

## A List of acronyms

$B\chi$ PT	baryonic chiral perturbation theory	LO	leading order
BCL	Bourenly-Caprini-Lellouch	LW	Lüscher-Weisz
BGL	Boyd-Grinstein-Lebed	MC	Monte Carlo
BK	Becirevic-Kaidalov	MM	minimal MOM
BSM	beyond standard model	MOM	momentum subtraction
BZ	Ball-Zwicky	$\overline{MS}$	modified minimal subtraction scheme
$\chi$ PT	chiral perturbation theory	NDR	naive dimensional regularization
CKM	Cabibbo-Kobayashi-Maskawa	nEDM	nucleon electric dipole moment
CLN	Caprini-Lellouch-Neubert	NGB	Nambu-Goldstone bosons
CP	charge-parity	NLO	next-to-leading order
CPT	charge-parity-time reversal	NME	nucleon matrix elements
CVC	conserved vector current	NNLO	next-to-next-to-leading order
DSDR	dislocation suppressing determinant ratio	NP	nonperturbative
DW	domain wall	npHQET	nonperturbative heavy-quark effective theory
DWF	domain wall fermion	NRQCD	nonrelativistic QCD
EDM	electric dipole moment	NSPT	numerical stochastic perturbation theory
EFT	effective field theory	OPE	operator product expansion
EM	electromagnetic	PCAC	partially-conserved axial current
ESC	excited state contributions	PDF	parton distribution function
EW	electroweak	PDG	particle data group
FCNC	flavour-changing neutral current	QCD	quantum chromodynamics
FH	Feynman-Hellman	QED	quantum electrodynamics
FSE	finite-size effects	QED <sub>L</sub>	formulation of QED in finite volume (see [1])
FV	finite volume	QED <sub>TL</sub>	formulation of QED in finite volume (see [2])
GF	gradient flow	RG	renormalization group
GGOU	Gambino-Giordano-Ossola-Uraltsev	RGI	renormalization group invariant
GRS	Gasser-Rusetsky-Scimemi	RH	R. Hill
HEX	hypercubic stout	RHQ	relativistic heavy-quark
HISQ	highly-improved staggered quarks	RHQA	relativistic heavy-quark action
HM $\chi$ PT	heavy-meson chiral perturbation theory	RI-MOM	regularization-independent momentum subtraction (also RI/MOM)
HMC	hybrid Monte Carlo	RI-SMOM	regularization-independent symmetric momentum (also RI/SMOM)
HMrS $\chi$ PT	heavy-meson rooted staggered chiral perturbation theory	RMS	root mean square
HQET	heavy-quark effective theory	S $\chi$ PT	staggered chiral perturbation theory
IR	infrared		
isoQCD	isospin-symmetric QCD		
LD	long distance		
LEC	low-energy constant		

SD	short distance
SF	Schrödinger functional
SIDIS	semi-inclusive deep-inelastic scattering
SM	standard model
SSF	step-scaling function
SUSY	supersymmetric
SW	Sheikholeslami-Wohlert
UT	unitarity triangle
UV	ultraviolet

## B Appendix

### B.1 Inclusion of electromagnetic effects

Electromagnetism on a lattice can be formulated using a naive discretization of the Maxwell action  $S[A_\mu] = \frac{1}{4} \int d^4x \sum_{\mu,\nu} [\partial_\mu A_\nu(x) - \partial_\nu A_\mu(x)]^2$ . Even in its noncompact form, the action remains gauge invariant. This is not the case for non-Abelian theories for which one uses the traditional compact Wilson gauge action (or an improved version of it). Compact actions for QED feature spurious photon-photon interactions which vanish only in the continuum limit. This is one of the main reason why the noncompact action is the most popular so far. It was used in all the calculations presented in this review. Gauge-fixing is necessary for noncompact actions because of the usual infinite measure of equivalent gauge orbits which contribute to the path integral. It was shown [3, 4] that gauge-fixing is not necessary with compact actions, including in the construction of interpolating operators for charged states.

