# Chapter 1

# COMMON THEORETICAL TOOLS

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## 1 QCD[1]

Quantum Chromodynamics (QCD) [1] is the sector of the Standard Model (SM) which is relevant for the strong interactions. It is obtained from the full SM by setting the weak and electromagnetic coupling constants to zero and freezing the scalar doublet to its vacuum expectation value. What remains is a Yang–Mills (YM) theory with local gauge group $SU(3)$ (colour) vectorially coupled to six Dirac fields (quarks) of different masses (flavours). The vector fields in the YM Lagrangian (gluons) live in the adjoint representation and transform like connections under the local gauge group whereas the quark fields live in the fundamental representation and transform covariantly. The QCD Lagrangian reads

$$\mathcal{L}_{\rm QCD} = -\frac{1}{4} F^a_{\mu\nu} F^{a\,\mu\nu} + \sum_{\{q\}} \bar{q}\,(i\gamma^\mu D_\mu - m_q)\,q\,, \tag{1.1}$$

where $\{q\} = u, d, s, c, b, t$, $F^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu + g f^{abc} A^b_\mu A^c_\nu$, $D_\mu = \partial_\mu - iT^a A^a_\mu$. $f^{abc}$ are the $SU(3)$ structure constants and $T^a$ form a basis of the fundamental representation of the $SU(3)$ algebra. When coupled to electromagnetism, gluons behave as neutral particles whereas $u$, $c$ and $t$ quarks have charges $+2/3$ and $d$, $s$ and $b$ quarks have charges $-1/3$.

The main properties of QCD follow:

- It is Poincaré, parity, time reversal and (hence) charge conjugation invariant. It is in addition invariant under $U(1)^6$ which implies individual flavour conservation.
- Being a non-Abelian gauge theory, the physical spectrum consists of colour singlet states only. The simplest of these states have the quantum numbers of quark–antiquark pairs (mesons) or of three quarks (baryons), although other possibilities are not excluded.
- The QCD effective coupling constant $\alpha_{\rm s}(q)$ decreases as the momentum transfer scale $q$ increases (asymptotic freedom) [2, 3]. This allows to make perturbative calculations in $\alpha_{\rm s}$ at high energies.
- At low energies it develops an intrinsic scale (mass gap), usually referred as $\Lambda_{\rm QCD}$, which provides the main contribution to the masses of most hadrons. At scales $q \sim \Lambda_{\rm QCD}$, $\alpha_{\rm s}(q) \sim 1$ and perturbation theory cannot be used. Investigations must be carried out using nonperturbative techniques, the best established of which is lattice QCD.
  Quarks are conventionally divided into light $m_q \ll \Lambda_{\rm QCD}$, $q = u, d, s$ and heavy $m_Q \gg \Lambda_{\rm QCD}$, $Q = c, b, t$

$$\begin{aligned} &m_u = 1.5 \div 4.0\,{\rm MeV}\,, \quad m_d = 4 \div 8\,{\rm MeV}\,, \quad m_s = 80 \div 130\,{\rm MeV}\,, \\ &m_c = 1.15 \div 1.35\,{\rm GeV}\,, \quad m_b = 4.1 \div 4.4\,{\rm GeV}\,, \quad m_t = 174.3 \pm 5.1\,{\rm GeV}\,. \end{aligned} \tag{1.2}$$

  These are $\overline{\rm MS}$ masses at scale 2 GeV, $m_c$ and $m_b$ for the light quarks, charm and bottom respectively. All values are taken from [4]. The extraction of the values of the heavy quark masses will be discussed in Chapter 6.

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– If light quark masses are neglected, the $U(1)^3$ flavour conservation symmetry of the QCD Lagrangian in this sector is enlarged to a $U(3) \otimes U(3)$ group. The axial $U(1)$ subgroup is explicitly broken by quantum effects (axial anomaly). The vector $U(1)$ subgroup provides light flavour conservation. The remaining $SU(3) \otimes SU(3)$ subgroup, known as chiral symmetry group, turns out to be spontaneously broken down to the diagonal $SU(3)$ (flavour symmetry). This produces eight Goldstone bosons, which, upon taking into account the explicit breaking of the symmetry due to the non-zero quark masses, acquire masses that are much smaller than $\Lambda_{\rm QCD}$.
– Hadrons containing heavy quarks have masses of the order of $m_Q$ rather than of the order $\Lambda_{\rm QCD}$. They enjoy particular kinematical features that allow for specific theoretical treatments. The study of hadrons containing two heavy quarks is the aim of this report.

## 2 EFFECTIVE FIELD THEORIES[2]

From the point of view of QCD the description of hadrons containing two heavy quarks is a rather challenging problem, which adds to the complications of the bound state in field theory those coming from a nonperturbative low-energy dynamics. A proper relativistic treatment of the bound state based on the Bethe–Salpeter equation [5] has proved difficult. Perturbative calculations have turned out unpractical at higher order and the method has been abandoned in recent QED calculations. Moreover, the entanglement of all energy modes in a fully relativistic treatment is more an obstacle than an advantage for the factorization of physical quantities into high-energy perturbative and low energy nonperturbative contributions. Partial semirelativistic reductions and models have been often adopted to overcome these difficulties at the price to introduce uncontrolled approximations and lose contact with QCD. The fully relativistic dynamics can, in principle, be treated without approximations in lattice gauge theories. This is in perspective the best founded and most promising approach. As we will detail in the following, it is not without difficulties at the present for heavy quarkonium.

A nonrelativistic treatment of the heavy quarkonium dynamics, which is suggested by the large mass of the heavy quarks, has clear advantages. The velocity of the quarks in the bound state provides a small parameter in which the dynamical scales may be hierarchically ordered and the QCD amplitudes systematically expanded. Factorization formulas become easier to achieve. A priori we do not know if a nonrelativistic description will work well enough for all heavy quarkonium systems in nature. For instance, the charm quark may not be heavy enough. The fact that most of the theoretical predictions presented in the report are based on such a nonrelativistic assumption and the success of most of them may be seen as a support to the assumption.

On the example of positronium in QED, a nonrelativistic bound state is characterized by at least three scales: the scale of the mass $m$ (called hard), the scale of the momentum transfer $p \sim mv$ (soft) and the scale of the kinetic energy of the quark and antiquark in the centre-of-mass frame $E \sim p^2/m \sim mv^2$ (ultrasoft). The scales $mv$ and $mv^2$ are dynamically generated, $v$ is the heavy-quark velocity in the centre-of-mass frame. In a nonrelativistic system: $v \ll 1$, and the above scales are hierarchically ordered: $m \gg mv \gg mv^2$. In perturbation theory $v \sim \alpha_{\rm s}$. Feynman diagrams will get contributions from all momentum regions associated with the scales. Since these momentum regions depend on $\alpha_{\rm s}$ each Feynman diagram contributes to a given observable with a series in $\alpha_{\rm s}$ and a non trivial counting. For energy scales close to $\Lambda_{\rm QCD}$ perturbation theory breaks down and one has to rely on nonperturbative methods. The wide span of energy scales involved makes also a lattice calculation in full QCD extremely challenging since one needs a space–time grid that is large compared to the largest length of the problem, $1/mv^2$, and a lattice spacing that is small compared to the smallest one, $1/m$. To simulate, for instance, a $b\bar{b}$ state where $m/mv^2 \sim 10$, one needs lattices as large as $100^4$, which are beyond present computing capabilities [6] (see also the next sections of the chapter).

