gauge action (same as Fig. 15) and at the 1-loop level otherwise. Data are from [69, 114].

malized continuum observable from the lattice action, is worth testing by precise MC computation.

Above we have discussed how one can add boundary terms to the *action* to systematically reduce the cutoff effects linear in a. Given the knowledge of the observables in perturbation theory at finite lattice spacing, we can go further and remove the cutoff-effects for arbitrary a/L, i.e. for instance including $\mathrm{O}((a/L)^2)$, *but up to a fixed order in* u. This is achieved by the *improvement of the observable* [69, 70, 97]

$$\Sigma^{(k)}(2,u,a/L) = \frac{\Sigma(2,u,a/L)}{1+\sum_{i=1}^{k}\delta_i(a/L)\,u^i}\,. \qquad \text{(II.2.9)}$$

The approach has been carried out with $k=2$ for the $N_{\mathrm{f}}=2$ data (Fig. 13) and is tested thoroughly for $N_{\mathrm{f}}=0$ in Fig. 15.

Recently, a nice universality test has been carried out by the CP-PACS collaboration [114]. Obviously the results in Fig. 16 are well compatible with an $a\to 0$ limit which is independent of the action. Similar results exist for the SU(2) theory [97]. These results leave little doubt that the continuum limit of the Schrödinger functional exists and is independent of the lattice action. In turn this also supports the statement that the Schrödinger functional is renormalized after the renormalization of the coupling constant.

We return to the extraction of σ in $N_{\mathrm{f}}=2$ QCD. Even though a-effects are not statistically significant, one has to be careful how one extracts the continuum limit. The worry does not so much concern the central values, but the correct estimate of their

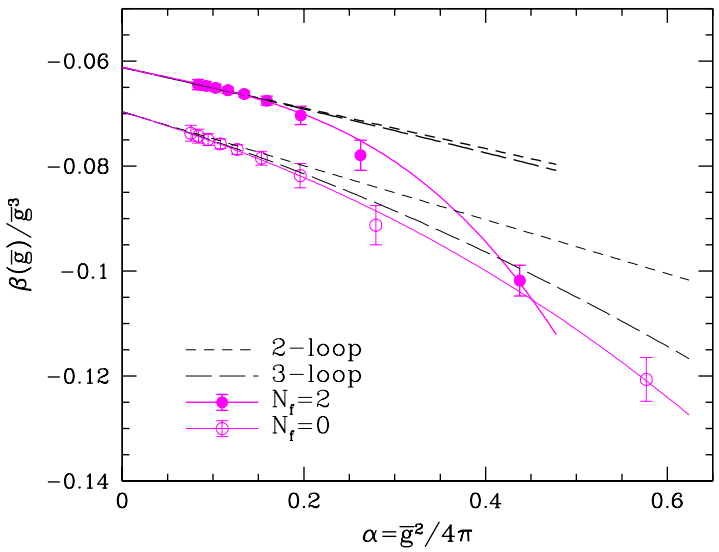


Figure 17: The QCD β–function in the SF scheme.

uncertainties. For example just averaging data at all values of a/L produces an unrealistically small statistical error, because one has then assumed that a-effects are entirely absent, although the data tell only that they are smaller than statistical uncertainties. One possible strategy for the continuum extrapolation is thus a fit to a constant that uses the lattices with $L/a = 6, 8$ only. As a check of this procedure, different variants of a combined continuum extrapolation of all the data sets, but excluding $L/a = 4$ were carried out. For example the ansatz

$$\Sigma^{(2)}(2, u, a/L) = \sigma(2, u) + \rho\, u^4\, (a/L)^2$$

with a constant ρ was fitted to the data. The final conclusion was that the simple fit to a constant (for $L/a = 6, 8$) yields realistic error estimates for the existing data set [70]. A further check of this procedure is Fig. 15 where the dotted lines represent the error band obtained in this way and the four points at smaller lattice spacing are in perfect agreement with this band.

After this long – but important – discussion of cutoff effects, we are convinced that we have continuum results for the step scaling function with realistic uncertainties. They are ready to be used to construct the running coupling and the Λ-parameter.

II.2.4 The running of the coupling

The numerical values of $\sigma(u)$ are next represented by a smooth interpolating function (a polynomial in u). With this function the running coupling $\bar{g}^2(2^{-i}L_{\max}) \equiv u_i$ can be constructed from the recursion

$$u_{\max} \equiv u_0 = \bar{g}^2(L_{\max})\,, \quad \sigma(u_{i+1}) = u_i\,,\ i = 0 \ldots n\,; \tag{II.2.10}$$

the result is shown in Fig. 18 for the (arbitrary) choice $u_{\max} = 5.5$. One can also set up a recursion for the β-function itself [70],

$$\beta(\sqrt{u_i}) = \sqrt{u_{i+1}/u_i}\,\sigma'(u_{i+1})\,\beta(\sqrt{u_{i+1}})\,. \tag{II.2.11}$$

Together with a start value for the β-function taken from perturbation theory (3-loop) at the weakest coupling ($\alpha \approx 0.08$) this yields the numerical results Fig. 17. Their agreement with perturbation theory is excellent at weak couplings $\alpha < 0.2$, while at the largest couplings significant deviations from perturbation theory are present for $N_{\rm f} = 2$. Indeed the difference between non-perturbative points and 3-loop can't be described by an effective 4-loop term *with a reasonable coefficient*. At the same time the perturbative series just by itself does not show signs of its failure at, say, $\alpha \approx 0.3$: instead successive orders yield smaller and smaller corrections.

We return to the running couplings shown in Fig. 18. In the zero flavor case, also the region of μ of around 250 MeV was investigated with a specifically adapted strategy [113]. In this region, the SF coupling shows the rapid growth expected from a strong coupling expansion.

Initially, the graphs Fig. 18 are obtained for μ in units of $\mu_{\min} = 1/L_{\max}$. One chooses $u_{\max}$ relatively large, but within the range covered by the non-perturbative computation of $\sigma(u)$. The artificial scale $L_{\max}$ has been replaced by the Λ parameter by use of eq. (II.1.4). We proceed to explain this step.

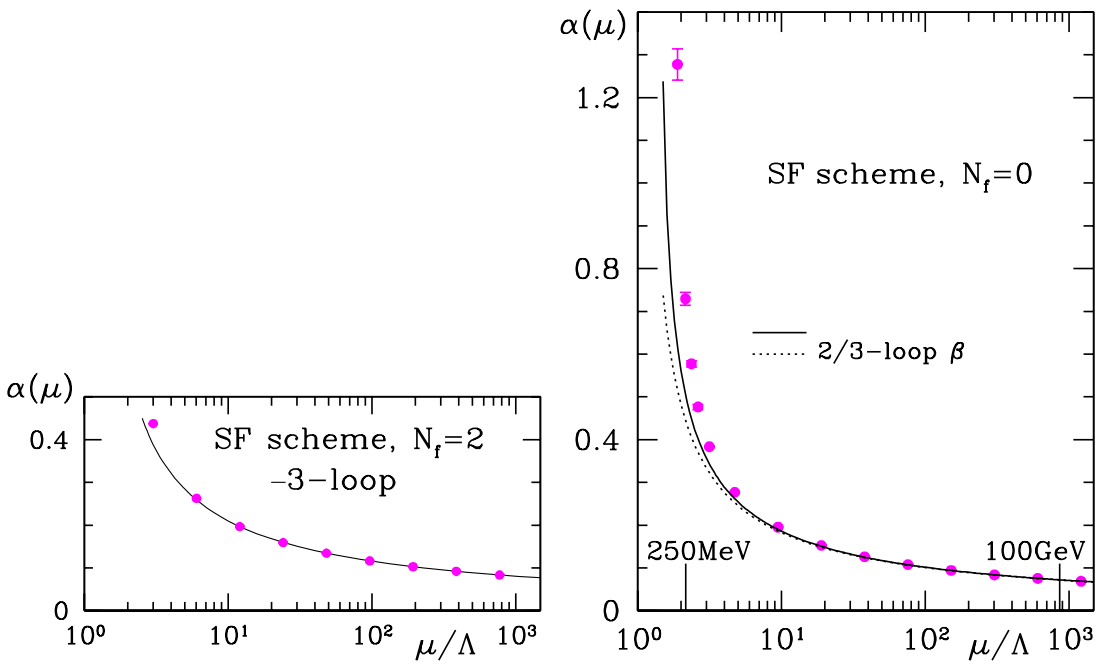


Figure 18: Running coupling for $N_{\rm f} = 2$ (left) and $N_{\rm f} = 0$ (right).

II.2.5 The Λ parameter

We may evaluate eq. (II.1.4) for the last few data points in Fig. 18 using the 3-loop approximation to the β-function in the SF-scheme. The resulting Λ-values are essentially independent of the starting point, since the data follow the perturbative running very accurately at large μ. This excludes a sizable contribution to the β-function beyond 3-loops in this region. Indeed, a typical estimate of a 4-loop term in the β-function would change the value of Λ by a tiny amount. The corresponding uncertainty can be neglected compared to the statistical errors.

Changing Λ from the SF scheme to the $\overline{\rm MS}$ scheme we then have

$$N_{\rm f} = 0\,, \qquad u_{\rm max} = 3.48 \;:\; \ln(\Lambda_{\overline{\rm MS}} L_{\rm max}) = -0.84(8)\,, \tag{II.2.12}$$

$$N_{\rm f} = 2\,, \qquad u_{\rm max} = 4.61 \;:\; \ln(\Lambda_{\overline{\rm MS}} L_{\rm max}) = -0.40(7)\,. \tag{II.2.13}$$

It remains to connect the artificially defined length scale $L_{\rm max}$ to an experimentally measurable low energy scale of QCD such as the proton mass or the kaon decay constant, $F_{\rm K}$.

So far it has been convenient to first evaluate $L_{\rm max}$ in units of the low energy scale r_0. This reference scale is precisely defined through the QCD static quark potential [47] but related to experiments only through potential models: $r_0 \approx 0.5\,\mathrm{fm}$. For $N_{\rm f} = 0$ a detailed investigation resulted in the continuum limit [93, 106]

$$N_{\rm f} = 0\,,\; u_{\rm max} = 3.48 \;:\; L_{\rm max}/r_0 = 0.738(16) \tag{II.2.14}$$

and thus

$$\Lambda^{(0)}_{\overline{\rm MS}} r_0 = 0.60(5)\,. \tag{II.2.15}$$

In the $N_{\rm f} = 2$ theory, the situation is illustrated in Table 2 which relies on results for r_0/a from [115, 116]. On the one hand, all the numbers in italic are consistent, indicating that lattice spacing effects are small, on the other hand the first column shows that a is not yet varied very much. At the moment

$$\Lambda^{(2)}_{\overline{\rm MS}} r_0 = 0.62(4)(4)$$

is quoted, where the second error generously covers the range of numbers in italic in Table 2 and the first one comes from eq. (II.2.13).

II.2.6 Discussion

The scale dependence of the SF coupling is close to perturbative below $\alpha_{\rm SF} = 0.2$ and becomes non-perturbative above $\alpha_{\rm SF} = 0.25$. In fact a strong coupling expansion suggests that *this* coupling grows exponentially for large L. In the $N_{\rm f} = 0$ theory it was possible to verify this behavior for L close to 1 fm [113] (Fig. 18). Apart from the determination of Λ, an achievement of this investigation is the confirmation that

		$u_{\max} = 3.65$		$u_{\max} = 4.61$	
$\beta = 6/g_0^2$	r_0/a	$L_{\max}/a$	$\Lambda_{\overline{\rm MS}} r_0$	$L_{\max}/a$	$\Lambda_{\overline{\rm MS}} r_0$
5.00	5.45(5)(20)	4.00(6)	0.655(27)	6.00(8)	*0.610(25)*
5.29	6.01(4)(22)	4.67(6)	*0.619(25)*	6.57(6)	*0.614(24)*
5.40	7.01(5)(15)	5.43(9)	*0.621(17)*	7.73(10)	*0.609(16)*

Table 2: Λ–parameter in units of r_0 for $N_{\rm f} = 2$ for different resolutions in the low energy part of the calculation. Two different values of $u_{\max}$ are considered, but $\Lambda_{\overline{\rm MS}} r_0$ should be independent of these when cutoff effects are small.

the transition between this non-perturbative region and the perturbative one is very smooth.

With some effort this transition region was also bridged for $\alpha_{\rm q\bar{q}}$ in the SU(3) pure gauge theory. As shown in Fig. 19, the non-perturbative continuum results agree reasonably well with the perturbative prediction at the largest μ (small r). The prediction is parameter free, since the Λ-parameter, eq. (II.2.15), can be changed to the q$\bar{\rm q}$-scheme, eq. (II.1.8), where also the 3-loop β-function is known [94, 117, 118]. The figure also illustrates that a reliable determination of Λ is not possible from $\alpha_{\rm q\bar{q}}$ because for the accessible μ the 3-loop contribution to the β-function is still very significant.

source	$\Lambda_{\overline{\rm MS}} r_0$			
	$N_{\rm f}$ =0	$N_{\rm f}$ =2	$N_{\rm f}$ =4	$N_{\rm f}$ =5
ALPHA [17, 70]	0.60(5)	0.62(6)		
world average [119]			0.74(10)	0.54(8)
DISNNLO [120]			0.57(8)	

Table 3: Results for $\Lambda_{\overline{\rm MS}} r_0$ for different number of flavors.

In Table 3 we compare our results for $\Lambda_{\overline{\rm MS}} r_0$ to selected phenomenological ones, where we set $r_0 = 0.5\,$fm. There appears to be an irregular $N_{\rm f}$-dependence, but we note that

1. the errors are not very small yet,
2. the 4-flavor Λ is obtained from the 5-flavor one by perturbation theory [121]. For this to be accurate, perturbation theory has to be accurate for $\mu \ll m_{\rm beauty}$, which is not completely obvious.

II.2.7 Improvements are necessary

The most urgently needed improvement of the present results is to eliminate the model dependence which is intrinsic in the use of r_0. So one should replace $L_{\max}/r_0$ by $F_{\rm K} \times$

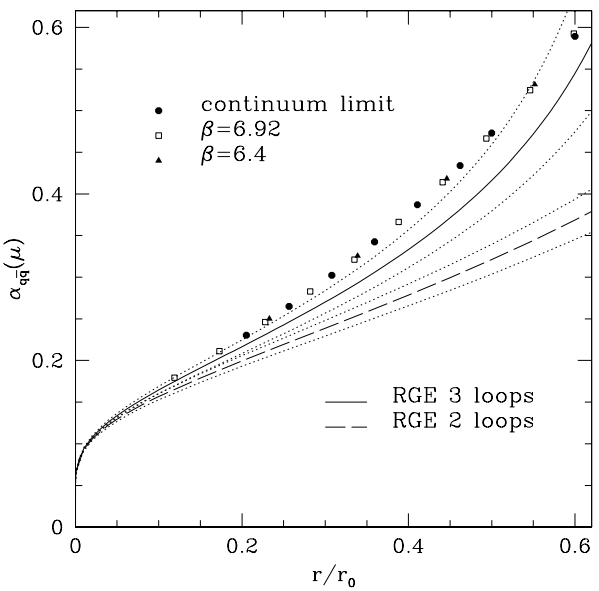


Figure 19: Running coupling in the q$\bar{\text{q}}$-scheme (eq. (II.1.8)). The perturbative prediction is given by the relation eq. (II.1.4) between the running coupling and $\Lambda^{(0)}_{q\bar{q}}$. The dotted lines show the uncertainty of Λ eq. (II.2.15).

$L_{\max}$ (computed at small enough light quark masses and small a) and an effort is presently being made. Also the strange quark sea has to be included ("2+1") and one should estimate the effects of the charm quark. Such 2+1 simulations are for example being carried out by JLQCD and CP-PACS, who have also studied the computation of the SF coupling with the gauge actions they are using [114].

These improvements will come and I am convinced that lattice results will yield the best controlled and most precise results for Λ in the long run. The reason is simple: I essentially described *all* the sources of systematic errors. The kind of assumptions one has to make are minimal.

Let me also mention that there is a large number of other results for α from lattice gauge theory, where $\alpha(\mu \sim a^{-1})$ is extracted from quantities related to the cutoff. Some of them cite a very small error [122]. As discussed in [31], it is not easy to estimate the systematic errors in these computations, mainly because one cannot separately discuss higher order perturbative corrections and discretization errors. We thus think it is very desirable to carry out the program of Fig. 11 with good precision and the relevant number of flavors.

II.3 Renormalization group invariant quark masses

The computation of running quark masses and the renormalization group invariant (RGI) quark mass proceeds in analogy to the computation of $\alpha(\mu)$. Since we are using a mass-independent renormalization scheme (cf. Sect. I.1.7.2), the renormalization (and thus the scale dependence) is independent of the flavor of the quark. When we consider "the" running mass below, any one flavor can be envisaged; the scale dependence is the same for all of them.

The renormalization group equation for the coupling eq. (II.1.2) is now accompanied by one describing the scale dependence of the mass,

$$\mu\frac{\partial\overline{m}}{\partial\mu} \;=\; \tau(\bar{g}) \;\;, \tag{II.3.1}$$

where τ has an asymptotic expansion

$$\tau(\bar{g}) \;\overset{\bar{g}\to 0}{\sim}\; -\bar{g}^2\left\{d_0+\bar{g}^2 d_1+\ldots\right\}\;, \qquad d_0 = 8/(4\pi)^2 \;\;, \tag{II.3.2}$$

with higher order coefficients d_i, $i>0$ which depend on the scheme.

