Subleading Shape Functions and the Determination of $|V_{ub}|$

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Abstract

It is argued that the dominant subleading shape-function contributions to the endpoint region of the charged-lepton energy spectrum in $B \to X_u l \nu$ decays can be related in a model-independent way to an integral over the $B \to X_s \gamma$ photon spectrum. The square root of the fraction of $B \to X_u l \nu$ events with charged-lepton energy above $E_0 = 2.2 \text{ GeV}$ can be calculated with a residual theoretical uncertainty from subleading shape-function effects that is safely below the 10% level. These effects have therefore a minor impact on the determination of $|V_{ub}|$. 
1. Introduction: One of the most promising strategies for the extraction of the Cabibbo–Kobayashi–Maskawa matrix element $|V_{ub}|$ relies on the measurement of the inclusive semileptonic $B \to X_u l \nu$ decay rate in the endpoint region of the charged-lepton energy spectrum, which is inaccessible to decays with a charm hadron in the final state [1]. Non-perturbative effects can be controlled systematically by using a twist expansion [2, 3] and soft-collinear factorization theorems [4, 5]. At leading order in $1/m_b$, bound-state effects are incorporated by a shape function accounting for the “Fermi motion” of the $b$ quark inside the $B$ meson. This function can be determined experimentally from the photon energy spectrum in inclusive radiative $B \to X_s \gamma$ decays [2].

Recently, there have been first discussions of the structure of subleading-twist contributions to the $B \to X_s \gamma$ and $B \to X_u l \nu$ spectra, which (at tree level) can be parameterized in terms of four subleading shape functions [6]. The phenomenological impact of these functions on the inclusive determination of $|V_{ub}|$ has been investigated in [7, 8]. These authors point out that certain $1/m_b$ corrections related to chromo-magnetic interactions appear to be enhanced by large numerical coefficients. They conclude that the ignorance about the functional form of the subleading shape functions would lead to a significant theoretical uncertainty in the determination of $|V_{ub}|$, which could only be reliably reduced if the lower cut on the lepton energy were taken below the region where Fermi-motion effects are important (i.e., below 2 GeV or so). For a value $E_0 = 2.2 \text{ GeV}$, as employed in a recent analysis reported by the CLEO collaboration [1], the resulting uncertainty on $|V_{ub}|$ was estimated to be at the 15% level [7]. While using simple models the correction was found to be negative, it was argued that the sign of the effect was uncertain in general [8].

In the present note we explore in more detail the origin of the “enhanced” corrections found in these papers. Our main point is that the first moments (but not higher moments) of the subleading shape functions give a large, non-vanishing contribution to the integral over the lepton spectrum even if the lower lepton-energy cut is taken out of the endpoint region. This effect corresponds to a calculable correction of order $\Lambda_{QCD}^2/(m_b \Delta E)$, where $\Delta E = M_B/2 - E_0$. The hadronic uncertainty inherent in the modeling of subleading shape functions must therefore be estimated with respect to this contribution. When this is done, the remaining theoretical uncertainty is found to be much less than what has been estimated in [7, 8]. We show how the effect of the first moments of the subleading shape functions can be isolated and expressed in a model-independent way in terms of the photon energy spectrum measured in $B \to X_s \gamma$ decays. We then estimate the numerical effect of the residual higher-twist corrections and find their impact on the $|V_{ub}|$ determination to be small, safely below the level of 10%.

2. Charged-lepton energy spectrum: The quantity of primary interest to the determination of $|V_{ub}|$ is the normalized fraction of $B \to X_u l \nu$ events with charged-lepton energy above a threshold $E_0$ chosen so as to kinematically suppress the background from
\[ B \to X_c l \nu \] decays,

\[ F_u(E_0) = \frac{1}{\Gamma(B \to X_u l \nu)} \int_{E_0}^{M_B/2} dE_l \frac{d\Gamma(B \to X_u l \nu)}{dE_l}. \tag{1} \]

When combined with a prediction for the total \( B \to X_u l \nu \) decay rate, knowledge of the function \( F_u(E_0) \) allows one to turn a measurement of the branching ratio for \( B \to X_u l \nu \) events with \( E_l > E_0 \) into a determination of \( |V_{ub}| \).