We may, however, also take advantage of the existence of a hierarchy of scales by substituting QCD with simpler but equivalent Effective Field Theories (EFTs). EFTs have become increasingly popular

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in particle physics during the last decades. They provide a realization of Wilson renormalization group ideas and fully exploit the properties of local quantum field theories. An EFT is a quantum field theory with the following properties: a) it contains the relevant degrees of freedom to describe phenomena that occur in certain limited range of energies and momenta and b) it contains an intrinsic energy scale $\Lambda$ that sets the limit of applicability of the EFT. The Lagrangian of an EFT is organized in operators of increasing dimension, hence, an EFT is in general non-renormalizable in the usual sense. In spite of this, it can be made finite to any finite order in $1/\Lambda$ by renormalizing (matching) the constants (matching coefficients) in front of the operators in the Lagrangian until that order. This means that one needs more renormalization conditions when the order in $1/\Lambda$ is increased. However, even if the only way of fixing the constants would be by means of experimental data, this would reduce but not spoil the predictive power of the EFT. If the data are abundant, the constants can be fit once for ever and used later on to make predictions on new experiments.

The prototype of EFT for heavy quarks is the Heavy Quark Effective Theory (HQET), which is the EFT of QCD suitable to describe systems with only one heavy quark [7]. These systems are characterized by two energy scales: $m$ and $\Lambda_{\rm QCD}$. HQET is obtained by integrating out the scale $m$ and built as a systematic expansion in powers of $\Lambda_{\rm QCD}/m$. As discussed above, bound states made of two heavy quarks are characterized by more scales. Integrating out only the scale $m$, which for heavy quarks can be done perturbatively, leads to an EFT, Nonrelativistic QCD (NRQCD) [6, 8, 9], that still contains the lower scales as dynamical degrees of freedom. Disentangling the remaining scales is relevant both technically, since it enables perturbative calculations otherwise quite complicate, and more fundamentally, since it allows to factorize nonperturbative contributions into the expectation values or matrix elements of few operators. These may be eventually evaluated on the lattice, extracted from the data or calculated in QCD vacuum models. In the last few years, the problem of systematically treating these remaining dynamical scales in an effective theory framework has been addressed by several groups and has now reached a solid level of understanding (a list of references to the original literature can be found in [10–12]). In one approach an additional effective theory (pNRQCD) very close to a quantum-mechanical description of the bound system, containing only the heavy quarkonium field and ultrasoft degrees of freedom, is matched to NRQCD [13–15]. An alternative approach, formulated only for the weak coupling case $mv^2 \gg \Lambda_{\rm QCD}$, does not involve matching from NRQCD, but instead matches a different effective theory (vNRQCD) to full QCD directly at the hard scale [16–18].

In the next section we will give a brief general introduction to NRQCD, since this is the framework for many applications reviewed in this report. More specific presentations of NRQCD can be found in Chapter 3, Section 2.2, Chapter 4, Section 3.1 and Chapter 5, Section 1.1. NRQCD on the lattice will be presented mainly in the following Section 3.2.3 and in Chapter 3, Section 2.1. In Chapter 4, Section 4.2 a short presentation of SCET, an EFT suited to describe collinear fields interacting with soft degrees of freedom, in combination with NRQCD may be found.

### 2.1 Nonrelativistic QCD

NRQCD is obtained by integrating out modes of energy and momentum $m$ from QCD Green functions describing heavy quark–antiquark pairs. It is characterized by an ultraviolet (UV) cut-off $\nu_{NR} = \{\nu_p, \nu_s\}$ that satisfies $E, p, \Lambda_{\rm QCD} \ll \nu_{NR} \ll m$; $\nu_p$ is the UV cut-off of the relative three-momentum of the heavy quark and antiquark; $\nu_s$ is the UV cut-off of the energy of the heavy quark and antiquark, and of the four-momenta of the gluons and light quarks. NRQCD is, therefore, designated to describe the dynamics of heavy quark–antiquark pairs (not necessarily of the same flavour) at energy scales in the centre-of-mass frame much smaller than their masses. At these energies quark–antiquark pairs cannot be created so it is enough to use Pauli spinors for both the heavy quark and the heavy antiquark degrees of freedom. Other degrees of freedom of the theory are gluons and light quarks of four momentum smaller than $\nu_s$.

The high-energy modes that have been integrated out have a relevant effect on the low-energy physics. This effect is not lost, but encoded into the matching coefficients $c$ and new local interactions of the NRQCD Lagrangian. In principle, there are infinite such terms to be included, in practice only few of

them are needed. Each operator can be counted in $v$. The velocity $v$ and $\alpha_{\rm s}$ (in the matching coefficients) are the two small expansion parameters of NRQCD. If we aim at an accuracy of order $(\alpha_{\rm s}^k\ v^n)$ we have to keep in the Lagrangian only terms and matching coefficients that contribute up to that order to the physical observable under study. The couplings $m$, $g$, $c$ are determined by the requirement that NRQCD reproduces the results of QCD up to order $(\alpha_{\rm s}^k\ v^n)$.

If the quark and antiquark have the same flavour, they can annihilate into hard gluons. In NRQCD their effect is encoded in the imaginary parts of the four-fermion matching coefficients (denoted by $f$ in the following). Their role in the description of heavy quarkonium annihilations in NRQCD will be discussed in Chapter 4.

In general, at each matching step the non-analytic behaviour in the scale that is integrated out becomes explicit in the matching coefficients. Since in this case we are integrating out the mass, it becomes an explicit parameter in the expansion in powers of $1/m$ in the Lagrangian, while the dependence in $\ln(m/\nu)$ is encoded into the matching coefficients.

Up to field redefinitions the NRQCD Lagrangian for one heavy flavour of mass $m$ and $n_f$ massless quarks at $\mathcal{O}(1/m^2)$, but including the kinetic energy term $\mathbf{D}^4/(8m^3)$, reads [8, 9, 19–21]:

$$\mathcal{L}_{\rm NRQCD} = \mathcal{L}_g + \mathcal{L}_l + \mathcal{L}_\psi + \mathcal{L}_\chi + \mathcal{L}_{\psi\chi}, \tag{1.3}$$

$$\mathcal{L}_g = -\frac{1}{4}F^{\mu\nu a}F^a_{\mu\nu} + c_1^g\frac{1}{4m^2}g f_{abc}F^a_{\mu\nu}F^{\mu\,b}{}_\alpha F^{\nu\alpha\,c}, \tag{1.4}$$

$$\begin{aligned}\mathcal{L}_l = {} & \sum_{i=1}^{n_f}\bar q_i i\not{D} q_i + c_1^{ll}\frac{g^2}{8m^2}\sum_{i,j=1}^{n_f}\bar q_i T^a\gamma^\mu q_i\ \bar q_j T^a\gamma_\mu q_j + c_2^{ll}\frac{g^2}{8m^2}\sum_{i,j=1}^{n_f}\bar q_i T^a\gamma^\mu\gamma_5 q_i\ \bar q_j T^a\gamma_\mu\gamma_5 q_j \\ & + c_3^{ll}\frac{g^2}{8m^2}\sum_{i,j=1}^{n_f}\bar q_i\gamma^\mu q_i\ \bar q_j\gamma_\mu q_j + c_4^{ll}\frac{g^2}{8m^2}\sum_{i,j=1}^{n_f}\bar q_i\gamma^\mu\gamma_5 q_i\ \bar q_j\gamma_\mu\gamma_5 q_j,\end{aligned} \tag{1.5}$$