Similarly to the Λ-parameter, we may define a renormalization group invariant quark mass, M, by the asymptotic behavior of $\overline{m}$,

$$M \;=\; \lim_{\mu\to\infty}\overline{m}(\mu)[2b_0\bar{g}(\mu)^2]^{-d_0/2b_0} \;\;. \tag{II.3.3}$$

It is an easy exercise to show that M does not depend on the renormalization scheme. It can be computed in the SF-scheme and used afterward to obtain the running mass in any other scheme by inserting the proper β- and τ-functions in the renormalization group equations.

To compute the scale evolution of the mass non-perturbatively, we introduce a new step scaling function,

$$\Sigma_{\rm P}(u,a/L) = \left.\frac{Z_{\rm P}(2L)}{Z_{\rm P}(L)}\right|_{\bar{g}^2(L)=u} \;\;, \tag{II.3.4}$$

with $Z_{\rm P}$ of eq. (I.1.41). Results for $\Sigma_{\rm P}$ at finite lattice spacing and the extracted continuum limit are displayed in Fig. 20. Details may be found in [23, 98].

Applying $\sigma_{\rm P}$ and σ recursively one then obtains the series,

$$\overline{m}(2^{-k}L_{\rm max})/\overline{m}(2L_{\rm max})\,,\;\; k=0,1,\ldots \;\;, \tag{II.3.5}$$

up to a largest value of k, which corresponds to the smallest $\bar{g}$ that was considered in Fig. 20. From there on, the perturbative 2-loop approximation to the τ-function and 3-loop approximation to the β-function (in the SF-scheme) may be used to integrate the renormalization group equations to infinite energy, or equivalently to $\bar{g}=0$. The result is the renormalization group invariant mass,

$$M = \overline{m}\,(2b_0\bar{g}^2)^{-d_0/2b_0}\exp\left\{-\int_0^{\bar{g}}{\rm d}g\left[\frac{\tau(g)}{\beta(g)}-\frac{d_0}{b_0 g}\right]\right\} \;\;. \tag{II.3.6}$$

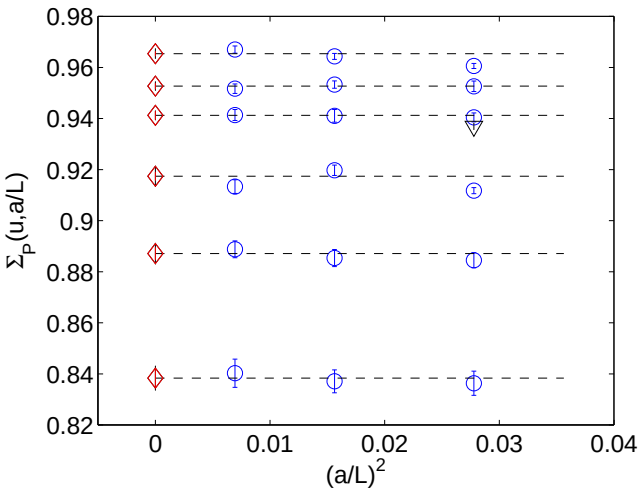


Figure 20: Lattice spacing dependence of the step scaling function for the quark mass for $N_f = 2$. The coupling u ranges from $u = 0.979$ to $u = 3.33$.

In this way, one is finally able to express the running mass $\overline{m}$ in units of the renormalization group invariant mass, M, as shown in Fig. 21. Remember that M has the same value in all renormalization schemes, in contrast to the running mass $\overline{m}$.

The *perturbative* evolution of the quark masses follows very accurately the non-perturbative results down to rather low energy scales. Of course, this result may not be generalized to running masses in other schemes.

The point at lowest scale μ in Fig. 21 corresponds to

$$M/\overline{m} = 1.296(16) \quad \text{at} \quad L = 2L_{\max} \ . \tag{II.3.7}$$

Remembering the very definition of the renormalized mass eq. (I.1.38), one can use this result to relate the renormalization group invariant mass and the bare current quark mass m on the lattice through

$$M = m \times 1.296(16) \times Z_A(g_0)/Z_P(g_0, 2L_{\max}/a) = Z_M(g_0)\, m \ . \tag{II.3.8}$$

In this last step, one then inserts the bare current quark mass, e.g. of the strange quark, and extrapolates the result to the continuum limit. The bare current quark masses themselves are the ones for which the appropriate pseudo scalar masses are fixed to their experimental values. The presently available results from this strategy are listed in Table 4. Note that the computation of the b-quark mass required a detour through Heavy Quark Effective Theory, the subject of the following lecture.

For the charm and the beauty quark masses determinations with $N_f > 0$ and NP renormalization are still missing. However, in our opinion it is even quite early concerning the determinations of the light quark masses. Although some N_f-dependence

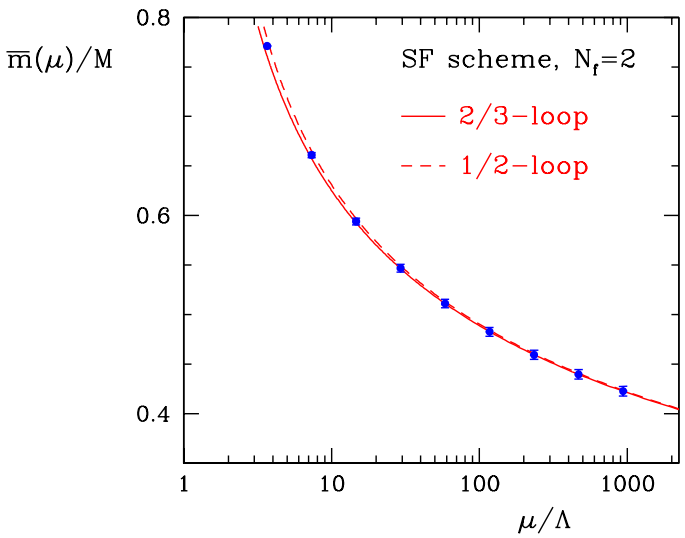


Figure 21: The running quark mass as a function of $\mu \equiv 1/L$ for $N_\mathrm{f} = 2$.

of the strange quark mass has been reported in the literature, one can presently not exclude that this is due to perturbative uncertainties or discretization errors. Note that the quark masses computed in the quenched approximation were in a similar stage in 1996 but very soon afterward the uncertainties shrunk by an order of magnitude due to NP renormalization and continuum extrapolations. This remains to be achieved for the real theory with $N_\mathrm{f} > 0$!

II.4 Renormalization scale dependence of other composite operators

Due to our definition of the renormalized quark mass, its scale dependence is given by the one of the composite operator $P^a(x)$. Other composite operators can be considered and indeed the strategy described here has been applied to 4-fermion operators in the weak effective Hamiltonian [11, 99–101], the HQET axial current [9, 10] and in the operator which yields $\langle x \rangle$ of the non-singlet structure functions [125–127]. It is worth pointing

i	N_f	input	M_i/GeV	ref.
strange	0	m_K, r_0	0.137(05)	[33]
strange	2	m_K, r_0	0.137(27)	[23]
charm	0	m_D, r_0	1.654(45)	[123]
beauty	0	$m_{\mathrm{B_s}}, m_{\mathrm{B_s^*}}, r_0$	6.771(99)	[124]

Table 4: Quark masses determined with full NP renormalization and continuum limit. We use $r_0 = 0.5\,\mathrm{fm}$.

out that the non-perturbative scale dependence disagrees more (and significantly) from the perturbative one in some of these cases. They provide examples which emphasize that a fully non-perturbative renormalization is necessary to control the associated uncertainties. We show two examples in Fig. 22. For details we have to refer to the cited papers.

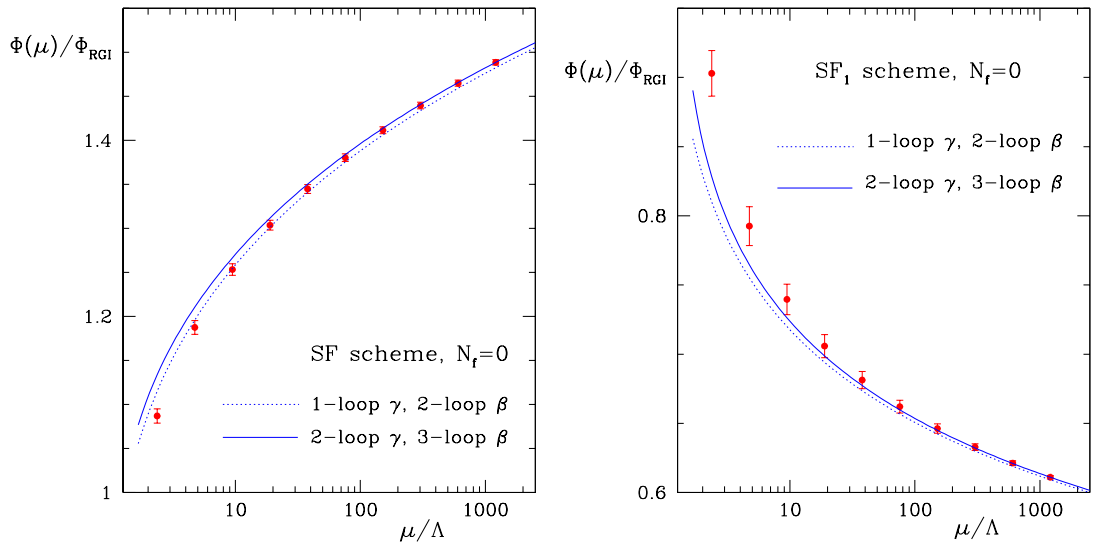


Figure 22: The running of the static-light axial current $\mu \equiv 1/L$ for $N_\mathrm{f} = 0$ (left) [10] and a left-left 4-fermion operator (right) [100].

However, we want to emphasize again one general feature, which was noted already for the $N_\mathrm{f} = 2$ running coupling. Significant differences between the perturbative and the non-perturbative result are present in cases, where the subsequent order of perturbation theory are very close to each other. The difference of 2/3-loop order running to the non-perturbative results can't be parameterized by the next order perturbative term with a reasonable coefficient.

Lecture III.

Non-perturbative Heavy Quark Effective Theory

III.1 Introduction

Similarly to the scale dependent renormalization covered in the previous lecture, the inclusion of heavy quarks in a lattice gauge theory simulation is a multi-scale problem. Such problems are always difficult and require the development of new techniques. By "heavy quark" we mean a quark whose mass is large compared to the intrinsic scale of QCD, $\Lambda_{\rm QCD}$. If we take $\Lambda_{\rm QCD} \approx 500\,\mathrm{MeV}$, the charm quark mass is about a factor 2 higher, but the bottom quark mass has

$$m_{\rm b} \approx 5\,\mathrm{GeV} \sim 10\Lambda_{\rm QCD}\,. \tag{III.1.1}$$

Here $m_{\rm b}$ is a quark mass defined at the scale $\mu = m_{\rm b}$, but the scheme is irrelevant at this point; we will continue to use the symbol $m_{\rm b}$ when this is the case. Since practical large volume simulations do not (yet) reach lattice spacings as small as $a = 1/(5\,\mathrm{GeV})$, we are faced with

$$am_{\rm b} > 1\,, \tag{III.1.2}$$

and a b-quark does not propagate properly on the lattice, at least when it is discretized with a standard relativistic QCD Lagrangian.

For the charm quark, values $am_{\rm c} \ll 1$ are achievable, but still care has to be taken. In Fig. 23 we show the RGI mass of the charm quark in the quenched approximation, computed for three definitions, which differ at finite lattice spacing. While an extrapolation to a common continuum value is convincing, it is already clear from this figure, that the four times heavier bottom quark can't be treated this way. In fact, the main point is that the cutoff-effects become entirely non-linear in a^2, when am is too large. This breakdown of the Symanzik expansion can be seen explicitly in perturbation theory [128]. In a 1-loop calculation, it has been estimated to happen around [128] $am_{\rm b} \approx 1/2$ or $aM_{\rm b} \approx 0.7$.

Various ways of coping with this problem have been proposed and investigated. Referring the reader to reviews for other approaches [129–131], we directly turn to HQET. Already in 1987 Estia Eichten suggested that to describe the non-perturbative dynamics of hadrons with a single heavy quark, it is a good approximation to consider this quark to be static, i.e. it propagates only in time (in the rest frame of the hadron) [132]. This static approximation describes the correct asymptotics of bound state properties as $m_{\rm b} \to \infty$ and corrections of order $1/m_{\rm b}$ can be included systematically. The expansion in $1/m_{\rm b}$ is then given by an effective field theory [133–135]. It has been extended to transition form factors, e.g. between B- and D-mesons, assuming that also the charm quark can be described by the effective field theory [134, 136, 137]. This is done by

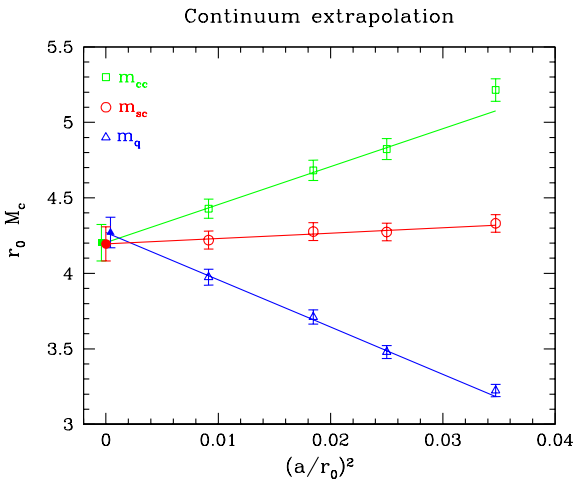


Figure 23: The RGI mass of the charm quark in units of r_0, evaluated with the O(a)-improved formulation, as a function of the lattice spacing [123]. The physical input is the mass of the D_s meson (and m_K, r_0). The RGI-mass at finite lattice spacing is defined through the PCAC-mass, eq. (I.2.21), of a charm-charm correlator (m_{cc}) or a charm-strange correlator (m_{sc}) and through the bare quark mass, m_q, and eq. (I.2.24).

considering heavy quark fields with finite velocities in the limit of large mass. We will here ignore this phenomenologically very interesting possibility and restrict ourselves to HQET at zero velocity (The formulation of HQET in Euclidean space and at non-zero velocity is more subtle [138]).

In this theory considerable progress has been made recently, which we want to explain. In particular, in order to compute $1/m_b$ corrections, one has to know the leading order (including its renormalization) non-perturbatively (Sect. III.3.1.2). This necessitates a so-called non-perturbative matching of effective theory and QCD. A strategy for this [139, 140] will be described in Sect. III.5 including results for $1/m_b$ corrections in a test case. The strategy solves at the same time the problem of a proper definition and computation of $1/m_b$-corrections, which is present in any regularization of the theory, and the problem of power divergences ($\sim a^{-n}$) in a theory with a hard cutoff such as the lattice regularization. After a more general introduction we will concentrate on the inclusion of $1/m_b$ corrections. Because of limitations of space we mention the also very relevant developments in the static approximation only rather briefly.

III.1.1 Derivation of the classical theory

We here go through some steps to derive the effective theory at the classical level. The main point is to see what assumptions have to be made and to present the explicit form of the Lagrangian. We follow the idea of [141], but work in Euclidean space since we are ultimately interested in the lattice theory.

