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# Unitarity and the heavy quark expansion in the determination of semileptonic form factors

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We discuss prospects for improving the $q^2$ extrapolation of the $B \to \pi l \nu$ form factors with model-independent constraints based on unitarity and heavy quark power-counting. As an illustration, we apply the method to preliminary results of calculations of the form factors, which we generated using the MILC gauge configurations and the Fermilab action for the heavy $b$-quark.

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## 1. Introduction and motivations

Lattice QCD calculations of semileptonic form factors provide valuable tests of lattice heavy-quark actions as well as critical input into the unitarity triangle analysis [1]. In general, $B$- and $D$-meson semileptonic decays aid in determining four CKM matrix elements; in particular, the decay $B \to \pi l \nu$ allows a measurement of $|V_{ub}|$.

The semileptonic decay $B \to \pi l \nu$ is parameterized by two form factors, $f_+(q^2)$ and $f_0(q^2)$:

$$\langle \pi(p_\pi) | \mathcal{V}^\mu | B(p_B) \rangle = f_+(E_\pi) \left[ p_B + p_\pi - \frac{m_B^2 - m_\pi^2}{q^2} q \right]^\mu + f_0(E_\pi) \frac{m_B^2 - m_\pi^2}{q^2} q^\mu , \tag{1.1}$$

where $q^2 = m_B^2 + m_\pi^2 - 2 E_\pi m_B$ is the squared momentum of the outgoing lepton and neutrino. Experimenters measure the differential decay rate, which is related to $f_+(q^2)$ as follows:

$$\frac{d\Gamma}{dq^2} = \frac{G_F^2 |V_{ub}|^2}{192 \pi^3 m_B^3} [(m_B^2 + m_\pi^2 - q^2)^2 - 4 m_B^2 m_\pi^2]^{3/2} | f_+(q^2)|^2 . \tag{1.2}$$

Because experiments can only determine the product $|V_{ub}|^2 | f_+(q^2)|^2$, lattice QCD calculations of the form factor normalization are needed in order to extract the CKM matrix element $|V_{ub}|$.

In principle, the procedure to determine $|V_{ub}|$ is straightforward. In practice, however, experiments measure the form factors most precisely at low $q^2$, whereas traditional lattice QCD can only accurately calculate form factors at high $q^2$ (low $E_\pi$). Thus the power of this method for determining $|V_{ub}|$ is limited by the poor overlap in $q^2$ of the lattice and experimental data. Various strategies to address this problem appear in the literature. The most conservative approach accepts the limitations of the available lattice techniques and only compares lattice and experiment in the $q^2$ region in which lattice data exists [2]. While certainly correct, this does not necessarily allow for the most precise possible determination of $|V_{ub}|$. The most common approach is to use an Ansatz to extrapolate lattice data to the low $q^2$ region where the experimental data is best. The standard functional form used in the literature is the BK parameterization [3]:

$$f_+(q^2) = f_+(0) \left(1 - q^2/m_{B^*}^2\right)^{-1} \left(1 - \alpha\, q^2/m_{B^*}^2\right)^{-1} . \tag{1.3}$$

This function has the merits that correctly incorporates the $B^*$ pole and fits the data well. Nevertheless, it is difficult to quantify the systematic errors in the $q^2$ extrapolation due to this particular choice for how treat higher-order poles. A novel approach is to generate lattice data at lower $q^2$ using an alternative method such as Moving NRQCD [4]. This, however, requires further work as well as the generation of additional lattice data.

Physical intuition suggests the correct shape of the $B \to \pi l \nu$ form factors, whatever it is, will be smooth. This intuition can be made quantitative through the use of analyticity, crossing-symmetry, and unitarity [5, 6]. It is well established that these general properties can be used to constrain the shape of form factors. In this work we explore the potential of these model-independent constraints to aid in lattice QCD calculations of the $B \to \pi l \nu$ semileptonic form factors.