$$\begin{aligned}\mathcal{L}_\psi = {} & \psi^\dagger\Bigg\{iD_0 + c_2\frac{\mathbf{D}^2}{2m} + c_4\frac{\mathbf{D}^4}{8m^3} + c_F\, g\frac{\boldsymbol{\sigma}\cdot\mathbf{B}}{2m} \\ & \quad + c_D\, g\frac{\mathbf{D}\cdot\mathbf{E} - \mathbf{E}\cdot\mathbf{D}}{8m^2} + i c_S\, g\frac{\boldsymbol{\sigma}\cdot(\mathbf{D}\times\mathbf{E} - \mathbf{E}\times\mathbf{D})}{8m^2}\Bigg\}\psi \\ & + c_1^{hl}\frac{g^2}{8m^2}\sum_{i=1}^{n_f}\psi^\dagger T^a\psi\ \bar q_i\gamma_0 T^a q_i + c_2^{hl}\frac{g^2}{8m^2}\sum_{i=1}^{n_f}\psi^\dagger\gamma^\mu\gamma_5 T^a\psi\ \bar q_i\gamma_\mu\gamma_5 T^a q_i \\ & + c_3^{hl}\frac{g^2}{8m^2}\sum_{i=1}^{n_f}\psi^\dagger\psi\ \bar q_i\gamma_0 q_i + c_4^{hl}\frac{g^2}{8m^2}\sum_{i=1}^{n_f}\psi^\dagger\gamma^\mu\gamma_5\psi\ \bar q_i\gamma_\mu\gamma_5 q_i,\end{aligned} \tag{1.6}$$

$$\mathcal{L}_\chi = \text{c.c. of } \mathcal{L}_\psi, \tag{1.7}$$

$$\begin{aligned}\mathcal{L}_{\psi\chi} = {} & \frac{f_1(^1S_0)}{m^2}O_1(^1S_0) + \frac{f_1(^3S_1)}{m^2}O_1(^3S_1) + \frac{f_8(^1S_0)}{m^2}O_8(^1S_0) + \frac{f_8(^3S_1)}{m^2}O_8(^3S_1), \\ & O_1(^1S_0) = \psi^\dagger\chi\,\chi^\dagger\psi, \qquad O_1(^3S_1) = \psi^\dagger\boldsymbol{\sigma}\chi\,\chi^\dagger\boldsymbol{\sigma}\psi, \\ & O_8(^1S_0) = \psi^\dagger \mathrm{T}^a\chi\,\chi^\dagger \mathrm{T}^a\psi, \qquad O_8(^3S_1) = \psi^\dagger \mathrm{T}^a\boldsymbol{\sigma}\chi\,\chi^\dagger \mathrm{T}^a\boldsymbol{\sigma}\psi,\end{aligned} \tag{1.8}$$

where $\psi$ is the Pauli spinor that annihilates the quark, $\chi$ is the Pauli spinor that creates the antiquark, $iD_0 = i\partial_0 - gA_0^a\,T^a$, $i\mathbf{D} = i\boldsymbol{\nabla} + g\mathbf{A}^a\,T^a$, $\mathbf{E}^i = F^{i0\,a}\,T^a$, $\mathbf{B}^i = -\epsilon_{ijk}F^{jk\,a}\,T^a/2$ and c.c. stands for charge conjugate. The allowed operators in the Lagrangian are constrained by the symmetries of QCD. However, due to the particular kinematical region we are focusing, Lorentz invariance is not linearly

realized in the heavy quark sector. In practice, Lorentz invariance is realized through the existence of relations between the matching coefficients, e.g., $c_2 = c_4 = 1$, $c_S = 2c_F - 1$ [19, 22–26].

The matching coefficients may be calculated in perturbation theory. For the heavy quark (antiquark) bilinear sector as well as for the purely gluonic sector up to $\mathcal{O}(1/m^2)$ the matching coefficients have been obtained at one loop in [19]. The complete LL running of these coefficients in the basis of operators (1.4)–(1.6) has been calculated in [20, 21][3]. For $c_F$ a NLL evaluation can be found in [28]. In the four heavy fermion sector the matching coefficients $f$ of the $1/m^2$ operators have been obtained at one loop in [29]. As discussed above, in this sector the matching coefficients have a non-zero imaginary part. Due to their relevance in heavy quarkonium decay processes, the calculation of corrections of higher order in $\alpha_{\rm s}$ has a long history [9, 30–36]. We summarize it in Section 3.1.1 of Chapter 4. An updated list of imaginary parts of four fermion matching coefficients may be found in [37].

Since several scales remain dynamical in NRQCD, it is not possible to give a homogeneous power counting for each operator without extra assumptions, i.e., the power counting in $v$ is not unambiguous. To obtain a better defined power counting one should go to EFTs of lower energy. It should be noticed that the importance of a given operator for a practical calculation does not depend only on its size, but also on the leading power of $\alpha_{\rm s}$ of the corresponding matching coefficient.

Finally, since modes of energy $m$ have been removed from the Lagrangian, NRQCD lattice simulations may use lattices that are coarser by about a factor $1/v^4$ ($\sim 100$ in the $b\bar{b}$ case) than those needed by full QCD [6]. We will come back to this in Section 3.2.3.

## 2.2 Lower energy EFTs

Effective field theories suited to describe the low energy modes of the heavy quarkonium dynamics that will be used in this report are pNRQCD and vNRQCD. Here we will not give details on these EFTs since specific introductions to pNRQCD can be found in Chapter 3, Section 2.2.1 and Chapter 4, Section 3.1.3, and to vNRQCD in Chapter 6, Section 5. For detailed recent reviews on effective field theories for heavy quarkonium we refer the reader to [10] and [11], which are mainly devoted to pNRQCD and vNRQCD respectively.

What we want to point out here is that in all these EFTs objects like potentials show up. For short range (or weakly coupled) quarkonia the potentials may be built order by order in perturbation theory. At higher order the pure potential picture breaks down and the interaction of the heavy quark fields with the low-energy gluons has to be taken into account (see the pNRQCD Lagrangian of Chapter 3, Eq. (3.9) and the vNRQCD Lagrangian of Chapter 6, Eqs. (6.20) and (6.21)). For long range (or strongly coupled) quarkonia the potentials are nonperturbative objects that may be expressed in terms of gluon fields expectation values. Noteworthy, the pNRQCD Lagrangian in the strong coupling regime reduces exactly, under some circumstances, to the simple case of a heavy quarkonium field interacting with a potential (see Chapter 3, Eq.(3.11)).

The potential picture that emerges from these EFTs is quite different from the one of traditional potential models and superior. Not only the potential is derived from QCD, but higher-order corrections can be systematically included without being plagued by divergences or *ad hoc* cut-offs; these are absorbed in the renormalization procedure of the EFT. Nevertheless, traditional potential models, which so much have contributed to the early understanding of the heavy quarkonium properties, may be still useful and will often appear in the report. First, a potential model can be seen, in absence of competitive lattice data, as a specific *ansatz* on the form of the low-energy QCD dynamics encoded in the potential defined by an EFT. Second, potential models still provide the only available tool to describe physical systems for which a suitable EFT has not been built yet. This is, for instance, the case of systems coupled to open flavour channels.

[3] After correcting a few misprints in the anomalous dimension matrix [27], the results of [21] agree with those of Ref. [20].