In this section, we keep the dependence of the fields on the space-time coordinates implicit and also drop the label b on the quark field and its mass. We start from the Dirac-Lagrangian of a b-quark with a large mass, m, in the continuum,

$$\begin{aligned} \mathcal{L} &= \overline{\psi}(D_\mu\gamma_\mu + m)\psi && \text{(III.1.3)} \\ &= \psi^\dagger \mathcal{D}\psi\,, \quad \mathcal{D} = m\gamma_0 + D_0 + \gamma_0 D_k \gamma_k\,. && \text{(III.1.4)} \end{aligned}$$

The light quark fields and gauge fields are not touched by our considerations. We write $\psi^\dagger$, but it is just another independent Grassmann integration variable in the path integral. Since we are considering the classical theory, we can assume that the fields are smooth. We can therefore perform an expansion in D_μ. More precisely, we have to refer to a special kinematical situation. We want to describe the dynamics of a hadron containing one heavy quark, where the hadron is at rest. For infinite mass, the heavy quark propagates only in time. Denoting the expansion parameter by ε, the dynamics thus dictates

$$D_0/m = \mathrm{O}(1)\,, \quad D_k/m = \mathrm{O}(\varepsilon)\,, \tag{III.1.5}$$

when these derivatives act on the heavy quark fields. This is often called a power counting scheme. In the quantum theory we will have $\varepsilon = \Lambda_{\mathrm{QCD}}/m$. Obviously quantities such as $F_{\mu\nu} = \mathrm{O}(1)$ are not touched by this consideration. At the lowest order in this expansion the ("large components") quark field ($P_\pm = \frac{1\pm\gamma_0}{2}$)

$$\psi_{\mathrm{h}} = P_+\psi\,, \quad \overline{\psi}_{\mathrm{h}} = \overline{\psi}P_+, \quad , \tag{III.1.6}$$

propagates forward in time, while the anti-quark field,

$$\psi_{\bar{\mathrm{h}}} = P_-\psi\,, \quad \overline{\psi}_{\bar{\mathrm{h}}} = \overline{\psi}P_-\,, \tag{III.1.7}$$

propagates backward. In a somewhat sloppy notation we will often write $\mathrm{O}(1/m)$ instead of $\mathrm{O}(\varepsilon)$. The $\mathrm{O}(1/m)$ terms in the Lagrangian

$$\begin{aligned} \mathcal{L} &= \mathcal{L}^{\mathrm{stat}}_{\mathrm{h}} + \mathcal{L}^{\mathrm{stat}}_{\bar{\mathrm{h}}} + \mathrm{O}(\tfrac{1}{m}) && \text{(III.1.8)} \\ \mathcal{L}^{\mathrm{stat}}_{\mathrm{h}} &= \overline{\psi}_{\mathrm{h}}(D_0 + m)\psi_{\mathrm{h}}\,, \quad \mathcal{L}^{\mathrm{stat}}_{\bar{\mathrm{h}}} = \overline{\psi}_{\bar{\mathrm{h}}}(-D_0 + m)\psi_{\bar{\mathrm{h}}}\,, && \text{(III.1.9)} \end{aligned}$$

connect quark and anti-quark fields. They can be decoupled through a Foldy-Wouthuysen rotation,

$$\begin{aligned} \mathcal{L} &= \phi^\dagger \mathcal{D}'\phi\,, \quad \phi = \mathrm{e}^S\psi\,,\ \phi^\dagger = \psi^\dagger \mathrm{e}^{-S} && \text{(III.1.10)} \\ & \mathcal{D}' = \mathrm{e}^S \mathcal{D}\mathrm{e}^{-S}\,, \quad S = \tfrac{1}{2m}D_k\gamma_k = -S^\dagger = \mathrm{O}(\tfrac{1}{m})\,, && \text{(III.1.11)} \end{aligned}$$

which yields explicitly

$$\begin{aligned} \mathcal{D}' &= \mathcal{D} + \tfrac{1}{2m}[D_k\gamma_k, \mathcal{D}] + \tfrac{1}{8m^2}[D_l\gamma_l, [D_k\gamma_k, \mathcal{D}]] + \mathrm{O}(\tfrac{1}{m^2}) && \text{(III.1.12)} \\ &= \mathcal{D} + \tfrac{1}{2m}[D_k\gamma_k, \mathcal{D}] - \tfrac{1}{4m}[D_l\gamma_l, \gamma_0 D_k\gamma_k] + \mathrm{O}(\tfrac{1}{m^2}) \\ &= \gamma_0\left\{\gamma_0 D_0 + m + \tfrac{1}{2m}(-D_k D_k - \frac{1}{2i}F_{kl}\sigma_{kl}) + \tfrac{1}{2m}F_{k0}\gamma_0\gamma_k\right\} + \mathrm{O}(\tfrac{1}{m^2})\,. \end{aligned}$$

The Lagrangian then reads

$$\mathcal{L} = \mathcal{L}_{\rm h}^{\rm stat} + \mathcal{L}_{\bar{\rm h}}^{\rm stat} + \left\{\mathcal{L}_{\rm h}^{(1)} + \mathcal{L}_{\bar{\rm h}}^{(1)} + \mathcal{L}_{\rm h\bar{h}}^{(1)}\right\} + {\rm O}(\tfrac{1}{m^2}) \qquad \text{(III.1.13)}$$

$$\mathcal{L}_{\rm h}^{(1)} = \tfrac{1}{2m}\overline{\psi}_{\rm h}(-D_kD_k - \frac{1}{2i}F_{kl}\,\sigma_{kl})\psi_{\rm h}\,, \qquad \text{(III.1.14)}$$

$$\sigma_{\mu\nu} = \frac{i}{2}[\gamma_\mu,\gamma_\nu]\,, \quad F_{kl} = [D_k, D_l]\,. \qquad \text{(III.1.15)}$$

For hadrons (or correlation functions) with a single b-quark (or anti-b-quark) only double insertions of $\mathcal{L}_{\rm h\bar{h}}^{(1)}$ contribute. These are of order $1/m^2$ and may be dropped at the order written explicitly.

For later convenience we introduce the short hand

$$\mathcal{L}_{\rm h}^{(1)} = -\tfrac{1}{2m}(\mathcal{O}_{\rm kin} + \mathcal{O}_{\rm spin})\,, \qquad \text{(III.1.16)}$$

$$\mathcal{O}_{\rm kin} = \overline{\psi}_{\rm h}\, D_kD_k\, \psi_{\rm h} = \overline{\psi}_{\rm h}\, \mathbf{D}^2\, \psi_{\rm h}\,, \qquad \text{(III.1.17)}$$

$$\mathcal{O}_{\rm spin} = \overline{\psi}_{\rm h}\, \frac{1}{2i}F_{kl}\,\sigma_{kl}\,\psi_{\rm h} = \overline{\psi}_{\rm h}\,\sigma\cdot\mathbf{B}\,\psi_{\rm h}\,. \qquad \text{(III.1.18)}$$

We note that $\mathcal{L}$, eq. (III.1.13) is a low energy effective Lagrangian [142–144]. It describes the long wave length modes of the fields accurately and makes truncation errors, which are of increasing relevance for shorter wave lengths. This becomes particularly apparent when we remove the mass terms from the static Lagrangian and define

$$\mathcal{L}_{\rm h}^{\rm stat} = \overline{\psi}_{\rm h}(D_0+\epsilon)\psi_{\rm h}\,, \quad \mathcal{L}_{\bar{\rm h}}^{\rm stat} = \overline{\psi}_{\bar{\rm h}}(-D_0+\epsilon)\psi_{\bar{\rm h}}\,, \qquad \text{(III.1.19)}$$

where the limit $\epsilon \to 0_+$ is to be understood in order to select the proper propagation in time. Replacing eq. (III.1.9) by eq. (III.1.19) corresponds *exactly* to an energy shift by an amount m of all states containing a single heavy quark or anti-quark. For Euclidean correlation functions it just leads to an additional factor of $\exp(-m\,(y_0 - x_0))$ for correlation functions where a quark propagates from x_0 to $y_0 \geq x_0$. (For the anti-quark there is a factor $\exp(+m\,(y_0 - x_0))$ with $y_0 \leq x_0$).

We note again that the essential assumption is eq. (III.1.5), namely the spatial covariant derivatives are counted as small compared to the mass term and the time derivative. This is the correct physical situation in a frame where the hadron is at rest and therefore at lowest order also the quark is at rest.

Instead of carrying out the expansion of the action, one could also expand the heavy quark propagator in terms of $1/m$.

Quantum fluctuations are not smooth and invalidate the above "derivation". However, one expects that they do not modify the structure of the effective Lagrangian, but rather only modify the coefficients of the various terms by non-trivial renormalizations due to these *short distance* fluctuations. After all, arguing heuristically, long wavelength terms have been identified correctly and are described by local interaction terms. In local quantum field theory, also effective local quantum field theory, such terms are renormalized by a renormalization of the coefficients of the local fields. Below, we will discuss this in some detail.

III.2 The effective quantum field theory

III.2.1 The static approximation and its symmetries

We start with the lowest order and just consider the heavy quark; the antiquark action and propagator is completely analogous. In continuum Euclidean space, the classic Lagrangian density $\mathcal{L}_{\rm h}^{\rm stat}$, eq. (III.1.19), contains local fields of a mass dimension $D \leq 4$. It is power counting renormalizable. The static effective field theory is thus expected to be renormalizable in the usual sense, i.e. by a finite number of counter-terms. The possible counter-terms are restricted by the symmetries. Apart from the usual ones (parity, gauge symmetry ...), there is a well known invariance under spin rotations [134, 136, 137, 148]. The infinitesimal variations of these transformations can be written as

$$\delta_\sigma^k \psi_{\rm h} = \sigma_k \psi_{\rm h}\,, \qquad \delta_\sigma^k \overline{\psi}_{\rm h} = -\overline{\psi}_{\rm h}\sigma_k\,, \qquad \sigma_k \equiv -\tfrac{1}{2}\epsilon_{ijk}\sigma_{ij}\,, \tag{III.2.1}$$

with $[\sigma_k, \sigma_l] = i\epsilon_{klm}\sigma_m$. In addition, the action is invariant under phase transformations,

$$\psi_{\rm h} \longrightarrow {\rm e}^{i\eta(\mathbf{x})}\,\psi_{\rm h}, \qquad \overline{\psi}_{\rm h} \longrightarrow \overline{\psi}_{\rm h}{\rm e}^{-i\eta(\mathbf{x})}, \tag{III.2.2}$$

with an arbitrary space- (but not time-) dependent parameter $\eta(\mathbf{x})$. This invariance corresponds to the local conservation of b-quark number, ensuring that the quark propagates only in time. The only counter-term of dimension $D \leq 4$, which involves $\psi_{\rm h}, \overline{\psi}_{\rm h}$ and is invariant under these symmetries is $\overline{\psi}_{\rm h}\psi_{\rm h}$. Denoting its coefficient by δm, the formal continuum quantum Lagrangian is thus simply

$$\mathcal{L}_{\rm h}^{\rm stat} = \overline{\psi}_{\rm h}(D_0 + \delta m)\psi_{\rm h}\,. \tag{III.2.3}$$

In order to discuss the equivalence of the effective theory and QCD for correlation functions, we introduce also the time component of the axial current in the effective theory,

$$A_0^{\rm stat}(x) = \overline{\psi}_{\rm l}(x)\gamma_0\gamma_5\psi_{\rm h}(x)\,, \tag{III.2.4}$$

as a prototype for a composite field. There is no other operator with its quantum numbers and with dimension $D \leq 3$. Hence $A_0^{\rm stat}(x)$ renormalizes multiplicatively.

III.2.1.1 Lattice formulation

Just like the continuum theory we formulate the lattice theory in terms of formally 4-component fields, satisfying

$$P_+\psi_{\rm h} = \psi_{\rm h}\,, \quad \overline{\psi}_{\rm h}P_+ = \overline{\psi}_{\rm h}\,. \tag{III.2.5}$$

The time-doubler is removed by choosing the lattice backward derivative

$$D_0^{\rm W}\psi_{\rm h}(x) = \frac{1}{a}\left[\psi_{\rm h}(x) - W^\dagger(x - a\hat{0}, 0)\psi_{\rm h}(x - a\hat{0})\right]\,, \tag{III.2.6}$$

in the action

$$S_{\rm h}^{\rm W} = a^4 \frac{1}{1 + a\,\delta m_{\rm W}} \sum_x \overline{\psi}_{\rm h}(x)(D_0^{\rm W} + \delta m_{\rm W})\psi_{\rm h}(x)\;. \qquad \text{(III.2.7)}$$

With $W(x,0) = U(x,0)$, the standard time-like links, this is the Eichten-Hill action [133]. For the Monte Carlo evaluation it is however of a considerable advantage to define the theory with more general parallel transporters $W(x,0)$, equivalent to $U(x,0)$ up to $\mathrm{O}(a^2)$. In this way statistical errors of correlation functions at large separation x_0 can be reduced exponentially (in x_0) and at the same time discretization errors have been found to be somewhat smaller [145, 146]. Concentrating on conceptual issues, we refer to the cited papers for details on this more practical issue.

It is an easy exercise to show that the static propagator in the presence of gauge fields is ($a\widehat{\delta m} = \ln(1 + a\delta m)$)

$$\begin{aligned} G_{\rm h}^{\rm W}(x,y) &= \theta(x_0 - y_0)\;\delta(\mathbf{x}-\mathbf{y})\;\exp\big(-\widehat{\delta m}_{\rm W}\,(x_0-y_0)\big)\;\mathcal{P}^{\rm W}(y,x)^\dagger\;P_+\;, \\ \mathcal{P}^{\rm W}(x,x) &= 1\;, \quad \mathcal{P}^{\rm W}(x,y+a\hat{\mu}) = \mathcal{P}^{\rm W}(x,y)W(y,\mu)\,, \end{aligned} \qquad \text{(III.2.8)}$$

when the fields are normalized as in eq. (III.2.7). Here $\theta(x_0), \delta(\mathbf{x})$ are straight forward lattice transcriptions of the continuum θ- and δ-functions. While in the continuum case, an ϵ-prescription is necessary to select the forward propagation $\theta(x_0 - y_0)$, the propagator of the lattice action with backward derivative, eq. (III.2.6), has this property automatically. The symmetries eq. (III.2.1) and eq. (III.2.2) are preserved by the lattice regularization eq. (III.2.7).

Improvement

With these symmetries one easily goes through the steps introduced in Sect. I.2.2 to find the structure of Symanzik's effective action. It turns out that the only allowed $\mathrm{O}(a)$ terms are proportional to the light quark masses [9]. They are therefore numerically not very relevant and in addition their coefficients vanish for $N_{\rm f} = 0$. It is interesting to note that through the static effective theory one can also give a convincing argument that the force between static quarks is free of linear a-effects, if the light quark action is $\mathrm{O}(a)$-improved [93].

For ease of notation we drop the sub- and superscript W from now on.

III.2.1.2 Renormalization

The only term needed for the renormalization of the action, δm, has been included above. The explicit form of the propagator shows that δm enters in a purely kinematical way, just as an energy shift by an amount $\widehat{\delta m}$ compared to the unrenormalized, $\delta m = 0$ case. Thus all masses of hadrons (we consider only those with a single heavy quark) have the same shift and their splittings can be predicted in static approximation up to $\Lambda_{\rm QCD}^2/m_{\rm b}$ corrections without adjusting any parameter except for those in the "light part of QCD". Obviously, the splittings are also the same if the b-quark is replaced by

the charm quark, but now up to $\Lambda^2_{\rm QCD}/m_{\rm c}$, if $m_{\rm c}$ is large enough for the $1/m_{\rm c}$ expansion to make sense.

But also in the static approximation non-trivial renormalizations occur as soon as hadronic matrix elements are considered. The most prominent example is the computation of the B-meson decay constant, $F_{\rm B}$. In QCD it can be obtained from the correlation function [21]

$$C_{\rm AA}(x_0) = Z_{\rm A}^2 a^3 \sum_{\mathbf{x}} \Big\langle A_0(x)(A_0)^\dagger(0)\Big\rangle \tag{III.2.9}$$

with the heavy-light axial current in QCD, $A_\mu = \overline{\psi}_{\rm l}\gamma_\mu\gamma_5\psi_{\rm b}$, and $A_\mu^\dagger = \overline{\psi}_{\rm b}\gamma_\mu\gamma_5\psi_{\rm l}$. In QCD, $Z_{\rm A}(g_0)$ is fixed by chiral Ward identities [20, 21], which shows that it does not depend on a renormalization scale. The decay constant may e.g. be obtained from (we use the finite volume normalization $\langle B|B\rangle = 1$ for the zero momentum state $|B\rangle$)

$$\begin{aligned}[\Phi^{\rm QCD}]^2 &\equiv F_{\rm B}^2\, m_{\rm B} \qquad\qquad\qquad\

The $1/m_{\rm b}$ Lagrangian then reads

$$\mathcal{L}_{\rm h}^{(1)}(x) = -(\omega_{\rm kin}\,\mathcal{O}_{\rm kin}(x) + \omega_{\rm spin}\,\mathcal{O}_{\rm spin}(x))\,. \tag{III.2.13}$$

Since these terms are fields of dimension five, the theory defined with a path integral weight $P \propto \exp(-a^4\sum_x[\mathcal{L}_{\rm light}(x) + \mathcal{L}_{\rm h}^{\rm stat}(x) + \mathcal{L}_{\rm h}^{(1)}(x)])$ is *not* renormalizable. In perturbation theory, new divergences will occur at each order in the loop expansion, which necessitate to introduce new counter-terms. The continuum limit of the lattice theory will then not exist. However, that effective theory is NRQCD not HQET. Since the effective theory is "only" supposed to reproduce the $1/m_{\rm b}$ expansion of the observables order by order in $1/m_{\rm b}$, we expand the weight P in $1/m_{\rm b}$, counting $\omega_{\rm kin} = {\rm O}(1/m_{\rm b}) = \omega_{\rm spin}$. This defines HQET. The same step has already been used in Symanzik's effective theory.

Up to and including ${\rm O}(1/m_{\rm b})$, expectation values in HQET are defined as

$$\begin{aligned}\langle\mathcal{O}\rangle &= \langle\mathcal{O}\rangle_{\rm stat} + \omega_{\rm kin}a^4\sum_x\langle\mathcal{O}\mathcal{O}_{\rm kin}(x)\rangle_{\rm stat} + \omega_{\rm spin}a^4\sum_x\langle\mathcal{O}\mathcal{O}_{\rm spin}(x)\rangle_{\rm stat}\\ &\equiv \langle\mathcal{O}\rangle_{\rm stat} + \omega_{\rm kin}\langle\mathcal{O}\rangle_{\rm kin} + \omega_{\rm spin}\langle\mathcal{O}\rangle_{\rm spin}\,,\end{aligned} \tag{III.2.14}$$

where

$$\langle\mathcal{O}\rangle_{\rm stat} = \frac{1}{\mathcal{Z}}\int_{\rm fields}\mathcal{O}\exp(-a^4\sum_x[\mathcal{L}_{\rm light}(x) + \mathcal{L}_{\rm h}^{\rm stat}(x)]) \tag{III.2.15}$$

is defined with respect to the lowest order action, which is power counting renormalizable. The path integral defining the average extends over all fields and the normalization $\mathcal{Z}$ is fixed by $\langle 1\rangle_{\rm stat} = 1$.

