

A Glossary

A.1 Lattice actions

In this appendix we give brief descriptions of the lattice actions used in the simulations and summarize their main features.

A.1.1 Gauge actions

The simplest and most widely used discretization of the Yang-Mills part of the QCD action is the Wilson plaquette action [1]:

$$S_G = \beta \sum_x \sum_{\mu < \nu} \left(1 - \frac{1}{3} \text{Re Tr } W_{\mu\nu}^{1 \times 1}(x) \right), \quad (404)$$

where $\beta \equiv 6/g_0^2$ (with g_0 the bare gauge coupling) and the plaquette $W_{\mu\nu}^{1 \times 1}(x)$ is the product of link variables around an elementary square of the lattice, i.e.,

$$W_{\mu\nu}^{1 \times 1}(x) \equiv U_\mu(x) U_\nu(x + a\hat{\mu}) U_\mu(x + a\hat{\nu})^{-1} U_\nu(x)^{-1}. \quad (405)$$

This expression reproduces the Euclidean Yang-Mills action in the continuum up to corrections of order a^2 . There is a general formalism, known as the ‘‘Symanzik improvement programme’’ [2, 3], which is designed to cancel the leading lattice artifacts, such that observables have an accelerated rate of convergence to the continuum limit. The improvement programme is implemented by adding higher-dimensional operators, whose coefficients must be tuned appropriately in order to cancel the leading lattice artifacts. The effectiveness of this procedure depends largely on the method with which the coefficients are determined. The most widely applied methods (in ascending order of effectiveness) include perturbation theory, tadpole-improved (partially resummed) perturbation theory, renormalization group methods, and the nonperturbative evaluation of improvement conditions.

In the case of Yang-Mills theory, the simplest version of an improved lattice action is obtained by adding rectangular 1×2 loops to the plaquette action, i.e.,

$$S_G^{\text{imp}} = \beta \sum_x \left\{ c_0 \sum_{\mu < \nu} \left(1 - \frac{1}{3} \text{Re Tr } W_{\mu\nu}^{1 \times 1}(x) \right) + c_1 \sum_{\mu, \nu} \left(1 - \frac{1}{3} \text{Re Tr } W_{\mu\nu}^{1 \times 2}(x) \right) \right\}, \quad (406)$$

where the coefficients c_0, c_1 satisfy the normalization condition $c_0 + 8c_1 = 1$. The *Symanzik-improved* [4], *Iwasaki* [5], and *DBW2* [6, 7] actions are all defined through Eq. (404) via particular choices for c_0, c_1 . Details are listed in Tab. 69 together with the abbreviations used in the summary tables. Another widely used variant is the *tadpole Symanzik-improved* [8, 9] action which is obtained by adding additional 6-link parallelogram loops $W_{\mu\nu\sigma}^{1 \times 1 \times 1}(x)$ to the action in Eq. (404), i.e.,

$$S_G^{\text{tadSym}} = S_G^{\text{imp}} + \beta \sum_x c_2 \sum_{\mu < \nu < \sigma} \left(1 - \frac{1}{3} \text{Re Tr } W_{\mu\nu\sigma}^{1 \times 1 \times 1}(x) \right), \quad (407)$$

where

$$W_{\mu\nu\sigma}^{1 \times 1 \times 1}(x) \equiv U_\mu(x) U_\nu(x + a\hat{\mu}) U_\sigma(x + a\hat{\mu} + a\hat{\nu}) U_\mu(x + a\hat{\sigma} + a\hat{\nu})^{-1} U_\nu(x + a\hat{\sigma})^{-1} U_\sigma(x)^{-1} \quad (408)$$

allows for 1-loop improvement [4].

Abbrev.	c_1	Description
Wilson	0	Wilson plaquette action
tlSym	-1/12	tree-level Symanzik-improved gauge action
tadSym	variable	tadpole Symanzik-improved gauge action
Iwasaki	-0.331	Renormalization group improved (“Iwasaki”) action
DBW2	-1.4088	Renormalization group improved (“DBW2”) action

Table 69: Summary of lattice gauge actions. The leading lattice artifacts are $\mathcal{O}(a^2)$ or better for all discretizations.

A.1.2 Light-quark actions

If one attempts to discretize the quark action, one is faced with the fermion doubling problem: the naive lattice transcription produces a 16-fold degeneracy of the fermion spectrum.

Wilson fermions

Wilson’s solution to the fermion doubling problem is based on adding a dimension-5 (irrelevant) operator to the lattice action. The Wilson-Dirac operator for the massless case reads [1, 10]

$$D_w = \frac{1}{2}\gamma_\mu(\nabla_\mu + \nabla_\mu^*) + a\nabla_\mu^*\nabla_\mu, \quad (409)$$

where ∇_μ, ∇_μ^* denote the covariant forward and backward lattice derivatives, respectively. The addition of the Wilson term $a\nabla_\mu^*\nabla_\mu$, results in fermion doublers acquiring a mass proportional to the inverse lattice spacing; close to the continuum limit these extra degrees of freedom are removed from the low-energy spectrum. However, the Wilson term also results in an explicit breaking of chiral symmetry even at zero bare quark mass. Consequently, it also generates divergences proportional to the UV cutoff (inverse lattice spacing), besides the usual logarithmic ones. Therefore the chiral limit of the regularized theory is not defined simply by the vanishing of the bare quark mass but must be appropriately tuned. As a consequence quark-mass renormalization requires a power subtraction on top of the standard multiplicative logarithmic renormalization. The breaking of chiral symmetry also implies that the nonrenormalization theorem has to be applied with care [11, 12], resulting in a normalization factor for the axial current which is a regular function of the bare coupling. On the other hand, vector symmetry is unaffected by the Wilson term and thus a lattice (point split) vector current is conserved and obeys the usual nonrenormalization theorem with a trivial (unity) normalization factor. Thus, compared to lattice fermion actions which preserve chiral symmetry, or a subgroup of it, the Wilson regularization typically results in more complicated renormalization patterns.

Furthermore, the leading-order lattice artifacts are of order a . With the help of the Symanzik improvement programme, the leading artifacts can be cancelled in the action by

adding the so-called ‘‘Clover’’ or Sheikholeslami-Wohlert (SW) term [13]. The resulting expression in the massless case reads

$$D_{\text{sw}} = D_{\text{w}} + \frac{ia}{4} c_{\text{sw}} \sigma_{\mu\nu} \widehat{F}_{\mu\nu}, \quad (410)$$

where $\sigma_{\mu\nu} = \frac{i}{2}[\gamma_\mu, \gamma_\nu]$, and $\widehat{F}_{\mu\nu}$ is a lattice transcription of the gluon field strength tensor $F_{\mu\nu}$. The coefficient c_{sw} can be determined perturbatively at tree-level ($c_{\text{sw}} = 1$; tree-level improvement or tISW for short), via a mean field approach [8] (mean-field improvement or mISW) or via a nonperturbative approach [14] (nonperturbatively improved or npISW). Hadron masses, computed using D_{sw} , with the coefficient c_{sw} determined nonperturbatively, will approach the continuum limit with a rate proportional to a^2 ; with tISW for c_{sw} the rate is proportional to $g_0^2 a$.

Other observables require additional improvement coefficients [13]. A common example consists in the computation of the matrix element $\langle \alpha | Q | \beta \rangle$ of a composite field Q of dimension- d with external states $|\alpha\rangle$ and $|\beta\rangle$. In the simplest cases, the above bare matrix element diverges logarithmically and a single renormalization parameter Z_Q is adequate to render it finite. It then approaches the continuum limit with a rate proportional to the lattice spacing a , even when the lattice action contains the Clover term. In order to reduce discretization errors to $\mathcal{O}(a^2)$, the lattice definition of the composite operator Q must be modified (or ‘‘improved’’), by the addition of all dimension- $(d+1)$ operators with the same lattice symmetries as Q . Each of these terms is accompanied by a coefficient which must be tuned in a way analogous to that of c_{sw} . Once these coefficients are determined nonperturbatively, the renormalized matrix element of the improved operator, computed with a npISW action, converges to the continuum limit with a rate proportional to a^2 . A tISW improvement of these coefficients and c_{sw} will result in a rate proportional to $g_0^2 a$.

It is important to stress that the improvement procedure does not affect the chiral properties of Wilson fermions; chiral symmetry remains broken.

Finally, we mention ‘‘twisted-mass QCD’’ as a method which was originally designed to address another problem of Wilson’s discretization: the Wilson-Dirac operator is not protected against the occurrence of unphysical zero modes, which manifest themselves as ‘‘exceptional’’ configurations. They occur with a certain frequency in numerical simulations with Wilson quarks and can lead to strong statistical fluctuations. The problem can be cured by introducing a so-called ‘‘chirally twisted’’ mass term. The most common formulation applies to a flavour doublet $\bar{\psi} = (u \ d)$ of mass-degenerate quarks, with the fermionic part of the QCD action in the continuum assuming the form [15]

$$S_{\text{F}}^{\text{tm;cont}} = \int d^4x \bar{\psi}(x) (\gamma_\mu D_\mu + m + i\mu_{\text{q}} \gamma_5 \tau^3) \psi(x). \quad (411)$$

Here, μ_{q} is the twisted-mass parameter, and τ^3 is a Pauli matrix in flavour space. The standard action in the continuum can be recovered via a global chiral field rotation. The physical quark mass is obtained as a function of the two mass parameters m and μ_{q} . The corresponding lattice regularization of twisted-mass QCD (tmWil) for $N_f = 2$ flavours is defined through the fermion matrix

$$D_{\text{w}} + m_0 + i\mu_{\text{q}} \gamma_5 \tau^3. \quad (412)$$

Although this formulation breaks physical parity and flavour symmetries, resulting in non-degenerate neutral and charged pions, it has a number of advantages over standard Wilson

fermions. Firstly, the presence of the twisted-mass parameter μ_q protects the discretized theory against unphysical zero modes. A second attractive feature of twisted-mass lattice QCD is the fact that, once the bare mass parameter m_0 is tuned to its “critical value” (corresponding to massless pions in the standard Wilson formulation), the leading lattice artifacts are of order a^2 without the need to add the Sheikholeslami-Wohlert term in the action, or other improving coefficients [16]. A third important advantage is that, although the problem of explicit chiral symmetry breaking remains, quantities computed with twisted fermions with a suitable tuning of the mass parameter μ_q , are subject to renormalization patterns which are simpler than the ones with standard Wilson fermions. Well known examples are the pseudoscalar decay constant and B_K .

Staggered Fermions

An alternative procedure to deal with the doubling problem is based on Kogut-Susskind fermions [17, 18] and is now known under the name “staggered” fermion formulation [19–21]. Here the degeneracy is only lifted partially, from 16 down to 4. It has become customary to refer to these residual doublers as “tastes” in order to distinguish them from physical flavours. Taste changing interactions can occur via the exchange of gluons with one or more components of momentum near the cutoff π/a . This leads to the breaking of the $SU(4)$ vector symmetry among tastes, thereby generating order a^2 lattice artifacts.

The residual doubling of staggered quarks (four tastes per flavour) is removed by taking a fractional power of the fermion determinant [22] — the “fourth-root procedure,” or, sometimes, the “fourth root trick.” This procedure would be unproblematic if the action had full $SU(4)$ taste symmetry, which would give a Dirac operator that was block-diagonal in taste space. However, the breaking of taste symmetry at nonzero lattice spacing leads to a variety of problems. In fact, the fourth root of the determinant is not equivalent to the determinant of any local lattice Dirac operator [23]. This in turn leads to violations of unitarity on the lattice [24–27].

According to standard renormalization group lore, the taste violations, which are associated with lattice operators of dimension greater than four, might be expected to go away in the continuum limit, resulting in the restoration of locality and unitarity. However, there is a problem with applying the standard lore to this nonstandard situation: the usual renormalization group reasoning assumes that the lattice action is local. Nevertheless, Shamir [28, 29] shows that one may apply the renormalization group to a “nearby” local theory, and thereby gives a strong argument that the desired local, unitary theory of QCD is reproduced by the rooted staggered lattice theory in the continuum limit.

A version of chiral perturbation that includes the lattice artifacts due to taste violations and rooting (“rooted staggered chiral perturbation theory”) can also be worked out [30–32] and shown to correctly describe the unitarity-violating lattice artifacts in the pion sector [25, 33]. This provides additional evidence that the desired continuum limit can be obtained. Further, it gives a practical method for removing the lattice artifacts from simulation results. Versions of rooted staggered chiral perturbation theory exist for heavy-light mesons with staggered light quarks but nonstaggered heavy quarks [34], heavy-light mesons with staggered light and heavy quarks [35, 36], staggered baryons [37], and mixed actions with a staggered sea [38, 39], as well as the pion-only version referenced above.

There is also considerable numerical evidence that the rooting procedure works as desired. This includes investigations in the Schwinger model [40–42], studies of the eigenvalues of the

Dirac operator in QCD [43–46], and evidence for taste restoration in the pion spectrum as $a \rightarrow 0$ [47, 48].