## 3 LATTICE INTRODUCTION[4]

Low energy nonperturbative QCD can either be modelled or simulated on the Lattice. Lattice gauge theory methods are particularly powerful in heavy quark physics when combined with effective field theories (EFTs). Lattice QCD input significantly increases the predictive power of EFTs as more and more low energy parameters can be calculated reliably directly from QCD and less fits to experimental data are required for this purpose. Past lattice QCD results were often obtained within the quenched approximation (neglecting sea quarks) or with unrealistically heavy up and down quarks and $n_f = 2$, rather than $n_f = 2 + 1$. At present these limitations are gradually being removed.

We shall only describe general aspects of lattice gauge theory simulations. Recent reviews of different aspects of Lattice QCD can for instance be found in Refs. [38–48]. Several books [49–54] on the subject have been written and the summary talks of the yearly proceedings of lattice conferences (see Ref. [55] for the most recent ones) provide an overview of the field. Ref. [56] contains collections of early papers.

Obviously there are infinitely many gauge invariant ways to discretize the continuum QCD action. We will summarise and define the actions most commonly used and address limitations of the method, before we discuss extrapolations and sources of systematic errors.

### 3.1 General aspects

Lattice simulations rely on stochastic (Monte Carlo) methods. Hence all results inevitably carry statistical errors which however are no problem of principle as they can be made arbitrarily small on (arbitrarily) big computers or by means of algorithmic and methodological improvements. In order to carry out path integral quantisation in a mathematically sound ways, the discretisation of space–time appears necessary. This also enables us to map continuous problems onto a finite computer. Discretisation, i.e., for instance replacing derivatives $\partial_t \phi(t)$ by $[\phi(t+a) - \phi(t-a)]/(2a)$ with "lattice spacing" $a$ and, in this example, lattice "errors" of $\mathcal{O}(a^2)$, inevitably carries the smell of *inexactness*. We stress however that the very nature of QCD itself requires us to introduce an ultra-violet regulator and, as we shall see below, lattice discretisation is one possible choice. Continuum results are then obtained by removing the regulator, $a \to 0$.

Observables are calculated ("measured") taking their expectation values in the path integral approach: this amounts to calculating averages over all possible "configurations" of gauge fields on the lattice, weighted with the respective exponent of the action. In simulations with sea quarks, producing these configurations is costly and the ILDG [57] (International Lattice Data Grid) is due to be set up, with the aim of standardising formats of organising and labelling such lattice data, in a way that allows for easy distributed storage, retrieval and sharing of such deposits among different lattice groups.

The typical observables are $n$-point Green functions. In order to determine a hadronic rest mass one has to construct an operator with the respective quantum numbers: spin $J$, parity $P$, charge conjugation $C$, isospin, flavour content etc. This is then projected onto zero momentum and the 2-point Green function calculated, creating the particle at time 0 and destroying it at time $t$. For large $t$ this will then decay exponentially, $\propto \exp(-mt)$, with $m$ being the ground state mass within the channel in question. There exist numerous "wave functions" with the right quantum numbers, some with better and some with inferior overlap to the physical ground state. It is a refined art to identify spatial "smearing" or "fuzzing" functions that maximise this overlap and allow to extract the mass at moderate $t$-values, where the signal still dominates over the statistical noise. The multi-exponential $t$-dependence of Green functions complicates the identification of excited states, i.e., sub-leading or sub-sub-leading exponents. By working with very precise data, realising a variational multi-state basis of test wave functions [58], and employing sophisticated fitting techniques [59, 60], it has however in some cases become possible to calculate moderately low lying radial excitations.

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Lattice QCD is formulated in Euclidean space time: in the continuum, this amounts to replacing Lorentz boosts and $O(3)$ rotational symmetry by $O(4)$ rotations. The reason for this is that a real (and bounded) action is required to allow for a probabilistic interpretation of the path integral measure and computer simulation. As an analytical continuation to Minkowski space time of a finite number of finite-precision data points is impossible, the predictive power is confined to quantities that have a Euclidean space time interpretation such as masses and matrix elements.

Lattice discretisation unavoidably breaks rotational $O(4)$ invariance, on the scale of the lattice spacing $a$. As the continuum limit $a \to 0$ is approached, any fixed physical correlation length $\xi$ will become much larger than the lattice spacing. Provided the interaction ranges that appear within the action are localised in space time, all physics will become independent of the underlying discretisation and a universal continuum limit will be reached, in which $O(4)$ invariance is restored. Asymptotic freedom implies that such a continuum limit is approached as the lattice coupling constant, $g \to 0$.

Replacing $O(4)$ invariance by its hypercubic subgroup means that in particular higher spin states are hard to identify. For instance $J = 4$ cannot easily be distinguished from $J = 0$ on a hypercubic lattice. At finite lattice spacing $a$, only discrete translations in space and imaginary time are possible. This results in the maximum modulus of Euclidean four-momentum components of $\pi/a$, providing the required ultraviolet regularisation. Although an infrared cut-off is not necessary in principle, on a finite computer only a finite number of lattice points can be realised. Typically toroidal boundary conditions are taken in all directions for the gauge fields while fermions, being Grassmann-valued fields, are antiperiodic in time. This results in quantisation of momentum components in steps of $2\pi/(La)$ where $L$ denotes the number of lattice points along the dimension in question: not all momenta can be realised and this leads to kinematic constraints when it comes to calculating decay matrix elements or to extracting a particle mass from a dispersion relation.

The temporal extent $aL_\tau$ of the lattice can also be interpreted as an inverse temperature (see e.g., Ref. [61]) and in this case QCD matter at high temperature can be simulated. There are some subtleties related to this approach. For instance the limit of infinite Euclidean time cannot be taken anymore. Details of thermal field theory are discussed in Chapter 7.

While the lattice regulator inevitably violates Poincaré invariance it preserves gauge invariance and most global symmetries of QCD. The exception was chiral symmetry which, one had to hope, would become restored in the continuum limit. However, within the past 10 years, formulations of chiral lattice fermions [62, 63] have evolved that implement an exact lattice chiral symmetry, which in the continuum limit corresponds to the continuum chiral symmetry. These are known as overlap fermions or domain wall fermions (which in some sense are a special case of the former) and in some literature (somewhat inaccurately) as Ginsparg–Wilson fermions since the lattice-Dirac operator used obeys the so-called Ginsparg–Wilson relation [64]. We shall refer to these implementations as chiral fermions.

At presently available light quark masses chiral fermions are typically two orders of magnitude more expensive to simulate than traditional formulations. As the quark mass is decreased chiral fermions become more competitive. Obvious advantages of chiral formulations are the applicability of chiral perturbation theory also at finite lattice spacing and a more continuum-like mixing between many lattice operators. With respect to quarkonia in which both valence quarks are heavy these new developments are at present of limited significance as light quark mass effects are usually sub-leading.

