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Status of lattice calculations of B-meson decays and mixing

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Abstract. The present status of lattice calculations of $f_{\rm B}$, $B_{\rm B}$ and SU(3) flavour breaking ratios such as $f_{\rm B_s}/f_{\rm B}$ is reviewed. Particular attention is devoted to systematic uncertainties, such as those arising from the lack of simulation data for dynamical quarks with realistic masses, and the related difficulties associated with chiral extrapolations. Global averages for decay constants and mixing parameters are presented (Table 1), and the procedures to obtain them are discussed in detail.

PACS. 11.30.Er CP violation – 12.38.Gc Lattice QCD calculations – 14.40.Nd Bottom mesons

1 Introduction

A lot of activity is currently devoted to pin down the elements of the CKM matrix $V_{\rm CKM}$. In the Standard Model $V_{\rm CKM}$ is unitary, which implies triangle relations like

$$V_{\rm ud}V_{\rm ub}^* + V_{\rm cd}V_{\rm cb}^* + V_{\rm td}V_{\rm tb}^* = 0. \qquad (1)$$

Any deviation from unitarity is interpreted as a signature of "new physics". In order to probe this scenario, experimental and theoretical inputs are being used to overconstrain the elements of $V_{\rm CKM}$. However, relations between measurable quantities and CKM matrix elements involving heavy quarks are usually afflicted with large hadronic uncertainties. A typical example are the mass differences $\Delta M_{\rm d}$ and $\Delta M_{\rm s}$ in the $B^0\,\bar{B}^0$ and $B_{\rm s}^0\,\bar{B}_{\rm s}^0$ systems:

$$\Delta M_{\rm d} = \frac{G_{\rm F}^2 M_{\rm W}^2}{6\pi^2}\eta_{\rm B} S(\tfrac{m_t}{M_{\rm W}})\, f_{\rm B}^2 \widehat{B}_{\rm B} |V_{\rm td}V_{\rm tb}^*|^2, \qquad (2)$$

$$\frac{\Delta M_{\rm s}}{\Delta M_{\rm d}} = \xi^2 \frac{m_{\rm B_s}}{m_{\rm B}}\frac{|V_{\rm ts}|^2}{|V_{\rm td}|^2}, \quad \xi = \frac{f_{\rm B_s}\sqrt{\widehat{B}_{\rm B_s}}}{f_{\rm B}\sqrt{\widehat{B}_{\rm B}}}. \qquad (3)$$

The limited accuracy with which the CKM elements on the rhs. are known comes from theoretical uncertainties in the decay constants $f_{\rm B}$, $f_{\rm B_s}$ and the B-parameters $B_{\rm B}$ and $B_{\rm B_s}$. These quantities have been computed using lattice calculations, an approach which was specifically designed for a systematic non-perturbative treatment of QCD. In order to chart the progress made and to provide global estimates for these quantities, the CKM-Lattice Working Group was founded in February 2002 [1,2]. Here I report on recent results and present global averages.

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2 Heavy quarks on the lattice

Systematic effects in lattice simulations, as well as the more specific problems of treating heavy quarks on the lattice have been described many times in the literature (see e.g. [3,4]).

The great majority of lattice results for heavy-light decay constants and B-parameters have to date been obtained in the quenched approximation, where quark loops are neglected in the evaluation of observables. The effects of non-zero lattice spacing a (lattice artefacts) have been studied extensively, though, and in many cases an extrapolation to the continuum limit was performed. In order to guarantee a smooth continuum behaviour, the non-perturbative renormalisation of quark bilinears and four-fermion operators in the discretised theory proved to be instrumental [5,6]. For some quantities, the level of precision that can be reached in the continuum limit in the quenched approximation is about 5%. This then implies that current estimates for decay constants are completely dominated by quenching effects. As a consequence, most collaborations now focus on simulations with $N_{\rm f} = 2$ or 3 dynamical quark flavours.