Issues with the rooting procedure have led Creutz [49–55] to argue that the continuum limit of the rooted staggered theory cannot be QCD. These objections have however been answered in Refs. [46, 56–62]. In particular, a claim that the continuum ’t Hooft vertex [63, 64] could not be properly reproduced by the rooted theory has been refuted [46, 58].

Overall, despite the lack of rigorous proof of the correctness of the rooting procedure, we think the evidence is strong enough to consider staggered QCD simulations on a par with simulations using other actions. See the following reviews for further evidence and discussion: Refs. [48, 57, 59, 62, 65].

Improved Staggered Fermions

An improvement program can be used to suppress taste-changing interactions, leading to “improved staggered fermions,” with the so-called “Asqtad” [66], “HISQ” [67], “Stout-smear” [68], and “HYP” [69] actions as the most common versions. All these actions smear the gauge links in order to reduce the coupling of high-momentum gluons to the quarks, with the main goal of decreasing taste-violating interactions. In the Asqtad case, this is accomplished by replacing the gluon links in the derivatives by averages over 1-, 3-, 5-, and 7-link paths. The other actions reduce taste changing even further by smearing more. In addition to the smearing, the Asqtad and HISQ actions include a three-hop term in the action (the “Naik term” [70]) to remove order a^2 errors in the dispersion relation, as well as a “Lepage term” [71] to cancel other order a^2 artifacts introduced by the smearing. In both the Asqtad and HISQ actions, the leading taste violations are of order $\alpha_S^2 a^2$, and “generic” lattices artifacts (those associated with discretization errors other than taste violations) are of order $\alpha_S a^2$. The overall coefficients of these errors are, however, significantly smaller with HISQ than with Asqtad. With the Stout-smear and HYP actions, the errors are formally larger (order $\alpha_S a^2$ for taste violations and order a^2 for generic lattices artifacts). Nevertheless, the smearing seems to be very efficient, and the actual size of errors at accessible lattice spacings appears to be at least as small as with HISQ.

Although logically distinct from the light-quark improvement program for these actions, it is customary with the HISQ action to include an additional correction designed to reduce discretization errors for heavy quarks (in practice, usually charm quarks) [67]. The Naik term is adjusted to remove leading $(am_c)^4$ and $\alpha_S(am_c)^2$ errors, where m_c is the charm-quark mass and “leading” in this context means leading in powers of the heavy-quark velocity v ($v/c \sim 1/3$ for D_s). With these improvements, the claim is that one can use the staggered action for charm quarks, although it must be emphasized that it is not obvious *a priori* how large a value of am_c may be tolerated for a given desired accuracy, and this must be studied in the simulations.

Ginsparg-Wilson fermions

Fermionic lattice actions, which do not suffer from the doubling problem whilst preserving chiral symmetry go under the name of “Ginsparg-Wilson fermions”. In the continuum the massless Dirac operator (D) anti-commutes with γ_5 . At nonzero lattice spacing a chiral

symmetry can be realized if this condition is relaxed to [72–74]

$$\{D, \gamma_5\} = aD\gamma_5D, \quad (413)$$

which is now known as the Ginsparg-Wilson relation [75]. The Nielsen-Ninomiya theorem [76], which states that any lattice formulation for which D anticommutes with γ_5 necessarily has doubler fermions, is circumvented since $\{D, \gamma_5\} \neq 0$.

A lattice Dirac operator which satisfies Eq. (411) can be constructed in several ways. The so-called “overlap” or Neuberger-Dirac operator [77] acts in four space-time dimensions and is, in its simplest form, defined by

$$D_N = \frac{1}{\bar{a}}(1 - \epsilon(A)), \quad \text{where} \quad \epsilon(A) \equiv A(A^\dagger A)^{-1/2}, \quad A = 1 + s - aD_w, \quad \bar{a} = \frac{a}{1+s}, \quad (414)$$

D_w is the massless Wilson-Dirac operator and $|s| < 1$ is a tunable parameter. The overlap operator D_N removes all doublers from the spectrum, and can readily be shown to satisfy the Ginsparg-Wilson relation. The occurrence of the sign function $\epsilon(A)$ in D_N renders the application of D_N in a computer program potentially very costly, since it must be implemented using, for instance, a polynomial approximation.

The most widely used approach to satisfying the Ginsparg-Wilson relation Eq. (411) in large-scale numerical simulations is provided by *Domain Wall Fermions* (DWF) [78–80] and we therefore describe this in some more detail. Following early exploratory studies [81], this approach has been developed into a practical formulation of lattice QCD with good chiral and flavour symmetries leading to results which contribute significantly to this review. In this formulation, the fermion fields $\psi(x, s)$ depend on a discrete fifth coordinate $s = 1, \dots, N$ as well as the physical 4-dimensional space-time coordinates x_μ , $\mu = 1 \dots 4$ (the gluon fields do not depend on s). The lattice on which the simulations are performed, is therefore a five-dimensional one of size $L^3 \times T \times N$, where L , T and N represent the number of points in the spatial, temporal and fifth dimensions respectively. The remarkable feature of DWF is that for each flavour there exists a physical light mode corresponding to the field $q(x)$:

$$q(x) = \frac{1+\gamma_5}{2}\psi(x, 1) + \frac{1-\gamma_5}{2}\psi(x, N) \quad (415)$$

$$\bar{q}(x) = \bar{\psi}(x, N)\frac{1+\gamma_5}{2} + \bar{\psi}(x, 1)\frac{1-\gamma_5}{2}. \quad (416)$$

The left and right-handed modes of the physical field are located on opposite boundaries in the 5th dimensional space which, for $N \rightarrow \infty$, allows for independent transformations of the left and right components of the quark fields, that is for chiral transformations. Unlike Wilson fermions, where for each flavour the quark-mass parameter in the action is fine-tuned requiring a subtraction of contributions of $\mathcal{O}(1/a)$ where a is the lattice spacing, with DWF no such subtraction is necessary for the physical modes, whereas the unphysical modes have masses of $\mathcal{O}(1/a)$ and decouple.

In actual simulations N is finite and there are small violations of chiral symmetry which must be accounted for. The theoretical framework for the study of the residual breaking of chiral symmetry has been a subject of intensive investigation (for a review and references to the original literature see, e.g., [82]). The breaking requires one or more *crossings* of the fifth dimension to couple the left and right-handed modes; the more crossings that are required the smaller the effect. For many physical quantities the leading effects of chiral symmetry breaking due to finite N are parameterized by a *residual* mass, m_{res} . For example, the PCAC relation (for degenerate quarks of mass m) $\partial_\mu A_\mu(x) = 2mP(x)$, where A_μ and P represent

the axial current and pseudoscalar density respectively, is satisfied with $m = m^{\text{DWF}} + m_{\text{res}}$, where m^{DWF} is the bare mass in the DWF action. The mixing of operators which transform under different representations of chiral symmetry is found to be negligibly small in current simulations. The important thing to note is that the chiral symmetry breaking effects are small and that there are techniques to mitigate their consequences.

The main price which has to be paid for the good chiral symmetry is that the simulations are performed in 5 dimensions, requiring approximately a factor of N in computing resources and resulting in practice in ensembles at fewer values of the lattice spacing and quark masses than is possible with other formulations. The current generation of DWF simulations is being performed at physical quark masses so that ensembles with good chiral and flavour symmetries are being generated and analysed [83]. For a discussion of the equivalence of DWF and overlap fermions see Refs. [84, 85].

A third example of an operator which satisfies the Ginsparg-Wilson relation is the so-called fixed-point action [86–88]. This construction proceeds via a renormalization group approach. A related formalism are the so-called “chirally improved” fermions [89].

Smearing

A simple modification which can help improve the action as well as the computational performance is the use of smeared gauge fields in the covariant derivatives of the fermionic action. Any smearing procedure is acceptable as long as it consists of only adding irrelevant (local) operators. Moreover, it can be combined with any discretization of the quark action. The “Asqtad” staggered quark action mentioned above [66] is an example which makes use of so-called “Asqtad” smeared (or “fat”) links. Another example is the use of n-HYP smeared [69, 90], stout smeared [91, 92] or HEX (hypercubic stout) smeared [93] gauge links in the tree-level clover improved discretization of the quark action, denoted by “n-HYP t1SW”, “stout t1SW” and “HEX t1SW” in the following.

In Tab. 70 we summarize the most widely used discretizations of the quark action and their main properties together with the abbreviations used in the summary tables. Note that in order to maintain the leading lattice artifacts of the actions as given in the table in nonspectral observables (like operator matrix elements) the corresponding nonspectral operators need to be improved as well.

A.1.3 Heavy-quark actions

Charm and bottom quarks are often simulated with different lattice-quark actions than up, down, and strange quarks because their masses are large relative to typical lattice spacings in current simulations; for example, $am_c \sim 0.4$ and $am_b \sim 1.3$ at $a = 0.06$ fm. Therefore, for the actions described in the previous section, using a sufficiently small lattice spacing to control generic $(am_h)^n$ discretization errors at the physical b -quark mass is computationally demanding and has so far not been possible, with the first exception being the calculation of FNAL/MILC in [94] which uses the HISQ action and a lattice spacing of $a \approx 0.03$ fm.

One alternative approach for lattice heavy quarks is direct application of effective theory. In this case the lattice heavy-quark action only correctly describes phenomena in a specific kinematic regime, such as Heavy-Quark Effective Theory (HQET) [95–97] or Nonrelativistic QCD (NRQCD) [98, 99]. One can discretize the effective Lagrangian to obtain, for example,

Abbrev.	Discretization	Leading lattice artifacts	Chiral symmetry	Remarks
Wilson	Wilson	$\mathcal{O}(a)$	broken	
tmWil	twisted-mass Wilson	$\mathcal{O}(a^2)$ at maximal twist	broken	flavour-symmetry breaking: $(M_{\text{PS}}^0)^2 - (M_{\text{PS}}^\pm)^2 \sim \mathcal{O}(a^2)$
tlSW	Sheikholeslami-Wohlert	$\mathcal{O}(g^2 a)$	broken	tree-level impr., $c_{\text{sw}} = 1$
n-HYP tlSW	Sheikholeslami-Wohlert	$\mathcal{O}(g^2 a)$	broken	tree-level impr., $c_{\text{sw}} = 1$, n-HYP smeared gauge links
stout tlSW	Sheikholeslami-Wohlert	$\mathcal{O}(g^2 a)$	broken	tree-level impr., $c_{\text{sw}} = 1$, stout smeared gauge links
HEX tlSW	Sheikholeslami-Wohlert	$\mathcal{O}(g^2 a)$	broken	tree-level impr., $c_{\text{sw}} = 1$, HEX smeared gauge links
mfSW	Sheikholeslami-Wohlert	$\mathcal{O}(g^2 a)$	broken	mean-field impr.
npSW	Sheikholeslami-Wohlert	$\mathcal{O}(a^2)$	broken	nonperturbatively impr.
KS	Staggered	$\mathcal{O}(a^2)$	$U(1) \times U(1)$ subgr. unbroken	rooting for $N_f < 4$
Asqtad	Staggered	$\mathcal{O}(g^2 a^2)$	$U(1) \times U(1)$ subgr. unbroken	Asqtad smeared gauge links, rooting for $N_f < 4$
HISQ	Staggered	$\mathcal{O}(g^2 a^2)$	$U(1) \times U(1)$ subgr. unbroken	HISQ smeared gauge links, rooting for $N_f < 4$
DW	Domain Wall	asymptotically $\mathcal{O}(a^2)$	remnant breaking exponentially suppr.	exact chiral symmetry and $\mathcal{O}(a)$ impr. only in the limit $N \rightarrow \infty$
oDW	optimal Domain Wall	asymptotically $\mathcal{O}(a^2)$	remnant breaking exponentially suppr.	exact chiral symmetry and $\mathcal{O}(a)$ impr. only in the limit $N \rightarrow \infty$
M-DW	Moebius Domain Wall	asymptotically $\mathcal{O}(a^2)$	remnant breaking exponentially suppr.	exact chiral symmetry and $\mathcal{O}(a)$ impr. only in the limit $N \rightarrow \infty$
overlap	Neuberger	$\mathcal{O}(a^2)$	exact	

Table 70: The most widely used discretizations of the quark action and some of their properties. Note that in order to maintain the leading lattice artifacts of the action in nonspectral observables (like operator matrix elements) the corresponding nonspectral operators need to be improved as well.

Lattice HQET [100] or Lattice NRQCD [101, 102], and then simulate the effective theory numerically. The coefficients of the operators in the lattice-HQET and lattice-NRQCD actions are free parameters that must be determined by matching to the underlying theory (QCD) through the chosen order in $1/m_h$ or v_h^2 , where m_h is the heavy-quark mass and v_h is the heavy-quark velocity in the heavy-light meson rest frame.