Lattice QCD is a *first principles* approach. No parameters apart from those that are inherent to QCD, i.e., strong coupling constant at a certain scale and quark masses, have to be introduced. In order to fix these $n_f + 1$ parameters $n_f + 1$ low energy quantities are matched to their experimental values. In simulations of quarkonia the lattice spacing $a(\beta, m_i)$, that corresponds to given values of the inverse lattice strong coupling, $\beta = 6/g^2$ and lattice quark masses $m_i$, is frequently obtained by matching to spin-averaged experimental level splittings. In simulations with un-realistic sea quark content one might hope that this increases the reliability of other predictions as the systematics are partly correlated. With realistic sea quark content the predictive power with respect to quarkonium physics can be enhanced by

using independent input such as the experimental proton mass $m_p$ or the pion decay constant, $f_\pi$, instead. A scale that cannot directly be accessed by experiment but which owes its popularity to the accuracy and ease with which it can be calculated is the Sommer scale $r_0$ [65], implicitly defined through,

$$r^2 \left. \frac{dV(r)}{dr} \right|_{r=r_0} = 1.65 \,, \tag{1.9}$$

where $V(r)$ denotes the static quark–antiquark potential and the numerical value on the right hand side is adjusted such that fits of the bottomonium spectrum to phenomenological or lattice potentials yield $r_0 \approx 0.5$ fm. $r_0$ is also well-defined in the theory with sea quarks and its model dependence is much smaller than that of the string tension. Within the quenched approximation scale uncertainties cannot be avoided anyway and hence such model dependence is admissible. In simulations with sea quarks this is different but $r_0$ still provides a convenient reference scale, that can be used to relate different lattice results with each other.

### 3.2 Actions and finite $a$ effects

We shall discuss the gauge and heavy quark actions that are usually employed. In simulations with sea quarks, in addition a light quark action needs to be specified.

Results from lattice simulations are inevitably obtained at a finite lattice spacing $a$. Ideally, they are then extrapolated to the physically relevant (and universal) continuum limit $a \to 0$. Within the quenched approximation, such extrapolations have become the standard while in simulations with light sea quarks a sufficient variation of the lattice spacing is often still prohibitively expensive in terms of computer time. The leading order $a$ behaviour depends on the choice of the discretisation.

One can follow Symanzik [66] and use a continuum effective field theory to show that the cutoff effects have the form $a^n(\ln \Lambda a)^m$, where $\Lambda$ denotes a low energy scale of the order of a few hundred MeV and $m \geq 0$. The leading power is usually (see below) $n = 1$ or 2 and within this leading term, $m = 0$. By changing the discretisation, the leading terms can be reduced or eliminated. This strategy is called "improvement", and it is used to hasten the approach to the continuum limit.

In a classical mechanical system improvement is straightforward. However, even in this case there exists a break-even point at which further improvement becomes computationally more expensive than the equivalent reduction of the lattice spacing, due to the exploding number of terms and interaction range. Typically this point is reached around $n \approx 5$. In a quantum field theory the situation is more complex. In QCD the (Wilson) coefficients of improvement terms obtain quantum corrections which can be obtained perturbatively as a power series in the strong coupling constant $g^2$, in a suitable scheme. Following an effective field theory philosophy, such calculations can be done and the size of next order corrections estimated. However, at sufficiently small $a$ any $c_1 g^{2n}(a)a + c_2 a^2$ expression will be dominated by the first term that, in this example, is proportional to $a$. To eliminate such terms the coefficient has to be determined nonperturbatively. Otherwise little is gained in a continuum limit extrapolation, other than a reduction of the slope of the leading order term. At a given finite $a$ value there is however still some gain from improvement as the results will be more continuum-like. Examples for a systematic nonperturbative improvement programme exist [67].

In the lattice literature often the word "scaling" is meant to imply that an effective continuum limit is reached: within the "scaling region" mass ratios appear to be independent of $a$, within statistical errors. If $a$ is reduced even further, eventually one will encounter "asymptotic scaling", i.e., lattice masses $a(g)m$ will depend on the coupling $g^2$ in the way expected from the perturbative two-loop $\beta$ function. It is quite clear by now that "asymptotic scaling" in terms of the bare lattice coupling might never be achieved on large lattices. However, asymptotic scaling has been verified for a particular choice of the coupling, as a function of the linear extent of tiny lattices, see e.g., Ref. [68].

### *3.2.1 Gauge actions*

In lattice simulations, $SU(3)$ group elements $U_{x,\mu}$ are typically represented as complex $3 \times 3$ matrices that live on directed links connecting a lattice site $x$ with the neighbouring site $x + a\hat{\mu}$. Traces of products of such "link variables" or "links" along closed paths (Wilson loops) are gauge invariant. The simplest non-trivial such example is a $1 \times 1$ square, an elementary "plaquette". The lattice action should preserve gauge invariance which means that it can be expressed as a sum over such loops. Fermion fields $\psi_x$ and $\bar{\psi}_x$ are living on the lattice sites and a quark can be "transported" from site $x + a\hat{\mu}$ to site $x$ by means of a left multiplication with $U_{x,\mu}$: the combination $\bar{\psi}_x U_{x,\mu} \psi_{x+a\hat{\mu}}$ is gauge invariant.

The simplest gauge action is the so-called Wilson action [69], which is proportional to the trace of the sum over all elementary plaquettes:

$$S_W = -\beta \sum_{x,\mu>\nu} \mathrm{Re}\,\mathrm{tr}\,\Pi_{x,\mu,\nu}, \tag{1.10}$$

where $x$ runs over all lattice sites and $\Pi_{x,\mu\nu} = U_{x,\mu} U_{x+a\hat{\mu},\nu} U^{\dagger}_{x+a\hat{\nu},\mu} U^{\dagger}_{x,\nu}$. Up to an irrelevant constant the Wilson action agrees with the Euclidean continuum action to $\mathcal{O}(a^2)$:

$$S_{\mathrm{YM}} = \int d^4x \, \frac{1}{4g^2} \sum_{a=1}^{8} F^a_{\mu\nu}(x) F^a_{\mu\nu}(x) = S_W + \text{const.} + \mathcal{O}(a^2)\,, \tag{1.11}$$

where we identify $\beta = 6/g^2$. Asymptotic freedom tells us that $a \to 0$ as $\beta \to \infty$. In simulations without sea quarks it has been established that $\beta = 6$ corresponds to a lattice spacing $a \approx 0.1\,\mathrm{fm} \approx (2\,\mathrm{GeV})^{-1}$. With sea quarks (using the same gluonic action) the same lattice spacing will be obtained at a somewhat smaller $\beta$-value as the running of $a(g)$ with the coupling $g$ will be somewhat slower. As mentioned above, perturbation theory in terms of the lattice coupling $g^2$ is not yet reliable around $g^2 \approx 1$, to describe the running of $a(g^2)$ (asymptotic scaling).

The $\mathcal{O}(a^2)$ artifacts within Eq. (1.11) can be replaced by $\mathcal{O}(a^4)$ lattice corrections, by adding two paths consisting of six links, for instance a $1 \times 2$ rectangle and a "chair". The result is known as the Symanzik–Weisz action [70] and the coefficients of the individual terms have been calculated to one loop [$\mathcal{O}(g^2)$] accuracy [71]. At tree level, only the coefficient of the rectangle assumes a non-trivial value. One (somewhat arbitrary) choice in the space of actions is the Iwasaki-action [72], again the sum of plaquette and rectangle, but with the relative weight fixed to a constant, originally motivated by demanding invariance of physical mass ratios under numerical renormalisation group transformations, within a certain $\beta$ window. In addition to simulations with these gauge actions [73–75], there have also been simulations employing a combination of the plaquette in the fundamental and in its adjoint representation [74] as well as simulations on anisotropic lattices, using an anisotropic Wilson action [76–78] or anisotropic variants of actions including Symanzik–Weisz style terms [79].

The main motivation for adding such extra terms to the action is to achieve a more continuum-like behaviour already at finite lattice spacing. It also turns out that simulations with chiral fermions benefit from such a choice which implies a "smoother" gauge field background.

