B Appendix

B.1 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 $B \to \pi\ell\nu$ 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 $B \to \pi\ell\nu$ All form factors are analytic functions of q^2 outside physical poles and inelastic threshold branch points; in the case of $B \to \pi\ell\nu$, 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 $B \to \pi\ell\nu$ semileptonic form factors that incorporates vector-meson dominance is the Bečirević-Kaidalov (BK) parameterization [1], which for the vector form factor reads:

$$f_+(q^2) = \frac{f(0)}{(1 - q^2/m_{B^*}^2)(1 - \alpha q^2/m_{B^*}^2)}\,. \tag{521}$$

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. (522) in order to mimic the effect of multiparticle states [2]. A similar idea, extending the use of effective poles also to $D \to \pi\ell\nu$ decays, is explored in Ref. [3]. Finally, yet another variant (RH) has been proposed by Hill in Ref. [4]. 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 [5–7], and angular momentum conservation constrains the asymptotic behaviour near thresholds—e.g., $\mathrm{Im}\, f_+(q^2) \sim (q^2 - t_+)^{3/2}$ (see, e.g., Ref. [8]). 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 [7, 9–14]. Any form factor f can be shown to admit a series expansion of the form

$$f(q^2) = \frac{1}{B(q^2)\phi(q^2, t_0)} \sum_{n=0}^{\infty} a_n(t_0)\, z(q^2, t_0)^n\,, \tag{522}$$

where the squared momentum transfer is replaced by the variable

$$z(q^2, t_0) = \frac{\sqrt{t_+ - q^2} - \sqrt{t_+ - t_0}}{\sqrt{t_+ - q^2} + \sqrt{t_+ - t_0}}\,. \tag{523}$$

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 $B \to \pi$ decays,

$$B(q^2) = \frac{z(q^2, t_0) - z(m_{B^*}^2, t_0)}{1 - z(q^2, t_0) z(m_{B^*}^2, t_0)} = z(q^2, m_{B^*}^2)\,. \tag{524}$$

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

$$\sum_{n=0}^{\infty} a_n^2 = \frac{1}{2\pi i} \oint \frac{dz}{z} \left| B(z)\phi(z)f(z) \right|^2 , \tag{525}$$

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

$$\begin{aligned} \phi(q^2, t_0) =& \sqrt{\frac{1}{32\pi\chi_{1^-}(0)}} \left(\sqrt{t_+ - q^2} + \sqrt{t_+ - t_0}\right) \\ & \times \left(\sqrt{t_+ - q^2} + \sqrt{t_+ - t_-}\right)^{3/2} \left(\sqrt{t_+ - q^2} + \sqrt{t_+}\right)^{-5} \frac{t_+ - q^2}{(t_+ - t_0)^{1/4}}\,, \end{aligned} \tag{526}$$

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 $B \to \pi\ell\nu$ decay amplitude to $\ell\nu \to B\pi$ inelastic scattering via crossing symmetry and reproducing the correct value of the inclusive $\ell\nu \to X_b$ amplitude. We will refer to the series parameterization with the outer function in Eq. (527) as Boyd, Grinstein, and Lebed (BGL). The perturbative and OPE truncations imply that the bound is not strict, and one should take it as

$$\sum_{n=0}^{N} a_n^2 \lesssim 1\,, \tag{527}$$

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. (527) 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. [8], which leads to a parameterization of the form

$$f_+(q^2) = \frac{1}{1 - q^2/m_{B^*}^2} \sum_{n=0}^{N} a_n^+(t_0) z(q^2, t_0)^n\,. \tag{528}$$

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

$$\sum_{j,k=0}^{N} B_{jk}(t_0)a_j^+(t_0)a_k^+(t_0) \leq 1\,. \tag{529}$$

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

$$t_0 = t_{\rm opt} = (m_B + m_\pi)(\sqrt{m_B} - \sqrt{m_\pi})^2\,, \tag{530}$$

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 $\mathrm{Im}\, f_+(q^2) \sim (q^2 - t_+)^{3/2}$ near threshold is satisfied, then the highest-order coefficient is further constrained as

$$a_N^+ = -\,\frac{(-1)^N}{N}\sum_{n=0}^{N-1}(-1)^n\, n\, a_n^+\,. \tag{531}$$

Substituting the above constraint on a_N^+ into Eq. (529) leads to the constrained BCL parameterization

$$f_+(q^2) = \frac{1}{1 - q^2/m_{B^*}^2}\sum_{n=0}^{N-1} a_n^+\left[z^n - (-1)^{n-N}\,\frac{n}{N}\,z^N\right]\,, \tag{532}$$