Another approach is to interpret a relativistic quark action such as those described in the previous section in a manner suitable for heavy quarks. One can extend the standard Symanzik improvement program, which allows one to systematically remove lattice cutoff effects by adding higher-dimension operators to the action, by allowing the coefficients of the dimension 4 and higher operators to depend explicitly upon the heavy-quark mass. Different prescriptions for tuning the parameters correspond to different implementations: those in common use are often called the Fermilab action [103], the relativistic heavy-quark action (RHQ) [104], and the Tsukuba formulation [105]. In the Fermilab approach, HQET is used to match the lattice theory to continuum QCD at the desired order in $1/m_h$.

More generally, effective theory can be used to estimate the size of cutoff errors from the various lattice heavy-quark actions. The power counting for the sizes of operators with heavy quarks depends on the typical momenta of the heavy quarks in the system. Bound-state dynamics differ considerably between heavy-heavy and heavy-light systems. In heavy-light systems, the heavy quark provides an approximately static source for the attractive binding force, like the proton in a hydrogen atom. The typical heavy-quark momentum in the bound-state rest frame is $|\vec{p}_h| \sim \Lambda_{\text{QCD}}$, and heavy-light operators scale as powers of $(\Lambda_{\text{QCD}}/m_h)^n$. This is often called “HQET power-counting”, although it applies to heavy-light operators in HQET, NRQCD, and even relativistic heavy-quark actions described below. Heavy-heavy systems are similar to positronium or the deuteron, with the typical heavy-quark momentum $|\vec{p}_h| \sim \alpha_S m_h$. Therefore motion of the heavy quarks in the bound state rest frame cannot be neglected. Heavy-heavy operators have complicated power counting rules in terms of v_h^2 [102]; this is often called “NRQCD power counting.”

Alternatively, one can simulate bottom or charm quarks with the same action as up, down, and strange quarks provided that (1) the action is sufficiently improved, and (2) the lattice spacing is sufficiently fine. These qualitative criteria do not specify precisely how large a numerical value of am_h can be allowed while obtaining a given precision for physical quantities; this must be established empirically in numerical simulations. At present, both the HISQ and twisted-mass Wilson actions discussed previously are being used to simulate charm quarks. Simulations with HISQ quarks have employed heavier-quark masses than those with twisted-mass Wilson quarks because the action is more highly improved, but neither action has been used to simulate at the physical am_b until the recent calculation of FNAL/MILC in [94], where a lattice spacing of $a \approx 0.03$ fm is available. All other calculations of heavy-light decay constants with these actions still rely on effective theories: the ETM collaboration interpolates between twisted-mass Wilson data generated near am_c and the static point [106], while the HPQCD collaboration, for the coarser lattice spacings, extrapolates HISQ data generated below am_b up to the physical point using an HQET-inspired series expansion in $(1/m_h)^n$ [107].

Heavy-quark effective theory

HQET was introduced by Eichten and Hill in Ref. [96]. It provides the correct asymptotic description of QCD correlation functions in the static limit $m_h/|\vec{p}_h| \rightarrow \infty$. Subleading effects are described by higher dimensional operators whose coupling constants are formally

of $\mathcal{O}((1/m_h)^n)$. The HQET expansion works well for heavy-light systems in which the heavy-quark momentum is small compared to the mass.

The HQET Lagrangian density at the leading (static) order in the rest frame of the heavy quark is given by

$$\mathcal{L}^{\text{stat}}(x) = \bar{\psi}_h(x) D_0 \psi_h(x) , \quad (417)$$

with

$$P_+ \psi_h = \psi_h , \quad \bar{\psi}_h P_+ = \bar{\psi}_h , \quad P_+ = \frac{1 + \gamma_0}{2} . \quad (418)$$

A bare quark mass $m_{\text{bare}}^{\text{stat}}$ has to be added to the energy levels E^{stat} computed with this Lagrangian to obtain the physical ones. For example, the mass of the B meson in the static approximation is given by

$$m_B = E^{\text{stat}} + m_{\text{bare}}^{\text{stat}} . \quad (419)$$

At tree-level $m_{\text{bare}}^{\text{stat}}$ is simply the (static approximation of the) b -quark mass, but in the quantized lattice formulation it has to further compensate a divergence linear in the inverse lattice spacing. Weak composite fields are also rewritten in terms of the static fields, e.g.,

$$A_0(x)^{\text{stat}} = Z_A^{\text{stat}} (\bar{\psi}(x) \gamma_0 \gamma_5 \psi_h(x)) , \quad (420)$$

where the renormalization factor of the axial current in the static theory Z_A^{stat} is scale-dependent. Recent lattice-QCD calculations using static b quarks and dynamical light quarks [106, 108] perform the operator matching at 1-loop in mean-field improved lattice perturbation theory [109, 110]. Therefore the heavy-quark discretization, truncation, and matching errors in these results are of $\mathcal{O}(a^2 \Lambda_{\text{QCD}}^2)$, $\mathcal{O}(\Lambda_{\text{QCD}}/m_h)$, and $\mathcal{O}(\alpha_s^2, \alpha_s^2 a \Lambda_{\text{QCD}})$.

In order to reduce heavy-quark truncation errors in B -meson masses and matrix elements to the few-percent level, state-of-the-art lattice-HQET computations now include corrections of $\mathcal{O}(1/m_h)$. Adding the $1/m_h$ terms, the HQET Lagrangian reads

$$\mathcal{L}^{\text{HQET}}(x) = \mathcal{L}^{\text{stat}}(x) - \omega_{\text{kin}} \mathcal{O}_{\text{kin}}(x) - \omega_{\text{spin}} \mathcal{O}_{\text{spin}}(x) , \quad (421)$$

$$\mathcal{O}_{\text{kin}}(x) = \bar{\psi}_h(x) \mathbf{D}^2 \psi_h(x) , \quad \mathcal{O}_{\text{spin}}(x) = \bar{\psi}_h(x) \boldsymbol{\sigma} \cdot \mathbf{B} \psi_h(x) . \quad (422)$$

At this order, two other parameters appear in the Lagrangian, ω_{kin} and ω_{spin} . The normalization is such that the tree-level values of the coefficients are $\omega_{\text{kin}} = \omega_{\text{spin}} = 1/(2m_h)$. Similarly the operators are formally expanded in inverse powers of the heavy-quark mass. The time component of the axial current, relevant for the computation of mesonic decay constants is given by

$$A_0^{\text{HQET}}(x) = Z_A^{\text{HQET}} \left(A_0^{\text{stat}}(x) + \sum_{i=1}^2 c_A^{(i)} A_0^{(i)}(x) \right) , \quad (423)$$

$$A_0^{(1)}(x) = \bar{\psi} \frac{1}{2} \gamma_5 \gamma_k (\nabla_k - \overleftarrow{\nabla}_k) \psi_h(x) , \quad k = 1, 2, 3 \quad (424)$$

$$A_0^{(2)} = -\partial_k A_k^{\text{stat}}(x) , \quad A_k^{\text{stat}} = \bar{\psi}(x) \gamma_k \gamma_5 \psi_h(x) , \quad (425)$$

and depends on two additional parameters $c_A^{(1)}$ and $c_A^{(2)}$.

A framework for nonperturbative HQET on the lattice has been introduced in Refs. [100, 111]. As pointed out in Refs. [112, 113], since $\alpha_s(m_h)$ decreases logarithmically with m_h , whereas corrections in the effective theory are power-like in Λ/m_h , it is possible that the

leading errors in a calculation will be due to the perturbative matching of the action and the currents at a given order $(\Lambda/m_h)^l$ rather than to the missing $\mathcal{O}((\Lambda/m_h)^{l+1})$ terms. Thus, in order to keep matching errors below the uncertainty due to truncating the HQET expansion, the matching is performed nonperturbatively beyond leading order in $1/m_h$. The asymptotic convergence of HQET in the limit $m_h \rightarrow \infty$ indeed holds only in that case.

The higher dimensional interaction terms in the effective Lagrangian are treated as space-time volume insertions into static correlation functions. For correlators of some multi-local fields \mathcal{Q} and up to the $1/m_h$ corrections to the operator, this means

$$\langle \mathcal{Q} \rangle = \langle \mathcal{Q} \rangle_{\text{stat}} + \omega_{\text{kin}} a^4 \sum_x \langle \mathcal{Q} \mathcal{O}_{\text{kin}}(x) \rangle_{\text{stat}} + \omega_{\text{spin}} a^4 \sum_x \langle \mathcal{Q} \mathcal{O}_{\text{spin}}(x) \rangle_{\text{stat}}, \quad (426)$$

where $\langle \mathcal{Q} \rangle_{\text{stat}}$ denotes the static expectation value with $\mathcal{L}^{\text{stat}}(x) + \mathcal{L}^{\text{light}}(x)$. Nonperturbative renormalization of these correlators guarantees the existence of a well-defined continuum limit to any order in $1/m_h$. The parameters of the effective action and operators are then determined by matching a suitable number of observables calculated in HQET (to a given order in $1/m_h$) and in QCD in a small volume (typically with $L \simeq 0.5$ fm), where the full relativistic dynamics of the b -quark can be simulated and the parameters can be computed with good accuracy. In Refs. [111, 114] the Schrödinger Functional (SF) setup has been adopted to define a set of quantities, given by the small volume equivalent of decay constants, pseudoscalar-vector splittings, effective masses and ratio of correlation functions for different kinematics, that can be used to implement the matching conditions. The kinematical conditions are usually modified by changing the periodicity in space of the fermions, i.e., by directly exploiting a finite-volume effect. The new scale L , which is introduced in this way, is chosen such that higher orders in $1/m_h L$ and in Λ_{QCD}/m_h are of about the same size. At the end of the matching step the parameters are known at lattice spacings which are of the order of 0.01 fm, significantly smaller than the resolutions used for large volume, phenomenological, applications. For this reason a set of SF-step scaling functions is introduced in the effective theory to evolve the parameters to larger lattice spacings. The whole procedure yields the nonperturbative parameters with an accuracy which allows to compute phenomenological quantities with a precision of a few percent (see Refs. [115, 116] for the case of the $B_{(s)}$ decay constants). Such an accuracy can not be achieved by performing the nonperturbative matching in large volume against experimental measurements, which in addition would reduce the predictivity of the theory. For the lattice-HQET action matched nonperturbatively through $\mathcal{O}(1/m_h)$, discretization and truncation errors are of $\mathcal{O}(a\Lambda_{\text{QCD}}^2/m_h, a^2\Lambda_{\text{QCD}}^2)$ and $\mathcal{O}((\Lambda_{\text{QCD}}/m_h)^2)$.

The noise-to-signal ratio of static-light correlation functions grows exponentially in Euclidean time, $\propto e^{\mu x_0}$. The rate μ is nonuniversal but diverges as $1/a$ as one approaches the continuum limit. By changing the discretization of the covariant derivative in the static action one may achieve an exponential reduction of the noise to signal ratio. Such a strategy led to the introduction of the $S_{\text{HYP}1,2}^{\text{stat}}$ actions [117], where the thin links in D_0 are replaced by HYP-smearred links [69]. These actions are now used in all lattice applications of HQET.

Nonrelativistic QCD

Nonrelativistic QCD (NRQCD) [101, 102] is an effective theory that can be matched to full QCD order by order in the heavy-quark velocity v_h^2 (for heavy-heavy systems) or in Λ_{QCD}/m_h (for heavy-light systems) and in powers of α_s . Relativistic corrections appear as higher-dimensional operators in the Hamiltonian.

As an effective field theory, NRQCD is only useful with an ultraviolet cutoff of order m_h or less. On the lattice this means that it can be used only for $am_h > 1$, which means that $\mathcal{O}(a^n)$ errors cannot be removed by taking $a \rightarrow 0$ at fixed m_h . Instead heavy-quark discretization errors are systematically removed by adding additional operators to the lattice Hamiltonian. Thus, while strictly speaking no continuum limit exists at fixed m_h , continuum physics can be obtained at finite lattice spacing to arbitrarily high precision provided enough terms are included, and provided that the coefficients of these terms are calculated with sufficient accuracy. Residual discretization errors can be parameterized as corrections to the coefficients in the nonrelativistic expansion, as shown in Eq. (427). Typically they are of the form $(a|\vec{p}_h|)^n$ multiplied by a function of am_h that is smooth over the limited range of heavy-quark masses (with $am_h > 1$) used in simulations, and can therefore be represented by a low-order polynomial in am_h by Taylor's theorem (see Ref. [118] for further discussion). Power-counting estimates of these effects can be compared to the observed lattice-spacing dependence in simulations. Provided that these effects are small, such comparisons can be used to estimate and correct the residual discretization effects.

An important feature of the NRQCD approach is that the same action can be applied to both heavy-heavy and heavy-light systems. This allows, for instance, the bare b -quark mass to be fixed via experimental input from Υ so that simulations carried out in the B or B_s systems have no adjustable parameters left. Precision calculations of the B_s -meson mass (or of the mass splitting $M_{B_s} - M_\Upsilon/2$) can then be used to test the reliability of the method before turning to quantities one is trying to predict, such as decay constants f_B and f_{B_s} , semileptonic form factors or neutral B mixing parameters.