In order to achieve full $\mathcal{O}(a^2)$ improvement the coefficients of the extra terms would have to be determined nonperturbatively, for instance by imposing continuum relations: in the pure gauge theory example above one could impose rotational invariance of the static quark potential at two distances, e.g., $V(3,0,0) = V(2,2,1), V(5,0,0) = V(3,4,0)$ to fix the two coefficients, or use dispersion relations of glueballs or torelons. This is laboursome and in general the fermions will not be nonperturbatively improved beyond $\mathcal{O}(a^2)$ anyway. So in practice, only approximate improvement has been implemented, either by using the perturbative coefficients at a given order or by employing a so-called "tadpole" improvement prescription.

The latter is motivated by two observations. The first one is that short-distance lattice quantities differ considerably from their continuum counterparts, even at lattice spacings at which one would, based

on the $\overline{\rm MS}$ scheme continuum experience, assume perturbation theory to be valid. For instance around $a^{-1} = 2\,\text{GeV}$ the numerical value for the plaquette with Wilson action reads $\Box = \frac{1}{3}\langle \text{tr}\,\Pi\rangle \approx 0.6$ while at $g = 0$ this should obviously be normalised to *one*. This is closely related to the breaking of continuum rotational symmetry on the scale of a lattice spacing $a$. Parisi [80] hypothesized that such ultra-violet effects could largely be factored out and put into commuting pre-factors. This mean-field improvement amounts to dividing links that appear within lattice operators by constant factors, e.g., $u_0 = \Box^{1/4}$. An independent observation is that lattice perturbation theory, whose convergence behaviour in terms of the lattice coupling $g^2$ is well known to be quite bad, differs from continuum perturbation theory largely by a class of lattice-specific tadpole diagrams which are numerically large. By normalising everything with respect to other "measured" observables like $u_0$ these contributions cancel at one loop order and one might hope that tadpole dominance and cancellation approximately generalises to higher orders as well [81].

Finally, there is the idea of (classically) "perfect" actions [82]. If one found an action that lies right on top of a renormalisation group trajectory then, independent of the lattice spacing $a$, one would obtain continuum results. Such actions can be identified by demanding independence of physical results under a change of the underlying scale. An action that contains a finite set of couplings is suggested and these are then optimised with respect to such constraints. In practice, one can of course at best construct an action that is close to such a trajectory in which case decreasing the lattice spacing still helps to reduce deviations of the nearly perfect action from a real renormalisation group trajectory which one attempts to approximate. An example of such an (approximately) perfect action and its construction can be found in Ref. [83].

### *3.2.2 Light quark actions*

The Dirac action is bi-linear in the quark fields. In the language of perturbation theory this amounts to the non-existence of vertices containing an odd number of quark fields. This means that the quark part of a lattice calculation can to some extent be separated from the gauge field evaluation: the gluon fields contain all information of the QCD vacuum, including sea quark loops, provided these are unquenched (see below). Hadronic $n$-point functions can be obtained from contractions of colour fields, $\Gamma$-matrices and quark-propagators, calculated on this gluonic background.

We denote a discretisation of the continuum Euclidean Dirac operator $[D_\mu\gamma_\mu + m_i]$ as $M_i[U]$. Each quark flavour $i$ now contributes a factor,

$$S_{f_i} = (\bar{\psi}, M_i[U]\psi), \tag{1.12}$$

to the action, where the scalar product $(\cdot,\cdot)$ is over all $V = L^3 l_\tau$ sites of Euclidean space time, colour and Dirac-spinor index. Note that $M_i$ depends on the gauge fields $U$. Components of $M_i^{-1}$ correspond to quark propagators. Often it is sufficient to calculate propagators that originate from only one source point. In this case only one space–time row of the otherwise $12V \times 12V$ matrix $M_i^{-1}$ needs to be calculated. As the non-diagonal contributions to the Dirac operator all originate from a first order covariant derivative, $M_i$ will be a sparse matrix with non-vanishing elements only in the vicinity of the (space time) diagonal. This tremendously helps to reduce the computational task. Quark propagators can be contracted into hadronic Green functions, expectation values (over gauge configurations) of which will decay with the mass in question in the limit of large Euclidean times.

One complication arises from the fermions as these are represented by anti-commuting Grassmann numbers. Realising these directly on a computer implies a factorial (with the number of lattice points) complexity [84] but fortunately they can be integrated out analytically as,

$$\int [d\psi][d\bar{\psi}] e^{(\bar{\psi}, M_i[U]\psi)} = \det M_i[U] = \int [d\phi][d\phi^+] e^{(\phi^+, M_i^{-1}[U]\phi)}, \tag{1.13}$$

where $\phi$ and $\phi^+$ are auxiliary Boson (pseudo-fermion) fields. The price one pays is that calculating $\det M_i[U]$ (or $M_i^{-1}$) involves effective interactions over several lattice sites. This renders simulations containing sea quark effects two to three orders of magnitude more expensive than using the quenched (or valence quark) approximation, $\det M_i[U] = \text{const.}$.

As one would expect ratios of light hadron masses from lattice simulations of quenched QCD have been found to be inconsistent with the observed spectrum [85]. However, the differences are typically smaller than 10 %, suggesting that the quenched approximation has some predictive power if cautiously consumed. Apart from the obvious shortcomings like a stable $\Upsilon(4S)$, the consequences of violating unitarity at light quark mass can become dramatic in some channels [86]. Roughly speaking as the axial anomaly does not exist in quenched QCD the $\eta'$ will be a surplus light Goldstone Boson or, more precisely, a ghost particle. The impact of this can be investigated in quenched chiral perturbation theory.

Ultimately, one needs to include sea quarks and there are three classes of light quark actions: staggered, Wilson-type, and chiral.

After trivially rescaling the quark fields, $\psi_x \to a^{-3/2}\psi_x, \bar{\psi} \to a^{-3/2}\bar{\psi}_x$, to allow for a representation as dimensionless numbers, a naïve discretisation of the Dirac action would read,

$$S_N = \sum_x \left\{ ma\bar{\psi}_x\psi_x + \frac{1}{2}\sum_\mu \gamma_\mu \bar{\psi}_x \left[ U_{x,\mu}\psi_{x+a\hat{\mu}} - U^\dagger_{x-a\hat{\mu},\mu}\psi_{x-a\hat{\mu}} \right] \right\}. \tag{1.14}$$

This action corresponds to the continuum action, up to $\mathcal{O}(a^2)$ terms, however, it turns out that it corresponds to 16 mass-degenerate species of Dirac fermions in the continuum limit, rather than to one: the famous fermion-doubling problem [89, 90]. In the lattice literature these species are now often called tastes, instead of flavours, to emphasize that they are unphysical.

It has been noted however that by means of a unitary transformation, the naïve action can be diagonalised in spinor-space, into four identical non-interacting terms, each corresponding to four continuum tastes. The result is the so-called Kogut–Susskind (KS) action [91], in which 16 spin-taste components are distributed within a $2^4$ hypercube, a construction that is known in the continuum as Kähler fermions. The advantage is that one taste of KS fermions corresponds to $n_f = 4$ continuum tastes rather than $n_f = 16$. Another nice feature is that even at finite lattice spacing one of the 15 $(n_f^2 - 1)$ pions will become exactly massless as $m \to 0$. The price that one pays is strong spin-taste mixing at finite lattice spacing and large coefficients accompanying the leading $\mathcal{O}(a^2)$ lattice artifacts. KS-type fermions are referred to as "staggered" and there are improved versions of them, most notably the Naik action [92], the AsqTad [93] ($a$ squared tadpole improved) action and HYP actions [94, 95] (in which parallel transporters are smeared "iteratively" within hypercubes). The latter two choices notably reduce the tastes mixing interactions.