In order to compute matrix elements or correlation functions in the effective theory, we also need the effective composite fields. At the classical level they can again be obtained from the Foldy-Wouthuysen rotation. In the quantum theory one adds all local fields with the proper quantum numbers and dimensions. For example the effective axial current (time component) is given by

$$A_0^{\rm HQET}(x) = Z_{\rm A}^{\rm HQET}\,[A_0^{\rm stat}(x) + c_{\rm A}^{\rm HQET}\delta A_0^{\rm stat}(x)]\,, \tag{III.2.16}$$

$$\delta A_0^{\rm stat}(x) = \overline{\psi}_{\rm l}(x)\frac{1}{2}(\overleftarrow{\nabla}_i + \overleftarrow{\nabla}_i^*)\gamma_i\gamma_5\psi_{\rm h}(x)\,. \tag{III.2.17}$$

Before entering into more details on the renormalization, we show some examples how the $1/m_{\rm b}$-expansion works.

III.2.2.1 $1/m_{\rm b}$-expansion of correlation functions and matrix elements

For now we assume that the coefficients

$$\begin{aligned}{\rm O}(1)\,: &\quad \delta m\,,\ Z_{\rm A}^{\rm HQET}\,,\\ {\rm O}(1/m_{\rm b})\,: &\quad \omega_{\rm kin}\,,\ \omega_{\rm spin}\,,\ c_{\rm A}^{\rm HQET}\,,\end{aligned} \tag{III.2.18}$$

are known as a function of the bare coupling g_0 and the quark mass $m_{\rm b}$. Their non-perturbative determination will be discussed later.

The rules of the $1/m_{\rm b}$-expansion are illustrated for of $C_{\rm AA}(x_0)$, eq. (III.2.9). One uses eq. (III.2.14) and the HQET representation of the composite field eq. (III.2.16). Then the expectation value is expanded consistently in $1/m_{\rm b}$, counting powers of $1/m_{\rm b}$ as in eq. (III.2.18). At order $1/m_{\rm b}$, terms proportional to $\omega_{\rm kin} \times c_{\rm A}^{\rm HQET}$ etc. are to be dropped. As a last step, we have to take the energy shift between HQET and QCD into account. Therefore the correlation function obtains an extra factor $\exp(-x_0 m_{\rm b})$, where the scheme dependence of $m_{\rm b}$ is compensated by a corresponding one in δm. One arrives at the expansion

$$\begin{aligned} C_{\rm AA}(x_0) &= {\rm e}^{-m_{\rm b}x_0}(Z_{\rm A}^{\rm HQET})^2 \Big[C_{\rm AA}^{\rm stat}(x_0) + c_{\rm A}^{\rm HQET}\, C_{\delta{\rm AA}}^{\rm stat}(x_0) \\ &\quad + \omega_{\rm kin}\, C_{\rm AA}^{\rm kin}(x_0) + \omega_{\rm spin}\, C_{\rm AA}^{\rm spin}(x_0)\Big] \end{aligned} \tag{III.2.19}$$

with (remember the definitions in eq. (III.2.14))

$$\begin{aligned} C_{\delta{\rm AA}}^{\rm stat}(x_0) &= \langle A_0^{\rm stat}(x)(\delta A_0^{\rm stat}(0))^\dagger\rangle_{\rm stat} + \langle \delta A_0^{\rm stat}(x)(A_0^{\rm stat}(0))^\dagger\rangle_{\rm stat}\,, \\ C_{\rm AA}^{\rm kin}(x_0) &= \langle A_0^{\rm stat}(x)(A_0^{\rm stat}(0))^\dagger\rangle_{\rm kin}\,, \\ C_{\rm AA}^{\rm spin}(x_0) &= \langle A_0^{\rm stat}(x)(A_0^{\rm stat}(0))^\dagger\rangle_{\rm spin}\,. \end{aligned} \tag{III.2.20}$$

It is now a straight forward exercise to obtain the expansion of the B-meson mass[22]

$$m_{\rm B} = m_{\rm b} + \widehat{\delta m} + E_{\rm stat} + \omega_{\rm kin}E_{\rm kin} + \omega_{\rm spin}E_{\rm spin}\,, \tag{III.2.21}$$

$$E_{\rm stat} = -\lim_{x_0\to\infty} \widetilde{\partial_0}\, \ln C_{\rm AA}^{\rm stat}(x_0)\Big|_{\delta m=0}\,, \tag{III.2.22}$$

$$E_{\rm kin} = -\lim_{x_0\to\infty} \widetilde{\partial_0}\, \rho_{\rm kin}(x_0)\,, \quad \rho_{\rm kin}(x_0) = \frac{C_{\rm AA}^{\rm kin}(x_0)}{C_{\rm AA}^{\rm stat}(x_0)}\,, \tag{III.2.23}$$

$$E_{\rm spin} = -\lim_{x_0\to\infty} \widetilde{\partial_0}\, \rho_{\rm spin}(x_0)\,, \quad \rho_{\rm spin}(x_0) = \frac{C_{\rm AA}^{\rm spin}(x_0)}{C_{\rm AA}^{\rm stat}(x_0)}\,, \tag{III.2.24}$$

and its decay constant

$$F_{\rm B}\sqrt{m_{\rm B}} = \lim_{x_0\to\infty} \{2\exp(m_{\rm B}x_0)\, C_{\rm AA}(x_0)\}^{1/2}\,, \tag{III.2.25}$$

$$\begin{aligned} &= Z_{\rm A}^{\rm HQET} \lim_{x_0\to\infty} \Phi^{\rm stat}\, \{1 + \tfrac{1}{2}x_0[\omega_{\rm kin}E_{\rm kin} + \omega_{\rm spin}E_{\rm kin}] \\ &\quad + \tfrac{1}{2}c_{\rm A}^{\rm HQET}\rho_{\delta{\rm A}}(x_0) + \tfrac{1}{2}\omega_{\rm kin}\rho_{\rm kin}(x_0) + \tfrac{1}{2}\omega_{\rm spin}\rho_{\rm spin}(x_0)\}\,, \end{aligned} \tag{III.2.26}$$

$$\Phi^{\rm stat} = \lim_{x_0\to\infty} \{2\exp(E_{\rm stat}x_0)\, C_{\rm AA}^{\rm stat}(x_0)\}^{1/2}\,, \quad \rho_{\delta{\rm A}}(x_0) = \frac{C_{\delta{\rm AA}}^{\rm stat}(x_0)}{C_{\rm AA}^{\rm stat}(x_0)}\,.$$

[22] It follows from the simple form of the static propagator that there is no dependence on δm except for the explicitly shown energy shift $\widehat{\delta m}$.

Using the transfer matrix formalism (with normalization $\langle B|B\rangle = 1$), one further observes that

$$\begin{aligned} E_{\rm kin} &= -\langle B|a^3\sum_{\mathbf{z}}\mathcal{O}_{\rm kin}(0,\mathbf{z})|B\rangle_{\rm stat}\,, \\ E_{\rm spin} &= -\langle B|a^3\sum_{\mathbf{z}}\mathcal{O}_{\rm spin}(0,\mathbf{z})|B\rangle_{\rm stat}\,. \end{aligned} \tag{III.2.27}$$

As expected, only the parameters of the action are relevant in the expansion of hadron masses.

A correct split of the terms in eq. (III.2.21) and eq. (III.2.26) into leading order and next to leading order pieces which *separately have a continuum limit* requires more thought on the renormalization of the $1/m_{\rm b}$-expansion. We turn to this now.

III.2.2.2 Renormalization and continuum limit

For illustration we first check the self consistency of eq. (III.2.19). The relevant question concerns renormalization, namely: are the "free" parameters $\delta m \ldots c_{\rm A}^{\rm HQET}$ sufficient to absorb all divergences on the r.h.s.? We consider the most difficult term, $C_{\rm AA}^{\rm kin}(x_0)$. According to the standard rules, it is renormalized as

$$\begin{aligned} \left(C_{\rm AA}^{\rm kin}\right)_{\rm R}(x_0) &= (Z_{\rm A}^{\rm stat})^2 \times \\ &\quad a^7\sum_{\mathbf{x},\,z}\left\langle A_0^{\rm stat}(x)\,(A_0^{\rm stat}(0))^\dagger\,(\mathcal{O}_{\rm kin})_{\rm R}(z)\right\rangle_{\rm stat} + \text{C.T.}\,, \end{aligned} \tag{III.2.28}$$

where C.T. denotes contact terms to be discussed shortly. The operator $(\mathcal{O}_{\rm kin})_{\rm R}(z)$ involves a subtraction of lower dimensional ones,

$$(\mathcal{O}_{\rm kin})_{\rm R}(z) = Z_{\mathcal{O}_{\rm kin}}(\mathcal{O}_{\rm kin}(z) + \frac{c_1}{a}\,\overline{\psi}_{\rm h}(z)D_0\psi_{\rm h}(z) + \frac{c_2}{a^2}\,\overline{\psi}_{\rm h}(z)\psi_{\rm h}(z))\,, \tag{III.2.29}$$

written here in terms of dimensionless c_i. Since we are interested in on-shell observables ($x_0 > 0$ in eq. (III.2.19)), we may use the equation of motion $D_0\psi_{\rm h}(z) = 0$ to eliminate the second term. The third one, $\frac{c_2}{a^2}\overline{\psi}_{\rm h}(z)\psi_{\rm h}(z)$, is equivalent to a mass shift and only changes δm, which is hence quadratically divergent [23]. Thus all terms which are needed for the renormalization of $\mathcal{O}_{\rm kin}$ are present in eq. (III.2.19).

It remains to consider the contact terms in eq. (III.2.28). They originate from singularities in the operator products $\mathcal{O}_{\rm kin}(z)A_0^{\rm stat}(x)$ as $z \to x$ (and $\mathcal{O}_{\rm kin}(z)(A_0^{\rm stat})^\dagger(0)$ as $z \to 0$), in complete analogy to the discussion in Sect. I.2.2.3. Using the operator product expansion they can be represented as linear combinations of $A_0^{\rm stat}(x)$ and $\delta A_0^{\rm stat}(x)$.

[23] Using the explicit form of the static propagator, eq. (III.2.8), one can check that indeed $a^3\sum_{\mathbf{x}}\left\langle A_0^{\rm stat}(x)\,(A_0^{\rm stat}(0))^\dagger a^4\sum_z\overline{\psi}_{\rm h}(z)\psi_{\rm h}(z)\right\rangle_{\rm stat} = x_0 C_{\rm AA}^{\rm stat}(x_0)$, which can be absorbed by a $1/m_{\rm b}$ correction to δm.

Such terms are contained in eq. (III.2.19) in the form of $C_{\rm AA}^{\rm stat}$ and $C_{\delta{\rm AA}}^{\rm stat}$. Indeed $A_0^{\rm stat}(x)$ and $\delta A_0^{\rm stat}(x)$ are the only operators of dimension 3 and 4 with the correct quantum numbers. Higher dimensional operators contribute only terms of order a.

Note that the coefficient of $A_0^{\rm stat}(x)$ in the expansion of the operator product $a^4\sum_z \mathcal{O}_{\rm kin}(z)A_0^{\rm stat}(x)$ is power divergent $\sim 1/a$, for simple dimensional reasons. This means that there is a power divergent contribution to $Z_{\rm A}^{\rm HQET}$. As this happens only at order $1/m_{\rm b}$, not at the lowest order, this contribution to $Z_{\rm A}^{\rm HQET}$ behaves like $\sim 1/(am_{\rm b})$ for small lattice spacing.

We conclude that all terms which are needed for the renormalization of $C_{\rm AA}^{\rm kin}(x_0)$ are present in eq. (III.2.19); the parameters may thus be adjusted to absorb all infinities and with properly chosen coefficients the continuum limit of the r.h.s. is expected to exist. The basic assumption of the effective field theory is that once the finite parts of the coefficients have been determined by matching a set of observables to QCD, these coefficients are applicable to any other observables.

III.2.2.3 The flavor currents in the effective theory

For later use we here give the expressions for the heavy-light currents. They are relevant in weak B-meson decays. For better readability, we include again the time component of the axial current.

Following our general rules for finding the HQET fields which represent the QCD ones we find

$$\begin{aligned}
A_0^{\rm HQET}(x) &= Z_{\rm A}^{\rm HQET}\left[A_0^{\rm stat}(x) + c_{\rm A}^{\rm HQET}\delta A_0^{\rm stat}(x)\right], && \text{(III.2.30)}\\
V_0^{\rm HQET}(x) &= Z_{\rm V}^{\rm HQET}\left[V_0^{\rm stat}(x) + c_{\rm V}^{\rm HQET}\delta V_0^{\rm stat}(x)\right], && \text{(III.2.31)}\\
V_k^{\rm HQET}(x) &= Z_{\mathbf{V}}^{\rm HQET}\left[V_k^{\rm stat}(x) + c_{\mathbf{V}}^{\rm HQET}\delta V_k^{\rm stat}(x)\right], && \text{(III.2.32)}\\
A_k^{\rm HQET}(x) &= Z_{\mathbf{A}}^{\rm HQET}\left[A_k^{\rm stat}(x) + c_{\mathbf{A}}^{\rm HQET}\delta A_k^{\rm stat}(x)\right]. && \text{(III.2.33)}
\end{aligned}$$

Ignoring that one can in principle simplify, for instance $\overline{\psi}_{\rm l}(x)\gamma_0\gamma_5\psi_{\rm h}(x) = -\overline{\psi}_{\rm l}(x)\gamma_5\psi_{\rm h}(x)$ due to $P_+\psi_{\rm h} = \psi_{\rm h}$, the basis fields are written in full analogy to the ones in QCD:

$$\begin{aligned}
V_0^{\rm stat} &= \overline{\psi}_{\rm l}\gamma_0\psi_{\rm h}\,, \quad A_0^{\rm stat} = \overline{\psi}_{\rm l}\gamma_0\gamma_5\psi_{\rm h}\,, && \text{(III.2.34)}\\
V_k^{\rm stat} &= \overline{\psi}_{\rm l}\gamma_k\psi_{\rm h}\,, \quad A_k^{\rm stat} = \overline{\psi}_{\rm l}\gamma_k\gamma_5\psi_{\rm h}\,, && \text{(III.2.35)}\\
\delta V_0^{\rm stat} &= \overline{\psi}_{\rm l}\frac{\overleftarrow{\nabla}_i + \overleftarrow{\nabla}_i^*}{2}\gamma_i\psi_{\rm h}\,, \quad \delta A_0^{\rm stat} = \overline{\psi}_{\rm l}\frac{\overleftarrow{\nabla}_i + \overleftarrow{\nabla}_i^*}{2}\gamma_i\gamma_5\psi_{\rm h}\,, && \text{(III.2.36)}\\
\delta V_k^{\rm stat} &= -\overline{\psi}_{\rm l}\frac{\overleftarrow{\nabla}_i + \overleftarrow{\nabla}_i^*}{2}\gamma_i\gamma_k\psi_{\rm h}\,, \quad \delta A_k^{\rm stat} = \overline{\psi}_{\rm l}\frac{\overleftarrow{\nabla}_i + \overleftarrow{\nabla}_i^*}{2}\gamma_i\gamma_k\gamma_5\psi_{\rm h}\,, && \text{(III.2.37)}
\end{aligned}$$

We have chosen the bare fields such that they are exactly related by spin rotations,[24]

$$\delta_\sigma^k[V_0^{\rm stat}] = iA_k^{\rm stat}\,, \quad \delta_\sigma^k[\delta V_0^{\rm stat}] = i\delta A_k^{\rm stat}\,,$$

[24] The unnatural $-$ sign in eq. (III.2.37) is present because we remain with the definition of $\delta A_0^{\rm stat}$ in [9] and do not want to introduce signs in eq. (III.2.38).
The other rotations look like $\delta_\sigma^j A_k^{\rm stat} = i\,\epsilon_{kjl}V_l^{\rm stat} - i\,\delta_{kj}A_0^{\rm stat}$.

$$\delta_\sigma^k[A_0^{\rm stat}] \;=\; iV_k^{\rm stat}\,, \quad \delta_\sigma^k[\delta A_0^{\rm stat}] = i\delta V_k^{\rm stat}\,. \tag{III.2.38}$$

In general, all Z-factors and coefficients $c^{\rm HQET}$ are functions of g_0 and $am_{\rm b}$ which are to be determined by matching non-perturbatively to QCD. Eq. (III.2.38) will be needed in Sect. III.3.1 when we discuss the static limit of the currents.

III.2.3 Schrödinger functional correlation functions

For an understanding of the details of the tests of HQET (Sect. III.4) as well as the non-perturbative matching to QCD (Sect. III.5) we will also need some Schrödinger functional correlation functions and their HQET expansion, which have not been defined yet. We give these details [140] now. The reader who is only interested in the general concepts may skip this section.