Given the same lattice-NRQCD heavy-quark action, simulation results will not be as accurate for charm quarks as for bottom ($1/m_b < 1/m_c$, and $v_b < v_c$ in heavy-heavy systems). For charm, however, a more serious concern is the restriction that am_h must be greater than one. This limits lattice-NRQCD simulations at the physical am_c to relatively coarse lattice spacings for which light-quark and gluon discretization errors could be large. Thus recent lattice-NRQCD simulations have focused on bottom quarks because $am_b > 1$ in the range of typical lattice spacings between ≈ 0.06 and 0.15 fm.

In most simulations with NRQCD b -quarks during the past decade one has worked with an NRQCD action that includes tree-level relativistic corrections through $\mathcal{O}(v_h^4)$ and discretization corrections through $\mathcal{O}(a^2)$,

$$S_{\text{NRQCD}} = a^4 \sum_x \left\{ \Psi_t^\dagger \Psi_t - \Psi_t^\dagger \left(1 - \frac{a\delta H}{2}\right)_t \left(1 - \frac{aH_0}{2n}\right)_t^n \right. \\ \left. \times U_t^\dagger(t-a) \left(1 - \frac{aH_0}{2n}\right)_{t-a}^n \left(1 - \frac{a\delta H}{2}\right)_{t-a} \Psi_{t-a} \right\}, \quad (427)$$

where the subscripts “ t ” and “ $t-a$ ” denote that the heavy-quark, gauge, \mathbf{E} , and \mathbf{B} -fields are on time slices t or $t-a$, respectively. H_0 is the nonrelativistic kinetic energy operator,

$$H_0 = -\frac{\Delta^{(2)}}{2m_h}, \quad (428)$$

and δH includes relativistic and finite-lattice-spacing corrections,

$$\begin{aligned} \delta H = & -c_1 \frac{(\Delta^{(2)})^2}{8m_h^3} + c_2 \frac{ig}{8m_h^2} \left(\nabla \cdot \tilde{\mathbf{E}} - \tilde{\mathbf{E}} \cdot \nabla \right) \\ & -c_3 \frac{g}{8m_h^2} \boldsymbol{\sigma} \cdot (\tilde{\nabla} \times \tilde{\mathbf{E}} - \tilde{\mathbf{E}} \times \tilde{\nabla}) \\ & -c_4 \frac{g}{2m_h} \boldsymbol{\sigma} \cdot \tilde{\mathbf{B}} + c_5 \frac{a^2 \Delta^{(4)}}{24m_h} - c_6 \frac{a(\Delta^{(2)})^2}{16nm_h^2}. \end{aligned} \quad (429)$$

m_h is the bare heavy-quark mass, $\Delta^{(2)}$ the lattice Laplacian, ∇ the symmetric lattice derivative and $\Delta^{(4)}$ the lattice discretization of the continuum $\sum_i D_i^4$. $\tilde{\nabla}$ is the improved symmetric lattice derivative and the $\tilde{\mathbf{E}}$ and $\tilde{\mathbf{B}}$ fields have been improved beyond the usual clover leaf construction. The stability parameter n is discussed in Ref. [102]. In most cases the c_i 's have been set equal to their tree-level values $c_i = 1$. With this implementation of the NRQCD action, errors in heavy-light-meson masses and splittings are of $\mathcal{O}(\alpha_s \Lambda_{\text{QCD}}/m_h)$, $\mathcal{O}(\alpha_s (\Lambda_{\text{QCD}}/m_h)^2)$, $\mathcal{O}((\Lambda_{\text{QCD}}/m_h)^3)$, and $\mathcal{O}(\alpha_s a^2 \Lambda_{\text{QCD}}^2)$, with coefficients that are functions of am_h . 1-loop corrections to many of the coefficients in Eq. (427) have now been calculated, and are starting to be included in simulations [119–121].

Most of the operator matchings involving heavy-light currents or four-fermion operators with NRQCD b -quarks and Asqtad or HISQ light quarks have been carried out at 1-loop order in lattice perturbation theory. In calculations published to date of electroweak matrix elements, heavy-light currents with massless light quarks have been matched through $\mathcal{O}(\alpha_s, \Lambda_{\text{QCD}}/m_h, \alpha_s/(am_h), \alpha_s \Lambda_{\text{QCD}}/m_h)$, and four-fermion operators through $\mathcal{O}(\alpha_s, \Lambda_{\text{QCD}}/m_h, \alpha_s/(am_h))$. NRQCD/HISQ currents with massive HISQ quarks are also of interest, e.g., for the bottom-charm currents in $B \rightarrow D^{(*)} l \nu$ semileptonic decays and the relevant matching calculations have been performed at 1-loop order in Ref. [122]. Taking all the above into account, the most significant systematic error in electroweak matrix elements published to date with NRQCD b -quarks is the $\mathcal{O}(\alpha_s^2)$ perturbative matching uncertainty. Work is therefore underway to use current-current correlator methods combined with very high order continuum perturbation theory to do current matchings nonperturbatively [123].

Relativistic heavy quarks

An approach for relativistic heavy-quark lattice formulations was first introduced by El-Khadra, Kronfeld, and Mackenzie in Ref. [103]. Here they showed that, for a general lattice action with massive quarks and non-Abelian gauge fields, discretization errors can be factorized into the form $f(m_h a)(a|\vec{p}_h|)^n$, and that the function $f(m_h a)$ is bounded to be of $\mathcal{O}(1)$ or less for all values of the quark mass m_h . Therefore cutoff effects are of $\mathcal{O}(a\Lambda_{\text{QCD}})^n$ and $\mathcal{O}((a|\vec{p}_h|)^n)$, even for $am_h \gtrsim 1$, and can be controlled using a Symanzik-like procedure. As in the standard Symanzik improvement program, cutoff effects are systematically removed by introducing higher-dimension operators to the lattice action and suitably tuning their coefficients. In the relativistic heavy-quark approach, however, the operator coefficients are allowed to depend explicitly on the quark mass. By including lattice operators through dimension n and adjusting their coefficients $c_{n,i}(m_h a)$ correctly, one enforces that matrix elements in the lattice theory are equal to the analogous matrix elements in continuum QCD through $(a|\vec{p}_h|)^n$, such that residual heavy-quark discretization errors are of $\mathcal{O}(a|\vec{p}_h|)^{n+1}$.

The relativistic heavy-quark approach can be used to compute the matrix elements of states containing heavy quarks for which the heavy-quark spatial momentum $|\vec{p}_h|$ is small compared to the lattice spacing. Thus it is suitable to describe bottom and charm quarks in

both heavy-light and heavy-heavy systems. Calculations of bottomonium and charmonium spectra serve as nontrivial tests of the method and its accuracy.

At fixed lattice spacing, relativistic heavy-quark formulations recover the massless limit when $(am_h) \ll 1$, recover the static limit when $(am_h) \gg 1$, and smoothly interpolate between the two; thus they can be used for any value of the quark mass, and, in particular, for both charm and bottom. Discretization errors for relativistic heavy-quark formulations are generically of the form $\alpha_s^k f(am_h)(a|\vec{p}_h|)^n$, where k reflects the order of the perturbative matching for operators of $\mathcal{O}((a|\vec{p}_h|)^n)$. For each n , such errors are removed completely if the operator matching is nonperturbative. When $(am_h) \sim 1$, this gives rise to nontrivial lattice-spacing dependence in physical quantities, and it is prudent to compare estimates based on power-counting with a direct study of scaling behaviour using a range of lattice spacings. At fixed quark mass, relativistic heavy-quark actions possess a smooth continuum limit without power-divergences. Of course, as $m_h \rightarrow \infty$ at fixed lattice spacing, the static limit is recovered and by then taking the continuum limit the corresponding power divergences are reproduced (see, e.g., Ref. [124]).

The relativistic heavy-quark formulations in use all begin with the asymmetric (or anisotropic) Sheikholeslami-Wohlert (“clover”) action [125]:

$$S_{\text{lat}} = a^4 \sum_{x,x'} \bar{\psi}(x') \left(m_0 + \gamma_0 D_0 + \zeta \vec{\gamma} \cdot \vec{D} - \frac{a}{2} (D^0)^2 - \frac{a}{2} \zeta (\vec{D})^2 + \sum_{\mu,\nu} \frac{ia}{4} c_{\text{SW}} \sigma_{\mu\nu} F_{\mu\nu} \right)_{x'x} \psi(x), \quad (430)$$

where D_μ is the lattice covariant derivative and $F_{\mu\nu}$ is the lattice field-strength tensor. Here we show the form of the action given in Ref. [104]. The introduction of a space-time asymmetry, parameterized by ζ in Eq. (428), is convenient for heavy-quark systems because the characteristic heavy-quark four-momenta do not respect space-time axis exchange ($\vec{p}_h < m_h$ in the bound-state rest frame). Further, the Sheikholeslami-Wohlert action respects the continuum heavy-quark spin and flavour symmetries, so HQET can be used to interpret and estimate lattice discretization effects [124, 126, 127]. We discuss three different prescriptions for tuning the parameters of the action in common use below. In particular, we focus on aspects of the action and operator improvement and matching relevant for evaluating the quality of the calculations discussed in the main text.

The meson energy-momentum dispersion relation plays an important role in relativistic heavy-quark formulations:

$$E(\vec{p}) = M_1 + \frac{\vec{p}^2}{2M_2} + \mathcal{O}(\vec{p}^4), \quad (431)$$

where M_1 and M_2 are known as the rest and kinetic masses, respectively. Because the lattice breaks Lorentz invariance, there are corrections proportional to powers of the momentum. Further, the lattice rest masses and kinetic masses are not equal ($M_1 \neq M_2$), and only become equal in the continuum limit.

The Fermilab interpretation [103] is suitable for calculations of mass splittings and matrix elements of systems with heavy quarks. The Fermilab action is based on the hopping-parameter form of the Wilson action, in which κ_h parameterizes the heavy-quark mass. In practice, κ_h is tuned such that the kinetic meson mass equals the experimentally-measured heavy-strange meson mass (m_{B_s} for bottom and m_{D_s} for charm). In principle, one could also tune the anisotropy parameter such that $M_1 = M_2$. This is not necessary, however, to obtain mass splittings and matrix elements, which are not affected by M_1 [126]. Therefore in the Fermilab action the anisotropy parameter is set equal to unity. The clover coefficient in the

Fermilab action is fixed to the value $c_{\text{SW}} = 1/u_0^3$ from mean-field improved lattice perturbation theory [8]. With this prescription, discretization effects are of $\mathcal{O}(\alpha_s a |\vec{p}_h|, (a |\vec{p}_h|)^2)$. Calculations of electroweak matrix elements also require improving the lattice current and four-fermion operators to the same order, and matching them to the continuum. Calculations with the Fermilab action remove tree-level $\mathcal{O}(a)$ errors in electroweak operators by rotating the heavy-quark field used in the matrix element and setting the rotation coefficient to its tadpole-improved tree-level value (see, e.g., Eqs. (7.8) and (7.10) of Ref. [103]). Finally, electroweak operators are typically renormalized using a mostly nonperturbative approach in which the flavour-conserving light-light and heavy-heavy current renormalization factors Z_V^l and Z_V^{hh} are computed nonperturbatively [128]. The flavour-conserving factors account for most of the heavy-light current renormalization. The remaining correction is expected to be close to unity due to the cancellation of most of the radiative corrections including tadpole graphs [124]; therefore it can be reliably computed at 1-loop in mean-field improved lattice perturbation theory with truncation errors at the percent to few-percent level.

The relativistic heavy-quark (RHQ) formulation developed by Li, Lin, and Christ builds upon the Fermilab approach, but tunes all the parameters of the action in Eq. (428) nonperturbatively [104]. In practice, the three parameters $\{m_0 a, c_{\text{SW}}, \zeta\}$ are fixed to reproduce the experimentally-measured B_s meson mass and hyperfine splitting ($m_{B_s^*} - m_{B_s}$), and to make the kinetic and rest masses of the lattice B_s meson equal [129]. This is done by computing the heavy-strange meson mass, hyperfine splitting, and ratio M_1/M_2 for several sets of bare parameters $\{m_0 a, c_{\text{SW}}, \zeta\}$ and interpolating linearly to the physical B_s point. By fixing the B_s -meson hyperfine splitting, one loses a potential experimental prediction with respect to the Fermilab formulation. However, by requiring that $M_1 = M_2$, one gains the ability to use the meson rest masses, which are generally more precise than the kinetic masses, in the RHQ approach. The nonperturbative parameter-tuning procedure eliminates $\mathcal{O}(a)$ errors from the RHQ action, such that discretization errors are of $\mathcal{O}((a |\vec{p}_h|)^2)$. Calculations of B -meson decay constants and semileptonic form factors with the RHQ action are in progress [130, 131], as is the corresponding 1-loop mean-field improved lattice perturbation theory [132]. For these works, cutoff effects in the electroweak vector and axial-vector currents will be removed through $\mathcal{O}(\alpha_s a)$, such that the remaining discretization errors are of $\mathcal{O}(\alpha_s^2 a |\vec{p}_h|, (a |\vec{p}_h|)^2)$. Matching the lattice operators to the continuum will be done following the mostly nonperturbative approach described above.