In order to bring down $n_f = 4$ to $n_f = 1$, as required to achieve $n_f = 2 + 1$, sometimes the determinant within Eq. (1.13) is replaced by its fourth positive root [96, 97]. It can be shown that within perturbation theory this indeed corresponds to replacing the $n_f$-factors accompanying sea quark loops by $n_f/4$. However, some caution is in place. The operator $\sqrt{M}$ is non-local [98] and if its non-locality altered $\sqrt{\det M} = \det\sqrt{M}$, universality could be lost in the continuum limit. One might argue that $A$ is not the only operator with the property $\det A = \sqrt{\det M}$ but also in the Schwinger model there exist some discouraging results for the behaviour of the topological winding number at small quark masses [99]. Moreover, the valence quark action automatically differs from the one used for the sea quarks as each taste of sea quarks will correspond to 4 tastes of valence quarks [100].

Nonetheless, large scale simulations with this action are pursued at present as the computational costs of going to light sea quark masses appear much smaller than with other actions. Moreover, as long as the sea quark masses are not too small, this approximation to QCD is not completely wrong and in fact likely to be more realistic than quenched QCD. Indeed, in quarkonium physics where light quark

mass effects are sub-leading, first results appear very encouraging [97]. There also exist first theoretical attempts of constructing a local representation of the $n_F < 4$ staggered action [101, 102].

Another "solution" to the fermion doubling problem are Wilson fermions [90]: the lattice analogue of the term, $-\frac{1}{2}aD_\mu D_\mu$, is added to the $M$ of Eq. (1.14). This increases the masses of the 15 doublers by amounts that are proportional to $a^{-1}$, removing the unwanted modes. Like in the case of staggered fermions the chiral symmetry that QCD classically enjoys at $m = 0$ is explicitly broken at any finite lattice spacing $a$. In addition, one encounters additive mass renormalisation and a rather awkward eigenvalue spectrum of the lattice Dirac operator as well as $\mathcal{O}(a)$ lattice terms. The latter can be removed by adding yet another counterterm to $M$: $\propto -ic_{sw}\sigma_{\mu\nu}F_{\mu\nu}$. The resulting action is known as the Sheikholeslami–Wohlert (SW) or clover action [103]. The $c_{sw}$ coefficient is known to one loop [$\mathcal{O}(g^2)$] in perturbation theory [103, 104] but has also been determined nonperturbatively in quenched QCD with Wilson gauge action [67], in $n_f = 2$ QCD with Wilson [105] and $n_f = 3$ QCD with Iwasaki gauge actions [106]. Another variant is the FLIC (fat link irrelevant clover) action [107]. Finally, there exists twisted mass QCD [108], in which an imaginary mass term is introduced into the Wilson action. Unfortunately, in this case there will be mixing between parity partners within Green functions, something that one also encounters in staggered formulations. However, the changed eigenvalue spectrum of $M$ renders smaller quark masses accessible. Moreover, in the case of a purely imaginary renormalized mass parameter, $\mathcal{O}(a)$ improvement holds.

Finally, formulations of chiral lattice fermions exist. These are automatically $\mathcal{O}(a)$ improved and do not suffer from the fermion doubling problem. Realisations of these fall into three categories: overlap fermions, based on the Neuberger action [62], domain wall fermions, which live on a five-dimensional lattice and become chiral as the size of the fifth dimension is sent to infinity [63] and perfect actions [82, 87, 88]. As always there is no free lunch and at presently accessible sea quark masses these formulations are around two orders of magnitude more expensive than the "traditional" quark actions, described above. For this reason, these formulations have not yet been applied to quarkonia (although one quenched study with "chiral" charm quarks exists [109]) but in the future as algorithmic and hardware development will reduce costs, gauge configurations with chiral sea quarks will become increasingly available, in particular also because at lighter quark masses chiral fermions will become more competitive.

### *3.2.3 Heavy quark actions*

To a very good approximation bottom quarks can be neglected from the sea as their presence will only affect the theory at very short distances. This is also true for charm quarks but, depending on the phenomenology one is interested in, to a somewhat lesser extent. In principle nothing speaks against employing the same quark actions as above to the heavy quark sector as well. With a naive treatment of cutoff effects, lattice corrections $\propto (ma)^n$ arise. This suggests that to make contact with the continuum limit, the condition $m < a^{-1}$ has to apply: as $m$ becomes large the lattice spacing has to be made finer and finer, the number of lattice points larger and larger and computational costs will explode, if not for charm then certainly for bottom.

One possible way out would be to introduce an anisotropy, $\xi = a_\sigma/a_\tau$ with a temporal lattice spacing $a_\tau \ll m^{-1}$ while the spatial lattice spacing can be kept coarser. An obvious application of anisotropic actions is finite temperature physics [110] but an anisotropy has also been employed successfully in investigations of pure gauge theories [79, 111] as well as in charmonium physics [76, 78]. Obviously, the anisotropy of the gauge action has to be matched to that of the light quark and heavy quark actions, in order to obtain a sensible continuum limit. This matching certainly becomes very expensive when sea quarks are included and even more so in the presence of improvement terms.

Another starting point are effective field theories, in particular NRQCD which relies on a power counting in terms of the relative heavy quark velocity, $v$. In addition, EFTs automatically provide the framework for factorisation of physical processes into nonperturbative low energy QCD and perturba-

tive high energy QCD contributions. The fermionic part of the $\mathcal{O}(v^4)$ Euclidean continuum NRQCD Lagrange density with quark fields $\psi$ and antiquark fields $\chi$ reads [6, 8],

$$\mathcal{L} = -\psi^\dagger \left[D_4 + H\right] \psi - \chi^\dagger [D_4 - H^\dagger] \chi + \mathcal{L}_{\psi\chi}, \tag{1.15}$$

with

$$\begin{aligned} H &= m + \delta m - c_2 \frac{\mathbf{D}^2}{2m} - c_F \frac{g\boldsymbol{\sigma}\cdot\mathbf{B}}{2m} - c_4 \frac{(\mathbf{D}^2)^2}{8m^3} \\ &- ic_D \frac{g(\mathbf{D}\cdot\mathbf{E} - \mathbf{E}\cdot\mathbf{D})}{8m^2} + c_S \frac{g\boldsymbol{\sigma}\cdot(\mathbf{D}\times\mathbf{E} - \mathbf{E}\times\mathbf{D})}{8m^2} + \cdots, \end{aligned} \tag{1.16}$$

where the matching coefficients $c_i(m/\mu, g^2) = 1 + \mathcal{O}(g^2)$, $\delta m = \mathcal{O}(g^2)$ are functions of the matching scale $\mu$ and coupling $g^2$. In the continuum $c_2 = c_4 = 1$, however, this is in general different on the lattice, where rotational invariance is broken and to $\mathcal{O}(v^4)$ an additional term $\propto a^2 \sum_i D_i^4/m$ appears. There are many obvious ways of discretising the above equation on the lattice and often the published expressions involve "tadpole" improvement factors $u_0 = 1 + \mathcal{O}(g^2)$. On a lattice with infinite temporal extent it is possible to use a discretisation of the above Hamiltonian within the kernel of a time-symmetric evolution equation [112] such that fields at time $t + a$ can be computed entirely from fields at time $t$ (and vice versa). This turns the computation of propagators particularly economical. In reality, computations are performed on a finite torus but as long as propagators fall off sufficiently fast in Euclidean time, the resulting error of this approximation will be small.