Another important systematic effect is the use of unphysical values of the light quark masses $m_{\rm u}$, $m_{\rm d}$, both in quenched and unquenched simulations. In particular, commonly used algorithms for dynamical quarks slow down considerably for masses smaller than about $m_{\rm s}/2$. Several proposals to address this problem have been made [7,8,9,10], but the effectiveness of each approach must be studied in more detail. In order to make contact with the chiral regime, one currently relies on extrapolations in the light quark mass, using Chiral Perturbation Theory (ChPT) as a guide. It has only been realised relatively recently that this can introduce large uncertainties, since chiral logarithms are not necessarily under control [11,12,13].

Whenever one deals with heavy quarks on a lattice of spatial extent L and lattice spacing a, one is faced with a multi-scale problem, in the sense that the following three inequalities cannot be satisfied simultaneously:

$$am_{\rm b} \ll 1, \quad m_\pi L \gg 1, \quad L/a \lesssim 50. \tag{4}$$

Violation of the first relation implies the presence of large lattice artefacts, the second inequality must be satisfied if one aims for small finite-volume effects, and the third is dictated by capacities of current computers.

Several strategies to deal with this problem have been applied over many years, among them the "static approximation" [14], the non-relativistic formulation (NRQCD) [15], the so-called "Fermilab-approach" [16], and extrapolations in the heavy quark mass.

3 Recent results

We now discuss results from several recent calculations, which will also illustrate some of the issues raised earlier.

The first topic is a recent benchmark calculation of $f_{\rm D_s}$ in the quenched approximation [17]. For lattice simulations, the $D_{\rm s}$ meson is particularly appealing, since both the charm and the strange quark can be treated directly, i.e. no extrapolations are required to make contact with the physical values of the valence quark masses. In ref. [17] the potentially large lattice artefacts arising from relativistic c-quarks are eliminated through an extrapolation to the continuum limit. By means of employing a lattice action in which the leading lattice artefacts of $\mathrm{O}(a)$ were removed non-perturbatively [18], the convergence of the results to the continuum could be accelerated. Furthermore, the authors used a non-perturbative estimate of the renormalisation factor which connects the axial current on the lattice with its continuum counterpart [19].

The main result in ref. [17] is the continuum result for $f_{\rm D_s}$ in units of the hadronic radius r_0 [20], namely $r_0 f_{\rm D_s} = 0.638 \pm 0.024$, which translates into

$$f_{\rm D_s} = 252 \pm 9\,\mathrm{MeV} \tag{5}$$

if the phenomenological value $r_0 = 0.5\,\mathrm{fm}$ is inserted. It is worth emphasising that the only remaining uncertainty is due to quenching. A crude estimate of the quenching error is obtained through the scale uncertainty, i.e. the fact that different quantities yield different estimates for the lattice scale in the quenched approximation. The typical size of this ambiguity is about 10% [21].

In another recent calculation by de Divitiis *et al.*[22] a new strategy to deal with the multi-scale problem was applied. Here the condition $m_\pi L \gg 1$ was sacrificed in favour of $am_{\rm b} \ll 1$. In this way one is able to accommodate a fully relativistic b-quark, and a physically meaningful result is obtained if one succeeds in determining the distortion due to the unphysically small volume. The key observation is that this can be achieved through a sequence of finite-size scaling steps, which relate the results obtained for several lattice sizes L_0, L_1, ...:

$$f_{\rm B}(L_0) \to f_{\rm B}(L_1) \to f_{\rm B}(L_2) \to \ \ldots \tag{6}$$

$$f_{\rm B}(L_{k+1}) = f_{\rm B}(L_k)\,\sigma_{\rm B}(L_k), \quad L_{k+1} > L_k \tag{7}$$