In [9] static quarks in the Schrödinger functional were discussed including Symanzik O(a)-improvement. It turns out that there are no dimension four composite fields which involve static quarks fields and which are compatible with the symmetries of the static action and the Schrödinger functional boundary conditions and which do not vanish by the equations of motion. Thus there are no O(a) boundary counter terms with static quark fields. For the same reason there are also no O($1/m_{\rm b}$) boundary terms in HQET. This then means the HQET expansion of the boundary quark fields $\zeta, \bar\zeta$ is trivial up to and including $1/m_{\rm b}$ terms.

In the spatial boundary condition of the fermion fields,

$$\psi(x+\hat{k}L) = {\rm e}^{i\theta}\psi(x)\,, \quad \overline{\psi}(x+\hat{k}L) = {\rm e}^{-i\theta}\overline{\psi}(x)\,, \tag{III.2.39}$$

the same phase θ is taken for all quark fields, whether relativistic or described by HQET.[25] In QCD, relevant correlation functions in the pseudo-scalar and vector channel are

$$f_{\rm A}(x_0,\theta) \;=\; -\frac{a^6}{2}\sum_{\mathbf{y},\mathbf{z}}\left\langle (A_{\rm I})_0(x)\,\overline{\zeta}_{\rm b}(\mathbf{y})\gamma_5\zeta_{\rm l}(\mathbf{z})\right\rangle\,, \tag{III.2.40}$$

$$k_{\rm V}(x_0,\theta) \;=\; -\frac{a^6}{6}\sum_{\mathbf{y},\mathbf{z},k}\left\langle (V_{\rm I})_k(x)\,\overline{\zeta}_{\rm b}(\mathbf{y})\gamma_k\zeta_{\rm l}(\mathbf{z})\right\rangle\,, \tag{III.2.41}$$

with the O(a) improved currents [139]

$$(A_{\rm I})_\mu \;=\; \overline{\psi}_{\rm l}\gamma_\mu\gamma_5\psi_{\rm b} + ac_{\rm A}\tilde{\partial}_\mu\overline{\psi}_{\rm l}\gamma_5\psi_{\rm b} \tag{III.2.42}$$

$$(V_{\rm I})_\mu \;=\; \overline{\psi}_{\rm l}\gamma_\mu\psi_{\rm b} + ac_{\rm V}\tilde{\partial}_\mu\overline{\psi}_{\rm l}i\sigma_{\mu\nu}\psi_{\rm b}\,. \tag{III.2.43}$$

[25] In principle we can easily have different θ for different fields, as long as they are quenched, so in particular for the heavy field. Since this freedom has not yet been used, we do not discuss it here. In applications with dynamical fermions it may well become relevant.

Furthermore we consider boundary to boundary correlation functions

$$f_1(\theta) = -\frac{a^{12}}{2L^6}\sum_{\mathbf{u},\mathbf{v},\mathbf{y},\mathbf{z}}\left\langle \overline{\zeta}_{\mathrm{l}}{}'(\mathbf{u})\gamma_5\zeta'_{\mathrm{b}}(\mathbf{v})\,\overline{\zeta}_{\mathrm{b}}(\mathbf{y})\gamma_5\zeta_{\mathrm{l}}(\mathbf{z})\right\rangle\,, \tag{III.2.44}$$

$$k_1(\theta) = -\frac{a^{12}}{6L^6}\sum_{\mathbf{u},\mathbf{v},\mathbf{y},\mathbf{z},k}\left\langle \overline{\zeta}_{\mathrm{l}}{}'(\mathbf{u})\gamma_k\zeta'_{\mathrm{b}}(\mathbf{v})\,\overline{\zeta}_{\mathrm{b}}(\mathbf{y})\gamma_k\zeta_{\mathrm{l}}(\mathbf{z})\right\rangle\,. \tag{III.2.45}$$

Their renormalization is standard [46], for example at vanishing light quark masses

$$[f_{\mathrm{A}}]_{\mathrm{R}}(x_0,\theta) = Z_{\mathrm{A}}\,(1+\tfrac{1}{2}b_{\mathrm{A}}am_{\mathrm{q,b}})Z_\zeta^2\,(1+b_\zeta am_{\mathrm{q,b}})f_{\mathrm{A}}(x_0,\theta)\,, \tag{III.2.46}$$

$$[f_1]_{\mathrm{R}}(\theta) = Z_\zeta^4\,(1+b_\zeta am_{\mathrm{q,b}})^2 f_1(\theta)\,, \tag{III.2.47}$$

with Z_ζ a renormalization factor of the relativistic boundary quark fields and b_ζ another improvement coefficient.

Their expansions to first order in $1/m_{\mathrm{b}}$ read

$$[f_{\mathrm{A}}]_{\mathrm{R}} = Z_{\mathrm{A}}^{\mathrm{HQET}}Z_{\zeta_{\mathrm{h}}}Z_\zeta \mathrm{e}^{-m_{\mathrm{b}}x_0}\left\{f_{\mathrm{A}}^{\mathrm{stat}} + c_{\mathrm{A}}^{\mathrm{HQET}}f_{\delta\mathrm{A}}^{\mathrm{stat}} + \omega_{\mathrm{kin}}f_{\mathrm{A}}^{\mathrm{kin}} + \omega_{\mathrm{spin}}f_{\mathrm{A}}^{\mathrm{spin}}\right\} \tag{III.2.48}$$

$$[k_{\mathrm{V}}]_{\mathrm{R}} = Z_{\mathrm{V}}^{\mathrm{HQET}}Z_{\zeta_{\mathrm{h}}}Z_\zeta \mathrm{e}^{-m_{\mathrm{b}}x_0}\left\{k_{\mathrm{V}}^{\mathrm{stat}} + c_{\mathrm{V}}^{\mathrm{HQET}}k_{\delta\mathrm{V}}^{\mathrm{stat}} + \omega_{\mathrm{kin}}k_{\mathrm{V}}^{\mathrm{kin}} + \omega_{\mathrm{spin}}k_{\mathrm{V}}^{\mathrm{spin}}\right\} \tag{III.2.49}$$

$$= -Z_{\mathrm{V}}^{\mathrm{HQET}}Z_{\zeta_{\mathrm{h}}}Z_\zeta \mathrm{e}^{-m_{\mathrm{b}}x_0}\{f_{\mathrm{A}}^{\mathrm{stat}} + c_{\mathrm{V}}^{\mathrm{HQET}}f_{\delta\mathrm{A}}^{\mathrm{stat}} + \omega_{\mathrm{kin}}f_{\mathrm{A}}^{\mathrm{kin}} - \tfrac{1}{3}\omega_{\mathrm{spin}}f_{\mathrm{A}}^{\mathrm{spin}}\}\,,$$

$$[f_1]_{\mathrm{R}} = Z_{\zeta_{\mathrm{h}}}^2 Z_\zeta^2 \mathrm{e}^{-m_{\mathrm{b}}T}\left\{f_1^{\mathrm{stat}} + \omega_{\mathrm{kin}}f_1^{\mathrm{kin}} + \omega_{\mathrm{spin}}f_1^{\mathrm{spin}}\right\}\,, \tag{III.2.50}$$

$$[k_1]_{\mathrm{R}} = Z_{\zeta_{\mathrm{h}}}^2 Z_\zeta^2 \mathrm{e}^{-m_{\mathrm{b}}T}\left\{f_1^{\mathrm{stat}} + \omega_{\mathrm{kin}}f_1^{\mathrm{kin}} - \tfrac{1}{3}\omega_{\mathrm{spin}}f_1^{\mathrm{spin}}\right\}\,. \tag{III.2.51}$$

Apart from

$$f_{\delta\mathrm{A}}^{\mathrm{stat}}(x_0,\theta) = -\frac{a^6}{2}\sum_{\mathbf{y},\mathbf{z}}\left\langle \delta A_0^{\mathrm{stat}}(x)\,\overline{\zeta}_{\mathrm{h}}(\mathbf{y})\gamma_5\zeta_{\mathrm{l}}(\mathbf{z})\right\rangle \tag{III.2.52}$$

the labeling of the different terms follows directly the one introduced in eq. (III.2.14). We have used identities such as $f_{\mathrm{A}}^{\mathrm{kin}} = -k_{\mathrm{V}}^{\mathrm{kin}}$, $f_{\mathrm{A}}^{\mathrm{spin}} = 3k_{\mathrm{V}}^{\mathrm{spin}}$. As a simple consequence of the spin symmetry of the static action, these are valid at any lattice spacing.

III.3 The scope of the theory

We are now in the position to discuss what can be done in the effective theory. This concerns also the continuum effective theory and in particular the question, where perturbation theory is sufficient to give an answer and where it is not.

III.3.1 A first example: the decay constant

III.3.1.1 Renormalization and matching in perturbation theory

The matrix element $\Phi^{\rm QCD}$, eq. (III.2.10), is scale independent, due to the chiral symmetry of QCD in the massless limit. But of course it depends on the mass of the b-quark. In the effective theory this symmetry is absent and, remaining a while at the lowest order in $1/m_{\rm b}$, $Z_{\rm A}^{\rm stat}$ depends on the renormalization scale, μ, used in the renormalization condition which defines the finite current. On the other hand, as long as the effective theory is considered by itself, $Z_{\rm A}^{\rm stat}$ does not depend on the mass of the b-quark in an obvious way. The mass-dependence comes in by choosing an appropriate finite renormalization such that the matrix elements of the current in the effective theory are equal to the ones of the QCD current (up to $\mathrm{O}(1/m_{\rm b})$). This step is called matching. Choosing to renormalize the current in the effective theory in the $\overline{\rm MS}$ scheme (any other scheme would of course be possible) we therefore have

$$\Phi^{\rm QCD} = C_{\rm match}(m_{\rm b},\mu) \times \Phi_{\overline{\rm MS}}(\mu) + \mathrm{O}(1/m_{\rm b}) \tag{III.3.1}$$

with

$$C_{\rm match}(m_{\rm b},\mu) = 1 + c_1(m_{\rm b}/\mu)\bar{g}^2_{\overline{\rm MS}}(\mu) + \ldots \tag{III.3.2}$$

The finite renormalization factor $C_{\rm match}$ is determined (usually in perturbation theory) such that eq. (III.3.1) holds for some particular matrix element of the current and will then be valid *for all matrix elements*. Obviously, the μ-dependence in eq. (III.3.1) is artificial, since we have a scale-independent quantity in QCD. Only the $m_{\rm b}$-dependence is for real.

The μ-dependence in eq. (III.3.1) is removed explicitly by changing from $\Phi_{\overline{\rm MS}}(\mu) \equiv Z^{\rm stat}_{\rm A,\overline{MS}}\langle 0|A_0|B\rangle_{\rm stat}$ to the RGI matrix element

$$\Phi_{\rm RGI} = \lim_{\mu\to\infty}\Big[2b_0\bar{g}^2(\mu)\Big]^{-\gamma_0/2b_0}\,\Phi_{\overline{\rm MS}}(\mu)\,. \tag{III.3.3}$$

Here, the lowest order coefficient of the β-function, b_0 enters as well as $\gamma_0 = -1/(4\pi^2)$ defined by

$$\gamma(\bar{g}) \equiv \frac{\mu}{Z_{\rm A}^{\rm stat}}\frac{\mathrm{d}}{\mathrm{d}\mu}Z_{\rm A}^{\rm stat} = -\gamma_0\bar{g}^2 + \mathrm{O}(\bar{g}^4)\,. \tag{III.3.4}$$

We can now write down the HQET-expansion of the QCD matrix element

$$\Phi^{\rm QCD} = C_{\rm PS}(M_{\rm b}/\Lambda_{\overline{\rm MS}}) \times \Phi_{\rm RGI} \;+\; \mathrm{O}(1/m_{\rm b})\,. \tag{III.3.5}$$

The relation between eq. (III.3.5) and eq. (III.3.1) is easily seen by using

$$\frac{\Phi_{\rm RGI}}{\Phi_{\overline{\rm MS}}(\mu)} = \Big[2b_0\bar{g}^2(\mu)\Big]^{-\gamma_0/2b_0}\exp\left\{-\int_0^{\bar{g}(\mu)}\mathrm{d}g\left[\frac{\gamma_{\overline{\rm MS}}(g)}{\beta_{\overline{\rm MS}}(g)} - \frac{\gamma_0}{b_0 g}\right]\right\} \tag{III.3.6}$$

setting the arbitrary renormalization point μ to m_b and identifying

$$\begin{aligned} C_\mathrm{PS}\left(\frac{M_\mathrm{b}}{\Lambda_{\overline{\mathrm{MS}}}}\right) &= C_\mathrm{match}(1)\frac{\Phi_{\overline{\mathrm{MS}}}(m_\mathrm{b})}{\Phi_\mathrm{RGI}} \\ &= \left[2b_0\bar{g}^2(m_\mathrm{b})\right]^{\gamma_0/2b_0}\exp\left\{\int_0^{\bar{g}(m_\mathrm{b})}\mathrm{d}g\left[\frac{\gamma_\mathrm{match}(g)}{\beta_{\overline{\mathrm{MS}}}(g)}-\frac{\gamma_0}{b_0 g}\right]\right\}, \end{aligned} \tag{III.3.7}$$

where $\bar{g}$ is taken in the $\overline{\mathrm{MS}}$ scheme. The last equation provides a definition of the anomalous dimension γ_match in the "matching scheme". Perturbatively, it has contributions from $\gamma_{\overline{\mathrm{MS}}}$ as well as from C_match, namely

$$\gamma_\mathrm{match}(\bar{g}) = -\gamma_0\bar{g}^2 - [\gamma_1^{\overline{\mathrm{MS}}} + 2b_0 c_1(1)]\bar{g}^4 + \dots\,. \tag{III.3.8}$$

Replacing the $\overline{\mathrm{MS}}$ coupling by a non-perturbative one, γ_match may also be defined beyond perturbation theory through eqs. (III.3.7,III.3.5).[26] Another advantage of eq. (III.3.7) (compared to eq. (III.3.1)) is that C_PS is independent of the arbitrary choice of renormalization scheme for the composite operators in the effective theory. Apart from the choice of the QCD coupling, the "convergence" of the series eq. (III.3.8) is dictated by the physics, nothing else.

Note further that (at leading order in $1/m_\mathrm{b}$) the conversion function C_PS contains the full (logarithmic) mass-dependence. The non-perturbative effective theory matrix elements, Φ_RGI, are mass independent numbers. Conversion functions such as C_PS are universal for all (low energy) matrix elements of their associated operator. Thus

$$C_\mathrm{AA}(x_0) \quad \overset{x_0\gg 1/m_\mathrm{b}}{\sim} \quad [C_\mathrm{PS}(\tfrac{M_\mathrm{b}}{\Lambda_{\overline{\mathrm{MS}}}})\, Z^\mathrm{stat}_\mathrm{A,RGI}]^2\langle A_0^\mathrm{stat}(x)^\dagger A_0^\mathrm{stat}(0)\rangle + \mathrm{O}(\tfrac{1}{m_\mathrm{b}}) \tag{III.3.9}$$

is a straight forward generalization of eq. (III.3.5). Here,
$Z^\mathrm{stat}_\mathrm{A,RGI} = \lim_{\mu\to\infty}\left[2b_0\bar{g}^2(\mu)\right]^{-\gamma_0/2b_0} Z^\mathrm{stat}_{\mathrm{A},\overline{\mathrm{MS}}}(\mu)$.

Analogous expressions for the conversion functions are valid for the time component of the axial current replaced by other composite fields, for example the space components of the vector current. Based on the work of [147–149] and recent efforts their perturbative expansion is known including the 3-loop anomalous dimension γ_match obtained from the 3-loop anomalous dimension $\gamma_{\overline{\mathrm{MS}}}$ [150] and the 2-loop matching function C_match [151–153]. Figure 24, taken from [154], illustrates that the remaining $\mathrm{O}(\bar{g}^6(m_\mathrm{b}))$ errors in C_PS seem to be relatively small.

We return to the full set of heavy-light flavor currents Sect. III.2.2.3. The bare fields satisfy the symmetry relations eq. (III.2.38). The same is then true for the RGI fields in static approximation. Furthermore, the axial currents are related to the vector

[26] Clearly the r.h.s. of eq. (III.3.7) is a function of $\bar{g}^2(m_\mathrm{b})$, i.e. a function of $m_\mathrm{b}/\Lambda_{\overline{\mathrm{MS}}}$. We prefer to write it as a function of the ratio of renormalization group invariants, $M_\mathrm{b}/\Lambda_{\overline{\mathrm{MS}}}$.