In the formal limit where the “energy window” \( \Delta E = M_B/2 - E_0 \) is such that \( \Lambda_{\text{QCD}} \ll \Delta E \ll m_b \), Fermi-motion effects can be neglected, and the function \( F_u(E_0) \) can be calculated using the operator product expansion. At tree level the result is

\[ F_u(E_0) = \frac{2}{m_b} \left( 2\Delta E - \bar{\Lambda} \right) - \frac{\lambda_1 + 33\lambda_2}{3m_b^2} + O[(\Delta E/m_b)^3], \tag{2} \]

where \( \bar{\Lambda} = M_B - m_b \), and \( 2\Delta E - \bar{\Lambda} = m_b - 2E_0 \) is twice the width of the energy window in the parton model. The hadronic parameters \( \lambda_1 \) and \( \lambda_2 \) measure the \( b \)-quark kinetic energy and chromo-magnetic interaction inside the \( B \) meson. Note that while the leading contribution in (2) is proportional to the width of the energy window, the power corrections are independent of \( \Delta E \). As a result, the relative size of the power corrections strongly increases as the energy cut \( E_0 \) is raised toward the kinematic endpoint (corresponding to \( \Delta E \to 0 \)). Although this simple analysis breaks down as \( \Delta E \sim \bar{\Lambda} \), it explains that the origin of the large power corrections found in [7, 8] is the kinematic suppression of the leading-order term.

For realistic values of the energy threshold the quantity \( \Delta E \) is of order \( \bar{\Lambda} \), and the operator product expansion must be replaced by the twist expansion [2, 3]. At subleading order in \( 1/m_b \) the tree-level expression for \( F_u(E_0) \) can then be written as

\[ F_u(E_0) = 2 \int_{-\bar{\Lambda}}^{2\Delta E - \bar{\Lambda}} d\omega \frac{2\Delta E - \bar{\Lambda} - \omega}{m_b - \omega} F_u(\omega), \tag{3} \]

where

\[ F_u(\omega) = f(\omega) + \frac{1}{m_b} \left[ \frac{t(\omega)}{2} - G_2(\omega) - 2\omega f(\omega) + 3H_2(\omega) - h_1(\omega) \right] + \ldots \]

\[ \equiv F_s(\omega) + \frac{2}{m_b} \left[ H_2(\omega) - h_1(\omega) \right] + \ldots \tag{4} \]

is a combination of the leading and subleading shape functions [7], and the dots denote higher-order terms in the expansion. The function \( F_s(\omega) \) defined by the second relation is related to the normalized photon energy spectrum in \( B \to X_s \gamma \) decays, \( S(E_\gamma) \), by (the factor 2 results from the Jacobian \( d\omega/dE \))

\[ 2F_s(m_b - 2E_\gamma) = S(E_\gamma) \equiv \frac{1}{\Gamma(B \to X_s \gamma)} \frac{d\Gamma(B \to X_s \gamma)}{dE_\gamma}. \tag{5} \]
It is important in this context that the shape of the $B \to X_s\gamma$ photon spectrum is largely insensitive to possible effects of New Physics \cite{9}, so $F_s(\omega)$ can be extracted from the data in a model-independent way. When we include radiative corrections below, $S(E_\gamma)$ will still denote the photon energy spectrum, normalized however on an interval $E_{\gamma\text{min}} < E_\gamma < M_B/2$, with $E_{\gamma\text{min}}$ sufficiently small to be out of the shape-function region.

The combination of subleading shape functions remaining in the last line of (4) parameterizes chromo-magnetic interactions in the $B$ meson. The moment expansion of these functions yields \cite{6}

$$H_2(\omega) - h_1(\omega) = -2\lambda_2 \delta'(\omega) - \frac{\rho_2}{2} \delta''(\omega) + \ldots,$$

where $\rho_2$ is a $B$-meson matrix element of a local dimension-6 operator. In the limit where $\Delta E \gg \bar{\Lambda}$, only the first moment yields a non-zero contribution to the function $F_u(E_0)$ in (4), because the weight function under the integral is linear in $\omega$ (to first order in $1/m_b$). On the other hand, near the endpoint of the lepton spectrum all moments of the shape functions become equally important \cite{2,3}. In between these two extremes there is a transition region, where only the first few moments of the shape functions give significant contributions.