Since the value of $f_{\rm B}$ for the smallest volume, i.e. $f_{\rm B}(L_0)$ and the so-called "step-scaling function" $\sigma_{\rm B}(L_k)$ can be computed in the continuum limit, one obtains a result for $f_{\rm B}$ for physically large volumes in a controlled manner. The main assumption, which was verified explicitly in ref. [22], is that the finite-size effects depend only weakly on the heavy quark mass. Starting from $L_0 = 0.4\,\mathrm{fm}$, a total of two scaling steps were performed, each time doubling the lattice size. The initial value of the decay constant in the continuum is $f_{\rm B}(L_0) = 471(2)\,\mathrm{MeV}$, and together with the continuum estimates for the step scaling functions, $\sigma_{\rm B}(L_0) = 0.400(3)$ and $\sigma_{\rm B}(L_1) = 0.92(4)$ one obtains

$$f_{\rm B} = 173 \pm 8 \pm 4\,\mathrm{MeV}, \tag{8}$$

at $L_2 = 1.6\,\mathrm{fm}$, which is large enough to be identified with the infinite volume limit. The quoted uncertainties cover all errors, except that due to quenching. In a similar way the authors of ref. [22] obtain

$$f_{\rm B_s} = 194 \pm 6 \pm 4\,\mathrm{MeV}, \tag{9}$$

$$f_{\rm D} = 217 \pm 7 \pm 5\,\mathrm{MeV}, \quad f_{\rm D_s} = 239 \pm 5 \pm 5\,\mathrm{MeV},$$

the result for $f_{\rm D_s}$ being compatible with ref. [17].

As mentioned earlier, the issue of chiral logarithms in SU(3)-flavour-breaking ratios such as $f_{\rm B_s}/f_{\rm B}$ or ξ has attracted a lot of attention recently. The dependence of heavy-light decay constants on the mass of the light quark has usually been modelled according to a naive linear ansatz, in which chiral logarithms, as well as analytic terms arising at NLO in ChPT, are neglected. The full expression at NLO reads

$$\frac{f_{\rm B_s}}{f_{\rm B}} - 1 = (m_{\rm K}^2 - m_\pi^2) f_2(\mu) - \frac{1+3g^2}{(4\pi f_\pi)^2}\left[\tfrac{1}{2} I_{\rm P}(m_{\rm K}) + \tfrac{1}{4} I_{\rm P}(m_\eta) - \tfrac{3}{4} I_{\rm P}(m_\pi)\right] \tag{10}$$

where $I_{\rm P}(m_{\rm PS}) = m_{\rm PS}^2 \ln(m_{\rm PS}^2/\mu^2)$ and f_2 is a low-energy constant. As was pointed out by Kronfeld & Ryan [11], the inclusion of chiral logarithms in the chiral extrapolation of lattice data for heavy-light decay constants can drastically change $f_{\rm B_s}/f_{\rm B}$ and consequently also ξ, which enters fits to the CKM parameters. By assuming $g^2 = g^2_{D^*D\pi} = 0.35$ [23] and $f_2 = 0.5(3)\,\mathrm{GeV}^{-2}$, Kronfeld and Ryan conclude that $\xi = 1.32 \pm 0.10$, which is more than 10% larger than the global estimate quoted by Ryan in 2001 [24]. It is somewhat ironic that the quantity ξ, which for a long time had been assumed to be only weakly sensitive to systematic effects, should be subjected to such a large uncertainty. Note that the corresponding ratio of B-parameters, $B_{\rm B_s}/B_{\rm B}$ is largely unaffected, since the coefficient of the chiral logarithm is $\propto (1-3g^2)$, which is close to zero.

The predicted enhancement of $f_{\rm B_s}/f_{\rm B}$ due to chiral logs seems plausible, since the corresponding ratio in the

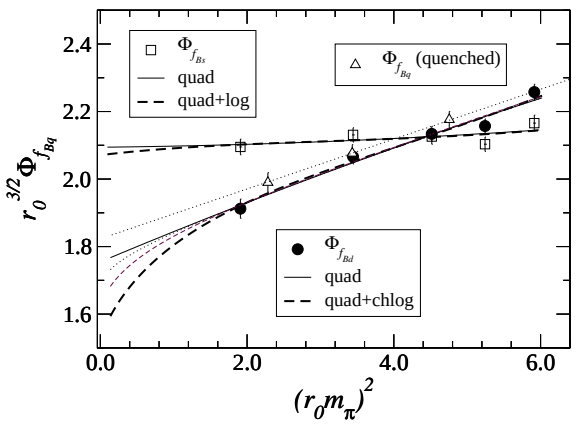

Fig. 1. Dependence of $\Phi_{f_{\rm B}}$ and $\Phi_{f_{\rm B_s}}$ on the light quark mass.