The Tsukuba heavy-quark action is also based on the Sheikholeslami-Wohlert action in Eq. (428), but allows for further anisotropies and hence has additional parameters: specifically the clover coefficients in the spatial (c_B) and temporal (c_E) directions differ, as do the anisotropy coefficients of the \vec{D} and \vec{D}^2 operators [105]. In practice, the contribution to the clover coefficient in the massless limit is computed nonperturbatively [133], while the mass-dependent contributions, which differ for c_B and c_E , are calculated at 1-loop in mean-field improved lattice perturbation theory [134]. The hopping parameter is fixed nonperturbatively to reproduce the experimentally-measured spin-averaged $1S$ charmonium mass [135]. One of the anisotropy parameters (r_t in Ref. [135]) is also set to its 1-loop perturbative value, while the other (ν in Ref. [135]) is fixed nonperturbatively to obtain the continuum dispersion relation for the spin-averaged charmonium $1S$ states (such that $M_1 = M_2$). For the renormalization and improvement coefficients of weak current operators, the contributions in the chiral limit are obtained nonperturbatively [136, 137], while the mass-dependent contributions are estimated using 1-loop lattice perturbation theory [138]. With these choices, lattice cutoff effects from the action and operators are of $\mathcal{O}(\alpha_s^2 a |\vec{p}|, (a |\vec{p}_h|)^2)$.

Light-quark actions combined with HQET

The heavy-quark formulations discussed in the previous sections use effective field theory to avoid the occurrence of discretization errors of the form $(am_h)^n$. In this section we describe methods that use improved actions that were originally designed for light-quark systems for B physics calculations. Such actions unavoidably contain discretization errors that grow as a power of the heavy-quark mass. In order to use them for heavy-quark physics, they must be improved to at least $\mathcal{O}(am_h)^2$. However, since $am_b > 1$ at the smallest lattice spacings available in current simulations, these methods also require input from HQET to guide the simulation results to the physical b -quark mass.

The ETM collaboration has developed two methods, the “ratio method” [139] and the “interpolation method” [140, 141]. They use these methods together with simulations with twisted-mass Wilson fermions, which have discretization errors of $\mathcal{O}(am_h)^2$. In the interpolation method Φ_{hs} and Φ_{hl} (or Φ_{hs}/Φ_{hl}) are calculated for a range of heavy-quark masses in the charm region and above, while roughly keeping $am_h \lesssim 0.5$. The relativistic results are combined with a separate calculation of the decay constants in the static limit, and then interpolated to the physical b quark mass. In ETM’s implementation of this method, the heavy Wilson decay constants are matched to HQET using NLO in continuum perturbation theory. The static limit result is renormalized using 1-loop mean-field improved lattice perturbation theory, while for the relativistic data PCAC is used to calculate absolutely normalized matrix elements. Both, the relativistic and static limit data are then run to the common reference scale $\mu_b = 4.5 \text{ GeV}$ at NLO in continuum perturbation theory. In the ratio method, one constructs physical quantities $P(m_h)$ from the relativistic data that have a well-defined static limit ($P(m_h) \rightarrow \text{const. for } m_h \rightarrow \infty$) and evaluates them at the heavy-quark masses used in the simulations. Ratios of these quantities are then formed at a fixed ratio of heavy-quark masses, $z = P(m_h)/P(m_h/\lambda)$ (where $1 < \lambda \lesssim 1.3$), which ensures that z is equal to unity in the static limit. Hence, a separate static limit calculation is not needed with this method. In ETM’s implementation of the ratio method for the B -meson decay constant, $P(m_h)$ is constructed from the decay constants and the heavy-quark pole mass as $P(m_h) = f_{hl}(m_h) \cdot (m_h^{\text{pole}})^{1/2}$. The corresponding z -ratio therefore also includes ratios of perturbative matching factors for the pole mass to $\overline{\text{MS}}$ conversion. For the interpolation to the physical b -quark mass, ratios of perturbative matching factors converting the data from QCD to HQET are also included. The QCD-to-HQET matching factors improve the approach to the static limit by removing the leading logarithmic corrections. In ETM’s implementation of this method (ETM 11 and 12) both conversion factors are evaluated at NLO in continuum perturbation theory. The ratios are then simply fit to a polynomial in $1/m_h$ and interpolated to the physical b -quark mass. The ratios constructed from f_{hl} (f_{hs}) are called z (z_s). In order to obtain the B meson decay constants, the ratios are combined with relativistic decay constant data evaluated at the smallest reference mass.

The HPQCD collaboration has introduced a method in Ref. [107] which we shall refer to as the “heavy HISQ” method. The first key ingredient is the use of the HISQ action for the heavy and light valence quarks, which has leading discretization errors of $\mathcal{O}(\alpha_s(v/c)(am_h)^2, (v/c)^2(am_h)^4)$. With the same action for the heavy- and light-valence quarks it is possible to use PCAC to avoid renormalization uncertainties. Another key ingredient at the time of formulation was the availability of gauge ensembles over a large range of

lattice spacings, in this case the library of $N_f = 2 + 1$ asqtad ensembles made public by the MILC collaboration which include lattice spacings as small as $a \approx 0.045$ fm. Since the HISQ action is so highly improved and with lattice spacings as small as 0.045 fm, HPQCD is able to use a large range of heavy-quark masses, from below the charm region to almost up to the physical b -quark mass with $am_h \lesssim 0.85$. They then fit their data in a combined continuum and HQET fit (i.e., using a fit function that is motivated by HQET) to a polynomial in $1/m_H$ (the heavy pseudoscalar-meson mass of a meson containing a heavy (h) quark).

This approach has been extended in recent work by the HPQCD and FNAL/MILC collaborations using the MILC-generated $N_f = 2+1+1$ HISQ ensembles with lattice spacings down to 0.03 fm [94]. These are being used by the HPQCD and the FNAL/MILC collaborations for their B-physics programmes and the corresponding analyses include heavy-quark masses at the physical b quark mass.

In Tab. 71 we list the discretizations of the quark action most widely used for heavy c and b quarks together with the abbreviations used in the summary tables. We also summarize the main properties of these actions and the leading lattice discretization errors for calculations of heavy-light meson matrix quantities with them. Note that in order to maintain the leading lattice artifacts of the actions as given in the table in nonspectral observables (like operator matrix elements) the corresponding nonspectral operators need to be improved as well.

A.2 Setting the scale

In simulations of lattice-QCD quantities such as hadron masses and decay constants are obtained in “lattice units” i.e., as dimensionless numbers. In order to convert them into physical units they must be expressed in terms of some experimentally known, dimensionful reference quantity Q . This procedure is called “setting the scale”. It amounts to computing the nonperturbative relation between the bare gauge coupling g_0 (which is an input parameter in any lattice simulation) and the lattice spacing a expressed in physical units. To this end one chooses a value for g_0 and computes the value of the reference quantity in a simulation: This yields the dimensionless combination, $(aQ)|_{g_0}$, at the chosen value of g_0 . The calibration of the lattice spacing is then achieved via

$$a^{-1} [\text{MeV}] = \frac{Q|_{\text{exp}} [\text{MeV}]}{(aQ)|_{g_0}}, \quad (432)$$

where $Q|_{\text{exp}}$ denotes the experimentally known value of the reference quantity. Common choices for Q are the mass of the nucleon, the Ω baryon or the decay constants of the pion and the kaon. Vector mesons, such as the ρ or K^* meson, are unstable and therefore their masses are not very well suited for setting the scale, despite the fact that they have been used over many years for that purpose.

Another widely used quantity to set the scale is the hadronic radius r_0 , which can be determined from the force between static quarks via the relation [142]

$$F(r_0)r_0^2 = 1.65. \quad (433)$$

If the force is derived from potential models describing heavy quarkonia, the above relation determines the value of r_0 as $r_0 \approx 0.5$ fm. A variant of this procedure is obtained [143] by using the definition $F(r_1)r_1^2 = 1.00$, which yields $r_1 \approx 0.32$ fm. It is important to realize that

Abbrev.	Discretization	Leading lattice artifacts and truncation errors for heavy-light mesons	Remarks
tmWil	twisted-mass Wilson	$\mathcal{O}((am_h)^2)$	PCAC relation for axial-vector current
HISQ	Staggered	$\mathcal{O}(\alpha_S(am_h)^2(v/c), (am_h)^4(v/c)^2)$	PCAC relation for axial-vector current; Ward identity for vector current
static	static effective action	$\mathcal{O}(a^2\Lambda_{\text{QCD}}^2, \Lambda_{\text{QCD}}/m_h, \alpha_s^2, \alpha_s^2 a \Lambda_{\text{QCD}})$	implementations use APE, HYP1, and HYP2 smearing
HQET	Heavy-Quark Effective Theory	$\mathcal{O}(a\Lambda_{\text{QCD}}^2/m_h, a^2\Lambda_{\text{QCD}}^2, (\Lambda_{\text{QCD}}/m_h)^2)$	Nonperturbative matching through $\mathcal{O}(1/m_h)$
NRQCD	Nonrelativistic QCD	$\mathcal{O}(\alpha_S\Lambda_{\text{QCD}}/m_h, \alpha_S(\Lambda_{\text{QCD}}/m_h)^2, (\Lambda_{\text{QCD}}/m_h)^3, \alpha_S a^2 \Lambda_{\text{QCD}}^2)$	Tree-level relativistic corrections through $\mathcal{O}(v_h^4)$ and discretization corrections through $\mathcal{O}(a^2)$
Fermilab	Sheikholeslami-Wohlert	$\mathcal{O}(\alpha_s a \Lambda_{\text{QCD}}, (a\Lambda_{\text{QCD}})^2)$	Hopping parameter tuned nonperturbatively; clover coefficient computed at tree-level in mean-field-improved lattice perturbation theory
RHQ	Sheikholeslami-Wohlert	$\mathcal{O}(\alpha_s^2 a \Lambda_{\text{QCD}}, (a\Lambda_{\text{QCD}})^2)$	Hopping parameter, anisotropy and clover coefficient tuned nonperturbatively by fixing the B_s -meson hyperfine splitting
Tsukuba	Sheikholeslami-Wohlert	$\mathcal{O}(\alpha_s^2 a \Lambda_{\text{QCD}}, (a\Lambda_{\text{QCD}})^2)$	NP clover coefficient at $ma = 0$ plus mass-dependent corrections calculated at 1-loop in lattice perturbation theory; ν calculated NP from dispersion relation; r_s calculated at 1-loop in lattice perturbation theory

Table 71: Discretizations of the quark action most widely used for heavy c and b quarks and some of their properties.

both r_0 and r_1 are not directly accessible in experiment, so that their values derived from phenomenological potentials are necessarily model-dependent. In spite of the inherent ambiguity whenever hadronic radii are used to calibrate the lattice spacing, they are very useful quantities for performing scaling tests and continuum extrapolations of lattice data. Furthermore, they can be easily computed with good statistical accuracy in lattice simulations.

More recently, the so-called gradient flow scales t_0 and w_0 have become popular, because they can be computed with very high statistical accuracy in lattice simulations without introducing any systematics due to the analysis. The scales are based on the gradient flow procedure [144] which evolves the gauge fields in field space along a fictitious flow time t according to a local diffusion equation. The field at finite flow time can be shown to be renormalized [145]. Expectation values of local gauge-invariant expressions of the field are physical quantities with a well-defined continuum limit and can hence be used to fix the scale. One example is provided by the gauge action density $E(t)$. Its expectation value is used to define the reference scale t_0 through the implicit equation [144]

$$\{t^2\langle E(t)\rangle\}_{t=t_0} = 0.3. \quad (434)$$

Another example is the related observable

$$W(t) = t \frac{d}{dt} \{t^2\langle E(t)\rangle\} \quad (435)$$

which is used to define the scale w_0 via the condition [146]

$$\{W(t)\}_{t=w_0^2} = 0.3. \quad (436)$$

Similarly to the hadronic radius, the values of t_0 and w_0 can not be determined from experiment, but only from within lattice QCD, yielding $\sqrt{t_0} \approx 0.14$ fm and $w_0 \approx 0.17$ fm (see, e.g., [147]). Nevertheless, they are very useful quantities for performing scaling tests and continuum extrapolations of lattice data.

A.3 Matching and running

The lattice formulation of QCD amounts to introducing a particular regularization scheme. Thus, in order to be useful for phenomenology, hadronic matrix elements computed in lattice simulations must be related to some continuum reference scheme, such as the $\overline{\text{MS}}$ -scheme of dimensional regularization. The matching to the continuum scheme usually involves running to some reference scale using the renormalization group.