Theoretical studies of the photon spectrum in $B \to X_s\gamma$ decays have shown that this transition region corresponds to values $E_0 \sim 2.0-2.3$ GeV (for yet lower values, Fermi-motion effects become unimportant) \cite{9}. To account for the effect of the first moment we define a new subleading shape function

$$s(\omega) = H_2(\omega) - h_1(\omega) + 2\lambda_2 f'(\omega),$$

whose normalization and first moment vanish, and whose contribution to the quantity $F_u(E_0)$ therefore vanishes for $\Delta E \gg \bar{\Lambda}$. Inserting this definition into relation (4), and using that $F_s(\omega) = f(\omega) + \ldots$ to leading order in $1/m_b$, we obtain from (6)

$$F_u(E_0) = 2 \int_{-\bar{\Lambda}}^{2\Delta E - \bar{\Lambda}} d\omega \left\{ \frac{2\Delta E - \bar{\Lambda} - \omega}{m_b - \omega} \left[ F_s(\omega) + \frac{2s(\omega)}{m_b} \right] - \frac{4\lambda_2}{m_b^2} F_s(\omega) \right\} + \ldots. \quad (8)$$

Taking into account the known $O(\alpha_s)$ corrections to the leading term in the twist expansion \cite{10,11}, and rewriting the contribution involving $F_s(\omega)$ as a weighted integral over the normalized photon energy spectrum in $B \to X_s\gamma$ decays, we get our final result

$$F_u(E_0) = \left(1 + \frac{2\Lambda_{\text{SL}}(E_0)}{m_b} \right) \int_{E_0}^{M_B/2} dE_\gamma w(E_\gamma, E_0) S(E_\gamma) + \ldots, \quad (9)$$

with the weight function

$$w(E_\gamma, E_0) = 2 \left(1 - \frac{E_0}{E_\gamma}\right) \left\{ 1 + \frac{\alpha_s(\mu)}{\pi} \left[ k_{\text{pert}}(E_{\gamma\text{min}}') - \frac{10}{9} \ln \left(1 - \frac{E_0}{E_\gamma}\right) \right] \right\} - \frac{8\lambda_2}{m_b^2}, \quad (10)$$

\footnote{Using an integration by parts, this result can be rewritten as a weighted integral over the fraction $F_s(E)$ of $B \to X_s\gamma$ events with photon energy above $E$, normalized such that $F_s(E_{\gamma\text{min}}') = 1$.}
and the subleading shape-function contribution

\[ \Lambda_{\text{SL}}(E_0) = \frac{\int_{-\Lambda}^{-\Lambda} d\omega (2\Delta E - \bar{\Lambda} - \omega) s(\omega)}{\int_{-\Lambda}^{-\Lambda} d\omega (2\Delta E - \bar{\Lambda} - \omega) f(\omega)} \].

(11)

The factor 2 in front of \( \Lambda_{\text{SL}}(E_0) \) in (9) is inserted so that \( \Lambda_{\text{SL}}(E_0)/m_b \) is the subleading shape-function correction to |\( V_{ub} \)|. We stress that, by definition, \( \Lambda_{\text{SL}}(E_0) \) is a parameter of order \( \Lambda_{\text{QCD}} \) that vanishes for \( \Delta E \gg \bar{\Lambda} \). It is thus a true measure of shape-function effects. On the contrary, the power corrections studied in [7, 8] arise predominantly from the \( \lambda_2/m_b^2 \) correction to the weight function.

The expression for the perturbative coefficient \( k_{\text{pert}} \) in (10) can be obtained from the results of [9, 12]. It reads

\[ k_{\text{pert}}(E_{\gamma}^{\text{min}}) = -\frac{35}{9} - \frac{2}{3} \ln^2 \delta - \frac{7}{3} \ln \delta + \sum_{i,j=2,7,8, i \geq j} \frac{C_i(\mu) C_j(\mu)}{[C_7(\mu)]^2} f_{ij}(\delta), \]

(12)

where \( \delta = 1 - E_{\gamma}^{\text{min}}/\langle E_{\gamma} \rangle \) depends on the lower boundary of the energy interval used to normalize the \( B \to X_s\gamma \) photon spectrum, \( C_i(\mu) \) are leading-order Wilson coefficients in the effective weak Hamiltonian for \( B \to X_s\gamma \) transitions, and the functions \( f_{ij}(\delta) \) can be found in [9]. In the definition of \( \delta \) we use the central value of the CLEO result for the average photon energy above 2 GeV, \( \langle E_{\gamma} \rangle = (2.346 \pm 0.034) \) GeV [13], as a substitute for \( m_b/2 \).