light quark sector, $f_{\rm K}/f_\pi$, is known to come out too small in quenched QCD, if only a naive linear quark mass dependence is assumed [25]. In ref. [13] it was argued that the chiral logarithms in $f_{\rm B_s}/f_{\rm B}$ and $f_{\rm K}/f_\pi$ are nearly of the same size, so that one would expect $f_{\rm B_s}/f_{\rm B} \approx f_{\rm K}/f_\pi = 1.22$, which is compatible with [11], but closer to previous global estimates. The key question for any future determination is whether or not the quark masses used in the simulation are light enough so that ChPT at NLO gives a good description. In the context of $f_{\rm B_s}/f_{\rm B}$ this was studied recently by the JLQCD Collaboration [26]. The dependence of $\Phi_{f_{\rm B}} = f_{\rm B}\sqrt{M_{\rm B}}$ and $\Phi_{f_{\rm B_s}}$ on the light quark mass is shown in Fig. 1. JLQCD conclude that chiral logarithms are not observed in the studied mass range. The modelling of the effect due to chiral logs yields a drop of up to 11% in $f_{\rm B}$ relative to $f_{\rm B_s}$. The corresponding enhancement of $f_{\rm B_s}/f_{\rm B}$ is of the same order of magnitude as that of ref. [11].

4 Global estimates: Strategies & Results

Before I present global averages for decay constants and B-parameters, I would like to outline the strategy which was used to obtain them. The main point to note is that a global analysis of lattice results is complicated by the fact that systematics can vary substantially among results from different collaborations. The main differences lie in the treatment of lattice artefacts, the choice of quantity that sets the lattice scale, the renormalisation procedure for currents and four-fermion operators on the lattice, and the details of extrapolations in the quark masses, either down to the chiral regime, or, where applicable, to the mass of the b-quark. Therefore, a straightforward global average of results is unreliable.

For the procedure applied here I have decided to focus on the quenched approximation: although unphysical, the quenched approximation is known to describe the light hadron spectrum at the level of 10% [21]. Furthermore, a wealth of results is available for $N_{\rm f} = 0$: the continuum limit has been taken in almost all recent quenched calculations, and other systematic effects have been studied thoroughly.

Simulations with dynamical quarks, either for $N_{\rm f} = 2$ or 3 have not yet reached the same level of maturity. The masses of the sea quarks are still quite large, so that their effects on observables are likely to be suppressed. Performing reliable continuum extrapolations is much more expensive, all of which implies that a clear separation of sea quark effects from lattice artefacts is very difficult. There are, however, attempts to expose the effects of unquenching by focusing on ratios in which systematic uncertainties other than quenching largely cancel. For instance, the CP-PACS [27] and MILC [28] collaborations have found $f_{\rm D_s}^{N_{\rm f}=2}/f_{\rm D_s}^{N_{\rm f}=0} \approx 1.10$ at $a \approx 0.1\,$fm, which implies a 10%-enhancement in $f_{\rm D_s}$ due to dynamical quark effects. No extrapolations in the valence quark masses are required, but it remains to be seen whether this number is stable against lattice artefacts and whether lighter sea quarks lead to a significant change.

As regards chiral logarithms in ratios like $f_{\rm B_s}/f_{\rm B}$ and ξ, their effects have not been quantified from first principles so far. In what follows, I shall therefore use results assuming the naive (LO) dependence on the light quark mass, but allow for a 10% *increase* in $f_{\rm B_s}/f_{\rm B}$ and $f_{\rm D_s}/f_{\rm D}$.