## 2. Unitarity and heavy quark constraints on form factors

Generically, all form factors are analytic functions of $q^2$ except at physical poles and threshold branch points. In the case of the $B \to \pi l \nu$ form factors, $f(q^2)$ is analytic below the $B\pi$ production

| | |
|---|---|
| $B \to \pi l \nu$ | $-0.34 < z < 0.22$ |
| $D \to \pi l \nu$ | $-0.17 < z < 0.16$ |
| $D \to K l \nu$ | $-0.04 < z < 0.06$ |
| $B \to D l \nu$ | $-0.02 < z < 0.04$ |

**Table 1:** Physical region in terms of the variable $z$ for various semileptonic decays given the choice $t_0 = 0.65 t_-$.



region except at the location of the $B^*$ pole. The fact that analytic functions can always be expressed as convergent power series allows the form factors to be written in a particularly useful manner.

Consider mapping the variable $q^2$ onto a new variable, $z$, in the following way:

$$z = \frac{\sqrt{1-q^2/t_+} - \sqrt{1-t_0/t_+}}{\sqrt{1-q^2/t_+} + \sqrt{1-t_0/t_+}}, \tag{2.1}$$

where $t_+ \equiv (m_B + m_\pi)^2$, $t_- \equiv (m_B - m_\pi)^2$, and $t_0$ is a free parameter. Although this mapping appears complicated, it actually has a simple interpretation in terms of $q^2$; this transformation maps $q^2 > t_+$ (the production region) onto $|z| = 1$ and maps $q^2 < t_+$ (which includes the semileptonic region) onto $z = [-1, 1]$. In terms of $z$, the form factors have a simple form:

$$P(t)\phi(t,t_0) f(t) = \sum_{k=0}^{\infty} a_k(t_0) z(t,t_0)^k, \tag{2.2}$$

where $P(t)$ is a function that vanishes at subthreshold (*e.g.* $B^*$) poles and $\phi(t,t_0)$ is an "arbitrary" analytic function whose choice only affects the particular values of the series coefficients ($a_k$'s). Given the choices for $P$ and $\phi$ used in Ref. [6], unitarity constrains the size of the series coefficients:

$$\sum_{k=0}^{N} a_K^2 \leq 1, \tag{2.3}$$

where this constraint holds for any value of N.

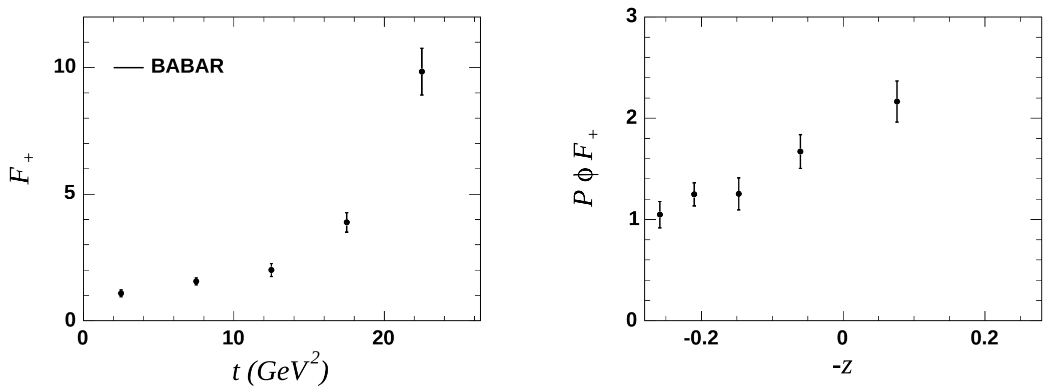
The free parameter $t_0$ can be chosen to make the maximum value of $|z|$ as small as possible in the semileptonic region; we choose $t_0 = 0.65 t_-$ as in Ref. [6]. For $B \to \pi l \nu$ semileptonic decays this maps the physical region onto:

$$0 < t < t_- \quad \to \quad -0.34 < z < 0.22.$$

The corresponding $z$-region for other decays is given in Table 1. The constraint on the size of the coefficients in the $z$-expansion in combination with the small numerical values of $|z|$ in the physical region ensures that, using the series expansion in $z$, one needs only a handful of parameters to obtain the form factors to a high degree of accuracy.