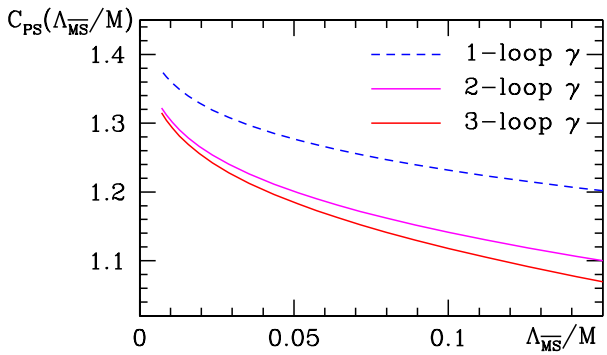


Figure 24: $C_{\rm PS}$ estimated in perturbation theory. For B-physics we have $\Lambda_{\overline{\rm MS}}/M_{\rm b} \approx 0.04$.

ones by a chiral rotation of the light quark fields [155]. It then follows that *in static approximation* the effective currents are given by

$$A_0^{\rm HQET} = C_{\rm PS}(M_{\rm b}/\Lambda_{\overline{\rm MS}})\, Z^{\rm stat}_{\rm A,RGI}(g_0)\, A_0^{\rm stat}\,, \qquad \text{(III.3.10)}$$

$$V_k^{\rm HQET} = C_{\mathbf{V}}(M_{\rm b}/\Lambda_{\overline{\rm MS}})\, Z^{\rm stat}_{\rm A,RGI}(g_0)\; V_k^{\rm stat}\,, \qquad \text{(III.3.11)}$$

$$V_0^{\rm HQET} = C_{\rm V}(M_{\rm b}/\Lambda_{\overline{\rm MS}})\, Z^{\rm stat}_{\rm A,RGI}(g_0)\, Z^{\rm stat}_{\rm V/A}(g_0)\, V_0^{\rm stat}\,, \qquad \text{(III.3.12)}$$

$$A_k^{\rm HQET} = C_{\mathbf{A}}(M_{\rm b}/\Lambda_{\overline{\rm MS}})\, Z^{\rm stat}_{\rm A,RGI}(g_0) Z^{\rm stat}_{\rm V/A}(g_0)\, A_k^{\rm stat}\,. \qquad \text{(III.3.13)}$$

The finite renormalization $Z^{\rm stat}_{\rm V/A}(g_0)$ can either be computed by a Ward identity [155] or, if one has a regularization with exact chiral symmetry, it is one. The factor $Z^{\rm stat}_{\rm A,RGI}(g_0)$ is analogous to $Z_{\rm M}(g_0)$ in eq. (II.3.8) and has been computed in a similar way [10]. It can be split into

$$Z^{\rm stat}_{\rm A,RGI}(g_0) = \frac{\Phi_{\rm RGI}}{\Phi(\mu)} \times Z^{\rm stat}_{\rm A}(g_0, 2L_{\rm max}/a)\Big|_{\mu=1/(2L_{\rm max})}\,, \qquad \text{(III.3.14)}$$

where the second factor depends on the lattice action, the first one does not. The first factor has been shown in Fig. 22 for a series of μ in the quenched approximation with a smallest scale of $\mu = 1/(2L_{\rm max})$.

We finally note that the bare pseudo scalar density, P, and the scalar density, S, are identical to $-A_0^{\rm stat}$ and $V_0^{\rm stat}$, respectively. This then also holds for the RGI ones; they are given by $-Z^{\rm stat}_{\rm A,RGI}(g_0)A_0^{\rm stat}$ and $Z^{\rm stat}_{\rm A,RGI}(g_0)\, Z^{\rm stat}_{\rm V/A}(g_0)V_0^{\rm stat}$.

For the renormalized $P^{\rm HQET}$ and $S^{\rm HQET}$, there is in principle an arbitrariness, since in QCD they depend on a scale and a scheme. This arbitrariness is fixed by considering the RGI fields in QCD. They satisfy the PCAC and PCVC relation with the RGI quark masses, for example ($M_{\rm l}$ is the mass of the light quark)

$$\partial_\mu (A_{\rm R})^{\rm QCD}_\mu = (M_{\rm b} + M_{\rm l}) P_{\rm RGI}\,. \qquad \text{(III.3.15)}$$

Taking the vacuum-to-B-meson matrix element of this relation (in static approximation)

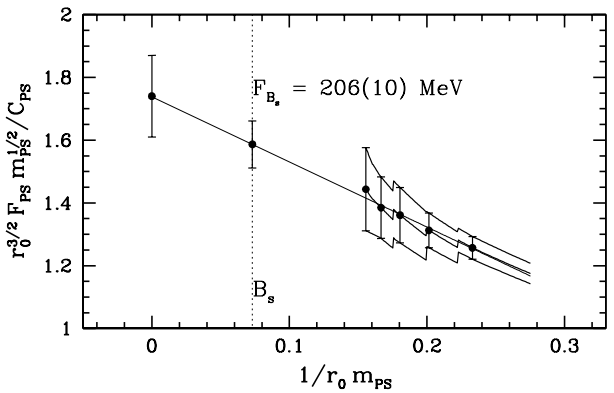


Figure 25: Example of an interpolation between a static result and results with $m_{\rm h} < m_{\rm b}$. Continuum extrapolations are done before the interpolation [156]. The point at $1/r_0 m_{\rm PS} = 0$ is given by $r_0^{3/2}\Phi_{\rm RGI}$.

fixes

$$P^{\rm HQET} = -C_{\rm PS}(M_{\rm b}/\Lambda_{\overline{\rm MS}})\,\frac{m_{\rm B}}{M_{\rm b}}\,Z^{\rm stat}_{\rm A,RGI}(g_0)A_0^{\rm stat}\,, \qquad \text{(III.3.16)}$$

$$S^{\rm HQET} = C_{\rm V}(M_{\rm b}/\Lambda_{\overline{\rm MS}})\,\frac{m_{\rm B}}{M_{\rm b}}\,Z^{\rm stat}_{\rm V/A}(g_0)\,Z^{\rm stat}_{\rm A,RGI}(g_0)\,V_0^{\rm stat} \qquad \text{(III.3.17)}$$

in static approximation. (Choosing a different matrix element would change $m_{\rm B} \to m_{\rm B} + {\rm O}(\Lambda_{\rm QCD})$.) We leave it as an exercise to verify these relations.

All conversion functions C are known up to (presumably small) $\alpha(m_{\rm b})^3$ errors. At least when the conversion functions are known with such high precision, the knowledge of the leading term in expansions such as eq. (III.3.5) is very useful to constrain the large mass behavior of QCD observables, computed on the lattice with unphysical quark masses $m_{\rm h} < m_{\rm b}$, typically $m_{\rm h} \approx m_{\rm charm}$. As illustrated in Fig. 25, one can then, with a reasonable smoothness assumption, interpolate to the physical point.

The relation between the RGI fields and the bare fields has so far been obtained for

- $Z^{\rm stat}_{\rm A,RGI}$ with both $N_{\rm f} = 0$ [10] and $N_{\rm f} = 2$ [157];
- the parity violating $\Delta B = 2$ four fermion operators [11, 158] for $N_{\rm f} = 0$ while $N_{\rm f} = 2$ has been started.

In the second case, the matrix elements of the two operators, evaluated in twisted mass QCD will give the standard model B-parameter for B-$\overline{\rm B}$ mixing.

Thus, soon one will be able to do interpolations such as Fig. 25 also for semi-leptonic decays such as $B \to \pi\, l\, \nu$ (close to zero recoil) and for the B-parameter.

III.3.1.2 Beyond the leading order: the need for non-perturbative conversion functions

Still, getting the continuum extrapolations of the data at finite heavy quark masses in Fig. 25 under control may represent a challenge when dynamical fermions are included.

Furthermore one should not forget that the functional form of the interpolation in that figure does essentially assume that the $1/m$ expansion remains reasonably accurate also significantly below m_b.

It is therefore natural to try to compute the $1/m_\mathrm{b}$ correction directly in HQET. However, if one wants to do this consistently, the leading order conversion functions such as C_PS have to be known non-perturbatively. This general problem in the determination of power corrections in QCD is seen in the following way. Consider the error made in eq. (III.3.7) (or eq. (III.3.1)) when the anomalous dimension has been computed at l loops and C_match at $l-1$ loop order. The conversion function C_PS is then known up to an *error*

$$\Delta(C_\mathrm{PS}) \propto [\bar{g}^2(m_\mathrm{b})]^l \sim \left\{\frac{1}{2b_0\ln(m_\mathrm{b}/\Lambda_\mathrm{QCD})}\right\}^l \overset{m_\mathrm{b}\to\infty}{\gg} \frac{\Lambda_\mathrm{QCD}}{m_\mathrm{b}}\,. \tag{III.3.18}$$

As m_b is made large, this perturbative error becomes dominant over the power correction one wants to determine. Taking a perturbative conversion function and adding power corrections to the leading order effective theory is thus a phenomenological approach, where one assumes that the coefficient of the $[\bar{g}^2(m_\mathrm{b})]^l$ term (as well as higher order ones) is small, such that the Λ/m_b corrections dominate over a certain mass interval. In such a phenomenological determination of a power correction, its size depends on the order of perturbation theory considered. A theoretically consistent evaluation of power corrections requires a fully non-perturbative formulation of the theory including a non-perturbative matching to QCD, see Sect. III.5.

Note for experts. Eq. (III.3.18) has little to do with renormalons. Rather it is due to the truncation of perturbation theory at a fixed order. Of course a renormalon-like growth of the perturbative coefficients does not help.

III.3.1.3 Splitting leading order (LO) and next to leading order (NLO)

We just learned that the very definition of a NLO correction to F_B means to take eq. (III.2.26) with all coefficients $Z_\mathrm{A}^\mathrm{HQET}\ldots c_\mathrm{A}^\mathrm{HQET}$ determined non-perturbatively. We want to briefly explain that the split between LO and NLO is not unique. This is fully analogous to the case of standard perturbation theory in α, where the split depends on the renormalization scheme used, or better on the experimental observable used to determine α in the first place.

Consider the lowest order. The only coefficient needed in eq. (III.2.26) is then $C_\mathrm{PS}Z^\mathrm{stat}_\mathrm{A,RGI} = \lim_{m_\mathrm{b}\to\infty} Z_\mathrm{A}^\mathrm{HQET}$. It has to be fixed by matching some matrix element of A_0^stat to the matrix element of A_0 in QCD. For example one may choose $\langle B'|A_0^\dagger|0\rangle$, with $|B'\rangle$ denoting the first pseudo-scalar excited state. Or one may take a finite volume matrix element $\langle B(L)|A_0^\dagger|\Omega(L)\rangle$, see Sect. III.4. Since the matching involves the QCD matrix element, there are higher order in $1/m_\mathrm{b}$ "pieces" in these equations. There is no reason for them to be independent of the particular matrix element. So from matching condition to matching condition, $C_\mathrm{PS}Z^\mathrm{stat}_\mathrm{A,RGI}$ differs by $\mathrm{O}(\Lambda_\mathrm{QCD}/m_\mathrm{b})$ terms.

The matrix element $F_{\rm B}$ in static approximation inherits this $O(\Lambda_{\rm QCD}/m_{\rm b})$ ambiguity. The $\Lambda_{\rm QCD}/m_{\rm b}$ corrections are hence not unique. Fixing a matching condition, the leading order $F_{\rm B}$ as well as the one including the corrections can be computed and has a continuum limit. Their difference can be defined as the $1/m_{\rm b}$ correction. However, what matters is not the ambiguous NLO term, but the fact that the uncertainty is reduced from $O(\Lambda_{\rm QCD}/m_{\rm b})$ in the LO term to $O(\Lambda^2_{\rm QCD}/m^2_{\rm b})$ in the sum.

III.3.2 A second example: mass formulae

Let us represent the formula for the meson mass, eq. (III.2.21), including also the vector meson as

$$m_{\rm B}^{\rm av} \equiv \frac{1}{4}[m_{\rm B} + 3m_{\rm B^*}] = m_{\rm b} + \widehat{\delta m} + E_{\rm stat} + \omega_{\rm kin} E_{\rm kin} + O(1/m_{\rm b}^2) \qquad \text{(III.3.19)}$$

and

$$\Delta m_{\rm B} \equiv m_{\rm B^*} - m_{\rm B} = \omega_{\rm spin} E_{\rm spin} + O(1/m_{\rm b}^2)\,, \qquad \text{(III.3.20)}$$

where the fact that $\mathcal{O}_{\rm spin}$ does not contribute in eq. (III.3.19) is a consequence of the exact spin symmetry of the lowest order. It is a simple exercise to verify the above equations explicitly by considering correlation functions of $V_k = \overline{\psi}_{\rm l}\gamma_k\psi_{\rm b}$ instead of A_0.

Usually these equations are written as [159]

$$m_{\rm B}^{\rm av} \sim m_{\rm b} + \overline{\Lambda} + \frac{1}{2m_{\rm b}}\lambda_1\,, \quad \Delta m_{\rm B} \sim -\frac{2}{m_{\rm b}}\lambda_2\,. \qquad \text{(III.3.21)}$$

We arrive at a similar form by defining power divergent subtractions for $E_{\rm kin}$ and $E_{\rm stat}$ vs.

$$m_{\rm B}^{\rm av} = m_{\rm b} + m_{\rm B}^{(0a)} + m_{\rm B}^{(0b)} + m_{\rm B}^{(1a)} + m_{\rm B}^{(1b)} + O(\Lambda^3_{\rm QCD}/m^2_{\rm b})\,, \qquad \text{(III.3.22)}$$

where we have split up as

$$O(\Lambda_{\rm QCD}) \quad : \quad m_{\rm B}^{(0a)} = \widehat{\delta m}^{\rm stat} + E_{\rm stat}^{\rm sub}\,, \quad m_{\rm B}^{(0b)} = E_{\rm stat} - E_{\rm stat}^{\rm sub}\,, \qquad \text{(III.3.23)}$$

$$O(\Lambda^2_{\rm QCD}/m_{\rm b}) \quad : \quad m_{\rm B}^{(1a)} = \widehat{\delta m}^{(1)} + \omega_{\rm kin} E_{\rm kin}^{\rm sub}\,, \quad m_{\rm B}^{(1b)} = \omega_{\rm kin}[E_{\rm kin} - E_{\rm kin}^{\rm sub}]\,. \qquad \text{(III.3.24)}$$

The subtraction terms (the Hamiltonian should be defined as $\mathbf{H} = -\frac{1}{a}\ln(\mathbf{T})$ in terms of the transfer matrix $\mathbf{T}$)

$$E_{\rm stat}^{\rm sub} = \langle\beta|\mathbf{H}|\beta\rangle_{\rm stat}|_{\delta m=0}\,, \quad E_{\rm kin}^{\rm sub} = \langle\beta| - a^3\sum_{\mathbf{x}}\mathcal{O}_{\rm kin}(x)|\beta\rangle_{\rm stat}\,. \qquad \text{(III.3.25)}$$

are chosen such that $m_{\rm B}^{(0a)} \ldots m_{\rm B}^{(1b)}$ are finite and have a continuum limit. This follows from our discussion of renormalization. By $\widehat{\delta m}^{\rm stat}$ we denote $\widehat{\delta m}$ in static approximation and by $\widehat{\delta m}^{(1)}$ the piece that is to be added when $\omega_{\rm kin} \neq 0$; it accounts for the term c_2/a^2 in eq. (III.2.29).

This rewriting exposes that the split up of the meson formulae into various orders of $1/m_{\rm b}$ is not unique. In the chosen form it depends on the arbitrary state $|\beta\rangle$. In other words: non-perturbatively, $\overline{\Lambda}$ and λ_1 can be defined exactly, but in many ways.[27]

Toward the end of this lecture we will see how the subtraction terms and $m_{\rm b} + \widehat{\delta m}$ can be defined such that they are computable in practice and the remaining error is reduced to $\mathrm{O}(\Lambda_{\rm QCD}^3/m_{\rm b}^2)$.

III.4 Non-perturbative tests of HQET

Although it is generally accepted that HQET is an effective theory of QCD, tests of this equivalence are rare and mostly based on phenomenological analysis of experimental results. A pure theory test can be performed if QCD including a heavy enough quark can be simulated on the lattice at lattice spacings which are small enough to be able to take the continuum limit. This has recently been achieved [154] and will be summarized below. We start with the QCD side of such a test. Lattice spacings such that $am_{\rm b} \ll 1$ can be reached if one puts the theory in a finite volume, $L^3 \times T$ with L, T not too large. We shall use $T = L$. For various practical reasons, Schrödinger functional boundary conditions are chosen. Equivalent boundary conditions are imposed in the effective theory. We then consider correlation functions such as $f_{\rm A}$ and f_1. The first one is the correlator of boundary quark fields ζ (located at $x_0 = 0$) and the time component of the axial current in the bulk ($0 < x_0 < T$). The second one describes the propagation of a quark-antiquark pair from the $x_0 = 0$ boundary to the $x_0 = T$ boundary. See Sect. III.2.3 for details.

We then take a ratio for which the renormalization factors of the boundary fields cancel,

$$\begin{aligned} Y_{\rm PS}(L, M_{\rm b}) \;&\equiv\; Z_{\rm A}\, \frac{f_{\rm A}(L/2)}{\sqrt{f_1}}\bigg|_{T=L} = \frac{\langle\Omega(L)|A_0|B(L)\rangle}{||\,|\Omega(L)\rangle\,||\;||\,|B(L)\rangle\,||}, \qquad \text{(III.4.1)} \\ &|B(L)\rangle = \mathrm{e}^{-L\mathbf{H}/2}|\varphi_{\rm B}(L)\rangle\,,\;\; |\Omega(L)\rangle = \mathrm{e}^{-L\mathbf{H}/2}|\varphi_0(L)\rangle\,. \end{aligned}$$

As shown in the above equations, $Y_{\rm PS}$ can be represented as a matrix element of the axial current between a normalized state $|B(L)\rangle$ with the quantum numbers of a B-meson and $|\Omega(L)\rangle$ which has vacuum quantum numbers. The time evolution $\mathrm{e}^{-L\mathbf{H}/2}$ ensures that both of these states are dominated by energy eigenstates with energies around $2/L$ and less (above $m_{\rm b}$). In other words, HQET is applicable if $1/L \ll m_{\rm b}$ (and of course $\Lambda_{\rm QCD} \ll m_{\rm b}$).