In principle, the matching factors which relate lattice matrix elements to the $\overline{\text{MS}}$ -scheme, can be computed in perturbation theory formulated in terms of the bare coupling. It has been known for a long time, though, that the perturbative expansion is not under good control. Several techniques have been developed which allow for a nonperturbative matching between lattice regularization and continuum schemes, and are briefly introduced here.

Regularization-independent Momentum Subtraction

In the *Regularization-independent Momentum Subtraction* (“RI/MOM” or “RI”) scheme [148] a nonperturbative renormalization condition is formulated in terms of Green functions involving quark states in a fixed gauge (usually Landau gauge) at nonzero virtuality. In this way one relates operators in lattice regularization nonperturbatively to the RI scheme.

In a second step one matches the operator in the RI scheme to its counterpart in the $\overline{\text{MS}}$ -scheme. The advantage of this procedure is that the latter relation involves perturbation theory formulated in the continuum theory. The use of lattice perturbation theory can thus be avoided, and the continuum perturbation theory, which is technically more feasible for higher order calculations, could be applied if more precision is required. A technical complication is associated with the accessible momentum scales (i.e., virtualities), which must be large enough (typically several GeV) in order for the perturbative relation to $\overline{\text{MS}}$ to be reliable. The momentum scales in simulations must stay well below the cutoff scale (i.e., 2π over the lattice spacing), since otherwise large lattice artifacts are incurred. Thus, the applicability of the RI scheme traditionally relies on the existence of a “window” of momentum scales, which satisfy

$$\Lambda_{\text{QCD}} \lesssim p \lesssim 2\pi a^{-1}. \quad (437)$$

However, solutions for mitigating this limitation, which involve continuum limit, nonperturbative running to higher scales in the RI/MOM scheme, have recently been proposed and implemented [149–152].

Within the RI/MOM framework one has some freedom in the choice of the external momenta used in the Green functions. In the choice made in the original work, the virtuality of each external leg is nonzero, but that of the momentum transfer between different legs can vanish [148]. This leads to enhanced nonperturbative contributions that fall as powers of p^2 . An alternative choice that reduces these issues is the symmetric MOM scheme, in which virtualities in all channels are nonzero [153]. This scheme is now widely used. To distinguish it from the original choice of virtualities, it is referred to as the RI/SMOM (or RI-SMOM) scheme, while the original choice is called the RI/MON (or RI-MOM) scheme.

Schrödinger functional

Another example of a nonperturbative matching procedure is provided by the Schrödinger functional (SF) scheme [154]. It is based on the formulation of QCD in a finite volume. If all quark masses are set to zero the box length remains the only scale in the theory, such that observables like the coupling constant run with the box size L . The great advantage is that the RG running of scale-dependent quantities can be computed nonperturbatively using recursive finite-size scaling techniques. It is thus possible to run nonperturbatively up to scales of, say, 100 GeV, where one is sure that the perturbative relation between the SF and $\overline{\text{MS}}$ -schemes is controlled.

Perturbation theory

The third matching procedure is based on perturbation theory in which higher order are effectively resummed [8]. Although this procedure is easier to implement, it is hard to estimate the uncertainty associated with it.

Mostly nonperturbative renormalization

Some calculations of heavy-light and heavy-heavy matrix elements adopt a mostly nonperturbative matching approach. Let us consider a weak decay process mediated by a current with quark flavours h and q , where h is the initial heavy quark (either bottom or charm) and

q can be a light ($\ell = u, d$), strange, or charm quark. The matrix elements of lattice current J_{hq} are matched to the corresponding continuum matrix elements with continuum current \mathcal{J}_{hq} by calculating the renormalization factor $Z_{J_{hq}}$. The mostly nonperturbative renormalization method takes advantage of rewriting the current renormalization factor as the following product:

$$Z_{J_{hq}} = \rho_{J_{hq}} \sqrt{Z_{V_{hh}^4} Z_{V_{qq}^4}} \quad (438)$$

The flavour-conserving renormalization factors $Z_{V_{hh}^4}$ and $Z_{V_{qq}^4}$ can be obtained nonperturbatively from standard heavy-light and light-light meson charge normalization conditions. $Z_{V_{hh}^4}$ and $Z_{V_{qq}^4}$ account for the bulk of the renormalization. The remaining correction $\rho_{J_{hq}}$ is expected to be close to unity because most of the radiative corrections, including self-energy corrections and contributions from tadpole graphs, cancel in the ratio [124, 127]. The 1-loop coefficients of $\rho_{J_{hq}}$ have been calculated for heavy-light and heavy-heavy currents for Fermilab heavy and both (improved) Wilson light [124, 127] and asqtad light [155] quarks. In all cases the 1-loop coefficients are found to be very small, yielding sub-percent to few percent level corrections.

In Tab. 72 we list the abbreviations used in the compilation of results together with a short description.

Abbrev.	Description
RI	regularization-independent momentum subtraction scheme
SF	Schrödinger functional scheme
PT1 ℓ	matching/running computed in perturbation theory at one loop
PT2 ℓ	matching/running computed in perturbation theory at two loops
mNPR	mostly nonperturbative renormalization

Table 72: The most widely used matching and running techniques.

A.4 Chiral extrapolation

As mentioned in the introduction, Symanzik’s framework can be combined with Chiral Perturbation Theory. The well-known terms occurring in the chiral effective Lagrangian are then supplemented by contributions proportional to powers of the lattice spacing a . The additional terms are constrained by the symmetries of the lattice action and therefore depend on the specific choice of the discretization. The resulting effective theory can be used to analyse the a -dependence of the various quantities of interest – provided the quark masses and the momenta considered are in the range where the truncated chiral perturbation series yields an adequate approximation. Understanding the dependence on the lattice spacing is of central importance for a controlled extrapolation to the continuum limit.

For staggered fermions, this program has first been carried out for a single staggered flavour (a single staggered field) [30] at $\mathcal{O}(a^2)$. In the following, this effective theory is

denoted by $S\chi\text{PT}$. It was later generalized to an arbitrary number of flavours [31, 156], and to next-to-leading order [32]. The corresponding theory is commonly called Rooted Staggered chiral perturbation theory and is denoted by $RS\chi\text{PT}$.

For Wilson fermions, the effective theory has been developed in [157–159] and is called $W\chi\text{PT}$, while the theory for Wilson twisted-mass fermions [160–162] is termed $tmW\chi\text{PT}$.

Another important approach is to consider theories in which the valence and sea quark masses are chosen to be different. These theories are called *partially quenched*. The acronym for the corresponding chiral effective theory is $PQ\chi\text{PT}$ [163–166].

Finally, one can also consider theories where the fermion discretizations used for the sea and the valence quarks are different. The effective chiral theories for these “mixed action” theories are referred to as $MA\chi\text{PT}$ [38, 167–172].

Finite-Volume Regimes of QCD

Once QCD with N_f nondegenerate flavours is regulated both in the UV and in the IR, there are $3 + N_f$ scales in play: The scale Λ_{QCD} that reflects “dimensional transmutation” (alternatively, one could use the pion decay constant or the nucleon mass, in the chiral limit), the inverse lattice spacing $1/a$, the inverse box size $1/L$, as well as N_f meson masses (or functions of meson masses) that are sensitive to the N_f quark masses, e.g., M_π^2 , $2M_K^2 - M_\pi^2$ and the spin-averaged masses of 1S states of quarkonia.

Ultimately, we are interested in results with the two regulators removed, i.e., physical quantities for which the limits $a \rightarrow 0$ and $L \rightarrow \infty$ have been carried out. In both cases there is an effective field theory (EFT) which guides the extrapolation. For the $a \rightarrow 0$ limit, this is a version of the Symanzik EFT which depends, in its details, on the lattice action that is used, as outlined in Sec. A.1. The finite-volume effects are dominated by the lightest particles, the pions. Therefore, a chiral EFT, also known as χPT , is appropriate to parameterize the finite-volume effects, i.e., the deviation of masses and other observables, such as matrix elements, in a finite-volume from their infinite volume, physical values. Most simulations of phenomenological interest are carried out in boxes of size $L \gg 1/M_\pi$, that is in boxes whose diameter is large compared to the Compton wavelength that the pion would have, at the given quark mass, in infinite volume. In this situation the finite-volume corrections are small, and in many cases the ratio $M_{\text{had}}(L)/M_{\text{had}}$ or $f(L)/f$, where f denotes some generic matrix element, can be calculated in χPT , such that the leading finite-volume effects can be taken out analytically. In the terminology of χPT this setting is referred to as the p -regime, as the typical contributing momenta $p \sim M_\pi \gg 1/L$. A peculiar situation occurs if the condition $L \gg 1/M_\pi$ is violated (while $L\Lambda_{\text{QCD}} \gg 1$ still holds), in other words if the quark mass is taken so light that the Compton wavelength that the pion would have (at the given m_q) in infinite volume, is as large or even larger than the actual box size. Then the pion zero-momentum mode dominates and needs to be treated separately. While this setup is unlikely to be useful for standard phenomenological computations, the low-energy constants of χPT can still be calculated, by matching to a re-ordered version of the chiral series, and following the details of the reordering such an extreme regime is called the ϵ - or δ -regime, respectively. Accordingly, further particulars of these regimes are discussed in Sec. 5.1 of this report.

A.5 Parameterizations of semileptonic form factors

In this section, we discuss the description of the q^2 -dependence of form factors, using the vector form factor f_+ of $B \rightarrow \pi \ell \nu$ decays as a benchmark case. Since in this channel the parameterization of the q^2 -dependence is crucial for the extraction of $|V_{ub}|$ from the existing measurements (involving decays to light leptons), as explained above, it has been studied in great detail in the literature. Some comments about the generalization of the techniques involved will follow.

The vector form factor for $B \rightarrow \pi \ell \nu$ All form factors are analytic functions of q^2 outside physical poles and inelastic threshold branch points; in the case of $B \rightarrow \pi \ell \nu$, the only pole expected below the $B\pi$ production region, starting at $q^2 = t_+ = (m_B + m_\pi)^2$, is the B^* . A simple ansatz for the q^2 -dependence of the $B \rightarrow \pi \ell \nu$ semileptonic form factors that incorporates vector-meson dominance is the Bećirević-Kaidalov (BK) parameterization [173], which for the vector form factor reads:

$$f_+(q^2) = \frac{f(0)}{(1 - q^2/m_{B^*}^2)(1 - \alpha q^2/m_{B^*}^2)}. \quad (439)$$

Because the BK ansatz has few free parameters, it has been used extensively to parameterize the shape of experimental branching-fraction measurements and theoretical form-factor calculations. A variant of this parameterization proposed by Ball and Zwicky (BZ) adds extra pole factors to the expressions in Eq. (437) in order to mimic the effect of multiparticle states [174]. A similar idea, extending the use of effective poles also to $D \rightarrow \pi \ell \nu$ decays, is explored in Ref. [175]. Finally, yet another variant (RH) has been proposed by Hill in Ref. [176]. Although all of these parameterizations capture some known properties of form factors, they do not manifestly satisfy others. For example, perturbative QCD scaling constrains the behaviour of f_+ in the deep Euclidean region [177–179], and angular momentum conservation constrains the asymptotic behaviour near thresholds—e.g., $\text{Im } f_+(q^2) \sim (q^2 - t_+)^{3/2}$ (see, e.g., Ref. [180]). Most importantly, these parameterizations do not allow for an easy quantification of systematic uncertainties.

A more systematic approach that improves upon the use of simple models for the q^2 behaviour exploits the positivity and analyticity properties of two-point functions of vector currents to obtain optimal parameterizations of form factors [179, 181–186]. Any form factor f can be shown to admit a series expansion of the form

$$f(q^2) = \frac{1}{B(q^2)\phi(q^2, t_0)} \sum_{n=0}^{\infty} a_n(t_0) z(q^2, t_0)^n, \quad (440)$$

where the squared momentum transfer is replaced by the variable

$$z(q^2, t_0) = \frac{\sqrt{t_+ - q^2} - \sqrt{t_+ - t_0}}{\sqrt{t_+ - q^2} + \sqrt{t_+ - t_0}}. \quad (441)$$

This is a conformal transformation, depending on an arbitrary real parameter $t_0 < t_+$, that maps the q^2 plane cut for $q^2 \geq t_+$ onto the disk $|z(q^2, t_0)| < 1$ in the z complex plane. The function $B(q^2)$ is called the *Blaschke factor*, and contains poles and cuts below t_+ — for instance, in the case of $B \rightarrow \pi$ decays,

$$B(q^2) = \frac{z(q^2, t_0) - z(m_{B^*}^2, t_0)}{1 - z(q^2, t_0)z(m_{B^*}^2, t_0)} = z(q^2, m_{B^*}^2). \quad (442)$$

Finally, the quantity $\phi(q^2, t_0)$, called the *outer function*, is some otherwise arbitrary function that does not introduce further poles or branch cuts. The crucial property of this series expansion is that the sum of the squares of the coefficients

$$\sum_{n=0}^{\infty} a_n^2 = \frac{1}{2\pi i} \oint \frac{dz}{z} |B(z)\phi(z)f(z)|^2, \quad (443)$$

is a finite quantity. Therefore, by using this parameterization an absolute bound to the uncertainty induced by truncating the series can be obtained. The aim in choosing ϕ is to obtain a bound that is useful in practice, while (ideally) preserving the correct behaviour of the form factor at high q^2 and around thresholds.