## 3. Strategy to combine lattice QCD and experiment

As shown in Figure 1, after remapping from $q^2$ to $z$ there is no visible curvature in the BABAR $B \to \pi l \nu$ experimental data [7]. This indicates that the curvature in the data is due to




(a) (b)

**Figure 1:** Experimental data for the $B \to \pi l \nu$ form factor $f_+$ from the BABAR collaboration [7]. Figure (a) shows the form factor versus $q^2$ while (b) shows $P\phi$ times the form factor versus the new variable $z$.

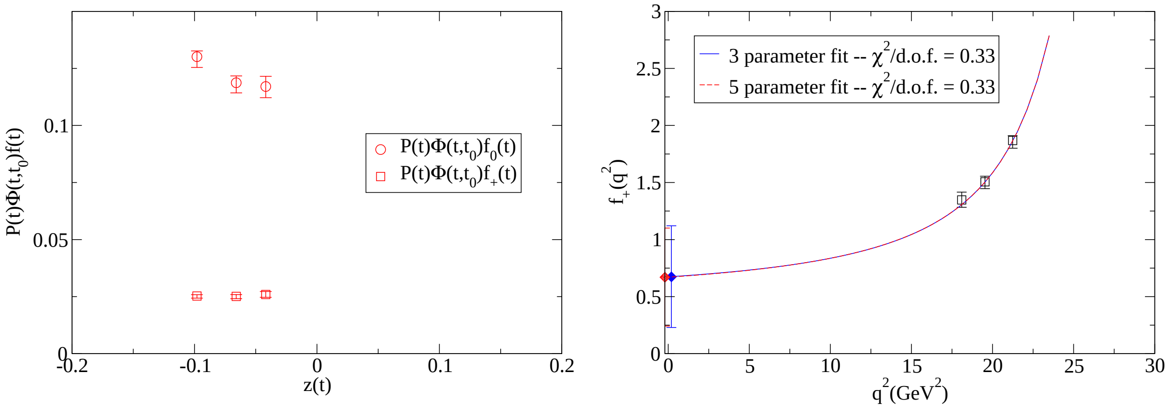
well-understood QCD effects (*i.e.*, the functions $P$ and $\phi$ in Eq. (2.2)). Consequently the experimental data should be well described by a normalization and a slope. The fact that, when expressed in terms of $z$, the form factor data is determined by only two parameters suggests the following approach for determining $|V_{ub}|$ from the decay $B \to \pi l \nu$:

1. Fit both experimental and lattice data in terms of the $z$ expansion
2. Determine and compare the slopes in $z$
3. Compare the normalizations to extract $|V_{ub}|$
4. Look for curvature

This approach has many positive features. It is practical because it requires a limited number of fit parameters. One can first quantify the agreement between the lattice QCD results and experimental data using the value of the slope before combining them to determine $|V_{ub}|$. Because the series in $z$ is convergent, and because the sizes of the series coefficients are bounded by Eq. (2.3), this $q^2$ extrapolation approach is well-suited to the method of constrained curve-fitting. One can constrain each coefficient with a prior, perform a fit to the data with more terms in the series than seems necessary, and simply let the data determine as many parameters as they can. The “extra" parameters will absorb the effects of the higher-order terms that have been omitted. Thus this method is systematically improvable – as the data become more precise they will reduce the error bars on the lower-order coefficients and begin to constrain additional higher-order coefficients. It is this quality that leads us to describe this method as *model-independent*.