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. (533); 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 $B \to \pi\ell\nu$ The discussion of the scalar $B \to \pi$ form factor is very similar. The main differences are the absence of a constraint analogue to Eq. (532) and the choice of the overall pole function. In our fits we adopt the simple expansion:

$$f_0(q^2) = \sum_{n=0}^{N-1} a_n^0\, z^n\,. \tag{533}$$

We do impose the exact kinematical constraint $f_+(0) = f_0(0)$ by expressing the a^0_{N-1} coefficient in terms of all remaining a^+_n and a^0_n coefficients. This constraint introduces important correlations between the a^+_n and a^0_n 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 $a^0_{0,1}$, while with $(N^+ = 3, N^0 = 4)$ we have $a^+_{0,1,2}$ and $a^0_{0,1,2}$ 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., $B_s \to K$ and $B_{(s)} \to D^{(*)}_{(s)}$, 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. [15]. Extending what has been discussed above for $B \to \pi$, the form factors for a generic $H \to L$ 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 $B \to \pi$, $B_s \to K$, or $\Lambda_b \to p$; and vector (resp. scalar) resonances in $B_c\pi$ scattering for the vector (resp. scalar) form factors of $B \to D$ or $\Lambda_b \to \Lambda_c$.[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 $B_s \to K\ell\nu$ and $B \to D\ell\nu$, 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 [16–18].

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

[1] 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.

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

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 $D \to \pi\ell\nu$ and $D \to K\ell\nu$, 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 $P_1 \to P_2$ (such as $B \to \pi$ or $B_s \to K$), the chiral and continuum extrapolations have often been performed in a different basis $f_\parallel$, $f_\perp$ given by [19]

$$\langle P_2(p')|V^\mu|P_1(p)\rangle = \sqrt{2M_1}[v^\mu f_\parallel(E_2) + p'^\mu_\perp f_\perp(E_2)]. \tag{534}$$

Here, $v^\mu = p^\mu/M_1$ is the initial-meson four-velocity, $p'^\mu_\perp = p'^\mu - (v\cdot p')v^\mu$ is the projection of the final-meson momentum in the direction perpendicular to v^μ, 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

$$f_0(q^2) = \frac{\sqrt{2M_1}}{M_1^2 - M_2^2}\big[(M_1 - E_2)f_\parallel(E_2) + (E_2^2 - M_K^2)f_\perp(E_2)\big], \tag{535}$$

$$f_+(q^2) = \frac{1}{\sqrt{2M_1}}\left[f_\parallel(E_2) + (M_1 - E_2)f_\perp(E_2)\right]. \tag{536}$$

The decomposition (535) 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 $B \to \pi$, heavy-meson chiral perturbation theory predicts, at leading-order in both the chiral and the heavy-quark expansion,

$$f_\perp(E_\pi) = \frac{1}{f_\pi}\frac{g_{B^*B\pi}}{E_\pi + \Delta_{B^*}}, \tag{537}$$

$$f_\parallel(E_\pi) = \frac{1}{f_\pi}, \tag{538}$$

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

$$f_\perp(E_2) = \frac{1}{E_2 + \Delta_\perp}\Big[...\Big] \tag{539}$$

and

$$f_\parallel(E_2) = \frac{1}{E_2 + \Delta_\parallel}\Big[...\Big] \qquad \text{or} \qquad f_\parallel(E_2) = \Big[...\Big] \tag{540}$$

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

$$f_+(E_2) = \frac{1}{E_2 + \Delta_+}\Big[...\Big] \tag{541}$$

and

$$f_0(E_2) = \frac{1}{E_2 + \Delta_0}\Big[...\Big] \qquad \text{or} \qquad f_0(E_2) = \Big[...\Big], \tag{542}$$

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. [20] found that this method (in the case of $B_s \to K$ 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.

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