The simplest form of the bound would correspond to $\sum_{n=0}^{\infty} a_n^2 = 1$. *Imposing* this bound yields the following “standard” choice for the outer function

$$\begin{aligned} \phi(q^2, t_0) = & \sqrt{\frac{1}{32\pi\chi_{1-}(0)}} \left(\sqrt{t_+ - q^2} + \sqrt{t_+ - t_0} \right) \\ & \times \left(\sqrt{t_+ - q^2} + \sqrt{t_+ - t_-} \right)^{3/2} \left(\sqrt{t_+ - q^2} + \sqrt{t_+} \right)^{-5} \frac{t_+ - q^2}{(t_+ - t_0)^{1/4}}, \end{aligned} \quad (444)$$

where $t_- = (m_B - m_\pi)^2$, and $\chi_{1-}(0)$ is the derivative of the transverse component of the polarization function (i.e., the Fourier transform of the vector two-point function) $\Pi_{\mu\nu}(q)$ at Euclidean momentum $Q^2 = -q^2 = 0$. It is computed perturbatively, using operator product expansion techniques, by relating the $B \rightarrow \pi\ell\nu$ decay amplitude to $\ell\nu \rightarrow B\pi$ inelastic scattering via crossing symmetry and reproducing the correct value of the inclusive $\ell\nu \rightarrow X_b$ amplitude. We will refer to the series parameterization with the outer function in Eq. (442) as Boyd, Grinstein, and Lebed (BGL). The perturbative and OPE truncations imply that the bound is not strict, and one should take it as

$$\sum_{n=0}^N a_n^2 \lesssim 1, \quad (445)$$

where this holds for any choice of N . Since the values of $|z|$ in the kinematical region of interest are well below 1 for judicious choices of t_0 , this provides a very stringent bound on systematic uncertainties related to truncation for $N \geq 2$. On the other hand, the outer function in Eq. (442) is somewhat unwieldy and, more relevantly, spoils the correct large q^2 behaviour and induces an unphysical singularity at the $B\pi$ threshold.

A simpler choice of outer function has been proposed by Bourrely, Caprini and Lellouch (BCL) in Ref. [180], which leads to a parameterization of the form

$$f_+(q^2) = \frac{1}{1 - q^2/m_{B^*}^2} \sum_{n=0}^N a_n^+(t_0) z(q^2, t_0)^n. \quad (446)$$

This satisfies all the basic properties of the form factor, at the price of changing the expression for the bound to

$$\sum_{j,k=0}^N B_{jk}(t_0) a_j^+(t_0) a_k^+(t_0) \leq 1. \quad (447)$$

The constants B_{jk} can be computed and shown to be $|B_{jk}| \lesssim \mathcal{O}(10^{-2})$ for judicious choices of t_0 ; therefore, one again finds that truncating at $N \geq 2$ provides sufficiently stringent bounds for the current level of experimental and theoretical precision. It is actually possible to optimize the properties of the expansion by taking

$$t_0 = t_{\text{opt}} = (m_B + m_\pi)(\sqrt{m_B} - \sqrt{m_\pi})^2, \quad (448)$$

which for physical values of the masses results in the semileptonic domain being mapped onto the symmetric interval $|z| \lesssim 0.279$ (where this range differs slightly for the B^\pm and B^0 decay channels), minimizing the maximum truncation error. If one also imposes that the asymptotic behaviour $\text{Im} f_+(q^2) \sim (q^2 - t_+)^{3/2}$ near threshold is satisfied, then the highest-order coefficient is further constrained as

$$a_N^+ = -\frac{(-1)^N}{N} \sum_{n=0}^{N-1} (-1)^n n a_n^+. \quad (449)$$

Substituting the above constraint on a_N^+ into Eq. (444) leads to the constrained BCL parameterization

$$f_+(q^2) = \frac{1}{1 - q^2/m_{B^*}^2} \sum_{n=0}^{N-1} a_n^+ \left[z^n - (-1)^{n-N} \frac{n}{N} z^N \right], \quad (450)$$

which is the standard implementation of the BCL parameterization used in the literature.

Parameterizations of the BGL and BCL kind, to which we will refer collectively as “ z -parameterizations”, have already been adopted by the BaBar and Belle collaborations to report their results, and also by the Heavy Flavour Averaging Group (HFAG, later renamed HFLAV). Some lattice collaborations, such as FNAL/MILC and ALPHA, have already started to report their results for form factors in this way. The emerging trend is to use the BCL parameterization as a standard way of presenting results for the q^2 -dependence of semileptonic form factors. Our policy will be to quote results for z -parameterizations when the latter are provided in the paper (including the covariance matrix of the fits); when this is not the case, but the published form factors include the full correlation matrix for values at different q^2 , we will perform our own fit to the constrained BCL ansatz in Eq. (448); otherwise no fit will be quoted. We however stress the importance of providing, apart from parameterization coefficients, values for the form factors themselves (in the continuum limit and at physical quark masses) for a number of values of q^2 , so that the results can be independently parameterized by the readers if so wished.

The scalar form factor for $B \rightarrow \pi \ell \nu$ The discussion of the scalar $B \rightarrow \pi$ form factor is very similar. The main differences are the absence of a constraint analogue to Eq. (447) and the choice of the overall pole function. In our fits we adopt the simple expansion:

$$f_0(q^2) = \sum_{n=0}^{N-1} a_n^0 z^n. \quad (451)$$

We do impose the exact kinematical constraint $f_+(0) = f_0(0)$ by expressing the a_{N-1}^0 coefficient in terms of all remaining a_n^+ and a_n^0 coefficients. This constraint introduces important

correlations between the a_n^+ and a_n^0 coefficients; thus only lattice calculations that present the correlations between the vector and scalar form factors can be used in an average that takes into account the constraint at $q^2 = 0$.

Finally we point out that we do not need to use the same number of parameters for the vector and scalar form factors. For instance, with $(N^+ = 3, N^0 = 3)$ we have $a_{0,1,2}^+$ and $a_{0,1}^0$, while with $(N^+ = 3, N^0 = 4)$ we have $a_{0,1,2}^+$ and $a_{0,1,2}^0$ as independent fit parameters. In our average we will choose the combination that optimizes uncertainties.

Extension to other form factors The discussion above largely extends to form factors for other semileptonic transitions (e.g., $B_s \rightarrow K$ and $B_{(s)} \rightarrow D_{(s)}^{(*)}$, and semileptonic D and K decays). Details are discussed in the relevant sections.

A general discussion of semileptonic meson decay in this context can be found, e.g., in Ref. [187]. Extending what has been discussed above for $B \rightarrow \pi$, the form factors for a generic $H \rightarrow L$ transition will display a cut starting at the production threshold t_+ , and the optimal value of t_0 required in z -parameterizations is $t_0 = t_+(1 - \sqrt{1 - t_-/t_+})$ (where $t_{\pm} = (m_H \pm m_L)^2$). For unitarity bounds to apply, the Blaschke factor has to include all sub-threshold poles with the quantum numbers of the hadronic current — i.e., vector (resp. scalar) resonances in $B\pi$ scattering for the vector (resp. scalar) form factors of $B \rightarrow \pi$, $B_s \rightarrow K$, or $\Lambda_b \rightarrow p$; and vector (resp. scalar) resonances in $B_c\pi$ scattering for the vector (resp. scalar) form factors of $B \rightarrow D$ or $\Lambda_b \rightarrow \Lambda_c$.¹ Thus, as emphasized above, the control over systematic uncertainties brought in by using z -parameterizations strongly depends on implementation details. This has practical consequences, in particular, when the resonance spectrum in a given channel is not sufficiently well-known. Caveats may also apply for channels where resonances with a nonnegligible width appear. A further issue is whether $t_+ = (m_H + m_L)^2$ is the proper choice for the start of the cut in cases such as $B_s \rightarrow K\ell\nu$ and $B \rightarrow D\ell\nu$, where there are lighter two-particle states that project on the current (B,π and B_c,π for the two processes, respectively).² In any such situation, it is not clear a priori that a given z -parameterization will satisfy strict bounds, as has been seen, e.g., in determinations of the proton charge radius from electron-proton scattering [188–190].

The HPQCD collaboration pioneered a variation on the z -parameterization approach, which they refer to as a “modified z -expansion,” that is used to simultaneously extrapolate their lattice simulation data to the physical light-quark masses and the continuum limit, and to interpolate/extrapolate their lattice data in q^2 . This entails allowing the coefficients a_n to depend on the light-quark masses, squared lattice spacing, and, in some cases the charm-quark mass and pion or kaon energy. Because the modified z -expansion is not derived from an underlying effective field theory, there are several potential concerns with this approach that have yet to be studied. The most significant is that there is no theoretical derivation relating the coefficients of the modified z -expansion to those of the physical coefficients measured in experiment; it therefore introduces an unquantified model dependence in the form-factor shape. As a result, the applicability of unitarity bounds has to be examined carefully. Related to this, z -parameterization coefficients implicitly depend on quark masses, and particular care should be taken in the event that some state can move across the inelastic threshold as quark

¹A more complicated analytic structure may arise in other cases, such as channels with vector mesons in the final state. We will however not discuss form-factor parameterizations for any such process.

²We are grateful to G. Herdoíza, R.J. Hill, A. Kronfeld and A. Szczepaniak for illuminating discussions on this issue.

masses are changed (which would in turn also affect the form of the Blaschke factor). Also, the lattice-spacing dependence of form factors provided by Symanzik effective theory techniques may not extend trivially to z -parameterization coefficients. The modified z -expansion is now being utilized by collaborations other than HPQCD and for quantities other than $D \rightarrow \pi \ell \nu$ and $D \rightarrow K \ell \nu$, where it was originally employed. We advise treating results that utilize the modified z -expansion to obtain form-factor shapes and CKM matrix elements with caution, however, since the systematics of this approach warrant further study.

A.6 Summary of simulated lattice actions

In the following Tabs. 73–78 we summarize the gauge and quark actions used in the various calculations with $N_f = 2, 2 + 1$ and $2 + 1 + 1$ quark flavours. The calculations with $N_f = 0$ quark flavours mentioned in Sec. 9 all used the Wilson gauge action and are not listed. Abbreviations are explained in Secs. A.1.1, A.1.2 and A.1.3, and summarized in Tabs. 69, 70 and 71.

Collab.	Ref.	N_f	gauge action	quark action
ALPHA 01A, 04, 05, 12, 13A	[191–195]	2	Wilson	npSW
Aoki 94	[196]	2	Wilson	KS
Bernardini 10	[197]	2	Wilson	npSW [†]
Bernardini 11	[198]	2	Wilson	npSW
Brandt 13	[199]	2	Wilson	npSW
Boucaud 01B	[200]	2	Wilson	Wilson
CERN-TOV 06	[201]	2	Wilson	Wilson/npSW
CERN 08	[202]	2	Wilson	npSW
CP-PACS 01, 04	[203, 204]	2	Iwasaki	mfSW
Davies 94	[205]	2	Wilson	KS
Dürr 11	[206]	2	Wilson	npSW
Engel 14	[207]	2	Wilson	npSW

[†] The calculation uses overlap fermions in the valence quark sector.

Table 73: Summary of simulated lattice actions with $N_f = 2$ quark flavours.

Collab.	Ref.	N_f	gauge action	quark action
ETM 07, 07A, 08, 09, 09A-D, 09G 10B, 10D, 10F, 11C, 12, 13, 13A	[139, 208–222]	2	tlSym	tmWil
ETM 10A, 12D	[223, 224]	2	tlSym	tmWil *
ETM 14D, 15A, 16C	[225–227]	2	Iwasaki	tmWil with npSW
ETM 15D, 16A, 17, 17B, 17C	[228–232]	2	Iwasaki	tmWil with npSW *
Gülpers 13, 15	[233, 234]	2	Wilson	npSW
Hasenfratz 08	[235]	2	tadSym	n-HYP tlSW
JLQCD 08, 08B	[236, 237]	2	Iwasaki	overlap
JLQCD 02, 05	[238, 239]	2	Wilson	npSW
JLQCD/TWQCD 07, 08A, 08C, 10	[240–243]	2	Iwasaki	overlap
Mainz 12, 17	[244, 245]	2	Wilson	npSW
QCDSF 06, 07, 12, 13	[246–249]	2	Wilson	npSW
QCDSF/UKQCD 04, 05, 06, 06A, 07	[250–254]	2	Wilson	npSW
RBC 04, 06, 07, 08	[255–258]	2	DBW2	DW
RBC/UKQCD 07	[259]	2	Wilson	npSW
RM123 11, 13	[260, 261]	2	tlSym	tmWil
RQCD 14, 16	[262, 263]	2	Wilson	npSW
SESAM 99	[264]	2	Wilson	Wilson

* The calculation uses Osterwalder-Seiler fermions [265] in the valence quark sector to treat strange and charm quarks.