## 4. Preliminary analysis of lattice QCD data

We now illustrate the method of extrapolating lattice QCD form factor data in $q^2$ using the $z$-expansion, Eq. (2.2). We use the same functions $P$ and $\phi$ and the same value of $t_0 = 0.65 t_-$ as in Ref. [6]. We use Bayesian priors to impose the unitarity constraints on the size of the coefficients




(a) (b)

**Figure 2:** Figure (a) shows our preliminary lattice form factor data multiplied by $P\phi$ plotted versus $z$. These same data are shown in all subsequent plots. Figure (b) shows the $q^2$ extrapolation of our data using a 3-parameter $z$-expansion (blue solid) and a 5-parameter $z$-expansion (red dashed). Also shown are the resulting bootstrap errors in the extrapolated value of $f_+(0)$.

in the $z$-expansion and calculate bootstrap errors in the resulting fit parameters. We emphasize that the work shown in these proceedings is exploratory: we have used data at only a single lattice spacing, $a = 0.12$ fm, and for a single quark mass, $am_{u,d} = 0.02$ and $am_s = 0.05$. Furthermore, we do not include any estimate of systematic errors. In principle, we should perform a chiral and continuum extrapolation using the appropriate staggered chiral perturbation theory expressions [8] before extrapolating in $q^2$, and we will add this in the upcoming paper.

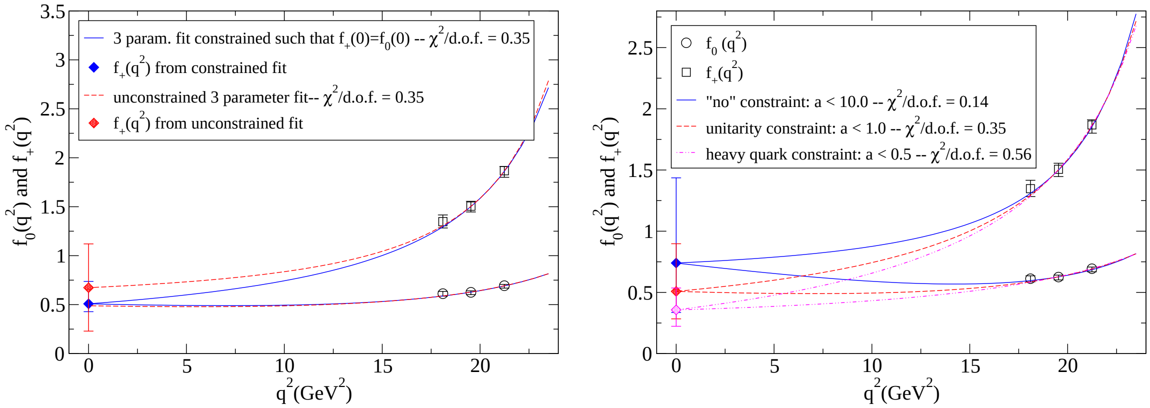
Figure 2(a) shows our lattice QCD data multiplied by the functions $P$ and $\phi$ and plotted versus the new variable $z$. Like the experimental data, it appears to be linear. We therefore expect to be able to fit the lattice $f_+$ data well using only 2-3 parameters, and an attempt to fit the data including more parameters should only lead to the higher-order parameters being poorly-determined. This is exactly what we observe. Figure 2(b) shows the results of both a 3-parameter and 5-parameter fit to $f_+(q^2)$ and the resulting bootstrap errors on the extrapolated value of $f_+(0)$. The resulting coefficients are

$$a_0 = 0.026 \pm 0.003, \qquad a_1 = 0.020 \pm 0.068, \qquad a_2 = 0.152 \pm 0.41 \tag{4.1}$$

for the 3-parameter fit and

$$a_0 = 0.026 \pm 0.003, \qquad a_1 = 0.020 \pm 0.068, \qquad a_2 = 0.148 \pm 0.45,$$
$$a_3 = -0.031 \pm 0.98, \qquad a_4 = 0.004 \pm 1$$

for the 5-parameter fit. The normalization ($a_0$) and slope ($a_1$) are consistent between fits; the curvature ($a_2$) is consistent with zero, and the higher-order coefficients are not constrained by the data.