The starting point for the global analysis is $f_{\rm D_s}$ in the quenched approximation ($N_{\rm f} = 0$). The recent benchmark calculation [17] demonstrates that the continuum value in quenched QCD (for a given quantity that sets the scale) is obtained with a total accuracy of 4%. The central value may vary between 225 and 255 MeV, depending on the chosen scale. Thus we have

$$f_{\rm D_s}^{N_{\rm f}=0} = 240 \pm 10\,({\rm stat}) \pm 15\,({\rm scale})\,{\rm MeV}. \qquad (11)$$

In order to estimate $f_{\rm D}$ one can divide this result by $f_{\rm D_s}/f_{\rm D} = 1.12 \pm 0.02^{+0.11}_{-0.00}$. This is the number quoted by Ryan [24] for $N_{\rm f} = 0$, except for the additional 10% asymmetric uncertainty due to chiral logs. This yields

$$f_{\rm D}^{N_{\rm f}=0} = 214 \pm 10\,({\rm stat}) \pm 13\,({\rm scale})^{+\ 0}_{-19}\,(\chi{\rm log})\,{\rm MeV}. \quad (12)$$

In Fig. 2 the quenched global estimates of eqs. (11) and (12) are compared with recent determinations from various groups, who have used either the Fermilab approach [29, 30, 31, 27, 28], or the O(a) improved Wilson action [32, 33, 34, 17, 22] to treat the heavy quark. Note that the results from different collaborations have not been converted to a common lattice scale. Without this conversion it is not clear whether the observed spread is just indicative of the scale ambiguity, or due to some other, possibly uncontrolled systematic effect.

The next step is to account for dynamical quarks. In my view the safest procedure is to multiply the quenched values of $f_{\rm D}$ and $f_{\rm D_s}$ by the ratio

$$f_{\rm P_q}^{N_{\rm f}=2}/f_{\rm P_q}^{N_{\rm f}=0} = 1.10 \pm 0.05, \quad P = D, B, \quad q = d, s, \quad (13)$$

in which some of the systematic errors can be expected to cancel. The number in eq. (13) is based on observations in ref. [27] that dynamical quarks enhance the values of

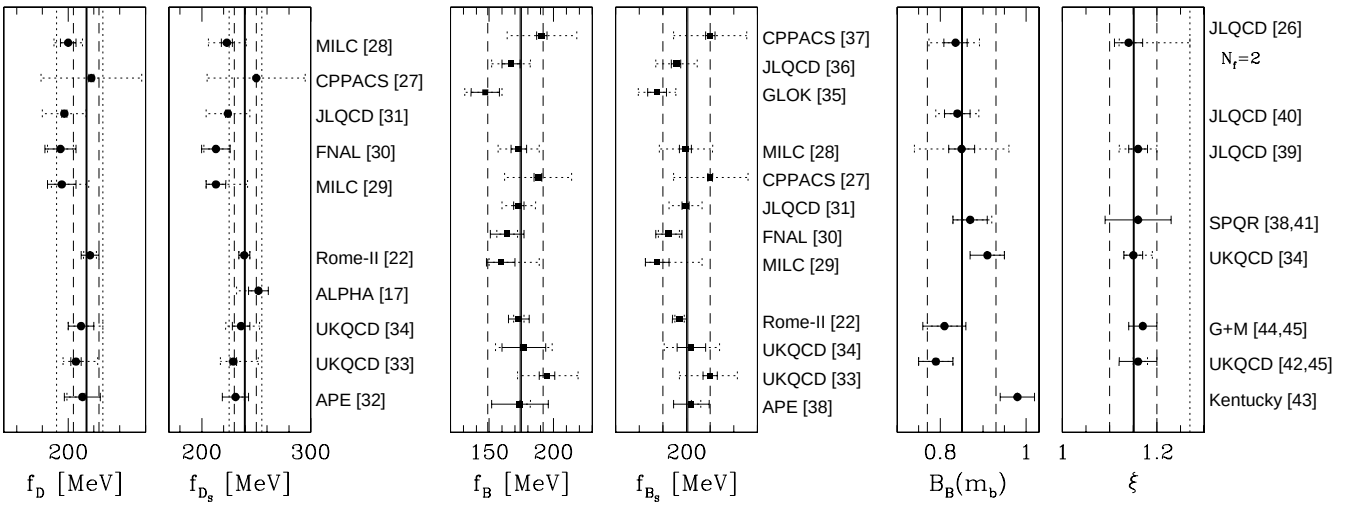

Fig. 2. Recent results for decay constants and B-parameters in the quenched approximation, compared to the global averages of eqs.(11), (12), (15), (17) and (18) (solid vertical lines). For D-mesons the dashed lines indicate the statistical error, while the systematic error is represented by the dotted lines. For the B-system the dashed vertical lines denote the total error, with the uncertainty due to chiral logs included in quadrature. Dotted error bars on individual determinations indicate the quoted systematic error. The result for $B_{\rm B}$ and ξ in [26] was obtained for $N_{\rm f} = 2$.