Table 73: (cntd.) Summary of simulated lattice actions with $N_f = 2$ quark flavours.

Collab.	Ref.	N_f	gauge action	quark action
Sternbeck 10, 12	[266, 267]	2	Wilson	npSW
SPQcdR 05	[268]	2	Wilson	Wilson
TWQCD 11, 11A	[269, 270]	2	Wilson	optimal DW
UKQCD 04	[259, 271]	2	Wilson	npSW
Wingate 95	[272]	2	Wilson	KS

Table 73: (cntd.) Summary of simulated lattice actions with $N_f = 2$ quark flavours.

Collab.	Ref.	N_f	gauge action	quark action
ALPHA 17	[273]	2 + 1	tlSym/Wilson	npSW
Aubin 08, 09	[274, 275]	2 + 1	tadSym	Asqtad [†]
Bazavov 12, 14	[276, 277]	2 + 1	tlSym	HISQ
Blum 10	[278]	2 + 1	Iwasaki	DW
BMW 10A-C, 11, 13, 15, 16, 16A	[150, 151, 279–284]	2 + 1	tlSym	2-level HEX tlSW
BMW 10, 11A	[285, 286]	2 + 1	tlSym	6-level stout tlSW
Boyle 14	[287]	2 + 1	Iwasaki, Iwasaki+DSDR*	DW
χ QCD 13A, 15	[288, 289]	2 + 1	Iwasaki	DW ⁺
χ QCD 15A	[290]	2 + 1	Iwasaki	M-DW ⁺
χ QCD 18	[291]	2 + 1	Iwasaki	DW, M-DW ⁺
CP-PACS/JLQCD 07	[292]	2 + 1	Iwasaki	npSW

[†] The calculation uses domain wall fermions in the valence-quark sector.

* An additional weighting factor known as the dislocation suppressing determinant ratio (DSDR) is added to the gauge action [83].

⁺ The calculation uses overlap fermions in the valence-quark sector.

Table 74: Summary of simulated lattice actions with $N_f = 2 + 1$ or $N_f = 3$ quark flavours.

Collab.	Ref.	N_f	gauge action	quark action
Engelhardt 12	[293]	2 + 1	tadSym	Asqtad [†]
FNAL/MILC 12, 12I	[294, 295]	2 + 1	tadSym	Asqtad
HPQCD 05, 05A, 08A, 13A	[296–299]	2 + 1	tadSym	Asqtad
HPQCD 10	[300]	2 + 1	tadSym	Asqtad *
HPQCD/UKQCD 06	[301]	2 + 1	tadSym	Asqtad
HPQCD/UKQCD 07	[302]	2 + 1	tadSym	Asqtad *
HPQCD/MILC/UKQCD 04	[303]	2 + 1	tadSym	Asqtad
Hudspith 15, 18	[304, 305]	2 + 1	Iwasaki, Iwasaki+DSDR ⁺	DW, M-DW
JLQCD 09, 10	[306, 307]	2 + 1	Iwasaki	overlap
JLQCD 11, 12, 12A, 14, 15A, 17, 18	[308–314]	2 + 1	Iwasaki (fixed topology)	overlap
JLQCD 15B-C, 16, 16B, 17A	[46, 315–317, 319]	2 + 1	tlSym	M-DW
JLQCD/TWQCD 08B, 09A	[320, 321]	2 + 1	Iwasaki	overlap
JLQCD/TWQCD 10	[243]	2 + 1, 3	Iwasaki	overlap
Junnarkar 13	[322]	2 + 1	tadSym	Asqtad [†]
Laiho 11	[323]	2 + 1	tadSym	Asqtad [†]
LHP 04, LHPC 05, 10	[324–326]	2 + 1	tadSym	Asqtad [†]
LHPC 12, 12A	[327, 328]	2 + 1	tlSym	2-level HEX tlSW

[†] The calculation uses domain wall fermions in the valence-quark sector.

⁺ An additional weighting factor known as the dislocation suppressing determinant ratio (DSDR) is added to the gauge action [83].

*

Table 74: (cntd.) Summary of simulated lattice actions with $N_f = 2 + 1$ or $N_f = 3$ quark flavours.

Collab.	Ref.	N_f	gauge action	quark action
Mainz 18	[329]	2 + 1	tlSym	npSW
Maltman 08	[330]	2 + 1	tadSym	Asqtad
Martin Camalich 10	[331]	2 + 1	Iwasaki	npSW
MILC 04, 07, 09, 09A, 09D, 10, 10A, 12C, 16	[47, 48, 303, 332–337]	2 + 1	tadSym	Asqtad
Nakayama 18	[338]	2 + 1	tlSym	M-DW
NPLQCD 06	[339]	2 + 1	tadSym	Asqtad [†]
PACS 18	[340]	2 + 1	Iwasaki	npSW
PACS-CS 08, 08A, 09, 09A, 10, 11A, 12, 13	[137, 341–347]	2 + 1	Iwasaki	npSW
QCDSF 11	[348]	2 + 1	tlSym	npSW
QCDSF/UKQCD 15, 16	[349, 350]	2 + 1	tlSym	npSW
RBC/UKQCD 07, 08, 08A, 10, 10A-B, 11, 12, 13, 16	[83, 152, 351–358]	2 + 1	Iwasaki, Iwasaki+DSDR*	DW
RBC/UKQCD 08B, 09B, 10D, 12E	[359–362]	2 + 1	Iwasaki	DW
RBC/UKQCD 14B, 15A, 15E	[304, 305, 363–365]	2 + 1	Iwasaki, Iwasaki+DSDR*	DW, M-DW
Shanahan 12	[366]	2 + 1	Iwasaki	npSW
Sternbeck 12	[267]	2 + 1	tlSym	npSW
SWME 10, 11, 11A, 13, 13A, 14A, 14C, 15A	[39, 367–373]	2 + 1	tadSym	Asqtad [†]
Takaura 18	[374, 375]	2 + 1	tlSym	M-DW
TWQCD 08	[376]	2 + 1	Iwasaki	DW

[†] The calculation uses domain wall fermions in the valence-quark sector.

* An additional weighting factor known as the dislocation suppressing determinant ratio (DSDR) is added to the gauge action [83].

⁺ The calculation uses HYP smeared improved staggered fermions in the valence-quark sector.

Table 74: (cntd.) Summary of simulated lattice actions with $N_f = 2 + 1$ or $N_f = 3$ quark flavours.

Collab.	Ref.	N_f	gauge action	quark action
ALPHA 10A	[377]	4	Wilson	npSW
CalLat 17, 18	[378, 379]	2 + 1 + 1	tadSym	HISQ *
ETM 10, 10E, 11, 11D, 12C, 13, 13A, 13D, 15E, 16	[221, 222, 380–387]	2 + 1 + 1	Iwasaki	tmWil
ETM 14A, 14B, 14E, 15, 15C, 17E	[387–392]	2 + 1 + 1	Iwasaki	tmWil ⁺
FNAL/MILC 12B, 12C, 13, 13C, 13E, 14A, 17, 18	[94, 393–399]	2 + 1 + 1	tadSym	HISQ
HPQCD 14A, 15B, 18	[400–402]	2 + 1 + 1	tadSym	HISQ
MILC 12C, 13A, 18	[336, 403, 404]	2 + 1 + 1	tadSym	HISQ
Perez 10	[405]	4	Wilson	npSW
PNDME 13, 15, 15A, 16, 18, 18A, 18B	[406–412]	2 + 1 + 1	tadSym	HISQ [†]

* The calculation uses Möbius domain-wall fermions (M-DW) in the valence sector.

⁺ The calculation uses Osterwalder-Seiler fermions [265] in the valence-quark sector.

[†] The calculation uses mean-field improved clover fermions (mfSW) in the valence-quark sector.

Table 75: Summary of simulated lattice actions with $N_f = 4$ or $N_f = 2 + 1 + 1$ quark flavours.

Collab.	Ref.	N_f	Gauge action	sea	Quark actions	
					light valence	heavy
ALPHA 11, 12A, 13, 14, 14B	[116, 413–416]	2	plaquette	npSW	npSW	HQET
ALPHA 13C	[417]	2	plaquette	npSW	npSW	npSW
Blossier 18	[418]	2	plaquette	npSW	npSW	npSW
Atoui 13	[419]	2	tlSym	tmWil	tmWil	tmWil
ETM 09, 09D, 11B, 12A, 12B, 13B, 13C	[139, 211, 420–424]	2	tlSym	tmWil	tmWil	tmWil
ETM 11A	[106]	2	tlSym	tmWil	tmWil	tmWil, static
TWQCD 14	[425]	2	plaquette	oDW	oDW	oDW

Table 76: Summary of lattice simulations $N_f = 2$ sea quark flavours and with b and c valence quarks.

Collab.	Ref.	N_f	Gauge action	sea	Quark actions light valence	heavy
χ QCD 14	[426]	2+1	Iwasaki	DW	overlap	overlap
Datta 17	[427]	2+1	Iwasaki, Iwasaki +DSDR ⁺	DW	DW	RHQ
Detmold 16	[428]	2+1	Iwasaki, Iwasaki +DSDR ⁺	DW	DW	RHQ
FNAL/MILC 04, 04A, 05, 08, 08A, 10, 11, 11A, 12, 13B	[294, 429–437]	2+1	tadSym	Asqtad	Asqtad	Fermilab
FNAL/MILC 14, 15C, 16	[438–440]	2+1	tadSym	Asqtad	Asqtad*	Fermilab*
FNAL/MILC 15, 15D, 15E	[441–443]	2+1	tadSym	Asqtad	Asqtad	Fermilab
HPQCD 06, 06A, 08B, 09, 13B	[444–448]	2+1	tadSym	Asqtad	Asqtad	NRQCD
HPQCD 12, 13E	[449, 450]	2+1	tadSym	Asqtad	HISQ	NRQCD
HPQCD 15	[451]	2+1	tadSym	Asqtad	HISQ [†]	NRQCD [†]
HPQCD 17	[452]	2+1	tadSym	Asqtad	HISQ	HISQ, NRQCD
HPQCD/UKQCD 07, HPQCD 10A, 10B, 11, 11A, 12A, 13C	[107, 302, 453–457]	2+1	tadSym	Asqtad	HISQ	HISQ
JLQCD 16	[317]	2+1	tlSym	M-DW	M-DW	M-DW
JLQCD 17B	[458]	2+1	tlSym	DW	DW	DW
Maezawa 16	[459]	2+1	tlSym	HISQ	HISQ	HISQ
Meinel 16	[460]	2+1	Iwasaki, Iwasaki + DSDR ⁺	DW	DW	RHQ
PACS-CS 11	[135]	2+1	Iwasaki	npSW	npSW	Tsukuba
RBC/UKQCD 10C, 14A	[108, 461]	2+1	Iwasaki	DW	DW	static
RBC/UKQCD 13A, 14, 15	[462–464]	2+1	Iwasaki	DW	DW	RHQ
RBC/UKQCD 17	[465]	2+1	Iwasaki	DW/M-DW	M-DW	M-DW
ETM 13E, 13F, 14E, 17D, 18	[390, 466–469]	2+1+1	Iwasaki	tmWil	tmWil	tmWil

* Asqtad for u , d and s quark; Fermilab for b and c quark.

⁺ An additional weighting factor known as the dislocation suppressing determinant ratio (DSDR) is added to the gauge action [83].

[†] HISQ for u , d , s and c quark; NRQCD for b quark.

Table 77: Summary of lattice simulations with $N_f = 2 + 1$ sea quark flavours and b and c valence quarks.

Collab.	Ref.	N_f	Gauge action	sea	Quark actions	
					light	valence heavy
ETM 16B	[470]	2+1+1	Iwasaki	tmWil	tmWil	tmWil ⁺
FNAL/MILC 12B, 13, 14A	[393, 395, 398]	2+1+1	tadSym	HISQ	HISQ	HISQ
FNAL/MILC 17	[94]	2+1+1	tadSym	HISQ	HISQ	HISQ
FNAL/MILC/TUMQCD 18	[471]	2+1+1	tadSym	HISQ	HISQ	HISQ
Gambino 17	[472]	2+1+1	Iwasaki	tmWil	tmWil	tmWil ⁺
HPQCD 13, 17A	[473, 474]	2+1+1	tadSym	HISQ	HISQ	NRQCD
HPQCD 17B	[475]	2+1+1	tadSym	HISQ	HISQ	HISQ, NRQCD
RM123 17	[476]	2+1+1	Iwasaki	tmWil	tmWil	tmWil ⁺

⁺ The calculation uses Osterwalder-Seiler fermions [265] in the valence quark sector.

Table 78: Summary of lattice simulations with $N_f = 2 + 1 + 1$ sea quark flavours and b and c valence quarks.

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