(a) (b)

**Figure 3:** Figure (a) shows the $q^2$ extrapolation in which the kinematic constraint $f_+(0) = f_0(0)$ is imposed (blue solid) and in which it is not (red dashed). Both extrapolations use a 3-parameter $z$-expansion for the form factors. Figure (b) shows the 3-parameter, kinematically-constrained $q^2$ extrapolation for three different bounds on the size of the coefficients in the $z$-expansion. The blue solid curve comes from a loose bound, the red dashed curve comes from the unitarity bound, and the magenta dot-dashed curve comes from the heavy quark bound.

Because lattice simulations can calculate both $B \to \pi l \nu$ form factors, the $q^2$ extrapolation of $f_+$ in Fig. 2 only uses part of the available lattice data. Kinematics constrain the two form factors to be equal at zero $q^2$, *i.e.* $f_+(0) = f_0(0)$; thus one can in principle extrapolate both $f_+$ and $f_0$ simultaneously while imposing the above kinematic constraint to improve the extrapolation error. This procedure is shown in Fig. 3(a). As expected, combining the $f_+$ and $f_0$ data reduces the error bars in the extrapolated value of $f_+(0)$.

The unitarity bound on the size of the coefficients in the $z$-expansion, Eq. (2.3) comes from fact that the decay rate to the exclusive channel $B \to \pi l \nu$ must be less than the inclusive $B$-meson decay rate. It is observed, however, that the coefficients are actually much smaller than what is predicted by the unitarity constraint alone. Becher and Hill explained the size of the series coefficients using heavy-quark power-counting arguments in Ref. [9]. The fact that, as the mass of $B$-meson increases, its branching fraction to any particular exclusive channel decreases, allowed them to calculate the branching fraction for the semileptonic decay $B \to \pi l \nu$ as a power of $\Lambda_{\text{QCD}}/m_B$. They used this result derive an even tighter bound on the size of the coefficients of the form factor $z$-expansion:

$$\sum_{k=0}^{N} a_K^2 \leq \left( \frac{\Lambda}{m_B} \right)^3, \tag{4.2}$$

where they estimate that $\Lambda/m_B \sim 0.1$. Using this estimate, one should need only 3-4 parameters to describe the form factors of the processes given in Table 1 to 1% accuracy. Figure 3(b) shows the 3-parameter $q^2$ extrapolation of $f_+$ and $f_0$ using three different constraints on the numerical size of the coefficients: a loose constraint, the unitarity constraint, and the heavy quark constraint (where we have allowed $\Lambda/m_B$ to be larger than the estimate in Ref. [9]). The three fits all have an acceptable $\chi^2$/d.o.f. and are consistent within 95% confidence level error bars.

One might notice that, in Fig. 3(b), the central value of $f_+(0)$ drifts downward as the constraints on the coefficients are tightened. There is nothing in principle wrong with this trend since tightening the constraints adds new physics information. Nevertheless, this trend could also be due to an unaccounted-for systematic error. A possible culprit is momentum-dependent discretization errors $\propto a^2 p_\pi^2$ in the lattice data, which, when included, should cause the size of the error bars to increase from right to left in Fig. 3(b). These errors should be incorporated *before* performing the $q^2$ extrapolation, and we are in the process of doing so.

## 5. Summary

Lattice QCD calculations of the $B \to \pi l \nu$ semileptonic form factors are important for determining the CKM matrix element $|V_{ub}|$. They are hindered, however, by the inability to accurately calculate form factors at low $q^2$. This is typically dealt with by using a model to restrict the shape of $f(q^2)$ vs. $q^2$, thereby introducing a source of systematic error that is difficult to quantify. Analyticity, unitarity, and heavy quark physics can be combined to constrain the shape of semileptonic form factors in a model-independent way using only a small number of fit parameters. We have studied the effect of these constraints on the $q^2$ extrapolation using data from a single ensemble and the results look promising. We will integrate continuum and chiral extrapolations and other systematic errors in the near future. Using this method, we can obtain the $B \to \pi l \nu$ semileptonic form factors to improved accuracy using the lattice QCD data that we already have.

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