Although discretization is straightforward, simulating QED in a finite volume is more challenging. Indeed, the long range nature of the interaction suggests that important finite-size effects have to be expected. In the case of periodic boundary conditions, the situation is even more critical: a naive implementation of the theory features an isolated zero-mode singularity in the photon propagator. It was first proposed in [5] to fix the global zero-mode of the photon field  $A_\mu(x)$  in order to remove it from the dynamics. This modified theory is generally named QED<sub>TL</sub>. Although this procedure regularizes the theory and has the right classical infinite-volume limit, it is nonlocal because of the zero-mode fixing. As first discussed in [6], the nonlocality in time of QED<sub>TL</sub> prevents the existence of a transfer matrix, and therefore a quantum-mechanical interpretation of the theory. Another prescription named QED<sub>L</sub>, proposed in [1], is to remove the zero-mode of  $A_\mu(x)$  independently for each time slice. This theory, although still nonlocal in space, is local in time and has a well-defined transfer matrix. Whether these nonlocalities constitute an issue to extract infinite-volume physics from lattice-QCD+QED<sub>L</sub> simulations is, at the time of this review, still an open question. However, it is known through analytical calculations of electromagnetic finite-size effects at  $\mathcal{O}(\alpha)$  in hadron masses [1, 6–12], meson leptonic decays [10, 12], and the hadronic vacuum polarization [13] that QED<sub>L</sub> does not suffer from a problematic (e.g., UV divergent) coupling of short- and long-distance physics due to its nonlocality, and is likely safe to use for these quantities. Another strategy, first proposed in [14] and used by the QCDSF collaboration, is to bound the zero-mode fluctuations to a finite range. Although more minimal, it is still a nonlocal modification of the theory and so far finite-size effects for this scheme have not been investigated. Two proposals for local formulations of finite-volume QED emerged. The first one described in [15] proposes to use massive photons to regulate zero-mode singularities, at the price of (softly) breaking gauge invariance. The second one presented in [4], based on earlier works [16, 17], avoids the zero-mode issue by using anti-periodic boundary conditions for  $A_\mu(x)$ . In this approach, gauge invariance requires the fermion field to undergo a charge conjugation transformation over a period, breaking electric charge conservation. These local approaches have the potential to constitute cleaner approaches to finite-volume QED. They have led to first numerical studies at unphysical masses [18, 19], but were not used in any calculation reviewed in this paper.

Once a finite-volume theory for QED is specified, there are various ways to compute QED effects themselves on a given hadronic quantity. The most direct approach, first used in [5], is to include QED directly in the lattice simulations and assemble correlation functions from

charged quark propagators. Another approach proposed in [7], is to exploit the perturbative nature of QED, and compute the leading-order corrections directly in pure QCD as matrix elements of the electromagnetic current. Both approaches have their advantages and disadvantages and as shown in [20], are not mutually exclusive. A critical comparative study can be found in [21].

Finally, most of the calculations presented here made the choice of computing electromagnetic corrections in the electro-quenched approximation. In this limit, one assumes that only valence quarks are charged, which is equivalent to neglecting QED corrections to the fermionic determinant. This approximation reduces dramatically the cost of lattice-QCD+QED calculations since it allows the reuse of previously generated QCD configurations. If QED is introduced perturbatively through current insertions, the electro-quenched approximation avoids computing disconnected contributions coming from the electromagnetic current in the vacuum, which are generally challenging to determine precisely. The electromagnetic contributions from sea quarks to hadron-mass splittings are known to be flavour-SU(3) and large- $N_c$  suppressed, thus electro-quenched simulations are expected to have an  $\mathcal{O}(10\%)$  accuracy for the leading electromagnetic effects. This suppression is in principle rather weak and results obtained from electro-quenched simulations might feature uncontrolled systematic errors. For this reason, the use of the electro-quenched approximation constitutes the difference between  $\star$  and  $\circ$  in the FLAG criterion for the inclusion of isospin-breaking effects.