3. Numerical results: The value of the coefficient \( k_{\text{pert}} \) is sensitive to the choice of the renormalization scale \( \mu \) and the value of the quark-mass ratio \( m_c/m_b \) used in the evaluation of charm-quark loops. We take \( \mu_b = m_b(m_b) = 4.2 \) GeV as our central value for the renormalization scale and vary \( \mu \) between \( \mu_b/2 \) and \( 2\mu_b \). We use a running charm-quark mass to evaluate the loop functions [14], taking \( m_c(\mu)/m_b(\mu) = 0.23 \pm 0.03 \). The results for \( k_{\text{pert}} \) corresponding to two different choices of \( E_{\gamma}^{\text{min}} \) are

\[ k_{\text{pert}} = \begin{cases} 
0.07 \pm 0.10; & E_{\gamma}^{\text{min}} = 1.5 \text{ GeV}, \\
-0.20 \pm 0.08; & E_{\gamma}^{\text{min}} = 1.75 \text{ GeV}.
\end{cases} \]

(13)

Since the effect of this correction is very small, one should not consider the small variation of \( k_{\text{pert}} \) as a measure of the perturbative uncertainty in the weight function [10]. Typically, we expect \( O(\alpha_s^2) \) corrections to contribute at the level of 5% of the tree-level term. A corresponding uncertainty will be included in our numerical analysis below.

The power correction to the weight function in (10) may be rewritten as

\[ \frac{8\lambda_2}{m_b^2} \approx \frac{m_{B^*}^2 - m_B^2}{2\langle E_{\gamma} \rangle^2} \approx 0.044. \]

(14)
Alternatively, using $\lambda_2 = (0.12 \pm 0.02) \text{GeV}^2$ and $m_b = (4.72 \pm 0.06) \text{GeV}$ we obtain the value $0.043 \pm 0.007$, which will be used in our numerical analysis. The size of this correction is not anomalously large; however, its impact is significant because it competes with terms proportional to the small difference $(1 - E_0/E_\gamma)$. In the endpoint region this difference scales like $\Lambda_{QCD}/m_b$, and so the $\lambda_2/m_b^2$ term is of relative order $1/m_b$.

Our final focus is on the subleading shape-function contribution $\Lambda_{SL}(E_0)$ defined in (11). Little is known about the function $s(\omega)$ except that its normalization and first moment vanish, and that its second moment, $M_2(\omega) = -\rho_2$, is given by a hadronic matrix element expected to be of order $(0.5 \text{GeV})^3$ with undetermined sign. As a result, the functional form and sign of $\Lambda_{SL}(E_0)$ cannot be predicted at present. However, the fact that $\Lambda_{SL}(E_0)$ must approach zero as $E_0$ is lowered to a value of about $2 \text{GeV}$ (below which shape-function effects from higher moments are irrelevant) ensures that its impact on the determination of $|V_{ub}|$ is small. To substantiate this claim we investigate several models for the subleading shape function in more detail. For the leading-order function we take the ansatz $3$

$$f(\omega) = \frac{1}{\Lambda} g_\omega(x), \quad \text{with } x = 1 + \frac{\omega}{\Lambda} \geq 0,$$

where $g_\omega(x) = [a^x/\Gamma(a)] x^{a-1} e^{-a x}$. The parameter $a$ must be larger than 1 and is fixed so that the second moment of $f(\omega)$ equals $-\lambda_1/3$ $2$, yielding $a = -3\Lambda^2/\lambda_1$. We assume that the subleading function $s(\omega)$ is finite everywhere in the interval $-\Lambda \leq \omega < \infty$, but we do not require that this function vanish at the endpoint.