decay constants by $5 - 15\,\%$, largely independent of the valence quark contents. Thus we find

$$\begin{aligned} f_{\rm D_s}^{N_{\rm f}=2} &= 264 \pm 11\,({\rm stat}) \pm 22\,({\rm quen})\,{\rm MeV} \qquad (14)\\ f_{\rm D}^{N_{\rm f}=2} &= 235 \pm 11\,({\rm stat}) \pm 19\,({\rm quen})\,^{+\,0}_{-21}\,(\chi{\rm log})\,{\rm MeV}\,, \end{aligned}$$

where I have combined the scale uncertainty and the error in eq. (13) into a total quenching error. Here we make no attempt to try and estimate the effects of a dynamical strange quark, and hence the above numbers are our final results for $f_{\rm D}$ and $f_{\rm D_s}$ which we list once more in Table 1.

The procedure to obtain estimates for $f_{\rm B}$ and $f_{\rm B_s}$ is entirely analogous, with one important difference: unlike the case of D-mesons, there is not yet a quenched benchmark calculation of $f_{\rm B_s}$, which would yield the total error within the quenched approximation. As a starting point we therefore use the "global representation" of quenched results quoted by Ryan [24], i.e.

$$f_{\rm B_s}^{N_{\rm f}=0} = 200 \pm 20\,{\rm MeV}. \qquad (15)$$

Here the error has been obtained by requiring consistency with a number of different results being subjected to different systematics. Dividing by [24]

$$f_{\rm B_s}/f_{\rm B} = 1.15 \pm 0.03^{+0.12}_{-0.00}\,(\chi{\rm log}) \qquad (16)$$

gives

$$f_{\rm B}^{N_{\rm f}=0} = 174 \pm 18\,^{+\,0}_{-17}\,(\chi{\rm log})\,{\rm MeV}, \qquad (17)$$

and multiplication with the ratio of eq. (13) yields the numbers listed in Table 1. In Fig. 2 the global quenched estimates are again compared to individual results obtained using NRQCD [35,36,37], the Fermilab approach [29,30,31,27,28], the finite-size scaling technique [22], as well as extrapolations in the heavy quark mass from the region of the charm quark mass [38,33,34].

Table 1. Global estimates for decay constants and B-parameters. The numbers are understood to refer to full QCD.

$f_{\rm D_s}$	$= 264 \pm 11 \pm 22\,({\rm quen})\,{\rm MeV}$
$f_{\rm D}$	$= 235 \pm 11 \pm 19\,({\rm quen})\,^{+\,0}_{-21}\,(\chi{\rm log})\,{\rm MeV}$
$f_{\rm B_s}$	$= 220 \pm 25\,{\rm MeV}$
$f_{\rm B}$	$= 191 \pm 23\,^{+\,0}_{-19}\,(\chi{\rm log})\,{\rm MeV}$
$\widehat{B}_{\rm B}$	$= \widehat{B}_{\rm B_s} = 1.34 \pm 0.12$
ξ	$= 1.15 \pm 0.05\,^{+0.12}_{-0.00}$
$f_{\rm B_s}\sqrt{\widehat{B}_{\rm B_s}}$	$= 255 \pm 31\,{\rm MeV}$
$f_{\rm B}\sqrt{\widehat{B}_{\rm B}}$	$= 221 \pm 28\,^{+\,0}_{-22}\,(\chi{\rm log})\,{\rm MeV}$