## B.2 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 [22], which for the vector form factor reads:

$$f_+(q^2) = \frac{f(0)}{(1 - q^2/m_{B^*}^2)(1 - \alpha q^2/m_{B^*}^2)}. \quad (516)$$

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. (516) in order to mimic the effect of multiparticle states [23]. A similar idea, extending the use of effective poles also to  $D \rightarrow \pi \ell \nu$  decays, is explored in Ref. [24]. Finally, yet another variant (RH) has been proposed by Hill in Ref. [25]. 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 [26–28], 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. [29]). 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 [28, 30–35]. Any form factor  $f$  can be shown to admit a series expansion of the form

$$f(q^2) = \frac{1}{B(q^2)\phi(q^2, t_0)} \sum_{n=0}^{\infty} a_n(t_0) z(q^2, t_0)^n, \quad (517)$$

where the squared momentum transfer is replaced by the variable

$$z(q^2, t_0) = \frac{\sqrt{t_+ - q^2} - \sqrt{t_+ - t_0}}{\sqrt{t_+ - q^2} + \sqrt{t_+ - t_0}}. \quad (518)$$

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,

$$B(q^2) = \frac{z(q^2, t_0) - z(m_{B^*}^2, t_0)}{1 - z(q^2, t_0)z(m_{B^*}^2, t_0)} = z(q^2, m_{B^*}^2). \quad (519)$$

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

$$\sum_{n=0}^{\infty} a_n^2 = \frac{1}{2\pi i} \oint \frac{dz}{z} |B(z)\phi(z)f(z)|^2, \quad (520)$$

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  $\phi$  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

$$\begin{aligned} \phi(q^2, t_0) = & \sqrt{\frac{1}{32\pi\chi_{1-}(0)}} \left( \sqrt{t_+ - q^2} + \sqrt{t_+ - t_0} \right) \\ & \times \left( \sqrt{t_+ - q^2} + \sqrt{t_+ - t_-} \right)^{3/2} \left( \sqrt{t_+ - q^2} + \sqrt{t_+} \right)^{-5} \frac{t_+ - q^2}{(t_+ - t_0)^{1/4}}, \end{aligned} \quad (521)$$

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. (521) as Boyd, Grinstein, and Lebed (BGL). The perturbative and OPE truncations imply that the bound is not strict, and one should take it as

$$\sum_{n=0}^N a_n^2 \lesssim 1, \quad (522)$$

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. (521) 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 Bourely, Caprini and Lellouch (BCL) in Ref. [29], which leads to a parameterization of the form

$$f_+(q^2) = \frac{1}{1 - q^2/m_{B^*}^2} \sum_{n=0}^N a_n^+(t_0) z(q^2, t_0)^n. \quad (523)$$

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

$$\sum_{j,k=0}^N B_{jk}(t_0) a_j^+(t_0) a_k^+(t_0) \leq 1. \quad (524)$$

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

$$t_0 = t_{\text{opt}} = (m_B + m_\pi)(\sqrt{m_B} - \sqrt{m_\pi})^2, \quad (525)$$

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

$$a_N^+ = -\frac{(-1)^N}{N} \sum_{n=0}^{N-1} (-1)^n n a_n^+. \quad (526)$$

Substituting the above constraint on  $a_N^+$  into Eq. (523) leads to the constrained BCL parameterization

$$f_+(q^2) = \frac{1}{1 - q^2/m_{B^*}^2} \sum_{n=0}^{N-1} a_n^+ \left[ z^n - (-1)^{n-N} \frac{n}{N} z^N \right], \quad (527)$$

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. (527); 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. (526) and the choice of the overall pole function. In our fits we adopt the simple expansion:

$$f_0(q^2) = \sum_{n=0}^{N-1} a_n^0 z^n. \quad (528)$$

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. [36]. 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  $\Lambda_b \rightarrow \Lambda_c$ .<sup>1</sup> Thus, as emphasized above, the control over systematic

<sup>1</sup>A 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.

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 ( $B, \pi$  and  $B_c, \pi$  for the two processes, respectively).<sup>2</sup> 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 [37–39].

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 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.