The model functions adopted in $3$ are such that $s(\omega)$ is set to zero, and so $\Lambda_{SL}(E_0)$ vanishes by construction. The model functions used in $8$ correspond to the ansatz

$$s(\omega) = \frac{2\lambda_2}{\Lambda^2} \left[ g_\omega'(x) - g_\omega'(x) \right] \quad \text{with } b \geq 2, \quad \text{(model 1)}$$

where the lower bound on the parameter $b$ is enforced by the requirements that $s(\omega)$ be finite at the endpoint $\omega = -\Lambda$ and have vanishing normalization and first moment. A property of this model is that also the second moment of $s(\omega)$ vanishes. Three alternative choices for $s(\omega)$ with non-zero second moment $M_2(s(\omega))$ are

$$s(\omega) = \frac{M_2(s(\omega))}{2\Lambda^3} \begin{cases} 2ab 
\left[ g_\omega(x) - g_\omega'(x) \right] & \text{with } b \geq 1, \\
 g_\omega''(x) & \text{with } b \geq 3, \\
 b^2 e^{-bx} \left( 1 - 2bx + \frac{b^2 x^2}{2} \right) & \text{with } b > 0. \end{cases} \quad \text{(model 2)}$$

$$s(\omega) = \frac{M_2(s(\omega))}{2\Lambda^3} \begin{cases} \left[ g_\omega(x) - g_\omega'(x) \right] & \text{with } b \geq 1, \\
 g_\omega''(x) & \text{with } b \geq 3, \\
 b^2 e^{-bx} \left( 1 - 2bx + \frac{b^2 x^2}{2} \right) & \text{with } b > 0. \end{cases} \quad \text{(model 3)}$$

$$s(\omega) = \frac{M_2(s(\omega))}{2\Lambda^3} \begin{cases} \left[ g_\omega(x) - g_\omega'(x) \right] & \text{with } b \geq 1, \\
 g_\omega''(x) & \text{with } b \geq 3, \\
 b^2 e^{-bx} \left( 1 - 2bx + \frac{b^2 x^2}{2} \right) & \text{with } b > 0. \end{cases} \quad \text{(model 4)}$$

Figure $4$ shows results for $\Lambda_{SL}(E_0)$ obtained in the various models, using $\tilde{\Lambda} = 0.5 \text{GeV}$, $\lambda_1 = -0.3 \text{GeV}^2$, and $M_2(s(\omega)) = (0.5 \text{GeV})^3$ as input parameters, and varying the parameter $b$ over a wide range of values. Although the details of the subleading shape function $s(\omega)$ are rather different in the four cases, all models exhibit the same general features. While
Figure 1: Model predictions for the subleading shape-function correction $\Lambda_{SL}(E_0)$ as a function of the cut $E_0$. For each model, the parameter $b$ is varied between the minimal allowed value (red) and 10 (blue) in steps of 1. The sign of $\Lambda_{SL}(E_0)$ is undetermined.

$\Lambda_{SL}(E_0)$ can be large close to the kinematic endpoint, it takes values of order $\bar{\Lambda}$ for $E_0 \sim 2.35\text{ GeV}$ and quickly decreases as $E_0$ is lowered below 2.3 GeV. For $E_0 = 2.2\text{ GeV}$ we find values of $\Lambda_{SL}(E_0)$ of at most 130 MeV (model 2), corresponding to a power correction to the extraction of $|V_{ub}|$ of less than 3%. Although our choice of model functions is meant as an illustration only, we believe the rapid decrease of $\Lambda_{SL}(E_0)$ for $E_0 < 2.3\text{ GeV}$ is a general result. It appears to be extremely unlikely that with a reasonable shape of $s(\omega)$ and a natural size of the second moment $M_2(s)$ the power correction $\Lambda_{SL}(E_0)/m_b$ could be as large as 10%.