One then expects (for fixed $L\Lambda_{\rm QCD}$)

$$Y_{\rm PS}(L, M_{\rm b})/C_{\rm PS}(M_{\rm b}/\Lambda) = X_{\rm RGI} + \mathrm{O}(1/z)\,, \quad z = M_{\rm b}L\,, \qquad \text{(III.4.2)}$$

[27] In phenomenological applications [160], one works in dimensional regularization where the subtraction terms can be omitted. One defines a perturbative scheme for $m_{\rm b}$. It is then clear that (for example) $\overline{\Lambda}$ depends on the order of perturbation theory as $[\bar{g}^2(m_{\rm b})]^{l+1}\, m_{\rm b}] \overset{m_{\rm b}\to\infty}{\gg} \Lambda_{\rm QCD}$ as in eq. (III.3.18). Quantities such as $\overline{\Lambda}$ are then *effective parameters*, not directly related to the asymptotic $1/m_{\rm b}$ expansion.

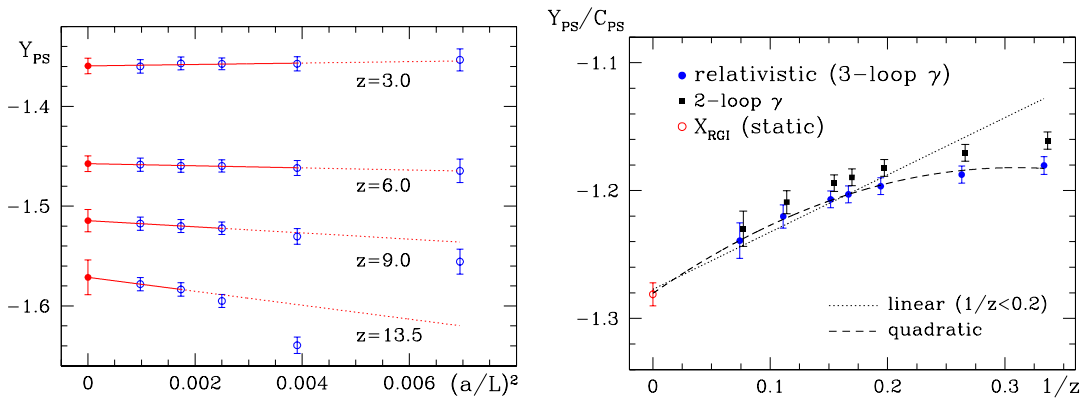


Figure 26: Testing eq. (III.4.2) through numerical simulations in the quenched approximation and for $L \approx 0.2\,\mathrm{fm}$ [154]. The physical mass of the b-quark corresponds to $z \approx 5$.

where the $1/m_\mathrm{b}$ corrections are written in the dimensionless variable $1/z$ and X_RGI is defined as Y_PS but at lowest order in the effective theory and normalized as in eq. (III.3.3). Of course such relations are expected after the continuum limit of both sides has been taken separately. For the case of $Y_\mathrm{PS}(L, M_\mathrm{b})$, this is done by the following steps:

- Fix a value u_0 for the renormalized coupling $\bar{g}^2(L)$ (in the Schrödinger functional scheme) at vanishing quark mass. In [154] u_0 is chosen such that $L \approx 0.2\,\mathrm{fm}$.
- For a given resolution L/a, determine the bare coupling from the condition $\bar{g}^2(L) = u_0$. This can easily be done since the relation between bare and renormalized coupling is known [98].
- Fix the bare quark mass m_q of the heavy quark such that $LM = z$ using the known renormalization factors Z_M, Z in $M = Z_\mathrm{M} Z\,(1 + a b_\mathrm{m} m_\mathrm{q})\,m_\mathrm{q}$, where Z was introduced in eq. (I.2.24) and Z_M in eq. (II.3.8).
- Evaluate Y_PS and repeat for better resolution a/L.
- Extrapolate to the continuum as shown in Fig. 26, left.

As can be seen in the figure, the continuum extrapolation becomes more difficult as the mass of the heavy quark is increased and $\mathrm{O}((a\,m)^2)$ discretization errors become more and more important. In contrast the continuum extrapolation in the static effective theory (Fig. 27) is much easier (once the renormalization factor relating bare current and RGI current is known [10]). After the continuum limit has been taken, the finite mass QCD observable $Y_\mathrm{PS}(L, M)$ turns smoothly into the prediction from the effective theory as illustrated in the r.h.s. of Fig. 26. Several such successful tests were performed in [154], two of them with the static ($M \to \infty$) limit known from the spin symmetry of HQET. For lack of space we do not show more examples but only note that the coefficient of the $1/z^n$ terms in fits to the finite mass results together with the static limit are roughly of order unity.

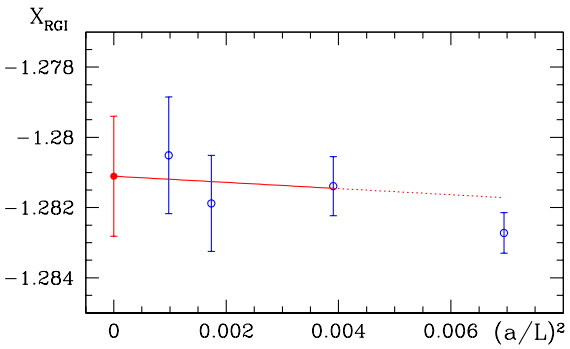


Figure 27: Continuum extrapolation of $X_{\rm RGI}$ [154].

Of course, finite mass lattice QCD results have been compared to the static limit over the years, see for example [161–173] and references therein. So what is new in the tests just discussed? The composite fields were renormalized non-perturbatively throughout and, by considering a small volume, the continuum limit could be taken at large quark masses.

III.5 Strategy for non-perturbative matching

Following Sect. III.3.1.2, the missing piece for a general computation including $1/m_{\rm b}$ corrections is a practical strategy for determining the parameters in the Lagrangian and in the effective fields beyond perturbation theory. Let us denote the number of parameters which have to be determined, not counting the parameters in the light sector of QCD, by $N_{\rm eff}$. For instance, including $1/m_{\rm b}$ terms but not considering matrix elements of any composite fields, we have $N_{\rm eff} = 3$, namely $\omega_{\rm kin}, \omega_{\rm spin}$ and $m_{\rm b} + \widehat{\delta m}$. Given these three parameters, all masses can be computed. If in addition we want to compute matrix elements of A_0, such as $F_{\rm B}$, we have $N_{\rm eff} = 5$, since also $Z_{\rm A}^{\rm HQET}, c_{\rm A}^{\rm HQET}$ are parameters of the theory.

III.5.1 Matching in small volume

Observables, e.g. dimensionless renormalized correlation functions or energies are denoted by $\Phi^{\rm HQET}$ in the effective theory and by $\Phi^{\rm QCD}$ in QCD. The $N_{\rm eff}$ unknown parameters can be determined from $\Phi_k^{\rm HQET} = \Phi_k^{\rm QCD}, k = 1 \ldots N_{\rm eff}$, provided the sensitivity of these conditions to the desired parameters is sufficient. In general the determination of $\Phi_k^{\rm QCD}$ will be very difficult because a b-quark has to be simulated and $\mathrm{O}((am_{\rm b})^2)$ cutoff effects will be large. The way around is once again to consider a finite volume, where small lattice spacings are accessible. In practice using furthermore Schrödinger functional boundary conditions is a good idea, since then the simulations can easily be done also with dynamical fermions. Given the experience of the tests of HQET (Sect. III.4), a good choice is $L = L_1 \approx 0.4\,\mathrm{fm}$. Then $1/z = 1/(LM_{\rm b}) \approx 1/10$ and the

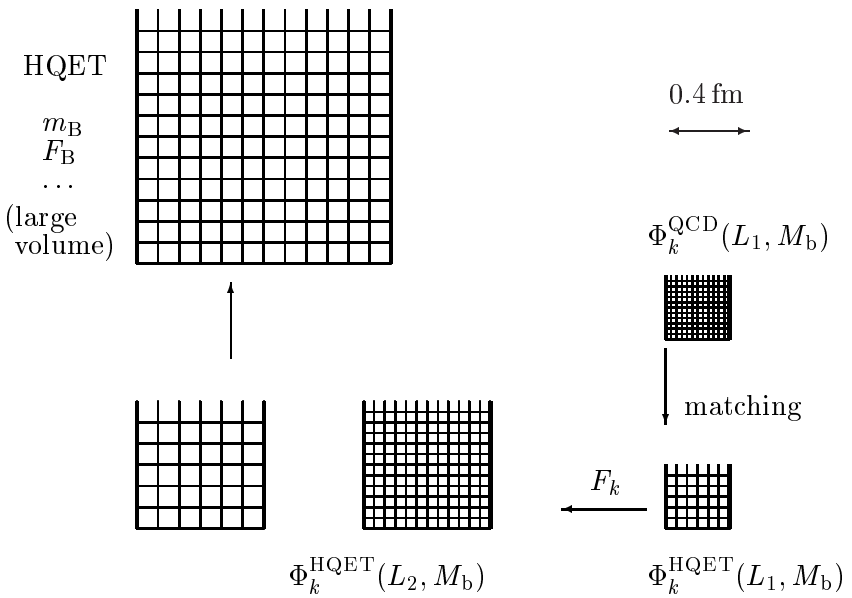


Figure 28: The strategy for a non-perturbative determination of the HQET-parameters from QCD simulations in a small volume. Steps indicated by arrows are to be repeated at smaller lattice spacings to reach a continuum limit.

HQET expansion is very accurate. So for the matching step we impose

$$\Phi_k^{\rm HQET}(L_1, M_{\rm b}) = \Phi_k^{\rm QCD}(L_1, M_{\rm b}), \quad k = 1, \ldots, N_{\rm eff}\,. \tag{III.5.1}$$

to determine the $N_{\rm eff}$ parameters in the effective theory (right hand side of Fig. 28). We assume that the observables $\Phi_k(L, M_{\rm b})$ have been made dimensionless by multiplication with appropriate powers of L. They should be chosen with care (e.g. no large momenta should appear) but the effect of variations in the matching conditions on the final results is in any case of a higher order in the $1/m_{\rm b}$ expansion.

III.5.2 Step scaling functions

The matching conditions, eq. (III.5.1), define the HQET parameters for any value of the lattice spacing (or equivalently bare coupling). In practice, for $L_1 \approx 0.4\,$fm, the parameters of the effective theory are then determined at rather small lattice spacings in a range of $a \approx 0.02\,$fm to $a \approx 0.05\,$fm. Large volumes as they are needed to compute the physical mass spectrum or matrix elements then require very large lattices ($L/a > 50$). A further step is needed to bridge the gap to practicable lattice spacings. A well-defined procedure is as follows (bottom part of Fig. 28). We define step scaling functions [37], F_k, by

$$\Phi_k^{\rm HQET}(sL, M) = F_k(\{\Phi_j^{\rm HQET}(L, M)\,,\ j = 1 \ldots N_{\rm eff}\})\,,\ \ k = 1 \ldots N_{\rm eff}\,, \tag{III.5.2}$$

where usually one uses scale changes of $s = 2$. These dimensionless functions describe the change of the complete set of observables $\{\Phi_k^{\rm HQET}\}$ under a scaling of $L \to sL$. In order to compute them one

i selects a lattice with a certain resolution a/L.

ii The specification of $\Phi_j^{\rm HQET}(L, M)$, $j = 1, \ldots, N_n$, then fixes all (bare) parameters of the theory.

iii The l.h.s. of eq. (III.5.2) is now computed, keeping the bare parameters fixed while changing $L/a \to L'/a = sL/a$.

iv The values for the continuum F_k are reached by extrapolating the resulting lattice numbers to $a/L \to 0$.

Starting from $L = L_1$ it turns out that a single step going to $L_2 = 2L_1$ is sufficient [140]. Then one can switch at fixed bare parameters to a large volume where finite size effects are negligible (left part of Fig. 28). This is done in full analogy to the steps i. . . iv above. One only computes the large volume quantities for the bare parameters fixed in step ii (with $L = L_2$). Again a continuum extrapolation can be carried out.

III.5.3 Example: The mass of the b quark

For illustration purposes we consider a simple example, the computation of the b-quark mass, starting from the observed (spin averaged) B-meson mass. For this calculation one obviously has to consider a range of masses $M_{\rm b}$ in eq. (III.5.1) and determine the physical point from the requirement $m_{\rm B}^{\rm av} = m_{\rm B}^{\rm av}|_{\rm experiment}$. It is thus the first computation to be carried out. Subsequently, one may directly choose the physical point in eq. (III.5.1).

III.5.3.1 Static approximation

Remembering eq. (III.3.23), we are after a precise definition and calculation of $E_{\rm stat}^{\rm sub}$ and $m_{\rm B}^{(0a)} = \widehat{\delta m}^{\rm stat} + E_{\rm stat}^{\rm sub}$. Already in the static approximation, a non-perturbative matching is required, if one wants to take the continuum limit. (Perturbatively one determines $\widehat{\delta m}^{\rm stat}$ with an in the continuum limit divergent error term of order $\Delta(\widehat{\delta m}^{\rm stat}) = c_{l+1} g_0^{2l+2}/a$.)

In eq. (III.5.1) we have the simple case $N_{\rm eff} = 1$. We omit the discussion of fixing the bare light quark masses and coupling. Obviously any finite volume energy in the b-sector, denoted by Γ, will do to fix $\widehat{\delta m}$. Two precise definitions are given in the following four equations. The reader who is only interested in the general concept may skip this detail.

The first choice which comes to mind is [60, 139, 140]

$$\Gamma^{\rm av}(L, \theta_0) = -\frac{\partial_0 + \partial_0^*}{2} F_{\rm av}(x_0, \theta_0) \text{ at } x_0 = L/2\,,\ T = L\,, \qquad \text{(III.5.3)}$$

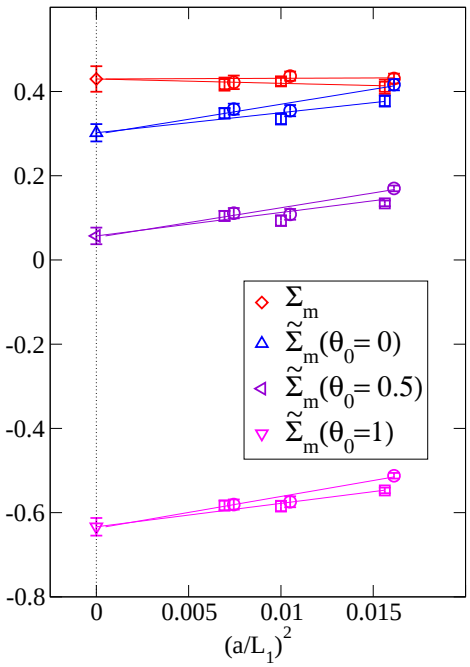


Figure 29: Continuum extrapolation of $\sigma_{\rm m} = \lim_{a/L\to 0} \Sigma_{\rm m}$ and $\tilde{\sigma}_{\rm m}$. Two different discretizations for the static quark action are used and extrapolated to a common continuum limit [140]. Dividing by L_2, the y-axes covers about an energy range of 300 MeV.

with (see Sect. III.2.3)

$$F_{\rm av}(x_0,\theta) = \frac{1}{4}\ln\left[-f_{\rm A}(x_0,\theta)\,(k_{\rm V}(x_0,\theta))^3\right]. \tag{III.5.4}$$

However, at order $1/m_{\rm b}$ the energy $\Gamma^{\rm av}$ depends on $c_{\rm A}^{\rm HQET}, c_{\rm V}^{\rm HQET}$. This is clearly inconvenient and can be avoided by choosing instead

$$\Gamma_1(L,\theta_0) = -\frac{\partial_T + \partial_T^*}{2} F_1(L,\theta_0) \text{ at } T = L/2\,, \tag{III.5.5}$$

with

$$F_1(L,\theta) = \frac{1}{4}\ln\left[f_1(\theta)\,(k_1(\theta))^3\right]. \tag{III.5.6}$$

A spin average is taken which will be relevant when we include the first order in $1/m_{\rm b}$. Both $\Gamma^{\rm av}$ and Γ_1 turn into $m_{\rm B}^{\rm av}$ when L and T are large.