**Choice of form-factor basis for chiral-continuum extrapolations** For pseudoscalar-to-pseudoscalar transitions  $P_1 \rightarrow P_2$  (such as  $B \rightarrow \pi$  or  $B_s \rightarrow K$ ), the chiral and continuum extrapolations have often been performed in a different basis  $f_{\parallel}, f_{\perp}$  given by [40]

$$\langle P_2(p') | V^\mu | P_1(p) \rangle = \sqrt{2M_1} [v^\mu f_{\parallel}(E_2) + p_{\perp}^{\prime\mu} f_{\perp}(E_2)]. \quad (529)$$

Here,  $v^\mu = p^\mu/M_1$  is the initial-meson four-velocity,  $p_{\perp}^{\prime\mu} = p^{\prime\mu} - (v \cdot p')v^\mu$  is the projection of the final-meson momentum in the direction perpendicular to  $v^\mu$ , and the form factors are taken to be functions of  $E_2 = v \cdot p'$  (the energy of the final-state meson in the initial-meson rest frame). After the chiral and continuum extrapolations, the standard form factors are then constructed as the linear combinations

$$f_0(q^2) = \frac{\sqrt{2M_1}}{M_1^2 - M_2^2} [(M_1 - E_2)f_{\parallel}(E_2) + (E_2^2 - M_K^2)f_{\perp}(E_2)], \quad (530)$$

$$f_+(q^2) = \frac{1}{\sqrt{2M_1}} [f_{\parallel}(E_2) + (M_1 - E_2)f_{\perp}(E_2)]. \quad (531)$$

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



The decomposition (529) is motivated by heavy-meson chiral perturbation theory and is also convenient for the extraction of the form factors from the correlation functions. For example, for  $B \rightarrow \pi$ , heavy-meson chiral perturbation theory predicts, at leading-order in both the chiral and the heavy-quark expansion,

$$f_{\perp}(E_{\pi}) = \frac{1}{f_{\pi}} \frac{g_{B^*B\pi}}{E_{\pi} + \Delta_{B^*}}, \quad (532)$$

$$f_{\parallel}(E_{\pi}) = \frac{1}{f_{\pi}}, \quad (533)$$

where  $\Delta_{B^*} = M_{B^*} - M_B$ . For a general transition  $P_1 \rightarrow P_2$ , the chiral and continuum extrapolations were therefore commonly performed by fitting functions of the form

$$f_{\perp}(E_2) = \frac{1}{E_2 + \Delta_{\perp}} \left[ \dots \right] \quad (534)$$

and

$$f_{\parallel}(E_2) = \frac{1}{E_2 + \Delta_{\parallel}} \left[ \dots \right] \quad \text{or} \quad f_{\parallel}(E_2) = \left[ \dots \right] \quad (535)$$

with  $\Delta_{\perp} = M_{1^-} - M_1$  and  $\Delta_{\parallel} = M_{0^+} - M_1$ , where  $M_{1^-}$  and  $M_{0^+}$  denote the masses of the bound states with  $J^P = 1^-$  and  $J^P = 0^+$  that couple to the weak current, and the ellipsis in the brackets denote terms describing the remaining dependence on the quark masses, lattice spacing, and kinematics. The terms in front of the brackets introduce poles at  $E_2 = -\Delta$ , which corresponds to  $q^2 \approx M_{J^P}^2$  for large  $M_1$ . Depending on the process, there may be no QCD-stable bound state with  $J^P = 0^+$ , in which case this pole factor for  $f_{\parallel}$  is usually omitted.

A problem with the above prescription is that, for finite heavy-quark mass, the  $J^P$  quantum numbers of the poles appearing in the form factors are definite only in the helicity basis of the form factors, with  $J^P = 1^-$  for  $f_+$  and  $J^P = 0$  for  $f_0$ . In particular, the form factor  $f_{\parallel}$ , being a linear combination of  $f_+$  and  $f_0$ , also has a pole at the lower mass  $M_{1^-}$  that is neglected when using the above functions. The alternative is to perform the chiral-continuum extrapolations for  $f_+$  and  $f_0$  using