In addition there are the four-fermion interaction terms $\mathcal{L}_{\psi\chi}$ which (in the case of flavour singlet quarkonia) are accompanied by factors $\propto \alpha_{\rm s}$ and have to be considered at $\mathcal{O}(v^4)$. In principle it is known how to do this in lattice simulations [112]. For the $B_c$ system, where annihilation is not possible, there will be further suppression of these terms by an additional factor $\alpha_{\rm s}$. Finally, due to integrating out heavy quark loops, two new purely gluonic operators are encountered [19, 29], accompanied by factors $1/m^2$. This "unquenching" of the heavy quark can in principle easily be implemented in lattice simulations too. However, this is obviously an effect, less important than achieving a realistic light flavour sea quark content.

Starting from a latticized NRQCD action there are in principle different ways to calculate quark propagators. Usually the full fermionic matrix that appears within a lattice discretisation of Eq. (1.16) is inverted, as described above, exploiting a Hamiltonian evolution equation. As an alternative one could also analytically expand the Green functions of interest in powers of $1/m$ and calculate the resulting coefficients individually. It is worthwhile to mention that in the continuum the expression "HQET" refers to heavy-light systems and "NRQCD" to quarkonia. In the lattice literature however, NRQCD is used for both, heavy-heavy and heavy-light system, indicating that the propagator is obtained as the inverse of the lattice NRQCD quark matrix. The term HQET implies an expansion of heavy quark propagators about the static limit. As these are somewhat smeared out in space, NRQCD propagators can be determined more accurately than HQET ones, however, with the invention of new "fat" static quark actions [94] that reduce $\delta m$ within Eq. (1.16) above this has recently changed.

The $m/\mu$ dependence of the matching coefficients $c_i$ has been calculated in the $\overline{\rm MS}$ scheme to various orders in perturbation theory but so far no result on the $ma$ dependence exists in lattice schemes. This seems to be changing, however [113]. Such corrections are important as in the Coulomb-limit, in which NRQCD power counting rules are formulated, $\alpha_{\rm s} = \mathcal{O}(v)$. The difference $\delta m$ between kinetic and rest mass can be determined nonperturbatively from the $\Upsilon$ dispersion relation.

The Fermilab method [114] constitutes a hybrid between heavy quark and light quark methods. It is based on an expansion in terms of the lattice spacing, starting from the Wilson quark action that encompasses the correct heavy quark symmetry. For $ma \ll 1$ this is equivalent to the Symanzik-improvement programme, the lowest order correction resembling the SW/clover term. However, at $ma > 1$ the result is interpreted in terms of the heavy quark terms that one obtains from a $1/m$ expansion. Evidently, the

light-quark clover term has the same structure as the $\sigma \cdot \mathbf{B}$ fine structure interaction, in particular on anisotropic lattices, where the difference can be attributed to the matching coefficients.

An extension of the Fermilab method is an effective field theory framework for describing discretization effects [115]. This theory lumps all discretization effects into short-distance coefficients of the NRQCD/HQET effective Lagrangian. Compared to the continuum HQET or NRQCD, the coefficients now depend on both short distances, $m_Q^{-1}$ and $a$. This theory is also a natural extension of Symanzik's theory of cutoff effects into the regime $m_Q a \not\ll 1$ [116]. The theory of heavy-quark cutoff effects is not limited to the Fermilab method and can be used to compare the relative size of cutoff effects in various ways of discretising the heavy-quark action [117].

Finally, it is possible to solve NRQCD on the lattice by computing static propagators with field strength insertions, in the spirit of the $1/m$ HQET expansion. This can either be done on the level of quarkonium Green functions (an approach that so far has never been attempted) or within the framework of static potentials and relativistic corrections derived from NRQCD [15, 118]. When constructing Green functions one has to keep the power counting in mind as well as the fact that the lowest order NRQCD Lagrangian goes beyond the static limit as the kinetic term is required. It is also possible to put pNRQCD [14] onto the lattice. In the limit $\Lambda < mv^2$ quarkonia are represented as colour singlet or colour octet states, propagating in the QCD vacuum [119]. This condition is only met for would-be toponium and to some extent for the lowest lying bottomonium states. However, this approach is conceptionally interesting and reduces the number of relevant decay matrix elements.

### 3.3 Extrapolations

In lattice simulations there are in general three kinds of effects: finite volume effects, lattice artifacts and errors due to wrong light quark masses. Within NRQCD there are additional error sources due to the truncation of the effective field theory at a fixed order in the velocity $v$ and determination of matching coefficients to a given accuracy in $\alpha_{\rm s}$. In addition to these controlled errors there are error sources that are not controlled by a small parameter like quenching or the use of ill-defined light quark actions. The statistical analysis of lattice data is not trivial but we shall not discuss the possible errors, caveats and pitfalls here as this would be too technical.

Due to the confinement phenomenon and screening of colour, finite size effects are usually quite benign and — once the lattice is sufficiently large — fall off at least like $1/(La)^3$. Because of this it is often sufficient to repeat simulations on 2-3 different volumes to check if finite size effects can be resolved within statistical errors, rather than to attempt proper infinite volume extrapolations. Obviously, higher lying states and charmonia are spatially more extended than lower lying states and bottomonia. In simulations with sea quarks the lattice size has to be large, compared to the pion mass. For instance the condition $La > 4/m_\pi$ yields $La > 5.7$ fm at physical pion mass. There are no large-volume lattice results as yet obtained at such light quark masses. To disentangle possible finite volume from other systematic effects, sequences of lattice simulations at different lattice spacings are often obtained at a volume that is fixed in physical units.

The power $n$ of the dominant finite lattice spacing effect $\mathcal{O}(a^n)$ is in general known and can be fitted to lattice data if sufficient leverage in $a$ is provided. In the context of "improvement" (to a given order of perturbation theory or *ad hoc*) sometimes the coefficient of the leading order term is small since it is suppressed by powers of $g^2$ such that the sub-leading term has to be accounted for as well. Within the context of effective field theories one cannot extrapolate to the continuum limit as the lattice spacing provides the cut-off scale but one can check independence of the results with respect to variations of $a$. Once the $ma$ dependences of the short range matching coefficients are determined, the scaling should improve. A notable exception is the Fermilab action which has a continuum limit. However, the functional form in the cross-over region between $ma > 1$ and $ma < 1$ is not as simple as $a^n(\ln a)^m$.

As computer power is limited, lattice sea quark masses are typically not much smaller than the strange quark mass but with the so-called AsqTad "$n_f = 2 + 1$" action values $m \approx 0.2\, m_s$ have been reported [97]. Lattice results have to be chirally extrapolated to the physical limit. Chiral corrections to quarkonium mass splittings are to leading order proportional to $m_\pi^2$ [120]. While within present-day lattice calculations of light hadronic quantities as well as of $B$ and $D$ physics, such finite mass effects are frequently the dominant source of systematic error, in the case of quarkonia, the dependence appears to be much milder, due to the absence of a light valence quark content.

If effective field theories are realised or simulations are only available at very few lattice spacings cut-off effects can be estimated by power counting rules and/or by varying the action(s). In the absence of fully unquenched results, some experience can be gained by comparing to experiment, on the likely effect of implementing a wrong number of sea quarks but this error source is not controllable from *first principles.* A real *ab initio* study must go beyond the valence quark approximation.

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