For the B-parameters $B_{\rm B}$, $B_{\rm B_s}$ and the ratio ξ, there are not so many results available, and only one recent calculation uses dynamical quarks [26]. It is then clear that systematics cannot be studied as thoroughly as for decay constants. In particular, the continuum limit has not been taken in any study so far. It turns out, though, that results for B-parameters and ξ are broadly consistent, regardless of whether NRQCD [39,40,26], relativistic heavy quarks [34,38,41] or the static approximation [42,43,44,45] are used in simulations. Apparently, dynamical quarks do not lead to a significant enhancement of $B_{\rm B}$ or $B_{\rm B_s}$ [26], contrary to what is observed for decay constants. Chiral logarithms in the SU(3)-flavour breaking ratio $B_{\rm B_s}/B_{\rm B}$ are suppressed, and a linear extrapolation in the light quark mass yields a value compatible with one. All published data are then consistent with the global representation:

$$\begin{aligned} B_{\rm B}(m_b) &= 0.85 \pm 0.08 \;\Rightarrow\; \widehat{B}_{\rm B}^{\rm NLO} = 1.34 \pm 0.12\\ B_{\rm B_s}(m_b) &= 0.85 \pm 0.08 \;\Rightarrow\; \widehat{B}_{\rm B_s}^{\rm NLO} = 1.34 \pm 0.12 \qquad (18)\\ B_{\rm B_s}/B_{\rm B} &= 1.00 \pm 0.03, \quad \xi = 1.15 \pm 0.05^{+0.12}_{-0.00}\,(\chi{\rm log}). \end{aligned}$$

The value of ξ is obtained by combining eq. (16) with the above result for $B_{\rm B_s}/B_{\rm B}$. The collection of global estimates in Table 1 is consistent with refs. [1,24,47].

5 Future studies

How can the current global estimates be improved in order to sharpen the constraints on CKM parameters? There are several areas in which progress can be made.

Future efforts must surely focus on dynamical simulations, but the quenched approximation remains helpful for the understanding of several issues. In my view, a quenched benchmark value of $f_{\rm B_s}$ is very important to quantify the uncertainties arising from discretisation and renormalisation effects. Although this is precisely the aim of the finite-size scaling method of [22], an independent check using a different method should be performed. Here one may think of an interpolation between results obtained in the static approximation and those obtained near $m_{\rm c}$, *after* the continuum limit has been taken. With the advent of methods that allow for precise non-perturbative determinations of the renormalisation factor for the axial current [48], as well as for a better signal/noise ratio in the static approximation [49], one can obtain results with much higher accuracy than previously possible [50]. This strategy may also be extended to B-parameters [51].

Obviously the most pressing problem is to simulate small dynamical quark masses more efficiently. The rôle of "improved staggered quarks" has been vigorously emphasised [9] in this context, with first results being reviewed in [52]. Eventually such efforts should yield not only estimates for, say, $f_{\rm B_s}^{N_{\rm f}=3}$, but should also settle the issue of chiral logarithms in $f_{\rm B_s}/f_{\rm B}$, ξ and $f_{\rm K}/f_\pi$. The latter is, in fact, explored separately by a number of groups using different algorithms and discretisations [53,26]. In this context, the so-called Grinstein ratio $(f_{\rm B_s}/f_{\rm B})\,/(f_{\rm D_s}/f_{\rm D})$ in which the chiral logarithms cancel [54], has been suggested as a more reliable way to determine $f_{\rm B_s}/f_{\rm B}$ on the lattice [26], once $f_{\rm D_s}$ and $f_{\rm D}$ have been measured at high-luminosity charm factories such as CESR-c [55]. This approach, however, can only succeed if the quark masses used in simulations are light enough so that the data are consistently described by ChPT at NLO.

Finally, one may think of better ways to obtain global averages. This may entail potentially laborious re-analyses of existing simulation data. In order to facilitate a comparison all results should be converted to a common scale, such as r_0. Systematic errors should best be quantified after an extrapolation to the continuum limit. Here on might concentrate on ratios like $f_{\rm B_s}/f_{\rm D_s}$ for fixed $N_{\rm f}$, or $f_{\rm D_s}^{N_{\rm f}=2}/f_{\rm D_s}^{N_{\rm f}=0}$. Thereby one has a better chance to expose the effects of replacing c by b-quarks and those due to dynamical quarks.

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