$$f_+(E_2) = \frac{1}{E_2 + \Delta_+} \left[ \dots \right] \quad (536)$$

and

$$f_0(E_2) = \frac{1}{E_2 + \Delta_0} \left[ \dots \right] \quad \text{or} \quad f_0(E_2) = \left[ \dots \right], \quad (537)$$

where  $\Delta_+ = M_{1^-} - M_1$  and  $\Delta_0 = M_{0^+} - M_1$  now truly correspond to the lowest pole in each form factor. The authors of Ref. [41] found that this method (in the case of  $B_s \rightarrow K$  form factors) yields significantly different results for the extrapolated  $f_0$  when compared to extrapolating  $f_{\parallel}$ ,  $f_{\perp}$  and then reconstructing  $f_+$  and  $f_0$ . Lattice determinations of the form factors based on extrapolations of  $f_{\parallel}$ ,  $f_{\perp}$  may therefore have an uncontrolled systematic error, and directly extrapolating  $f_+$  and  $f_0$  appears to be the better choice.

### B.3 Explicit parameterizations used in the form factor fits

In order to reconstruct the form factors from the results of fits performed using a  $z$ -parameterization it is necessary not only to use the correct version of the parameterization but also to adopt *exactly* the same numerical values for all ancillary quantities that enter the fit (e.g., location of poles). In particular, users must avoid utilizing the most updated numerical inputs for these quantities with  $z$ -coefficients extracted using older values. The purpose of this appendix is to eliminate all ambiguities in the implementation of the fit results presented in Secs. 7 and 8.

#### B.3.1 $D \rightarrow K$ form factors

BCL parameterization:

$$f_+(q^2) = \frac{1}{1 - q^2/m_{D_s^*}^2} \sum_{n=0}^{N^+-1} a_n^+ \left[ z^n - (-1)^{n-N^+} \frac{n}{N^+} z^N \right], \quad (538)$$

$$f_0(q^2) = \frac{1}{1 - q^2/m_{D_s^*(0^+)}^2} \sum_{n=0}^{N^0-1} a_n^0 z^n. \quad (539)$$

The kinematical constraint  $f_+(0) = f_0(0)$  is implemented expressing  $a_{N^0-1}^0$  in terms of the other coefficients. We use  $t_+ = (m_D + m_K)^2$ ,  $t_- = (m_D - m_K)^2$  and  $t_0 = t_+ - \sqrt{t_+(t_+ - t_-)}$ . The numerical inputs are:  $m_D = 1.87265$  GeV,  $m_{D_s^*} = 2.1122$  GeV,  $m_{D_s^*(0^+)} = 2.317$  GeV, and  $m_K = 0.495644$  GeV.

#### B.3.2 $B \rightarrow \pi$ form factors

BCL parameterization:

$$f_+(q^2) = \frac{1}{1 - q^2/m_{B^*}^2} \sum_{n=0}^{N^+-1} a_n^+ \left[ z^n - (-1)^{n-N^+} \frac{n}{N^+} z^N \right], \quad (540)$$

$$f_0(q^2) = \sum_{n=0}^{N^0-1} a_n^0 z^n. \quad (541)$$

The kinematical constraint  $f_+(0) = f_0(0)$  is implemented expressing  $a_{N^0-1}^0$  in terms of the other coefficients. We use  $t_+ = (m_B + m_\pi)^2$  and  $t_0 = (m_B + m_\pi)(\sqrt{m_B} - \sqrt{m_\pi})$ . The numerical inputs are:  $m_{B^*} = 5.32471$  GeV,  $m_B = 5.27934$  GeV and  $m_\pi = 0.1349768$  GeV.

Results for the form factor  $f_T$  are taken directly from Ref. [42] where we refer the reader for details on the parameterization.