In the numerical evaluation we chose $\theta_0 = 0$. We require matching, $\Phi_1^{\rm QCD}(L_1, M_{\rm b}) = \Phi_1^{\rm HQET}(L_1, M_{\rm b})$, with

$$\Phi_1^{\rm QCD}(L_1, M_{\rm b}) \equiv L_1\,\Gamma_1(L_1,\theta_0)\,, \tag{III.5.7}$$

$$\Phi_1^{\rm HQET}(L_1, M_{\rm b}) \equiv L_1\,(\Gamma_1^{\rm stat}(L_1,\theta_0) + m_{\rm b})\,. \tag{III.5.8}$$

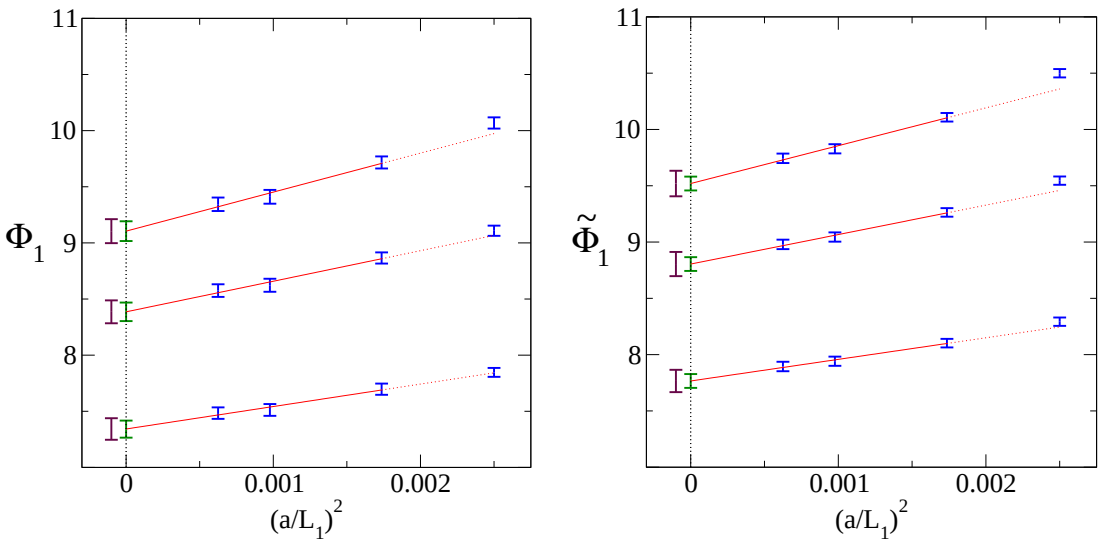


Figure 30: Continuum extrapolation of $\Phi_1(L_1, M_\mathrm{b})$, for $z = 10.4\,,\ 12.1\,,\ 13.3$ from bottom to top [140]. On the right, the equivalent in the alternative strategy is shown with $\theta_0 = 1/2$. Dividing by L_1, the y-axes covers about a range of 2 GeV.

Here Γ_1^{stat} refers to eq. (III.5.5) at the lowest order in $1/m_\mathrm{b}$. Eq. (III.5.2) can then be written in the simple form,

$$\Phi_1^{\mathrm{HQET}}(2L, M_\mathrm{b}) = 2\Phi_1^{\mathrm{HQET}}(L, M_\mathrm{b}) + \sigma_\mathrm{m}\left(\bar{g}^2(L)\right)\,, \tag{III.5.9}$$

$$\sigma_\mathrm{m}\left(\bar{g}^2(L)\right) \equiv 2L\,[\,\Gamma_1^{\mathrm{stat}}(2L, \theta_0) - \Gamma_1^{\mathrm{stat}}(L, \theta_0)\,]\,. \tag{III.5.10}$$

In σ_m the divergent δm as well as the mass shift m_b cancel. Its continuum extrapolation is illustrated in Fig. 29.

We now see immediately that

$$m_\mathrm{B}^{\mathrm{av}} = m_\mathrm{B}^{(0a)} + m_\mathrm{B}^{(0b)} + \mathrm{O}(\Lambda_{\mathrm{QCD}}^2/m_\mathrm{b}) \tag{III.5.11}$$

$$m_\mathrm{B}^{(0b)} = \underbrace{E_{\mathrm{stat}} - \Gamma_1^{\mathrm{stat}}(L_2, \theta_0)}_{a\to 0 \text{ in HQET}} \tag{III.5.12}$$

$$m_\mathrm{B}^{(0a)} = \underbrace{\Gamma_1^{\mathrm{stat}}(L_2, \theta_0) - \Gamma_1^{\mathrm{stat}}(L_1, \theta_0)}_{a\to 0 \text{ in HQET}} + \frac{1}{L_1}\underbrace{\Phi_1^{\mathrm{QCD}}(L_1, M_\mathrm{b})}_{a\to 0 \text{ in QCD}}, \tag{III.5.13}$$

where the first term in eq. (III.5.13) (in dimensionless form) is given by eq. (III.5.10) and E_{stat} is the infinite volume energy of a B-meson in static approximation introduced earlier. It is often called the static binding energy. As indicated, the continuum limit can be taken in each individual step; a numerical example for the last term is shown in Fig. 30.

After obtaining all pieces in eq. (III.5.11), the equation is numerically solved for $z_\mathrm{b} = M_\mathrm{b} L_1$, see Fig. 31. Since also the size of L_1 in units of r_0 [47] is known, one can

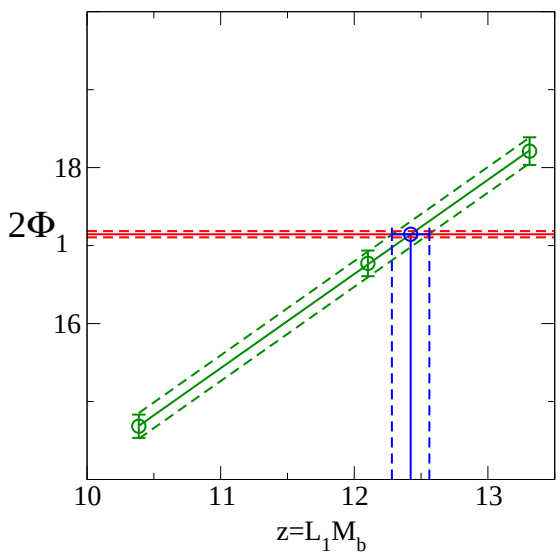


Figure 31: Graphical solution of eq. (III.5.11). Data points are $2\Phi_1$ and the horizontal error band is $L_2 m_{\rm B}^{\rm av} - \sigma_{\rm m} - L_2[E^{\rm stat} - \Gamma_1^{\rm stat}(L_2, \theta_0)]$.

quote

$$r_0 M_{\rm b}^{(0)} = 17.25(20) \;\rightarrow\; M_{\rm b}^{(0)} = 6.806(79)\,\text{GeV}\,, \tag{III.5.14}$$

where $r_0 = 0.5\,\text{fm}$ is used. This result is in the quenched approximation but includes the lowest non-trivial order in $1/m_{\rm b}$ and a continuum limit. In the form of eq. (III.3.22), we have defined the subtraction $E_{\rm stat}^{\rm sub} = \Gamma_1^{\rm stat}(L_2)$. The term $m_{\rm B}^{(0a)}$ is then given entirely by the finite volume computations while $m_{\rm B}^{(0b)}$ results from the large volume $E_{\rm stat}$ and $\Gamma_1^{\rm stat}(L_2)$. We proceed to discuss the $1/m_{\rm b}$ corrections.

III.5.3.2 Including $1/m_{\rm b}$ corrections.

Both the spin average $m_{\rm B}^{\rm av}$ and the finite volume energy Γ_1 are constructed such that $\omega_{\rm spin}$ drops out of their $1/m_{\rm b}$ expansion. Furthermore, Γ_1 does not obtain any $1/m_{\rm b}$-terms due to the expansion of composite fields, a convenient property of the Schrödinger functional boundary fields. Thus, for the particular problem of relating $m_{\rm B}^{\rm av}$ to the mass of the quark, only one more matching observable has to be defined, to determine $\omega_{\rm kin}$.

The choice in [140] was

$$\Phi_2(L, M_{\rm b}) = R_1(L, \theta_1, \theta_2) - R_1^{\rm stat}(L, \theta_1, \theta_2)\,, \tag{III.5.15}$$

$$R_1(L, \theta_1, \theta_2) = F_1(L, \theta_1) - F_1(L, \theta_2) \;\text{ at } T = L/2\,, \tag{III.5.16}$$

$$R_1^{\rm stat}(L, \theta_1, \theta_2) = \ln\left[f_1^{\rm stat}(\theta_1)/f_1^{\rm stat}(\theta_2)\right],\; \text{at } T = L/2 \tag{III.5.17}$$

where the static piece $R_1^{\rm stat}$ is subtracted such that Φ_2 is proportional to $\omega_{\rm kin}$. It is now a matter of simple algebra to compute the step scaling functions and finally the $1/m_{\rm b}$-correction to eq. (III.5.14). In the numerical evaluation three combinations $(\theta_1, \theta_2) =$

θ_0	$r_0\, M_{\rm b}^{(0)}$	$r_0\, M_{\rm b} = r_0\, (M_{\rm b}^{(0)} + M_{\rm b}^{(1a)} + M_{\rm b}^{(1b)})$		
		$\theta_1 = 0$	$\theta_1 = 1/2$	$\theta_1 = 1$
		$\theta_2 = 1/2$	$\theta_2 = 1$	$\theta_2 = 0$
		Main strategy		
0	17.25(20)	17.12(22)	17.12(22)	17.12(22)
		Alternative strategy		
0	17.05(25)	17.25(28)	17.23(27)	17.24(27)
1/2	17.01(22)	17.23(28)	17.21(27)	17.22(28)
1	16.78(28)	17.17(32)	17.14(30)	17.15(30)

Table 5: RGI results of $M_{\rm b}$ in the static approximation and of the $1/m_{\rm b}$ correction for the alternative strategy.

$(0, 1/2)$, $(1/2, 1)$, $(0, 1)$ were chosen. The $1/m_{\rm b}$-correction, split as in eq. (III.3.22), but for the quark mass, turned out to be about independent of θ_1, θ_2 with (after continuum extrapolation)

$$r_0\, M_{\rm b}^{(1a)} = -0.06(3)\,, \quad r_0\, M_{\rm b}^{(1b)} = -0.06(8) \;\to\; r_0 M_{\rm b} = 17.12(22). \tag{III.5.18}$$

Indeed since for our choice of matching condition the static approximation is independent of θ_1, θ_2, the values for $r_0\, M_{\rm b}^{(1)}$ have to be independent up to small $r_0\, \Lambda_{\rm QCD}^3/m_{\rm b}^2$ terms. This is so because the result including all terms has this precision.

With $\Lambda_{\overline{\rm MS}} r_0 = 0.602(48)$ [17, 93], the 4-loop β function and the mass anomalous dimension [174–177], we translate $M_{\rm b} = M_{\rm b}^{(0)} + M_{\rm b}^{(1)}$ to the mass in the $\overline{\rm MS}$ scheme,

$$\overline{m}_{\rm b}(\overline{m}_{\rm b}) = 4.347(48){\rm GeV}\,; \tag{III.5.19}$$

the associated perturbative uncertainty can safely be neglected. In the $\overline{\rm MS}$ scheme the $1/m_{\rm b}$ term amounts to $-27(22)$MeV.

III.5.3.3 An alternative strategy.

Also an alternative strategy has been tested. It is based on $\Gamma^{\rm av}$, eq. (III.5.3). It hence also involves the $1/m_{\rm b}$-corrections to the currents, but only in the combination $c_{\rm av}^{\rm HQET} = (c_{\rm A}^{\rm HQET} + 3c_{\rm V}^{\rm HQET})/4$. Three matching observables are necessary. They can be found in [140]. Here we only mention that again three angles $\theta_0, \theta_1, \theta_2$ appear, but now in nine different combinations. Together with the above discussed strategy, there are 12 different matching conditions.

At lowest order in $1/m_{\rm b}$, the equations relating quark mass and the spin-averaged B-meson mass remain unchanged. Only the step scaling function $\sigma_{\rm m}$ is replaced by $\tilde{\sigma}_{\rm m}$, and Φ_1 is replaced by $\tilde{\Phi}_1$. Both depend on the angle θ_0, but not on θ_1, θ_2. A comparison is shown in Fig. 29, Fig. 30. Dividing by L_1 and L_2 respectively, one

observes differences of about 250 MeV in these quantities. According to the HQET counting they are expected to be of order $\Lambda_{\rm QCD}$. In the combination, which leads to $M_{\rm b}^{(0)}$, these differences are reduced to $O(\Lambda_{\rm QCD}^2/m_{\rm b})$.

In the table shown, such differences are barely visible in the lowest order results, where one would estimate $O(\Lambda_{\rm QCD}^2/m_{\rm b}^2) \sim 1\%$ effects. After including the $1/m_{\rm b}$ corrections no signs of differences remain. Indeed one would estimate them to be $O((\Lambda_{\rm QCD}/m_{\rm b})^3) \sim 0.1\%$, quite below our statistical precision. We conclude that the expansion works very well, as expected.

We finally note that the overall uncertainty of the b-quark mass is dominated by the renormalization factors in relativistic QCD, i.e. by the relation between the bare mass and the RGI mass in QCD. The second most important contribution to the errors is the large volume $E_{\rm kin}$. This quantity contains a quadratic divergence. Once $E_{\rm kin}^{\rm sub}$ is subtracted, the remaining finite piece has errors which grow fast as one approaches the continuum limit. However, the methods of [178] have not yet been applied and we expect to reduce this source of error.

III.6 More literature

Before summarizing and discussing the perspectives for HQET on the lattice, let us attempt to give a brief guide to literature on subjects which we did not cover.

Early numerical computations have been summarized in reviews [162, 179, 180]. The power divergent mixing of operators of different dimensions was seen in an explicit perturbative computation [181]. The $\mathrm{B}^* - \mathrm{B}$ mass splitting, which is a $1/m_{\rm b}$ effect given at lowest order by $E_{\rm spin}$ has been investigated with perturbative $\omega_{\rm spin}$ by [182–185].

In static approximation, the four fermion operators responsible for $\mathrm{B} - \overline{\mathrm{B}}$ mixing with Wilson fermions require the subtraction of operators with different chiralities, which was attempted with perturbatively estimated mixing coefficients [184,186]. Later it was realized that the mixing is completely avoided with an action with exact chiral symmetry (and spin symmetry) [187] and a calculation of $\mathrm{B} - \overline{\mathrm{B}}$ mixing was carried out with perturbative renormalization [188].

The dependence of heavy-light meson properties on the mass of the light quark can be described by a suitable chiral effective theory [189, 190]. Its Lagrangian involves the $\mathrm{B}^*\mathrm{B}\pi$ coupling as a low energy constant. This was estimated in a static computation [191]. Also an exploratory computation of the Isgur-Wise functions $\tau_{1/2}, \tau_{3/2}$ at zero recoil has been carried out [192, 193]. These functions give the form factors for transitions between heavy-light mesons of different orbital angular momentum.

Finally, the formulation of HQET at a finite velocity has been investigated by Aglietti et al. We refer to [138, 194] and references therein. Both perturbative investigations of the renormalization [193, 195] and numerical simulations [192, 196] have been carried out.

III.7 Summary and perspectives

Non-perturbative HQET at the leading order in $1/m_{\rm b}$ has reached a satisfactory status. To underline this statement, we comment briefly on the progress made in recent years. The ground breaking work of [132, 197, 198] was followed by intense activity leading to a computation where (within the quenched approximation) all error sources were investigated and controlled as well as possible in the middle of the nineties [199]. For the B decay constant, the authors estimated three sources of errors between 7% and 12% each, one of them due to an estimated precision of the perturbative renormalization.

It took almost a decade until a non-perturbative method for the renormalization in the effective theory was fully developed [9, 10], but meanwhile a total error of 4% in the $\rm B_s$-meson decay constant has been reached [200], including the continuum extrapolation. In reaching this accuracy also the reduction of statistical errors [145, 146] was relevant.

Also the standard model B-parameter for B-$\overline{\rm B}$ mixing is well on its way [11,158,201]. In these cases, bare perturbation theory is now avoided by non-perturbative renormalization of the lattice operators. As explained in Sect. III.3.1, all static-light bilinears require only one common renormalization factor $Z^{\rm stat}_{\rm A,RGI}$. As this is known [10], also semi-leptonic decay form factors can be computed with non-perturbative renormalization. For completeness we note that a source of a perturbative error remains in $C_{\rm PS}$, Fig. 24, and its relatives for other bilinears, but here high order continuum perturbation theory is available [150–153] and is applied at the b-scale. This error is under reasonable control. Applying these methods to the theory with dynamical fermions is straight forward; "only" the usual problems of simulations with light quarks have to be solved.

By themselves such lowest order (in $1/m_{\rm b}$) results are not expected to have an interesting precision for phenomenological applications, but certainly they can constrain the large mass behavior computed with other methods [161–173]. An interesting application has been the combination of the approach of [172, 173] with the large mass behavior computed via HQET [200].

The $1/m_{\rm b}$ corrections can also be computed directly in the effective theory. Here, the necessary steps have been carried out in detail for the mass of the b-quark in the quenched approximation. The resulting precision is rather satisfactory and higher order $1/m_{\rm b}$-corrections can be neglected. The latter has also been verified explicitly by comparing the results following from a number of different matching conditions. No significant differences were found.

An extension of this computation to full QCD has been started by the ALPHA collaboration. This is of particular interest because for full QCD it is of course more difficult to reach the small lattice spacings needed for computations with relativistic quarks of masses around $m_{\rm charm}$ – the basis of the alternatives mentioned above. It is time to address other observables such as the B-meson decay constant in this direct approach!

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