4. Conclusion: In summary, we have studied the impact of subleading shape functions on the determination of $|V_{ub}|$ from the combination of weighted integrals over energy
Table 1: Illustrative theoretical predictions for the fraction $F_u(E_0)$ of $B \to X_u l \nu$ events with charged-lepton energy $E_l > E_0$, assuming a perfect measurement of the $B \to X_s \gamma$ photon spectrum (see text for explanation).

| $E_0$ [GeV] | LO       | NLO          | 1/$m_b$ | total       | residual error |
|------------|----------|--------------|--------|-------------|----------------|
| 2.0        | 0.271    | 0.041 ± 0.014 | -0.040 ± 0.006 | 0.273 ± 0.015 | ±0.003         |
| 2.1        | 0.195    | 0.033 ± 0.010 | -0.037 ± 0.006 | 0.191 ± 0.011 | ±0.005         |
| 2.2        | 0.126    | 0.024 ± 0.006 | -0.033 ± 0.005 | 0.117 ± 0.008 | ±0.006         |
| 2.3        | 0.068    | 0.015 ± 0.004 | -0.026 ± 0.004 | 0.057 ± 0.006 | ±0.008         |

spectra in inclusive $B \to X_u l \nu$ and $B \to X_s \gamma$ decays. We have argued that for a lower energy cut $E_0 = 2.2$ GeV as employed in a recent CLEO analysis one is in a transition region, where Fermi-motion effects are dominated by the first few moments of the leading and subleading shape functions. The dominant power correction (the only one that remains when the cut is lowered below about 2 GeV) results from the first moment of the subleading shape function, which is known in terms of the hadronic parameter $\lambda_2$.

Our main result is given in (9) and (10). To exhibit its features, let us assume that a perfect measurement of the $B \to X_s \gamma$ photon spectrum is available in the energy range above $E_{\gamma}^{\text{min}} = 1.5$ GeV. (For the purpose of illustration, we use a fit to the CLEO data in [13].) We then calculate the fraction of $B \to X_u l \nu$ events with charged-lepton energy above $E_0$ for different values of the cut. The results are summarized in Table 1. Columns 2, 3, and 4 show the contributions from the tree-level term, the $O(\alpha_s)$ corrections, and the power correction to the weight function in (10), including theoretical uncertainties from input parameter variations as detailed above. The next column shows the total result, while the final column gives an estimate of the residual uncertainty from subleading shape-function effects, as parameterized by the term $2\Lambda_{SL}(E_0)/m_b$ in (9). We show the largest uncertainty obtained in the four classes of models considered earlier. We observe that the power correction to the weight function has a significant impact, which as anticipated is by far the dominant effect of subleading shape functions. For $E_0 = 2.2$ GeV, the power correction leads to a reduction of the predicted value for $F_u(E_0)$ by $(26 \pm 6)\%$, corresponding to a 13% enhancement of the extracted value of $|V_{ub}|$. This is in good agreement with the estimate given in [7].

The most important implication of our analysis is that subleading shape-function effects do not entail a significant limitation on the extraction of $|V_{ub}|$. This assessment differs from the conclusion reached in [7, 8], where it was argued that these effects could not be controlled reliably unless the cut $E_0$ could be lowered outside the shape-function region. The new element of our analysis is that we identify the first moment of the subleading shape-function as the dominant source of power corrections and show how its contribution can be expressed in terms of an integral over the $B \to X_s \gamma$ photon
spectrum. We have estimated the residual uncertainty on $|V_{ub}|$ from subleading shape-function effects by using four different classes of model functions and found corrections of at most 3% (with $E_0 = 2.2$ GeV). The smallness of this effect can be understood on the basis that it is a power correction of the form $\Lambda_{SL}(E_0)/m_b$ with a hadronic parameter $\Lambda_{SL}(E_0) = O(\Lambda_{QCD})$ that vanishes as $E_0$ is lowered below about 2 GeV. We thus conclude that, very conservatively, the residual uncertainty on $|V_{ub}|$ is less than 10%.

The main result of this letter is the new expression for the weight function in (10), which now includes the leading power correction. Perhaps the largest uncertainty in this method for determining $|V_{ub}|$ is due to (largely unknown) corrections from violations of quark–hadron duality, and from spectator-dependent effects such as weak annihilation and Pauli interference [15, 16] (see also [8], where a 6–8% correction on $|V_{ub}|$ was obtained for $E_0 = 2.2$ GeV using a simple model for spectator effects). In these references, several strategies have been developed that could help to determine the magnitude of these corrections using experimental data.

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