#### B.3.3 $B_s \rightarrow K$ form factors

BCL parameterization:

$$f_+(q^2) = \frac{1}{1 - q^2/m_{B_s^*}^2} \sum_{n=0}^{N^+-1} a_n^+ \left[ z^n - (-1)^{n-N^+} \frac{n}{N^+} z^N \right], \quad (542)$$

$$f_0(q^2) = \frac{1}{1 - q^2/m_{B_s^*(0^+)}^2} \sum_{n=0}^{N^0-1} a_n^0 z^n. \quad (543)$$

The kinematical constraint  $f_+(0) = f_0(0)$  is implemented expressing  $a_{N^0-1}^0$  in terms of the other coefficients. We use  $t_+ = (m_B + m_\pi)^2$ ,  $t_- = (m_{B_s} - m_K)^2$  and  $t_0 = t_+ - \sqrt{t_+(t_+ - t_-)}$ . The numerical inputs are:  $m_B = 5.27931$  GeV,  $m_{B^*} = 5.3251$  GeV,  $m_{B_s} = 5.36688$  GeV,  $m_{B^*(0^+)} = 5.68$  GeV,  $m_K = 0.493677$  GeV and  $m_\pi = 0.1349766$  GeV.

### B.3.4 $B \rightarrow K$ form factors

BCL parameterization:

$$f_+(q^2) = \frac{1}{1 - q^2/m_{B_s^*}^2} \sum_{n=0}^{N^+-1} a_n^+ \left[ z^n - (-1)^{n-N^+} \frac{n}{N^+} z^N \right], \quad (544)$$

$$f_0(q^2) = \frac{1}{1 - q^2/m_{B_s^*(0^+)}^2} \sum_{n=0}^{N^0-1} a_n^0 z^n, \quad (545)$$

$$f_T(q^2) = \frac{1}{1 - q^2/m_{B_s^*}^2} \sum_{n=0}^{N^T-1} a_n^T z^n. \quad (546)$$

The kinematical constraint  $f_+(0) = f_0(0)$  is implemented expressing  $a_{N^0-1}^0$  in terms of the other coefficients. We use  $t_+ = (m_B + m_K)^2$  and  $t_0 = (m_B + m_K)(\sqrt{m_B} - \sqrt{m_K})$ . The numerical inputs are:  $m_B = 5.27931$  GeV,  $m_{B_s^*} = 5.4154$  GeV,  $m_{B_s^*(0^+)} = 5.718$  GeV and  $m_K = 0.493677$  GeV.

### B.3.5 $B \rightarrow D$ form factors

BCL parameterization:

$$f_+(q^2) = \sum_{n=0}^{N^+-1} a_n^+ \left[ z^n - (-1)^{n-N^+} \frac{n}{N^+} z^N \right], \quad (547)$$

$$f_0(q^2) = \sum_{n=0}^{N^0-1} a_n^0 z^n. \quad (548)$$

The kinematical constraint  $f_+(0) = f_0(0)$  is implemented expressing  $a_{N^0-1}^0$  in terms of the other coefficients. We use  $t_+ = (m_B + m_D)^2$  and  $t_0 = (m_B + m_D)(\sqrt{m_B} - \sqrt{m_D})$ . The numerical inputs are:  $m_B = 5.27931$  GeV and  $m_D = (1.86483 + 1.86965)/2$  GeV.

### B.3.6 $B_s \rightarrow D_s$ form factors

Results for the form factors are taken directly from Table VIII of Ref. [43] where we refer the reader for details on the parameterization.

### B.3.7 $B \rightarrow D^*$ form factors

We adopt the BGL parameterization used in Ref. [44]: the form factors are given in Eqs. (63) and (64), the poles for the Blaschke factors are given in Table 9, the four outer functions in Eqs. (67)–(70) and the remaining numerical inputs in Table 10. We impose the kinematic constraints at zero and max recoil (see Eqs.(72) and (73) of Ref. [44]) by eliminating the coefficients  $a_0^{F_1}$  and  $a_0^{F_2}$ .

### B.3.8 $B_s \rightarrow D_s^*$ form factors

We adopt the same BGL parameterization described in Sec. B.3.7. Both the outer functions and the location of the poles are identical to the  $B \rightarrow D^*$  case, and the kinematical constraints are imposed in the same way. The only difference are the masses  $m_{B_s} = 5.36688$  GeV and  $m_{D_s^*} = 2.112$  GeV.

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